Design, synthesis, docking, MD simulations, and anti-proliferative evaluation of thieno[2,3-*d*]pyrimidine derivatives as new EGFR inhibitors

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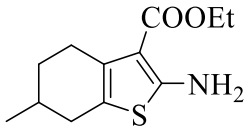
1. Chemistry

All commercially available materials were purchased from commercial sources and used without further purification. All reactions were performed in a temperature-controlled oil/wax bath. Reactions were monitored by analytical thin layer chromatography (TLC), using aluminum-backed plates, cut to size. TLC visualization was achieved by UV. ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker AVANCE 400 MHz spectrometers at ambient temperature. Spectral data is reported in ppm, coupling constants (*J*) in Hz. IR spectra were recorded as KBr pellets on a PerkinElmer Spectrum one FT-IR spectrometer. Mass spectroscopy (MS) was performed at NAWAH scientific Mass Spectroscopy Centre on Advion compact mass spectrometer (CMS) NY | USA for APCI. All melting points were taken on a Gallenkamp melting point apparatus and are uncorrected. Nomenclature was determined using ChemBioDraw Ultra 14.0.

Ethyl 2-amino-6-methyl-4,5,6,7-tetrahydro[1]benzothiophene-3-carboxylate (2)

A mixture of 4-methylcyclohexanone (**1**) (4.48 g, 40 mmol), ethyl cyanoacetate (4.52 g, 40 mmol), sulphur (1.28 g, 40 mmol) and morpholine (5 mL) in absolute ethanol (25 mL) was heated on water-bath at 40℃ for 4 h. The reaction mixture was allowed to cool to room temperature, the formed solid was filtered, dried and crystallized from ethanol to give **2.**



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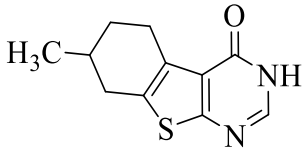
6-Methyl-5,6,7,8-tetrahydro[1]benzothieno[2,3-d]pyrimidin-4(3H)-one (3)

A mixture of ethyl 2-amino-6-methyl-4,5,6,7-tetrahydro[1]benzothiophene-3-carboxylate (**2**) (0.24 g, 1 mmol) and formamide (99.5%) (15 mL) was heated under reflux for 5 h. The solvent was then evaporated under reduced pressure and the residue was crystallized isopropanol.



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2. Biological testing

2.1.**In vitro antiproliferative activity**

The *in vitro* antiproliferative activities of all the synthesized compounds against a panel of four human tumor cell lines namely, A549 and MCF-7cell were evaluated quantitatively as described in the literature, using MTT assay protocol. two commercially available drugs (erlotinib) were used in this test as positive controls. The anti-proliferative activity was assessed quantitatively as follows.

Human cancer cell lines were dropped in 96-well plates at a density of 3-8 × 10^3 cells/well. Next, the wells were incubated for 12 h in a 5% CO_2 incubator at 37 ℃. Then, for each well, the growth medium was exchanged with 0.1 ml of fresh medium containing graded concentrations of the test compounds to be or equal DMSO and incubated for two days. Then 10 µl MTT solution (5 µg/ml) was added to each well, and the cells were incubated for additional 4 h. The crystals of MTT-formazan were dissolved in 100 µl of DMSO; the absorbance of each well was measured at 490 nm using an automatic ELISA reader system (TECAN, CHE). The IC_{50} values were calculated using the nonlinear regression fitting models (Graph Pad, Prism Version 5). The data represented the mean of three independent experiments in triplicate and were expressed as means ± SD. The IC_{50} value was defined as the concentration at which 50% of the cells could survive.

2.2.**Safety assay**

The normal cell lines, W138, were utilized. MTT assay was applied as described before.

2.3.*In vitro* EGFR inhibition

The tested compounds were examined for their inhibitory activities against both $EGFR^{WT}$ and $EGFR^{T790M}$. Homogeneous time resolved fluorescence (HTRF) assay was applied in this test. $EGFR^{WT}$, $EGFR^{T790M}$ (Sigma). firstly, the $EGFR^{WT}$ and/or $EGFR^{T790M}$ and their substrates were incubated with the tested compounds in enzymatic buffer for 5 min. ATP (1.65 µM) was added into the reaction mixture to allow starting the enzymatic reaction. The assay was conducted for 30 min at room temperature. The reaction was stopped by addition of detection reagents which contain EDTA. The detection step continued for 1 h, and then the IC_{50} values were determined by GraphPad Prism 5.0. Three independent experiments were performed for each concentration.

2.4.Cell cycle analysis

A549 cells were exposed to compound **5b** at a concentration of 17.79 µM µM for 72h. Then, the tested cells were collected by trypsinization and washed in PBS. Ice-cold absolute ethanol was used for fixation of the collected cells. The cells were stained with Cycle TESTTM PLUS DNA Reagent Kit (BD Biosciences, San Jose, CA) according to the manufacturer's instructions. Cell-cycle distribution was evaluated using a flow cytometer.

2.5.Apoptosis analysis

To detect the apoptosis induced by compound **5b**, A549 cells were seeded and incubated overnight and then treated with compound **5b** at concentrations of 17.79 µM for 72 h. DMSO was chosen as the negative control. After that, the cells were collected and washed with PBS two successive times. The cells were exposed to centrifugation. Apoptosis detection kit (BD Biosciences, San Jose, CA) was used in this test. According to the manufacturer's protocol the cells were stained by Annexin V-FITC and propidium iodide (PI) in the binding buffer for 20min at room temperature in the dark. Using a flow cytometer, Annexin V-FITC and PI binding were analyzed. flowjo software was used to analyze the frequencies in all quadrants.

2.6.Quantitative Real Time Reverse-Transcriptase PCR technique (determination of BAX and Bcl-2)

The quantity of BAX and Bcl-2 mRNA in control and compound 5b (at the IC_{50} concentration)-treated A549 cells was assessed by qRT-PCR (reference). Total RNA from vehicle-treated control (0.01% DMSO) and 10k-treated HepG2 cells were extracted as-per the manufacturer instructions (RNeasy mini kit, Qiagen, Germany). After RNA extraction, cDNA was prepared

using the Revert Aid First Strand cDNA Synthesis kit (Thermo Scientific, USA). Amplification of target cDNA for apoptosis markers and GAPDH [as a normalization (housekeeping) gene] was done using one-step RT-PCR SYBR® Green kit Master Mix (Bio-Rad Laboratories, USA) on Rotor-Gene Q real-time PCR thermal cycler instrument. cDNA (2 µl aliquots) was mixed with 1 µl of forward primer, 1 µl reverse primer, 10 µl master mixture, and the reaction volume was completed to 20 µl with nuclease-free water. All experiments were performed in triplicates.

The sequences for primers used in quantitative Real Time Reverse-Transcriptase PCR (qRT-PCR)

Gene	Primer sequence
BAX	F: 5'- CCCGAGAGGTCTTTTTCCGAG -3'
	R: 5'- CCAGCCCATGATGGTTCTGAT -3'
Bcl-2	F: 5'- TTGTGGCCTTCTTTGAGTTCGGTG -3'
	R: 5'- GGTGCCGGTTCAGGTACTCAGTCA -3'
GABDH	F: 5'- GACCCCTTCAT GACCTCAAC -3'
	R: 5'- CTTCTCCATGGTGGT GAAGA -3'

3. *In silico* studies

3.1.Docking studies

The crystal structures of the target enzymes $EGFR^{WT}$ (PDB ID: 4HJO, resolution 2.75 Å and $EGFR^{T790M}$ (PDB ID: 3W2O, resolution 2.35 Å) were downloaded from Protein Data Bank (http://www.pdb.org). Molecular Operating Environment (MOE) was used for the docking analysis [91]. In these studies, the free energies and binding modes of the designed molecules against $EGFR^{WT}$ and $EGFR^{T790M}$ were determined. At first, the water molecules were removed from the crystal structures of $EGFR^{WT}$ and $EGFR^{T790M}$, retaining only one chain in each enzyme. Erlotinib and TAK-285 (The co-crystallized ligands) were utilized as references in the docking processes against both $EGFR^{WT}$ and $EGFR^{T790M}$, respectively. After that, in order to prepare the target molecules for binding with the designed compounds, the target proteins were subjected to protonation step. Then, the hydrogen atoms were hidden to make the areas

of interaction clearer. Next, the energy of all systems was minimized followed by identification the binding pockets of the target proteins.

The structures of the designed compounds and the co-crystallized ligands, erlotinib and TAK-285 were drawn using ChemBioDraw Ultra 14.0 and saved as SDF format. Then, the saved files were opened using MOE and 3D structures were protonated. Next, the energy of the molecules was minimized. Validation process was performed for each target by running the docking process for only the co-crystallized ligand. Low RMSD values between docked and crystal conformations indicate valid performance. The docking procedures were carried out utilizing a default protocol. In each case, 10 docked structures were generated using genetic algorithm searches. The output from of MOE was further analyzed and visualized using Discovery Studio 4.0 software.

3.2.M D simulations

Molecular dynamics simulation of the protein-ligand complexes was performed using GROMACS 2021 and Linux 5.4 package. The GROMOS96 54a7 forcefield was selected as the force field for proteins and the ligand topologies were generated from the PRODRG server. All the complexes were solvated using simple point charge (SPC) water molecules in a rectangular box. To make the simulation system electrically neutral, required number of Na^+ and Cl^- ions were added while 0.15 mol/L salt concentrations were set in all the systems. Using the steepest descent method, all the solvated systems were subjected to energy minimization for 5000 steps. Afterwards, NVT (constant number of particles, volume, and temperature) series, NPT (constant number of particles, pressure, and temperature) series, and the production run were conducted in the MD simulation. The NVT and the NPT series were conducted at a 300 K temperature and 1 atm pressure for the duration of 300 ps. V-rescale thermostat and Parrinello-Rahman barostat were selected of the performed simulation. Finally, the production run was performed at 300 K for a duration of 100 ns (nanoseconds). Thereafter, a comparative analysis was performed measuring root mean square deviation (RMSD), root mean square fluctuation (RMSF), radius of gyration (Rg), solvent accessible surface area (SASA) and hydrogen bonds to analyze their stability. The Xmgrace program was used to represent the analyses in the form of plots.

3.3.MM-GBSA

The g_mmpbsa package of GROMACS was utilized to calculate the MM/PBSA (Molecular Mechanics/Poisson Boltzmann Surface Area) binding free energies followed by final MD production run to get a detailed overview of the molecular interactions between the protein and ligand. The free solvation energy (polar and nonpolar solvation energies) and potential energy (electrostatic and Van der Waals interactions) of each protein-ligand complex were analyzed to determine the total ΔG_{bind} of the complex. The binding energies were calculated using the following equation in this method:

$$\Delta G_{binding} = G_{complex} - (G_{protein} + G_{ligand})$$

Here, the $\Delta G_{binding}$ = the total binding energy of the protein-ligand complex, $G_{protein}$ = the binding energy of free protein, and G_{ligand} = the binding energy of unbounded ligand.

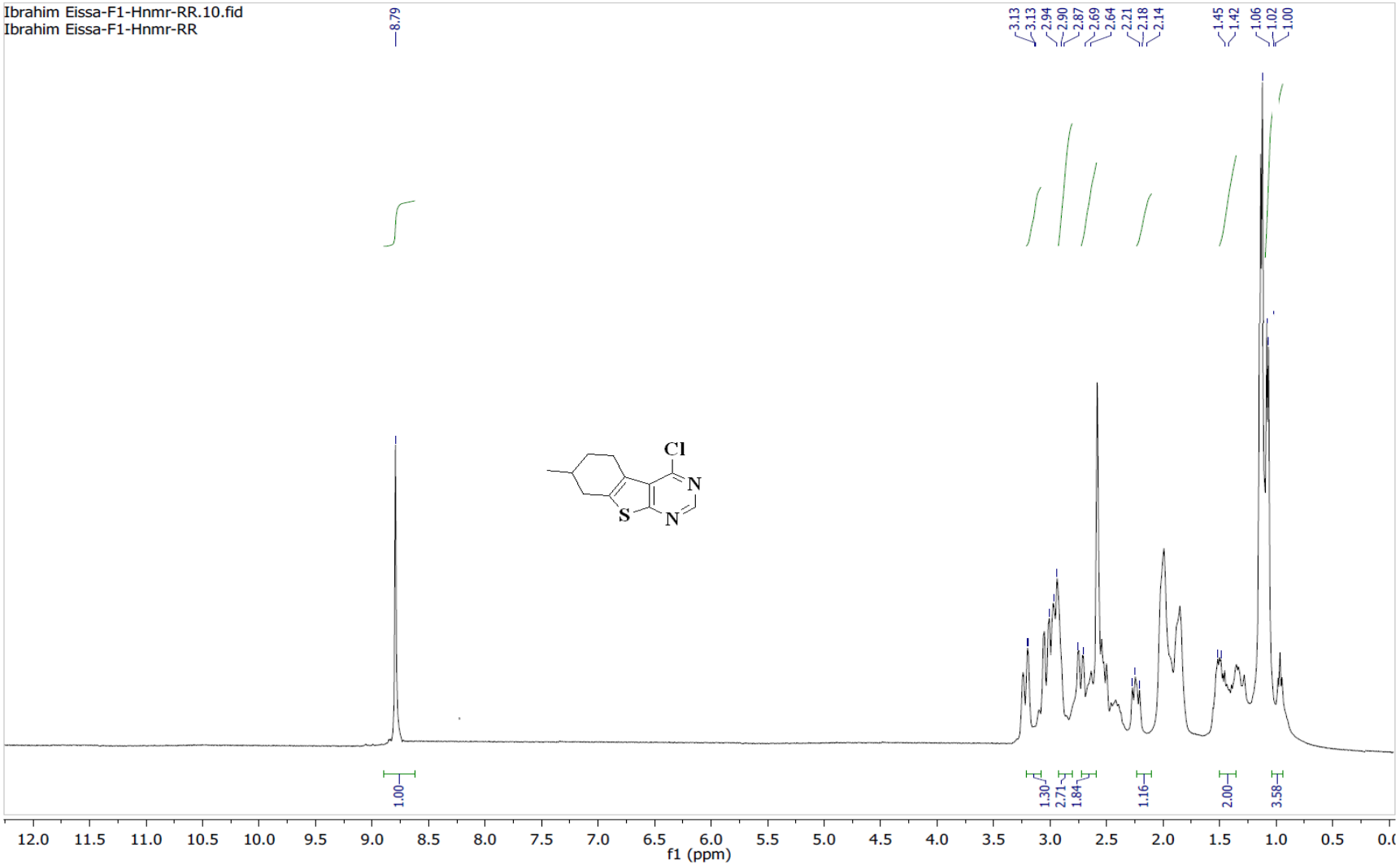
3.4.ADMET studies

ADMET descriptors (absorption, distribution, metabolism, excretion and toxicity) of the tested compounds were determined using Discovery studio 4.0. At first, the CHARMM force field was applied then the tested compounds were prepared and minimized according to the preparation of small molecule protocol. Then ADMET descriptors protocol was applied to carry out these studies.

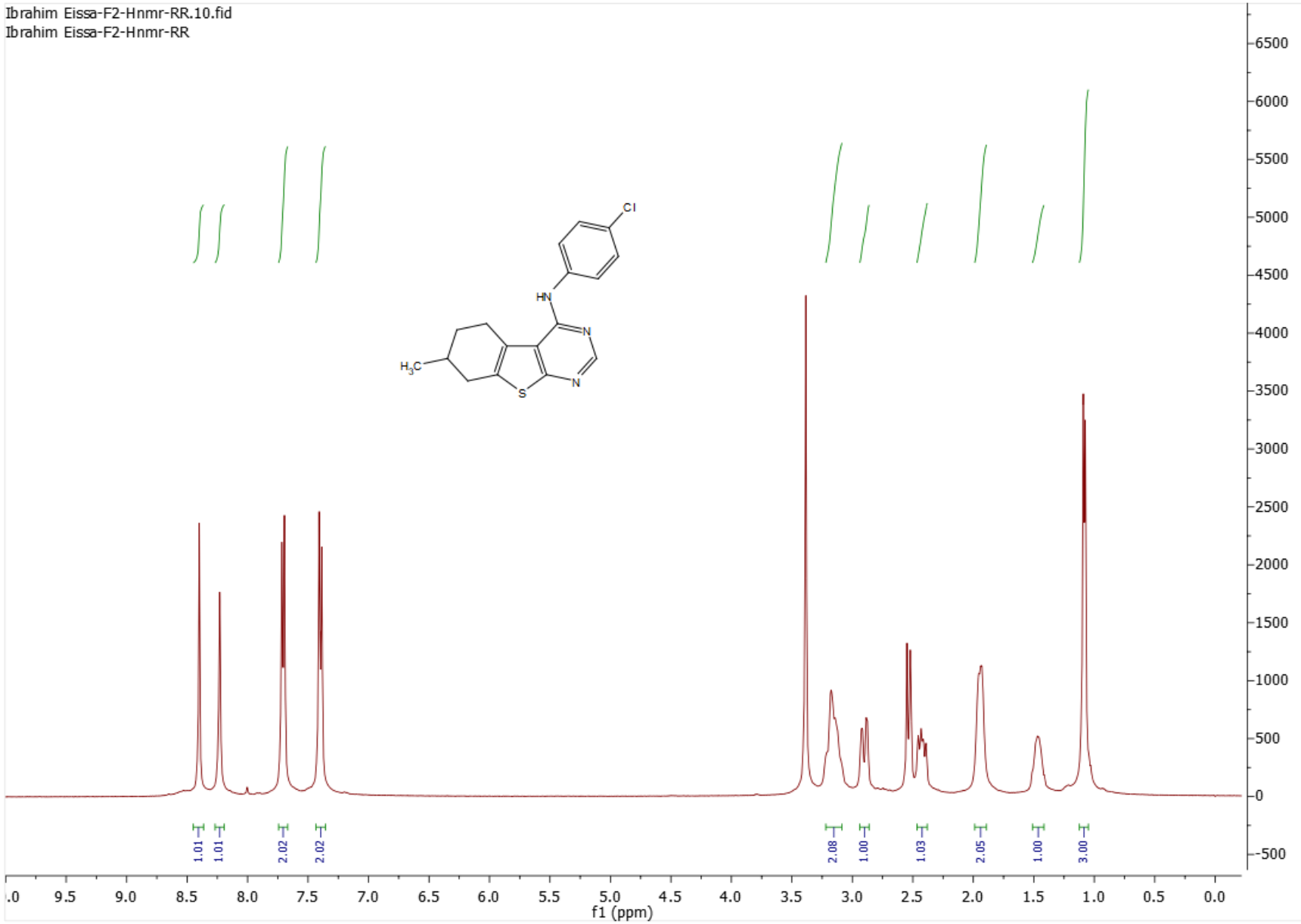
3.5.**Toxicity studies**

The toxicity parameters of the synthesized compounds were calculated using Discovery studio 4.0. Sorafenib was used as a reference drug. At first, the CHARMM force field was applied then the compounds were prepared and minimized according to the preparation of small molecule protocol. Then different parameters were calculated from toxicity prediction (extensible) protocol.

H^1 NMR of compound 4



H^1 NMR of compound 5a



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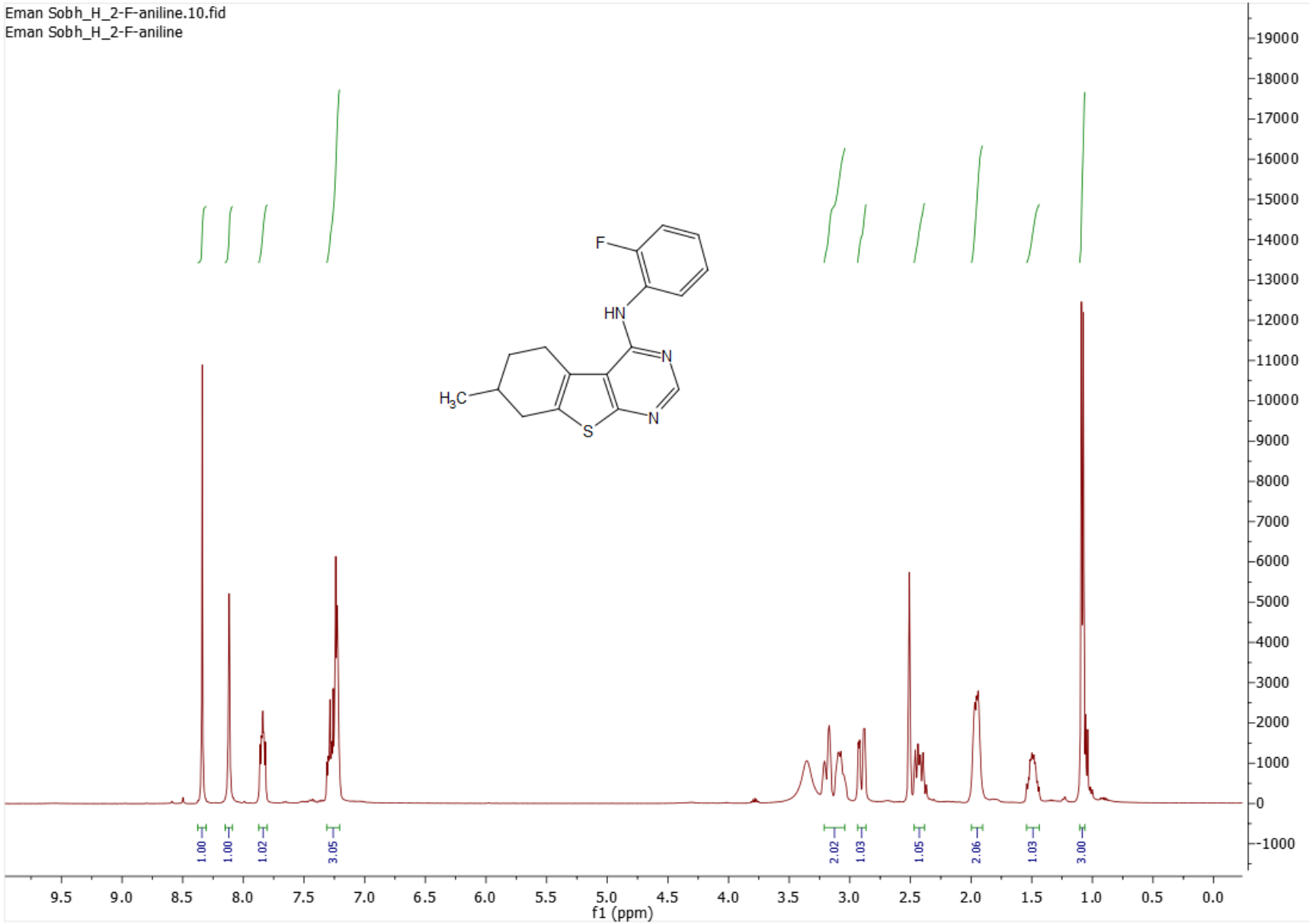

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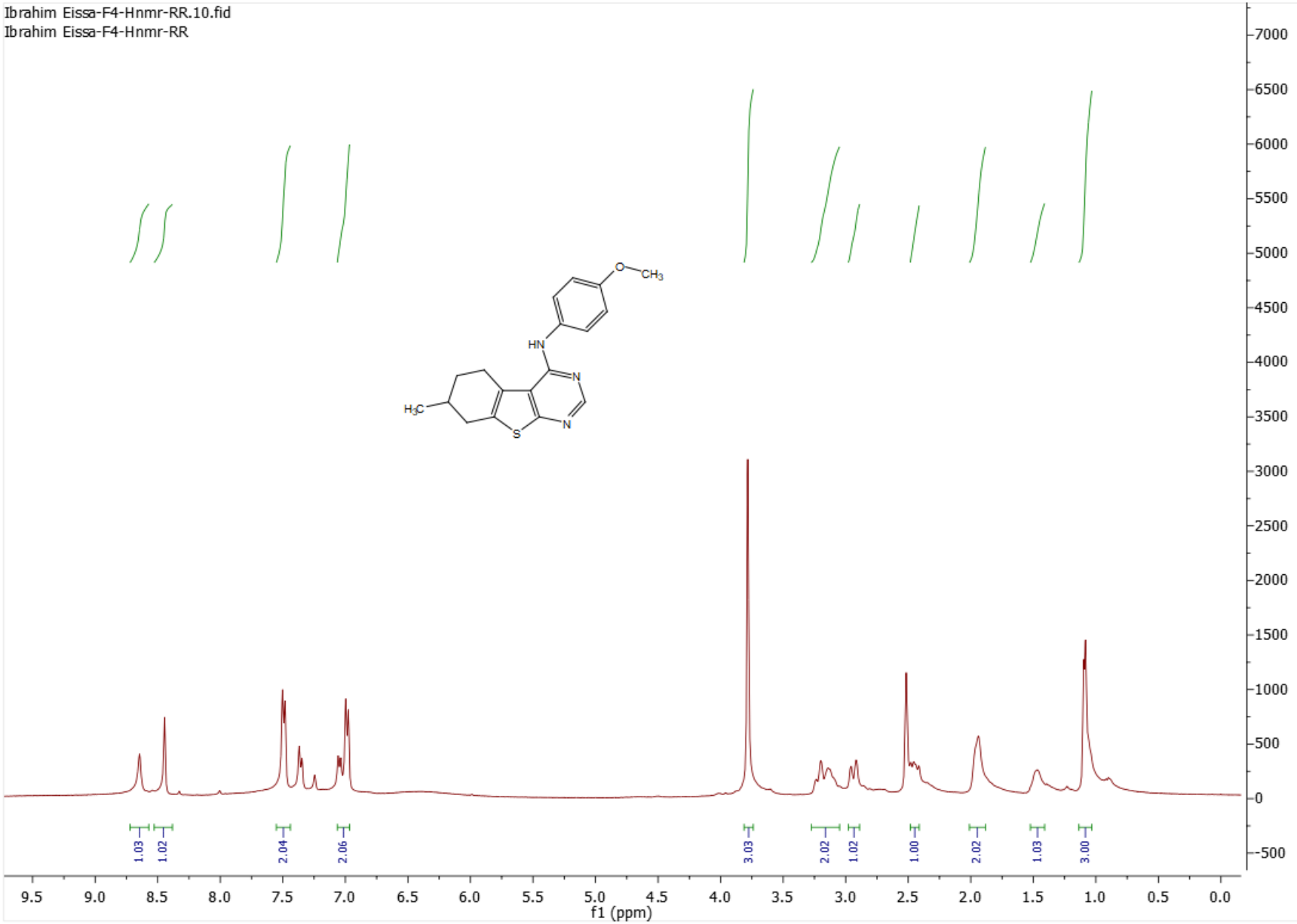

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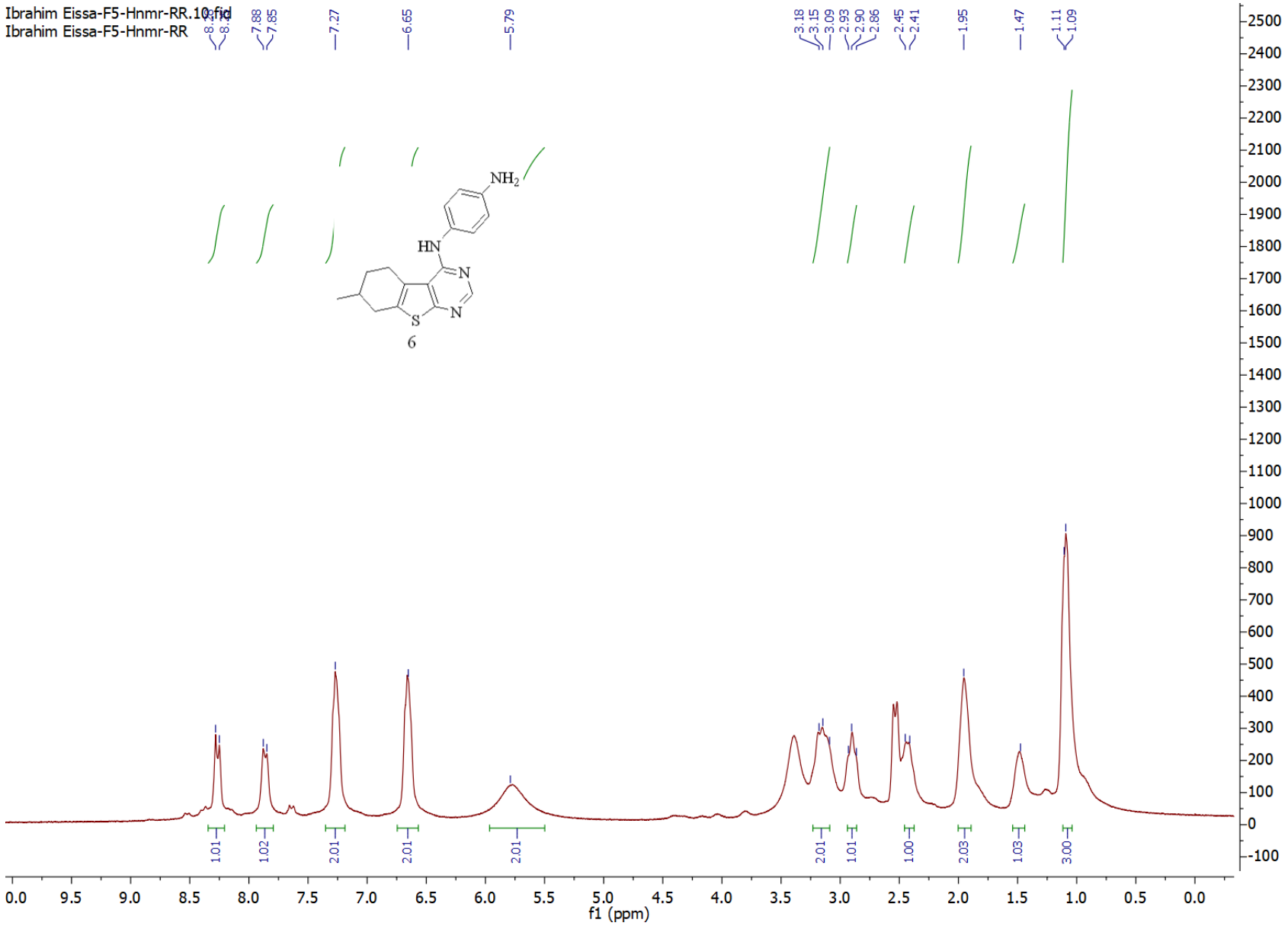

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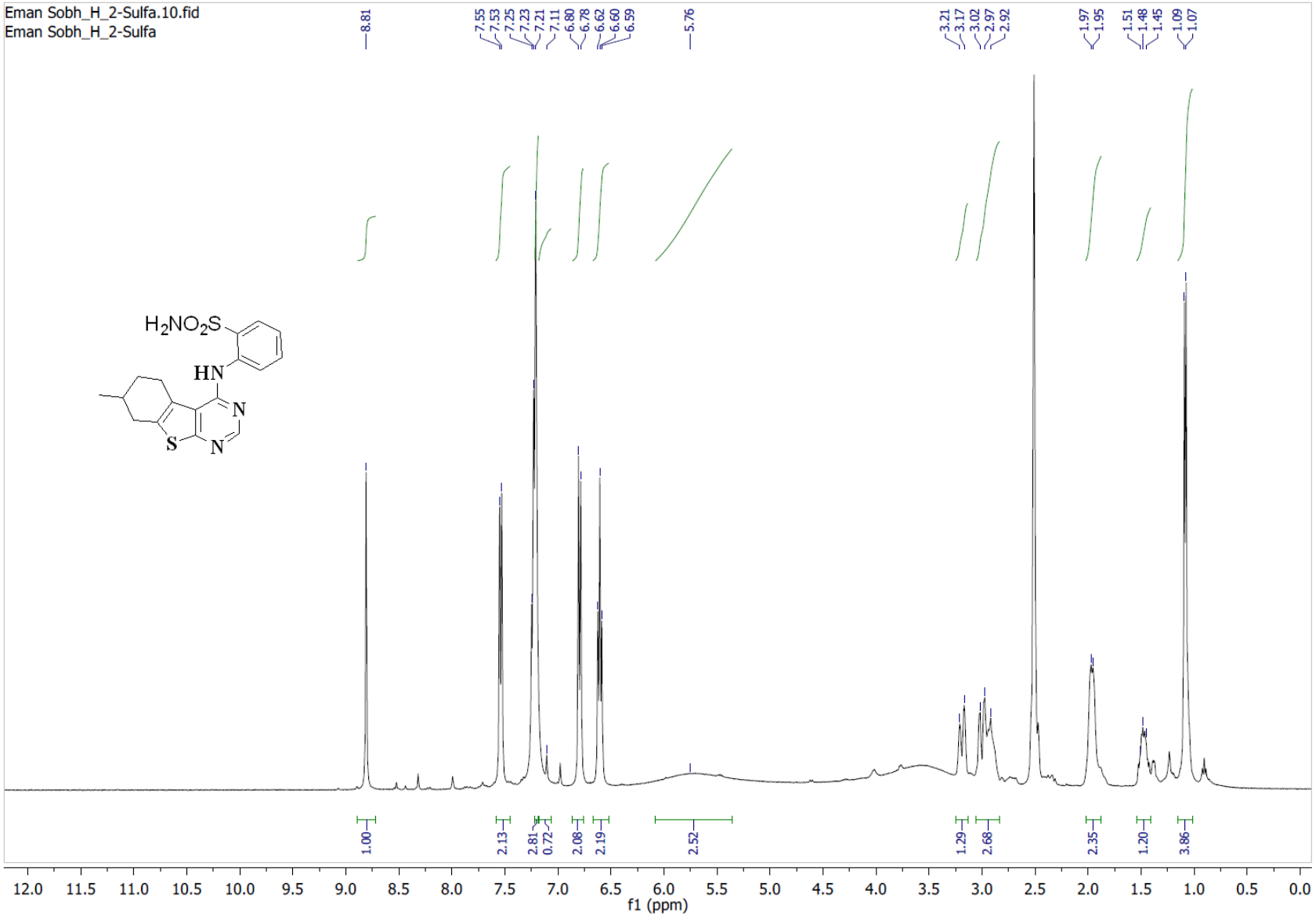

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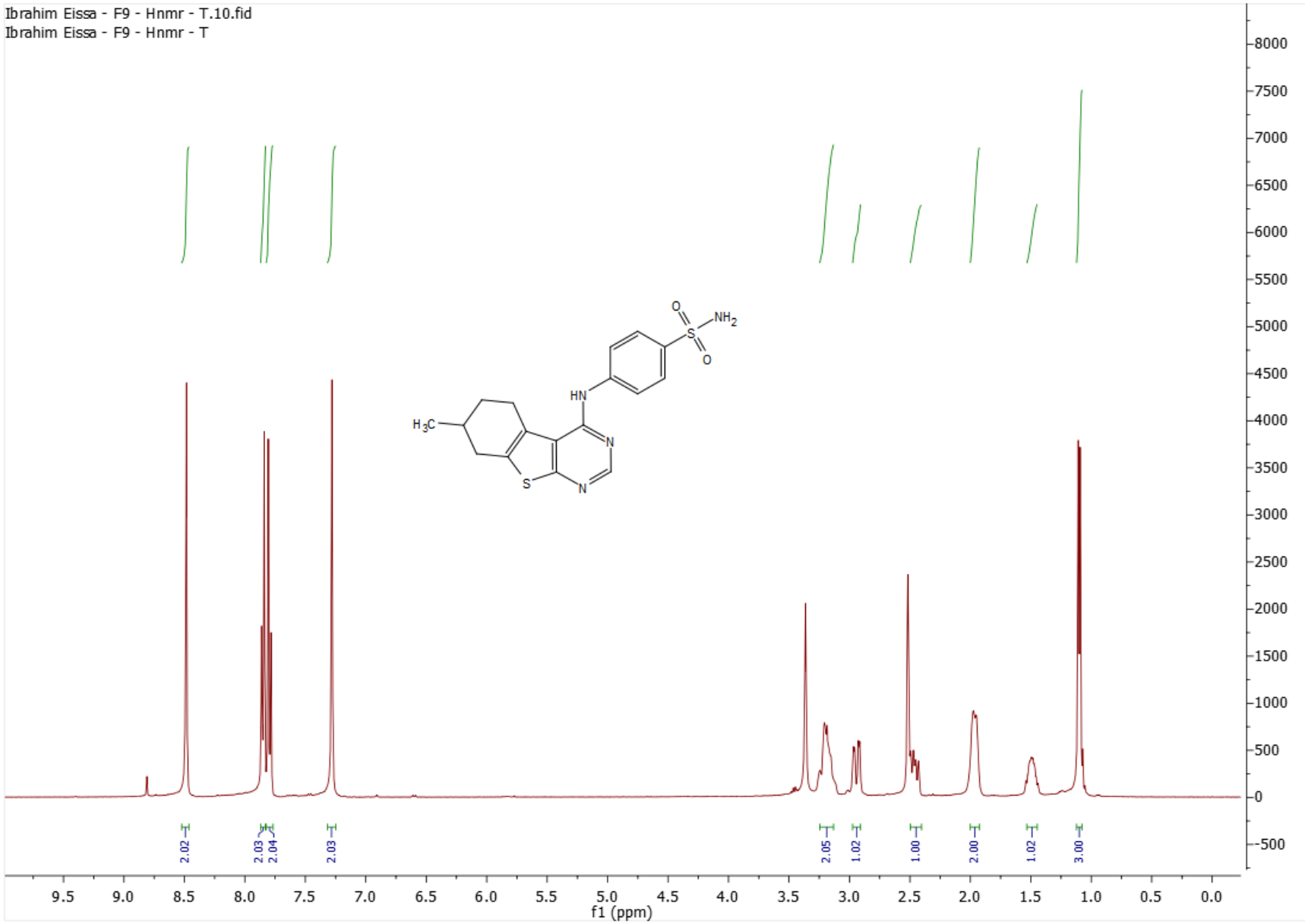
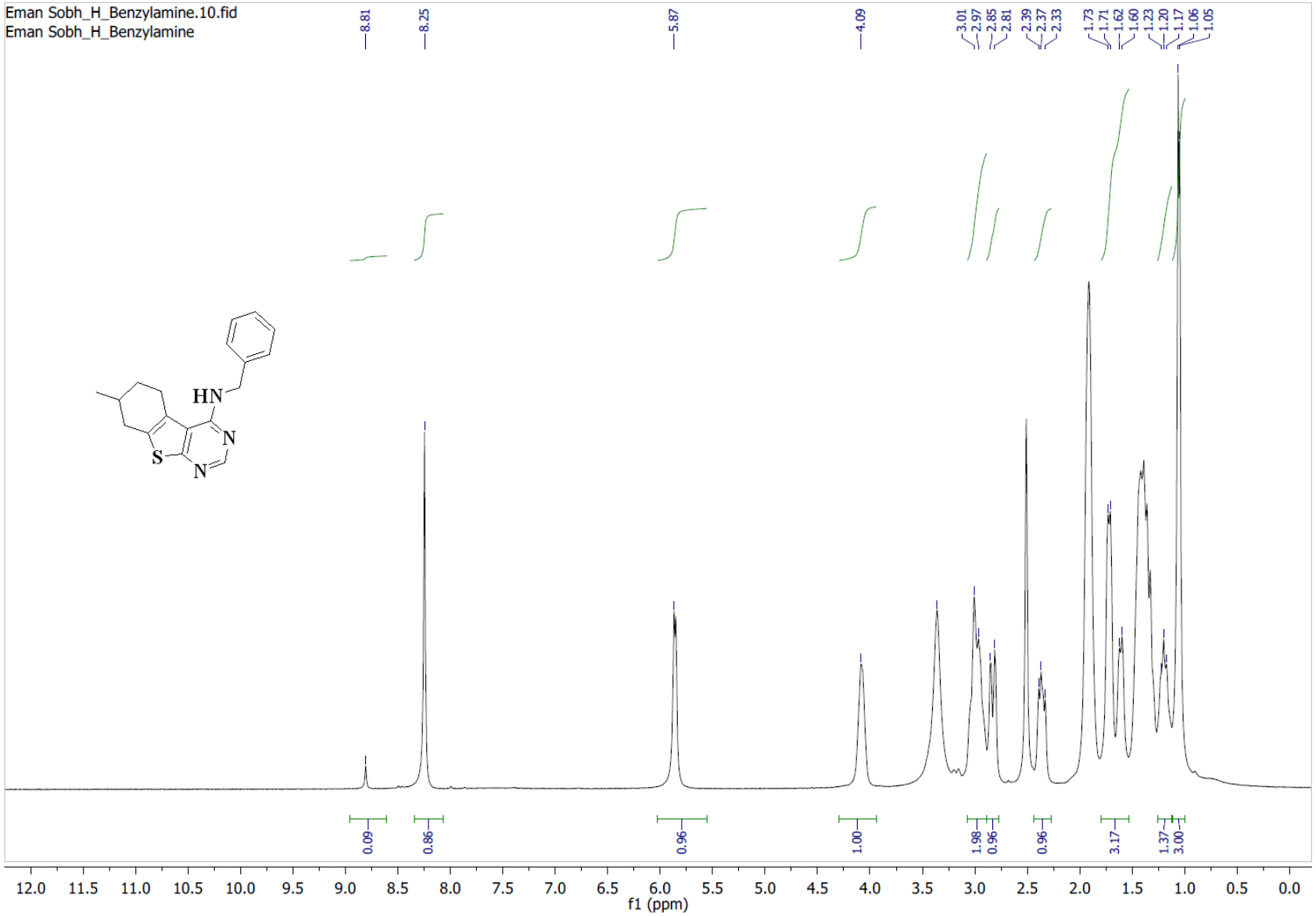


H1 NMR of compound 6



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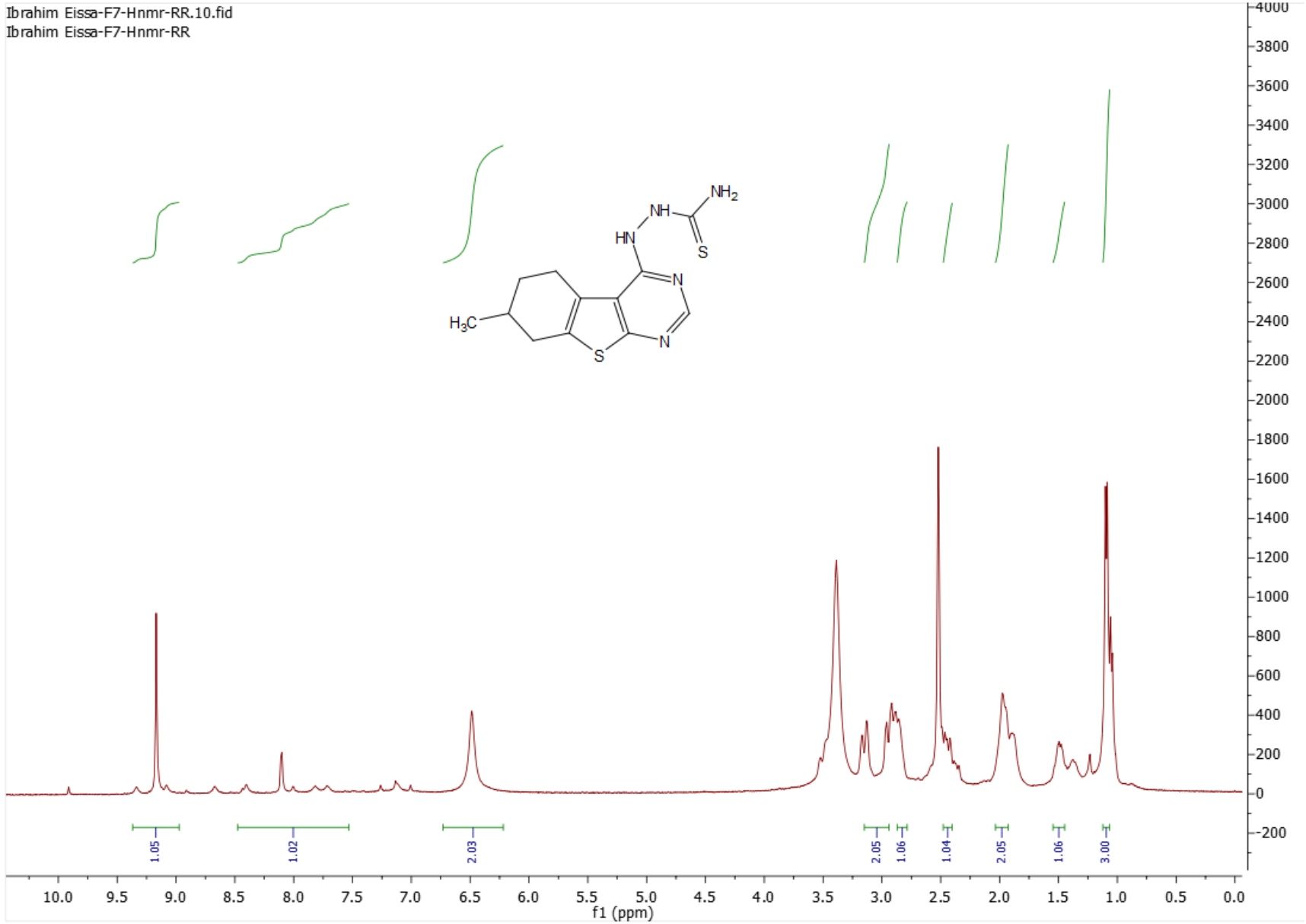

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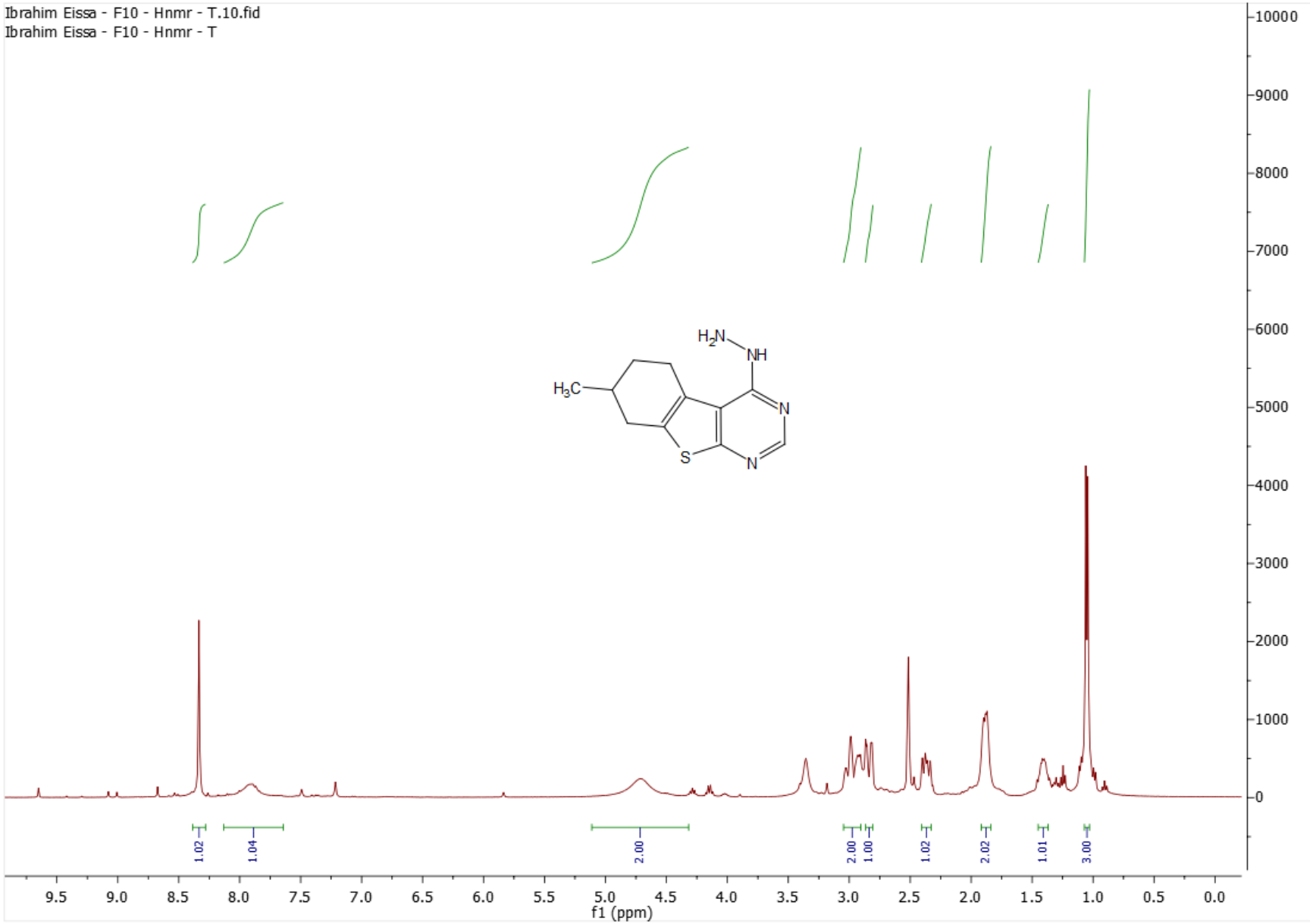
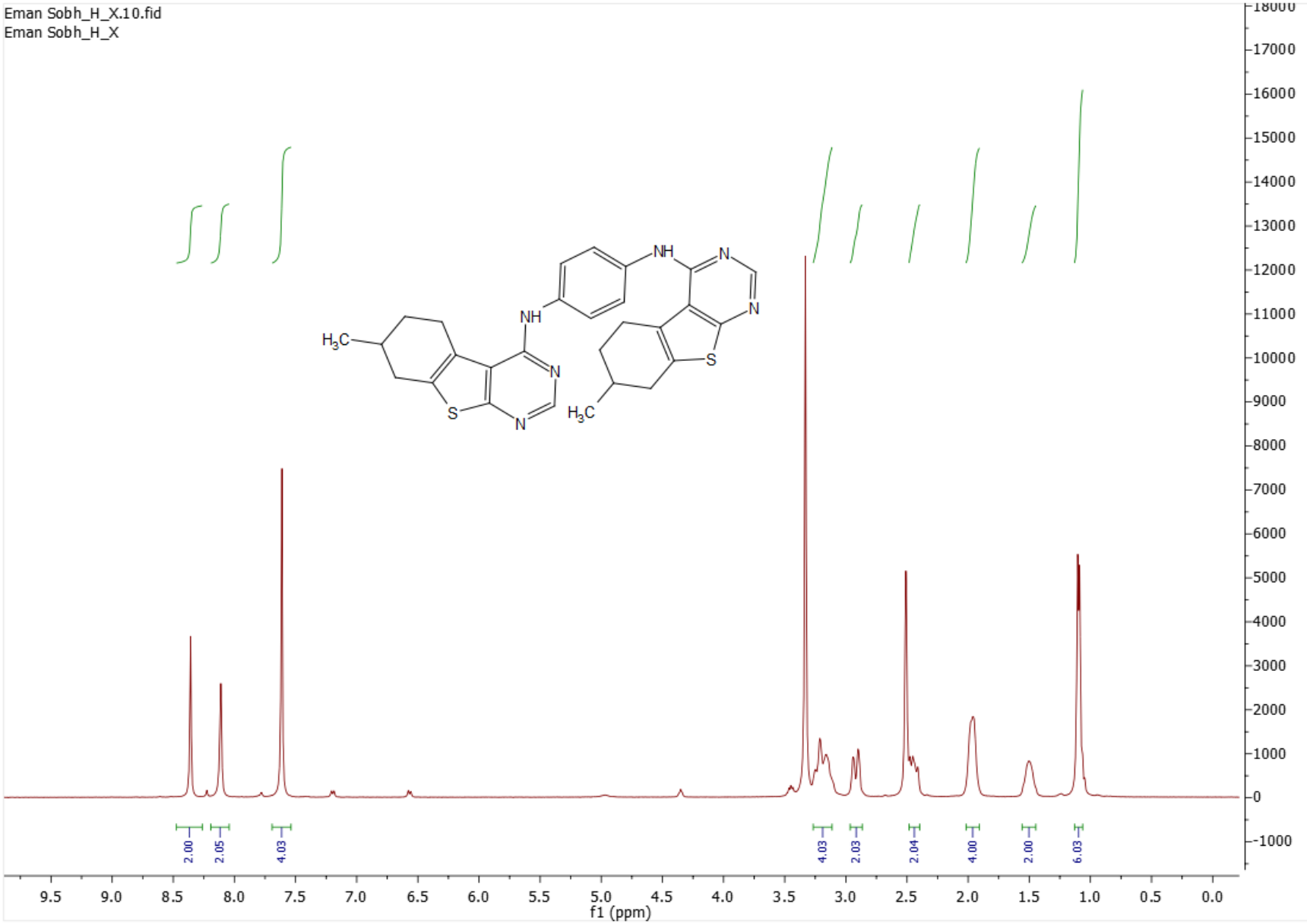


H1 NMR of compound 8



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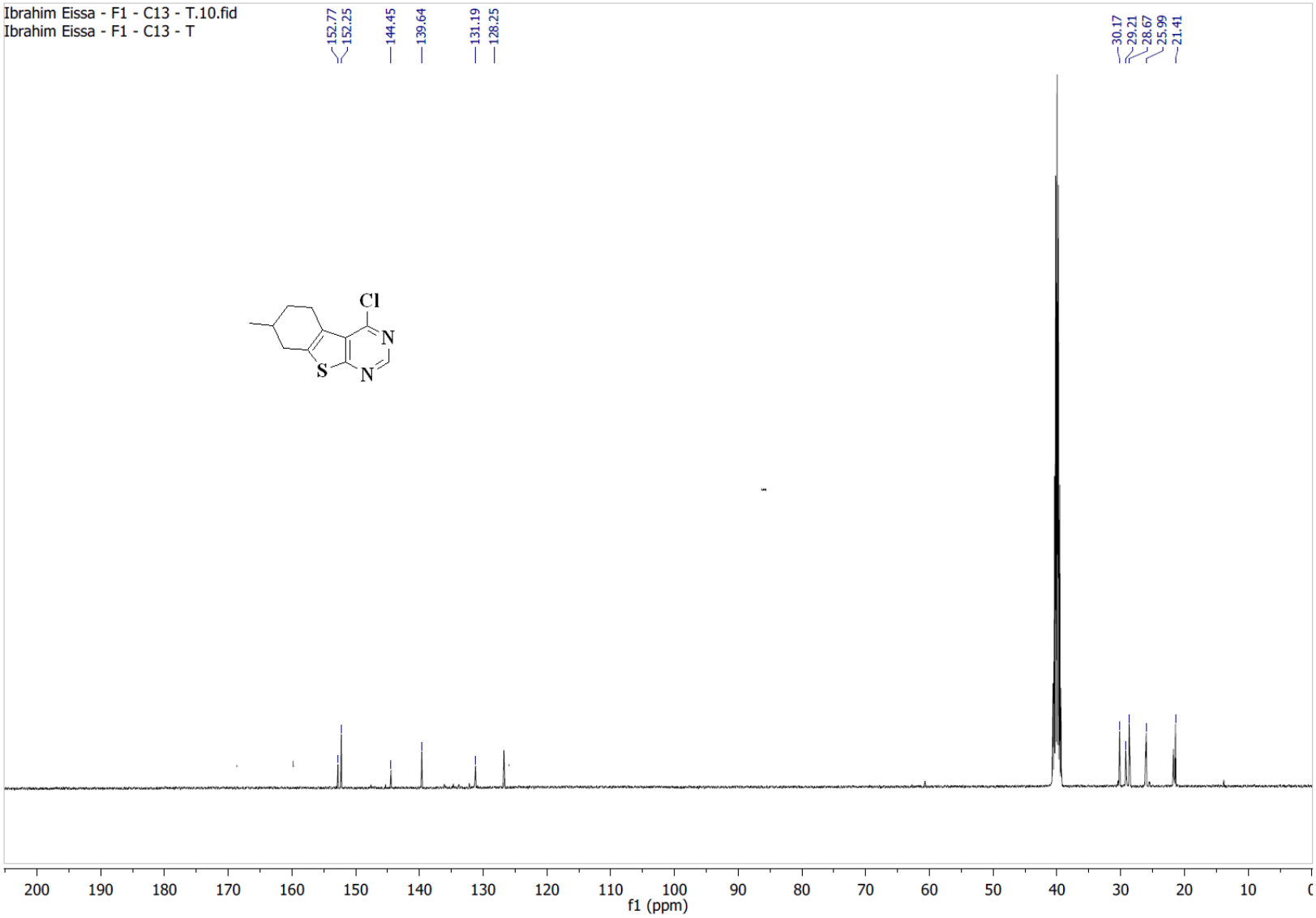

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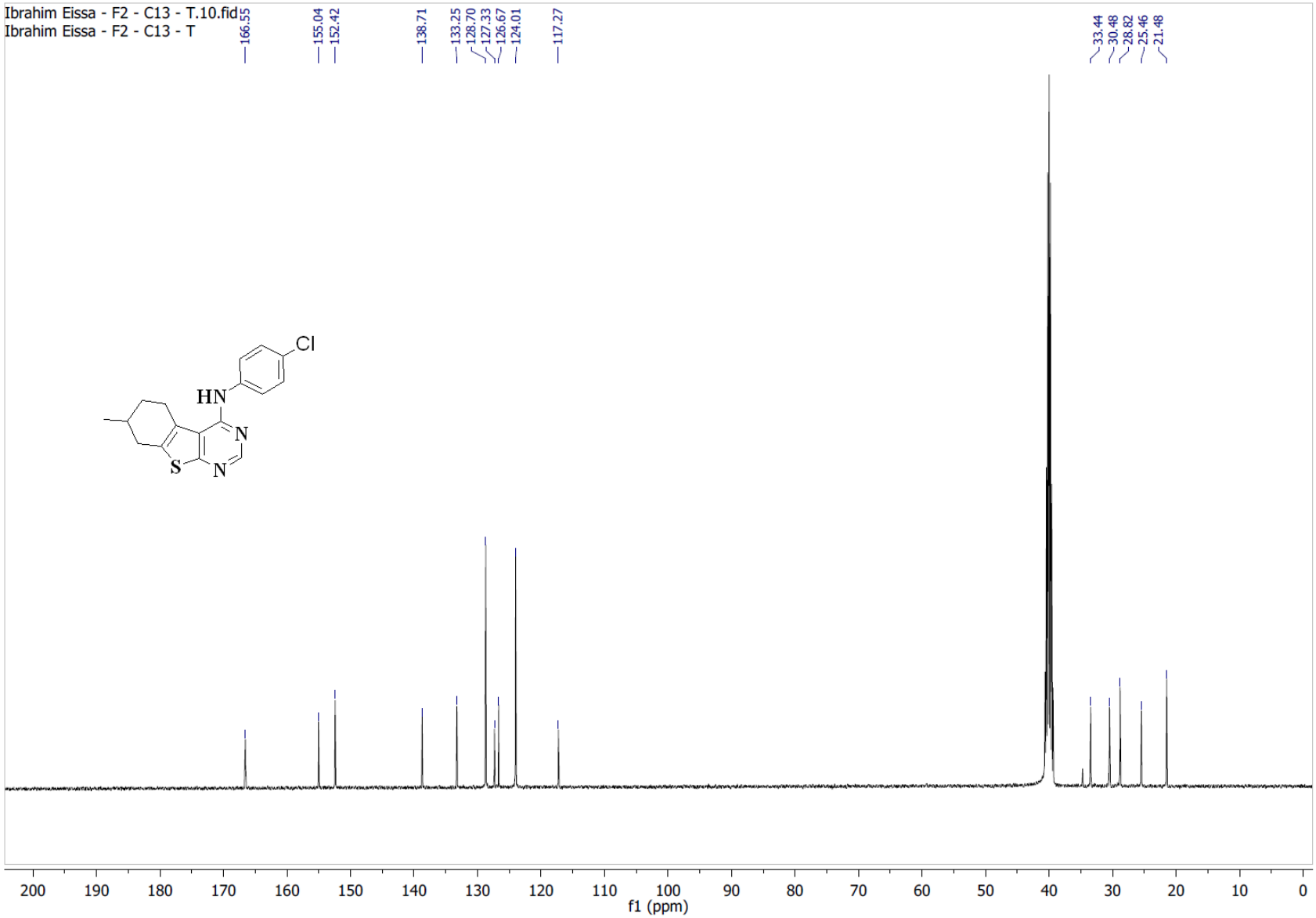

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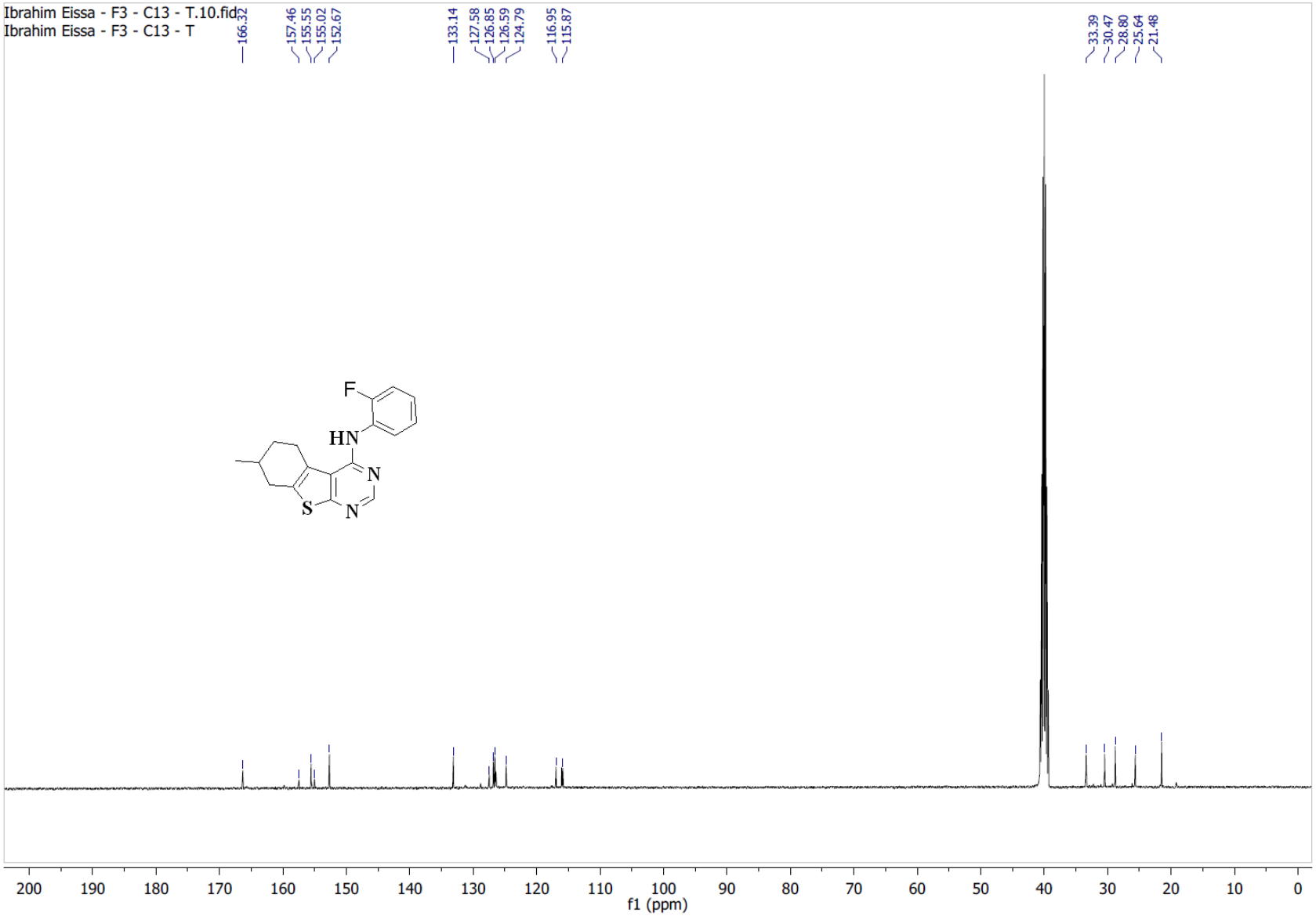

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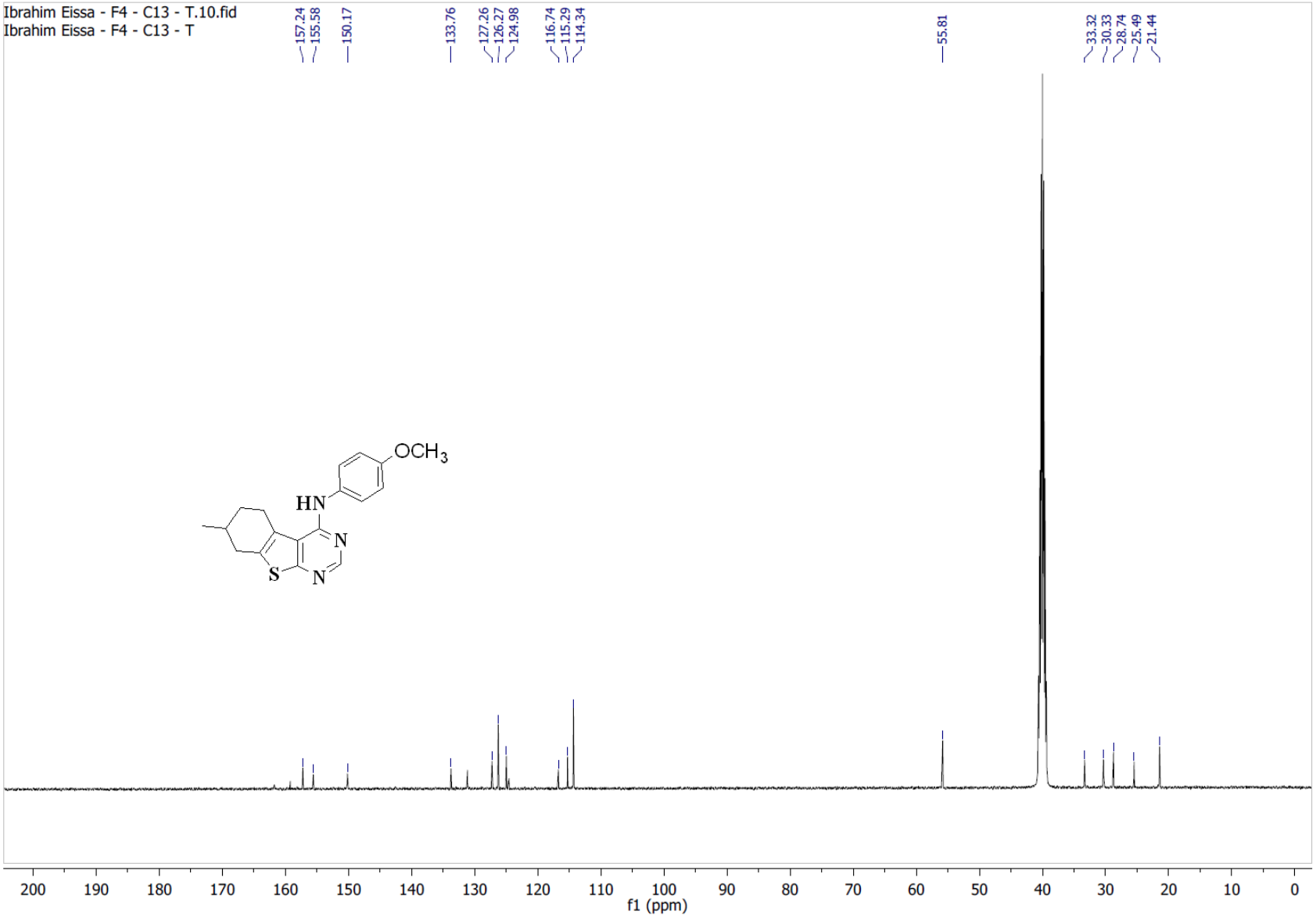

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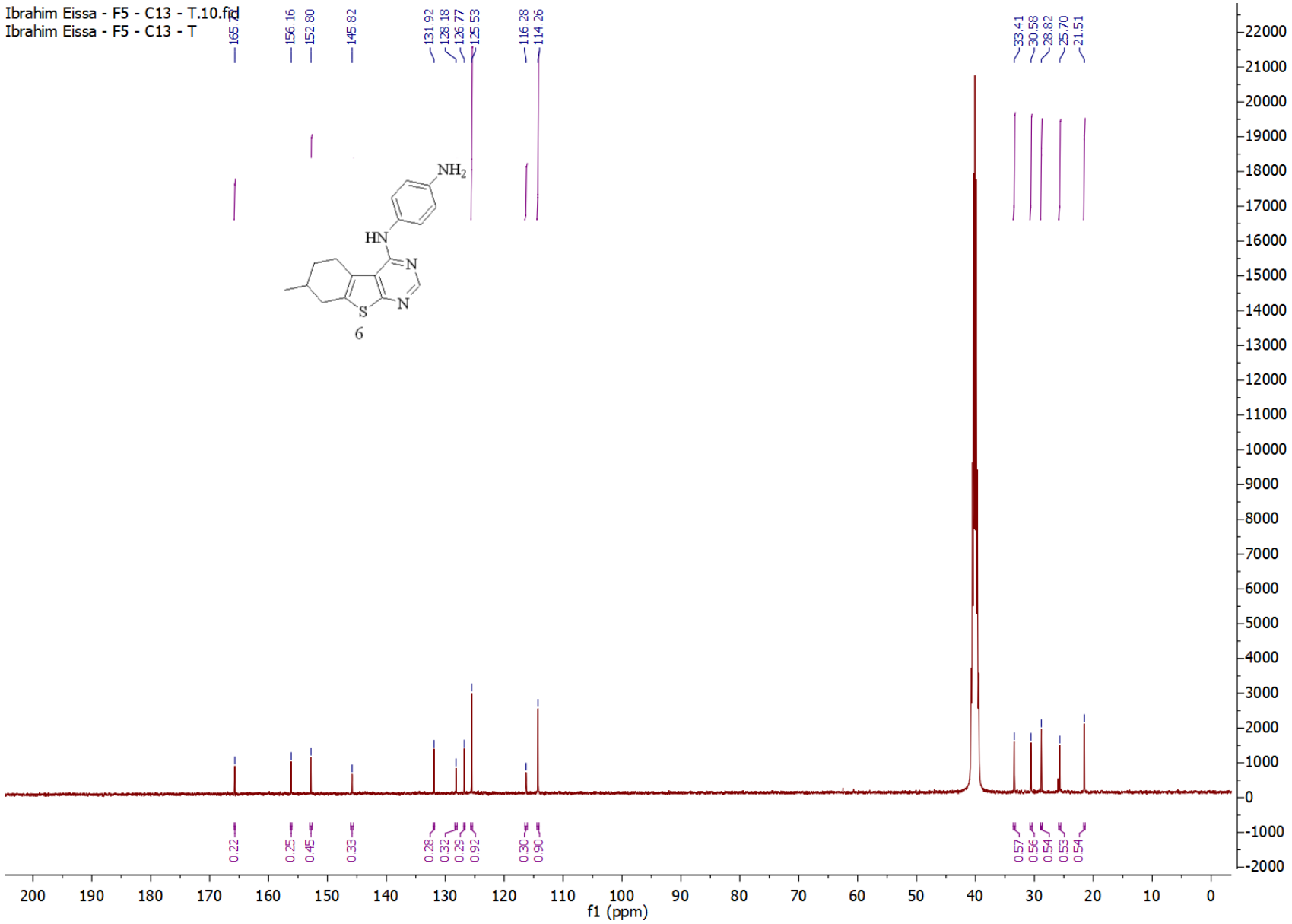

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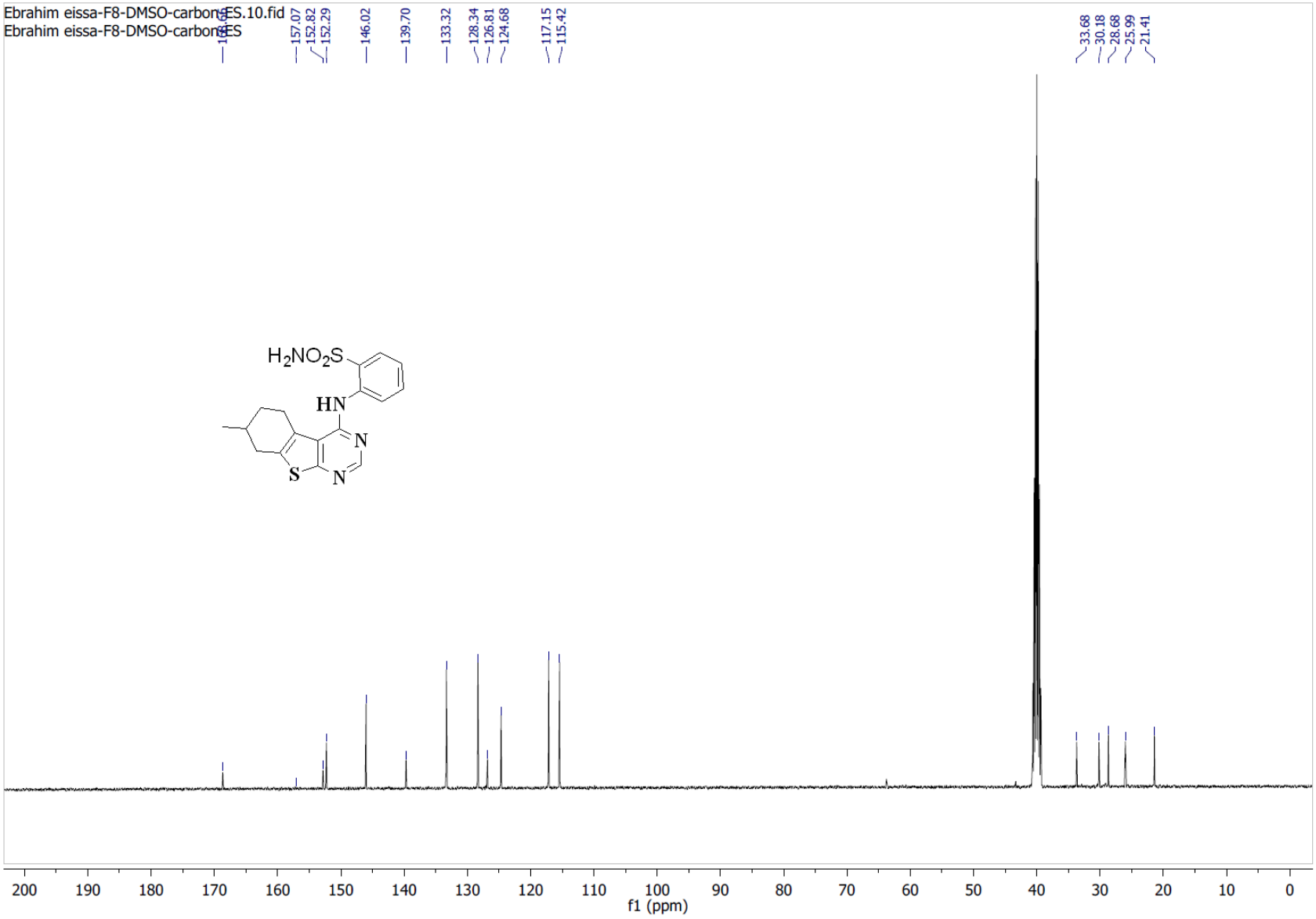

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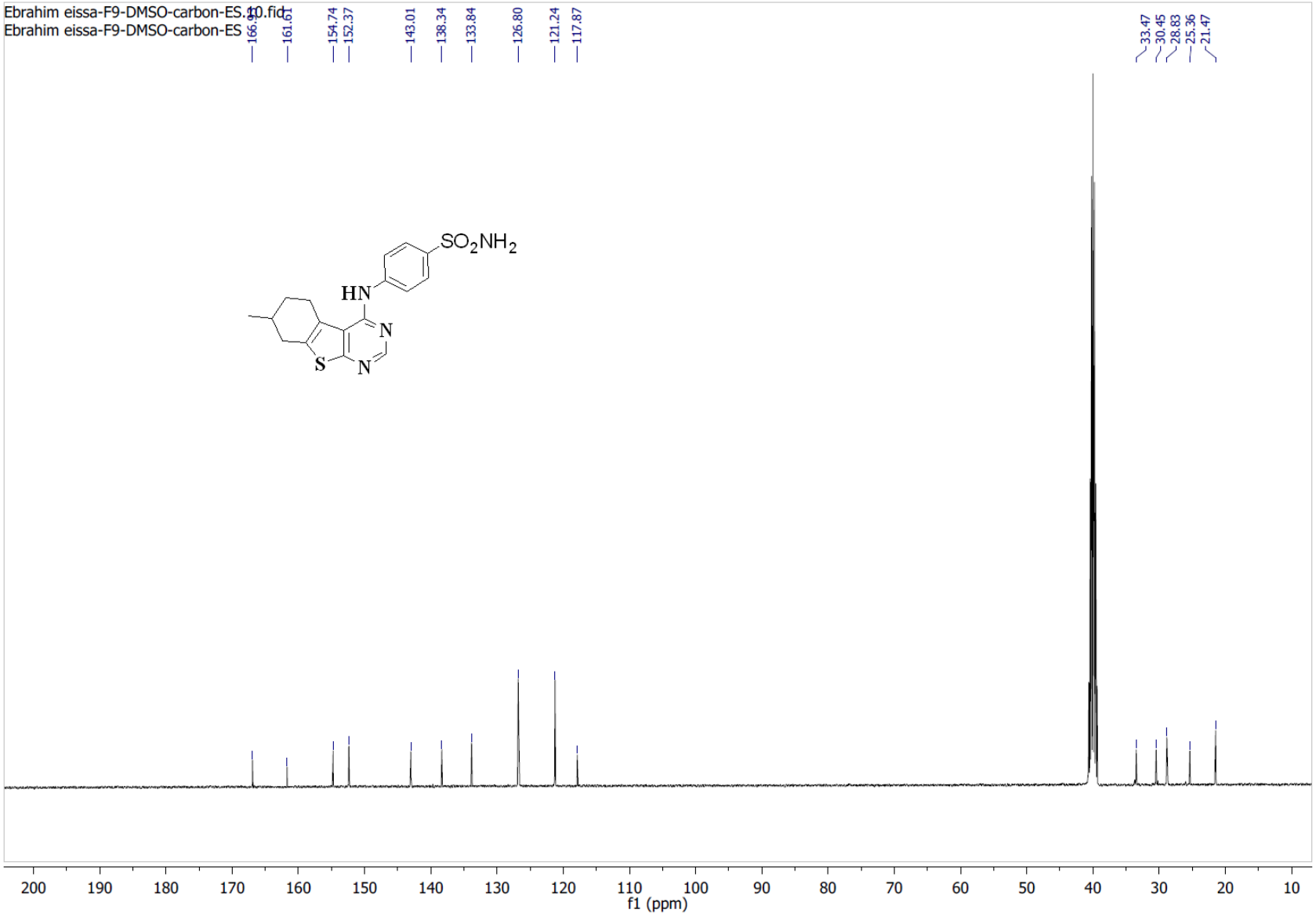

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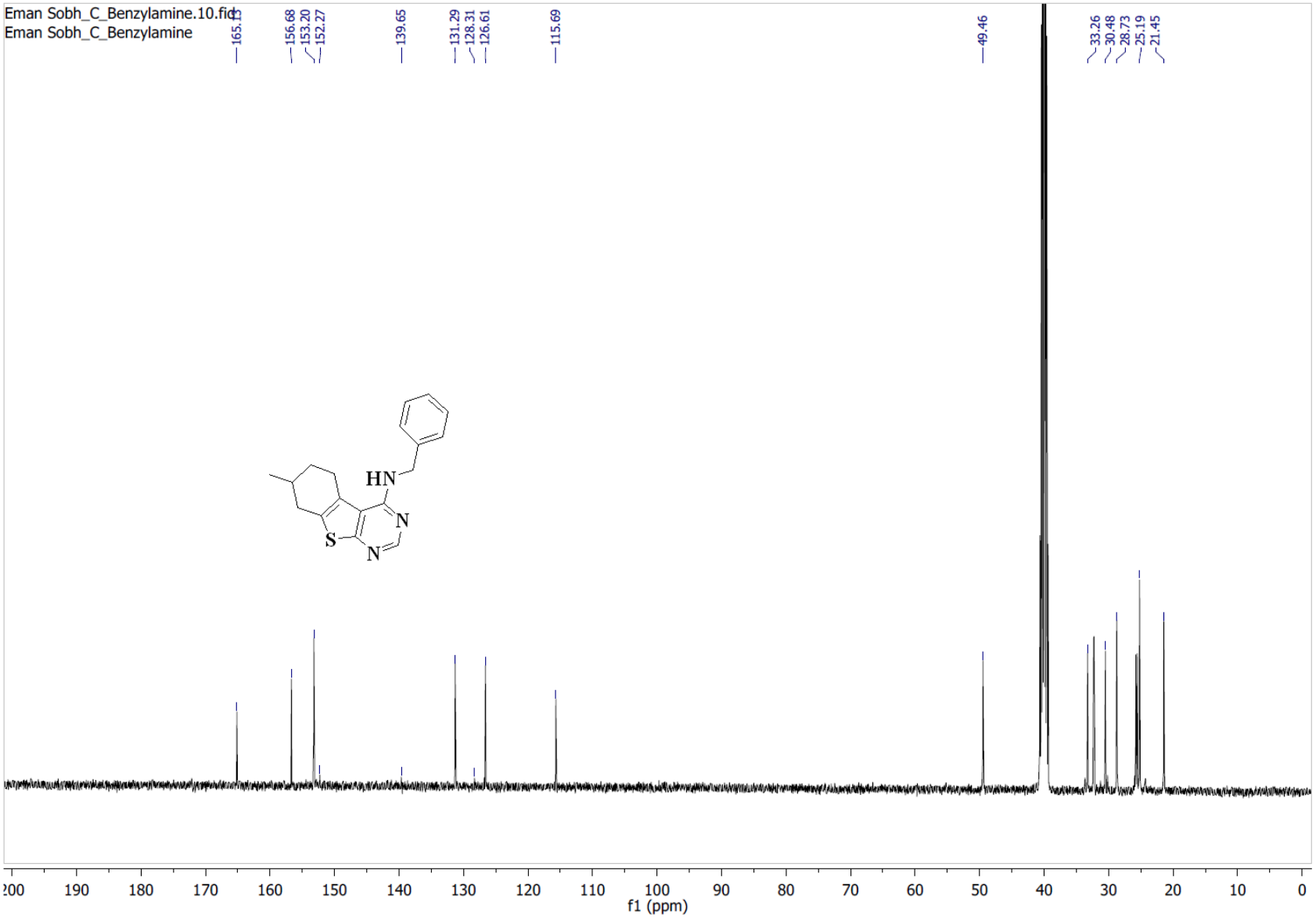

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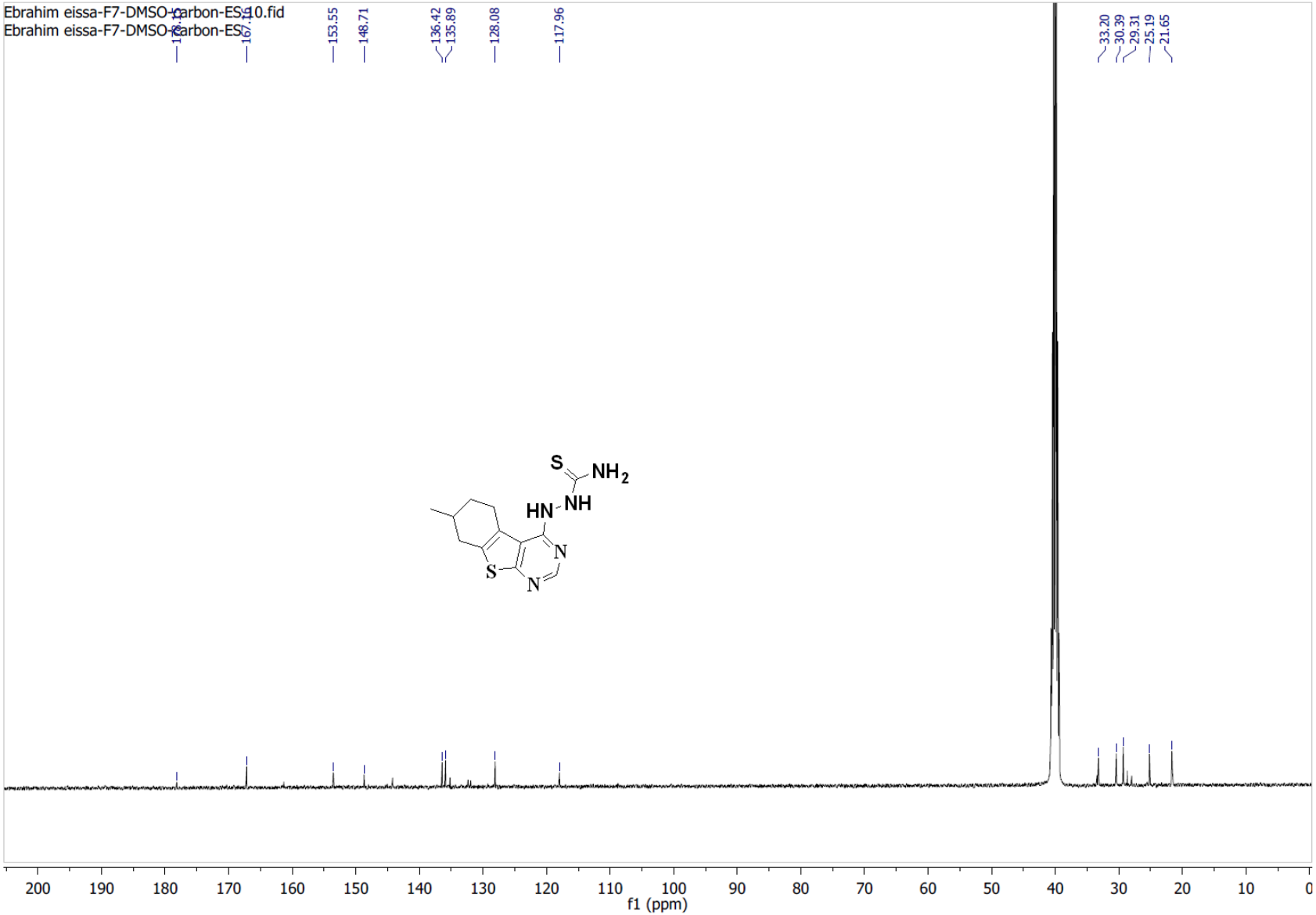

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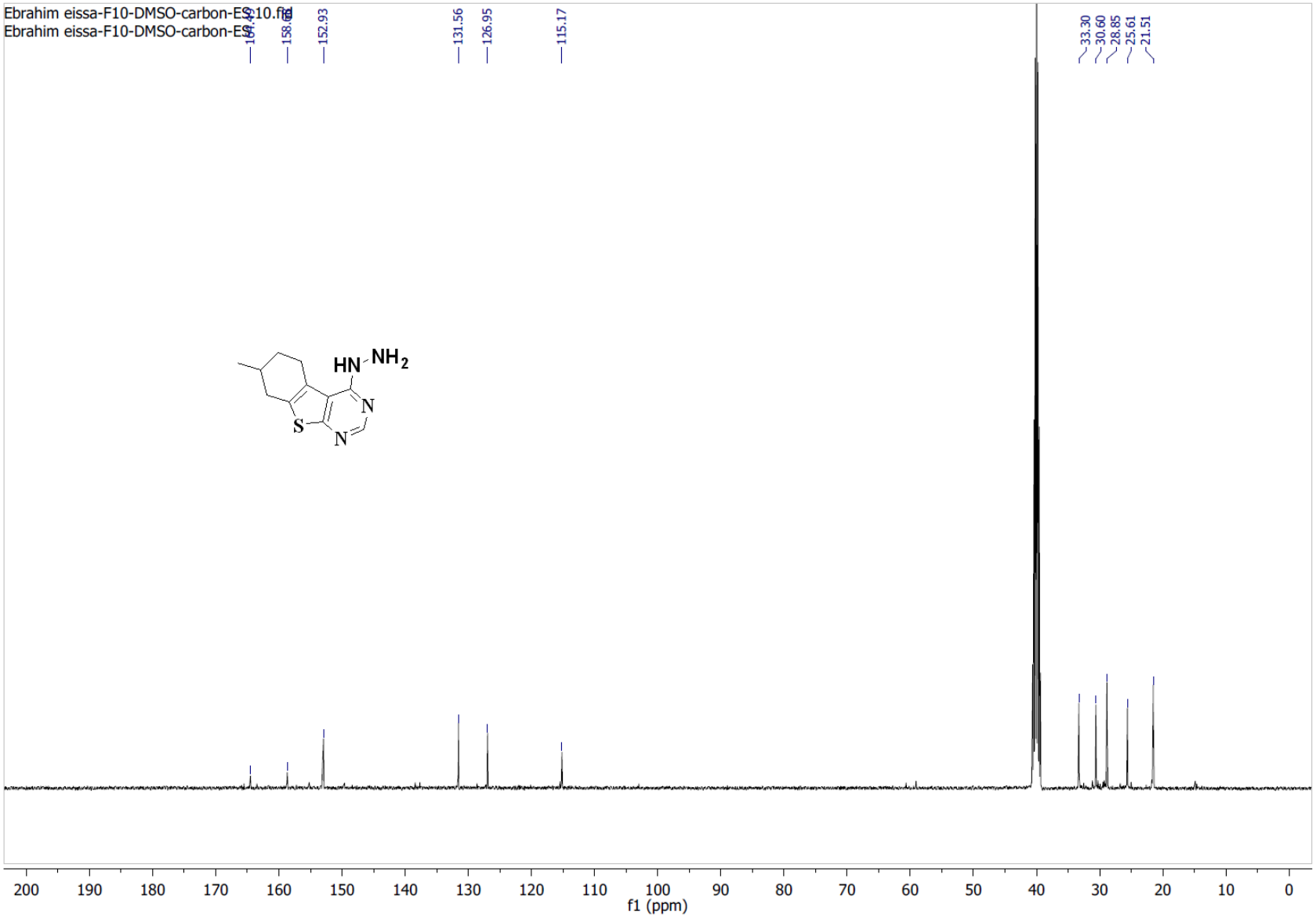

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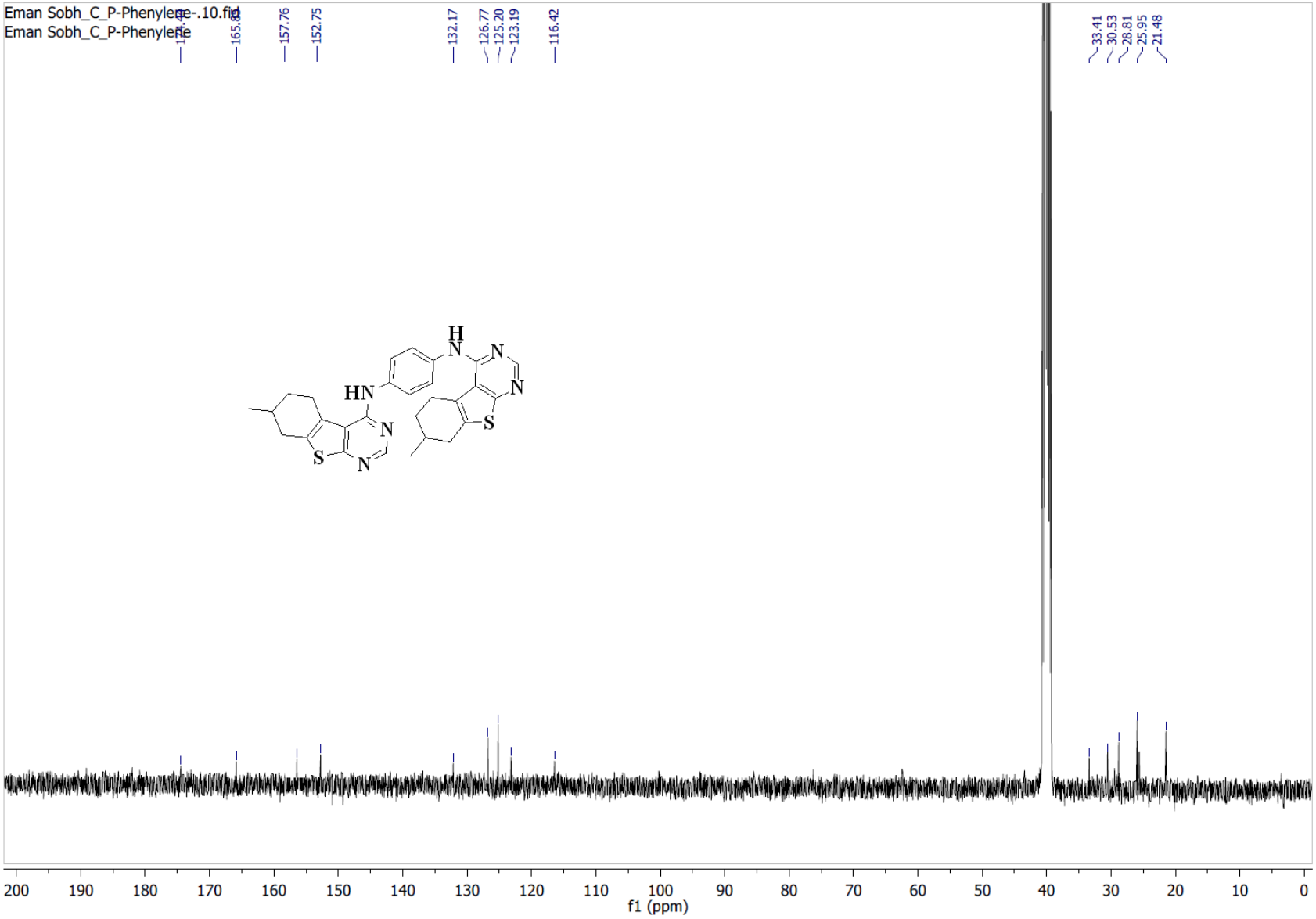
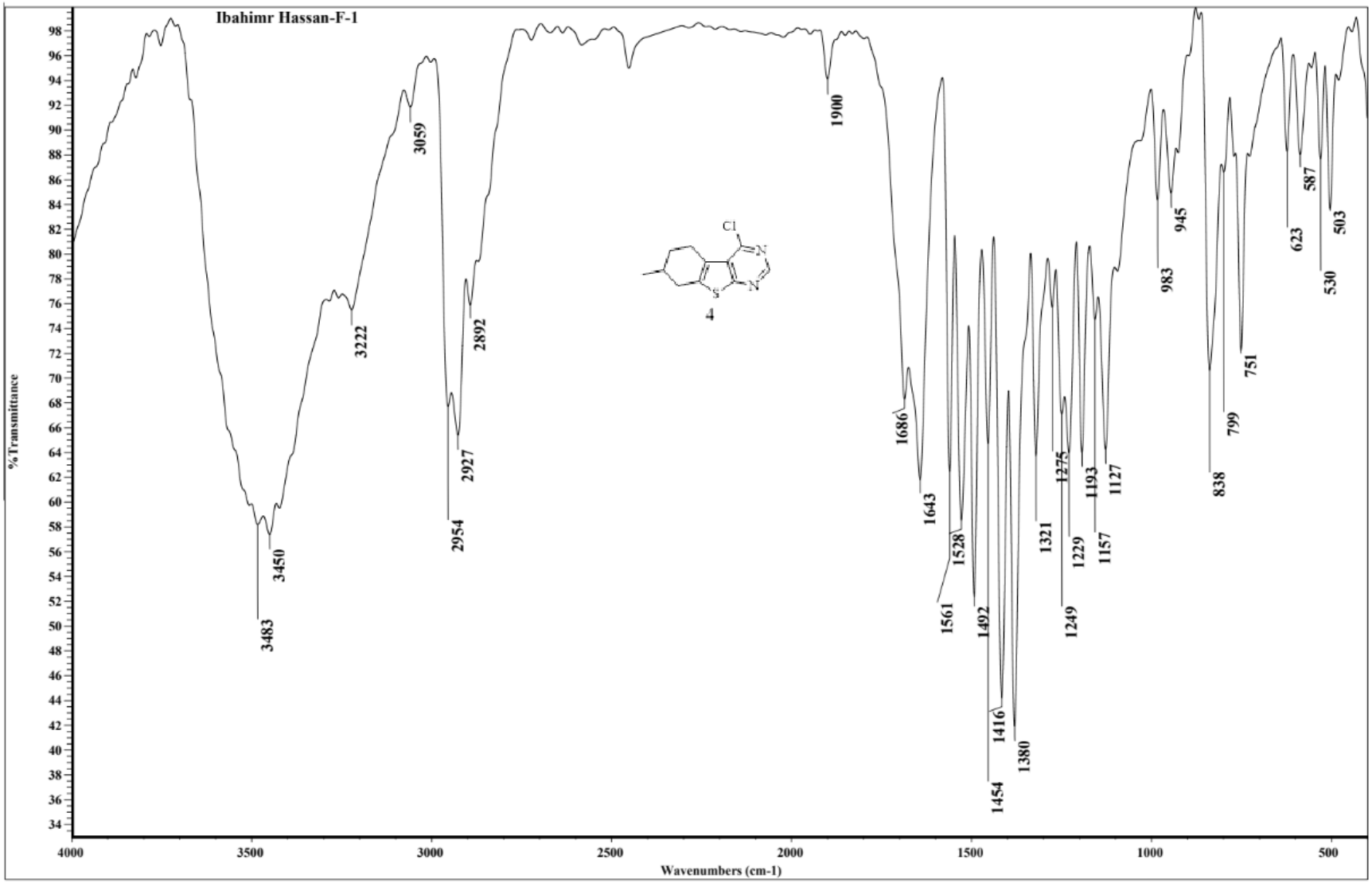
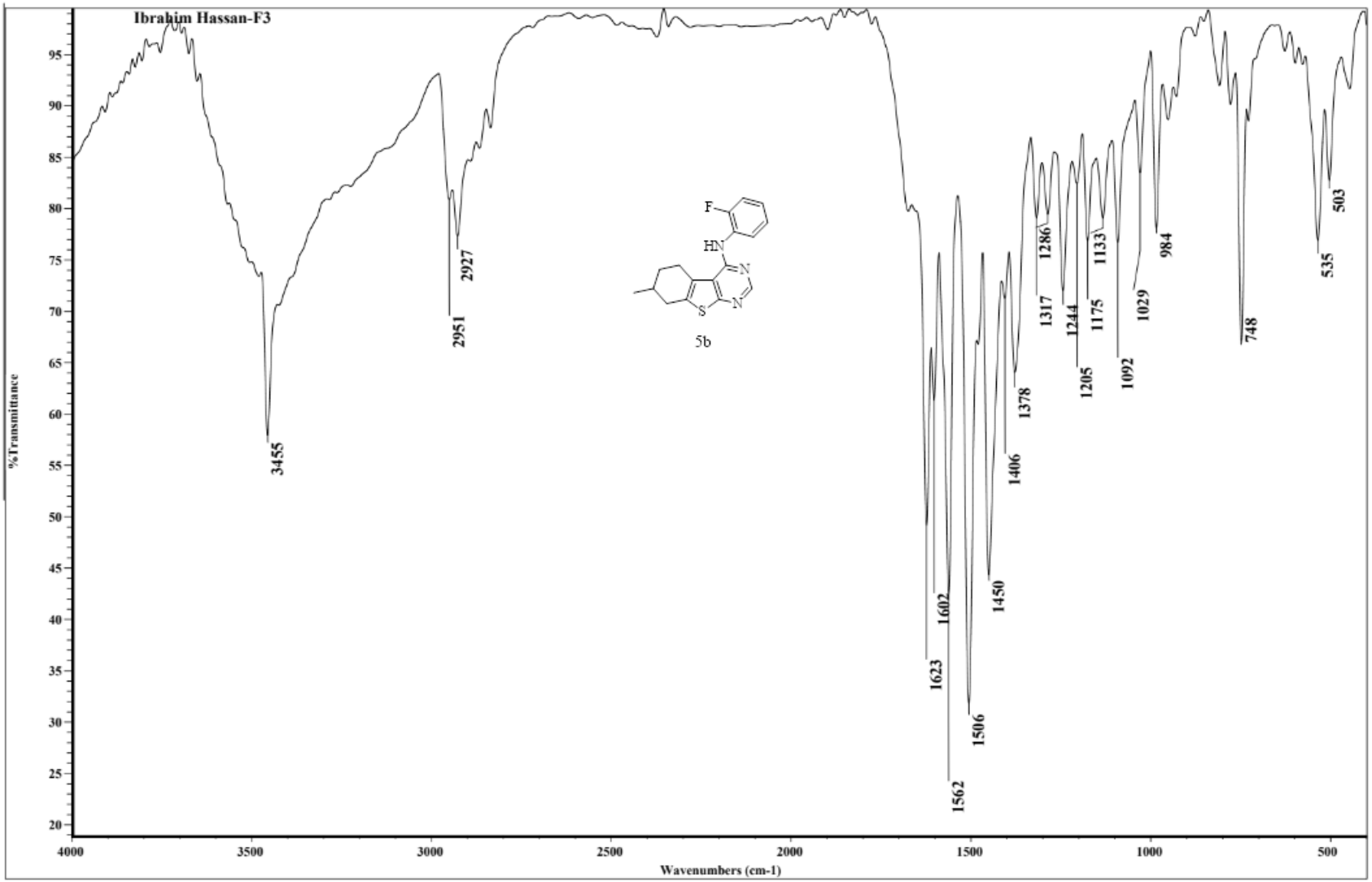


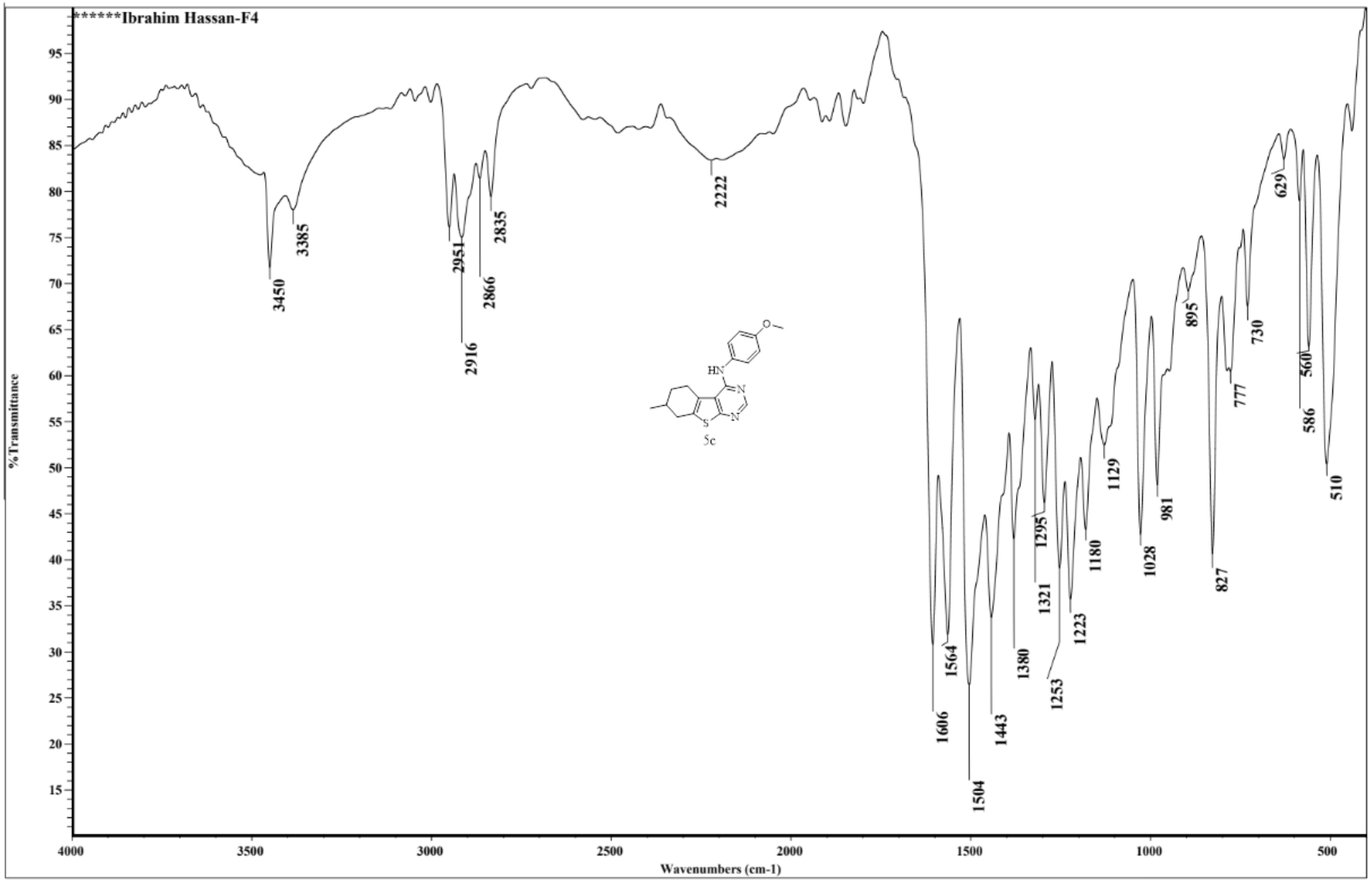
IR spectra of compound 4



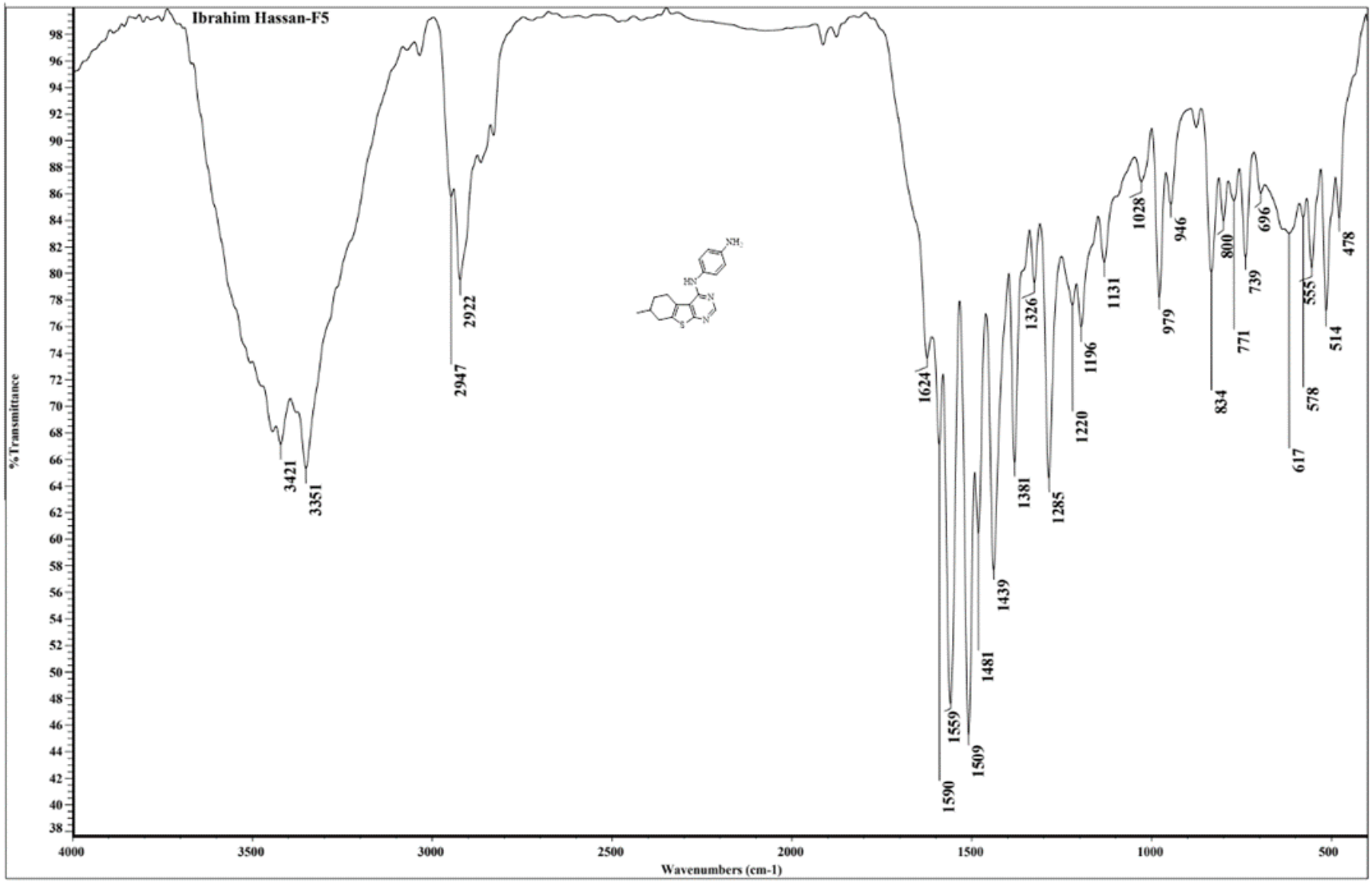
IR spectra of compound 5b



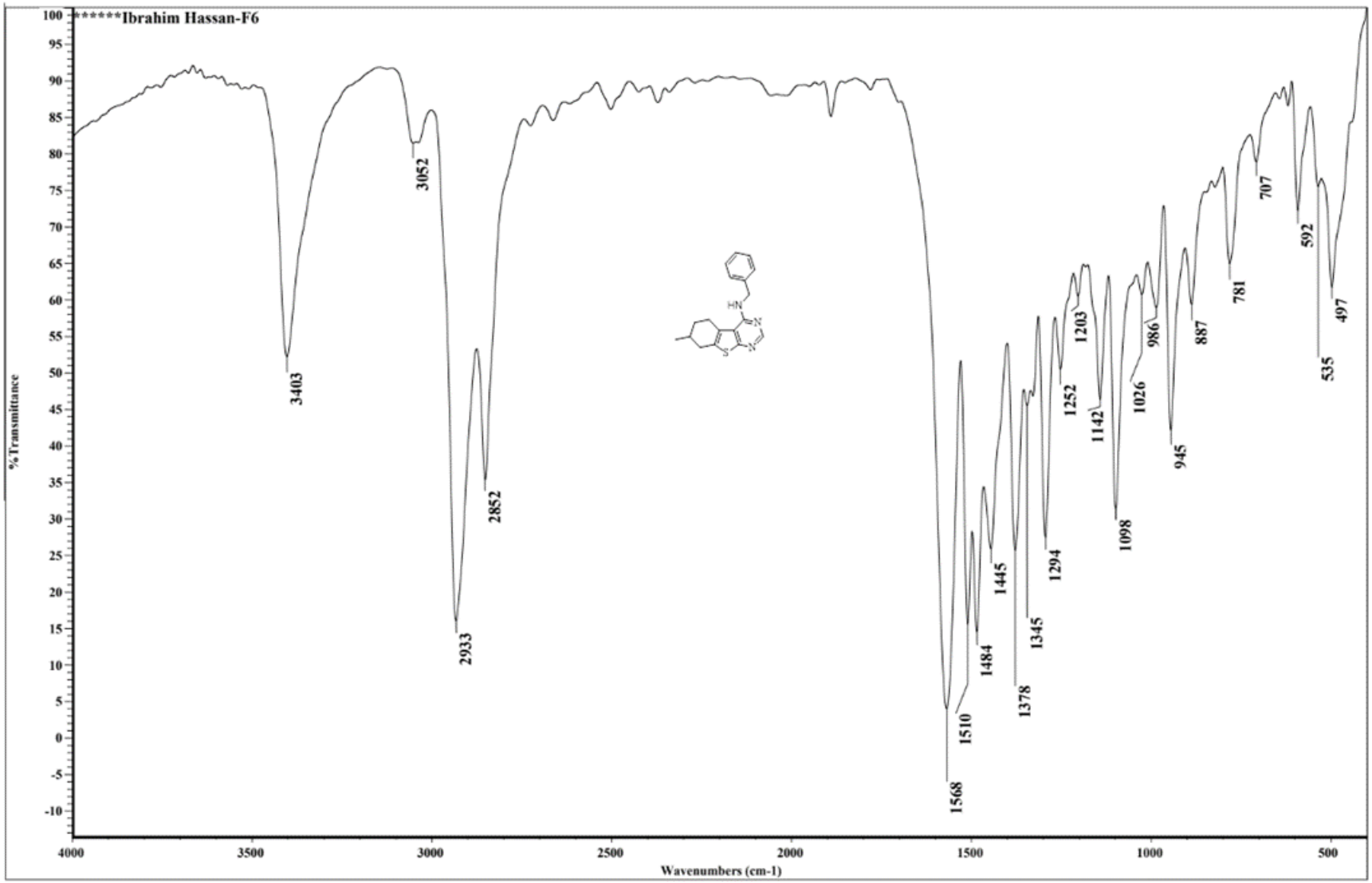
IR spectra of compound 5c



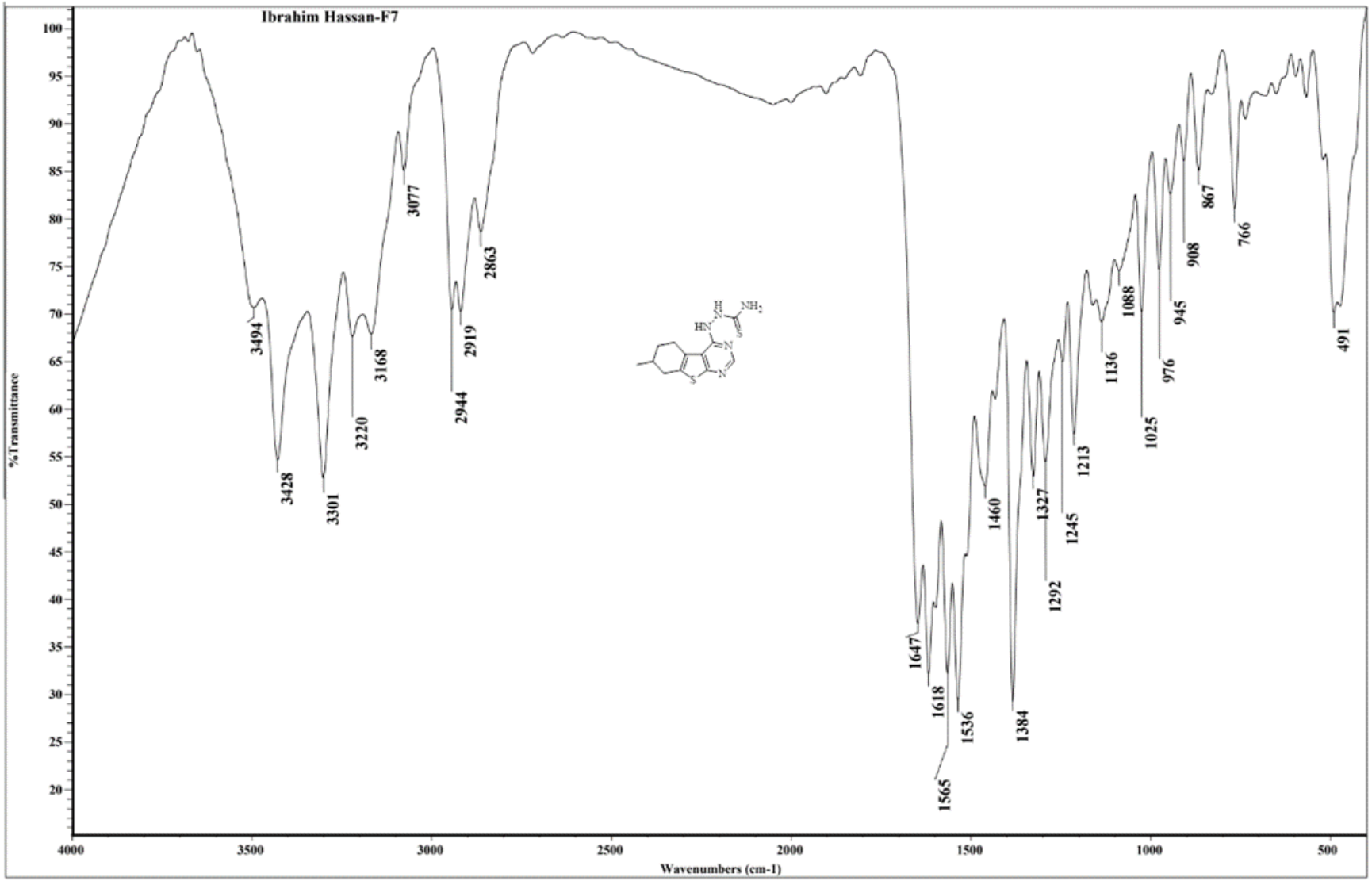
IR spectra of compound 5d



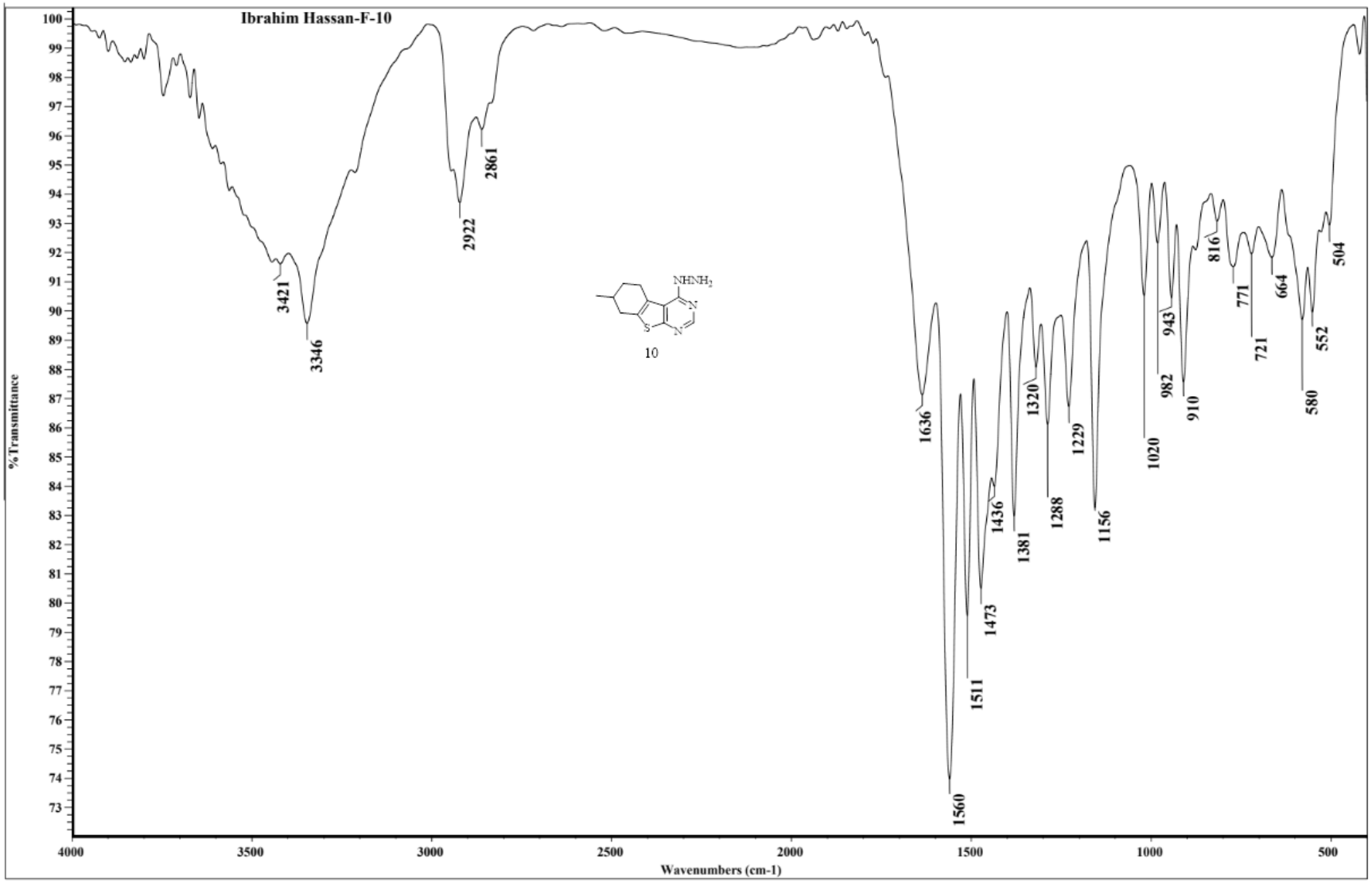
IR spectra of compound 6



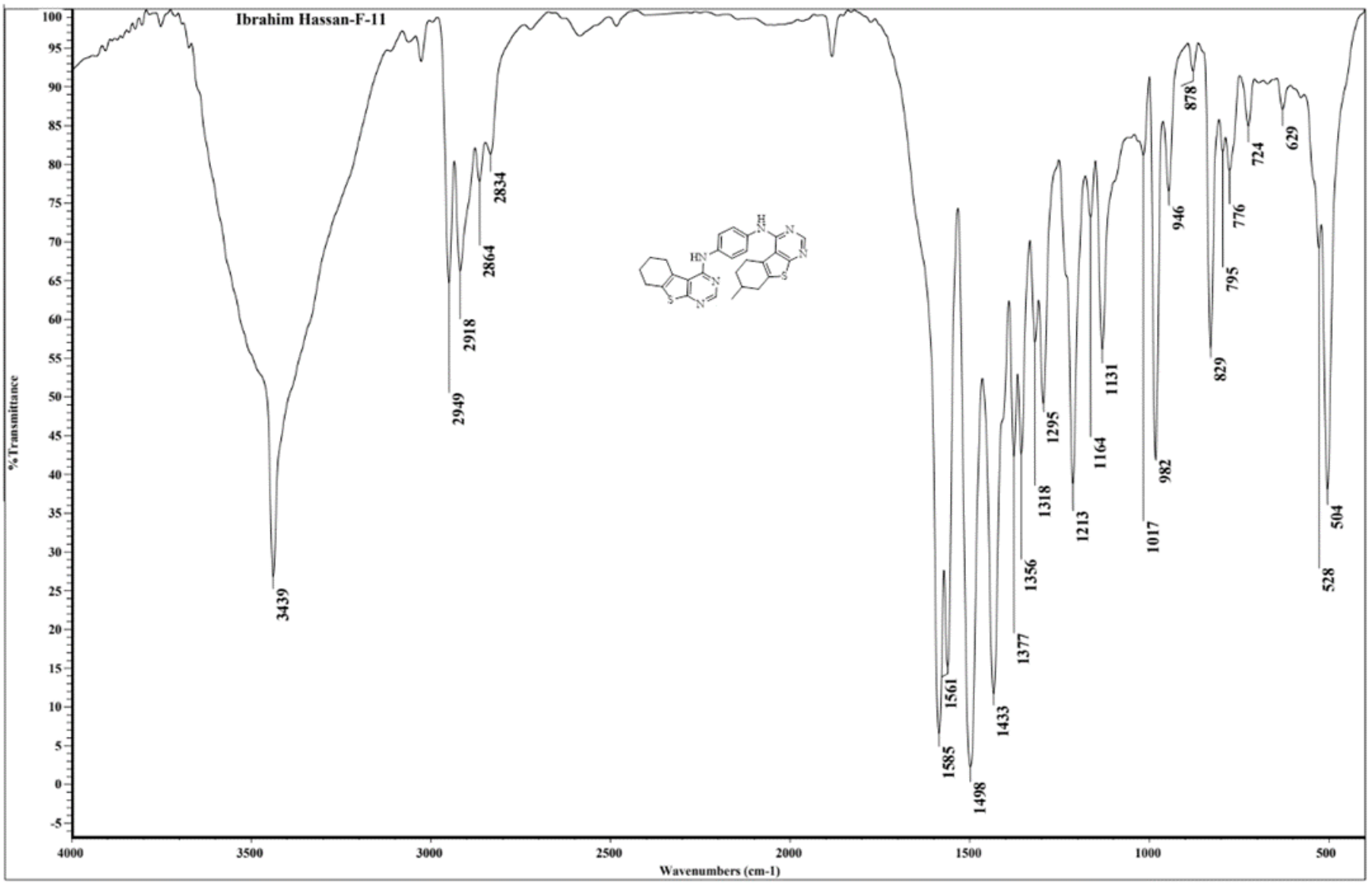
IR spectra of compound 7a



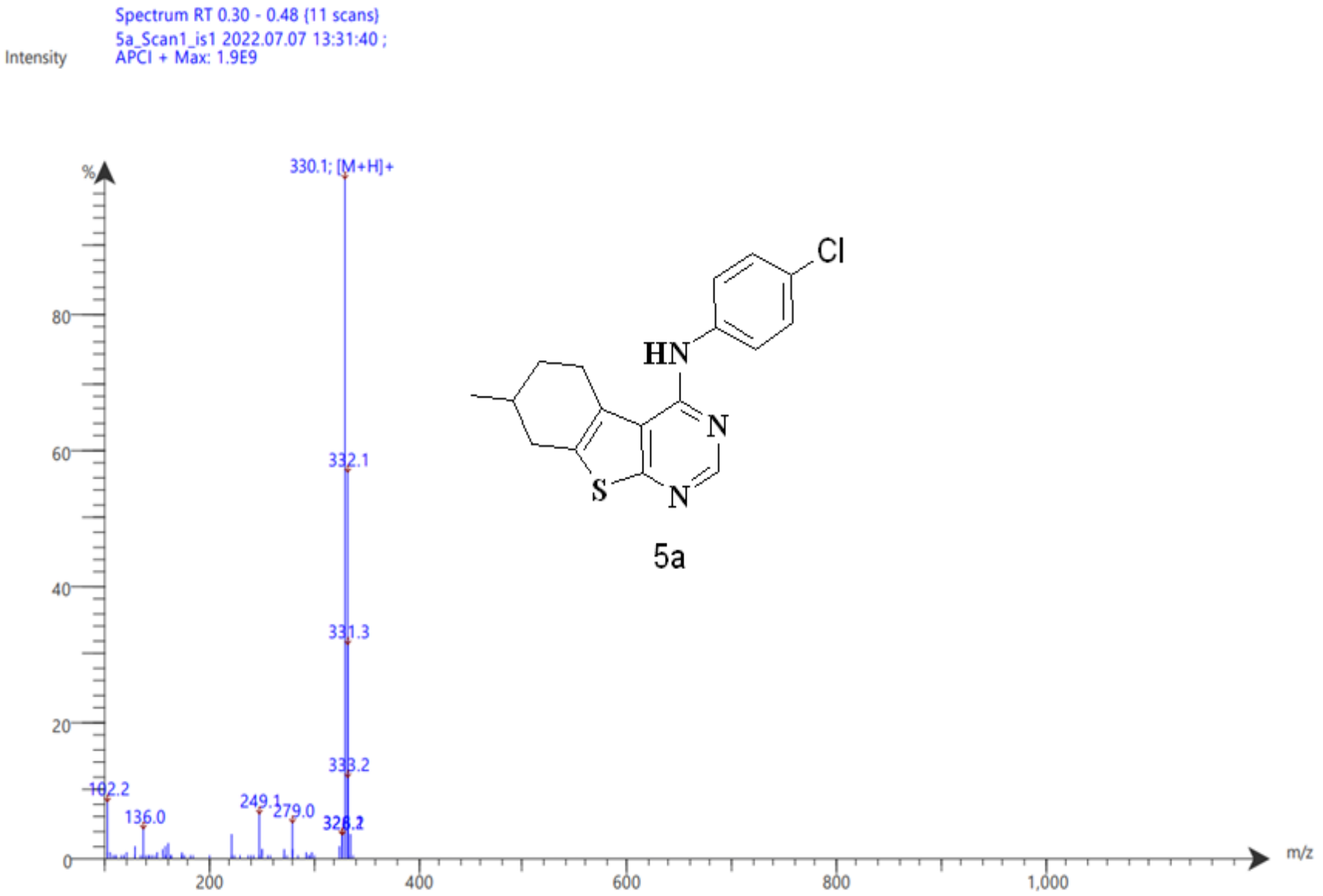
IR spectra of compound 7b



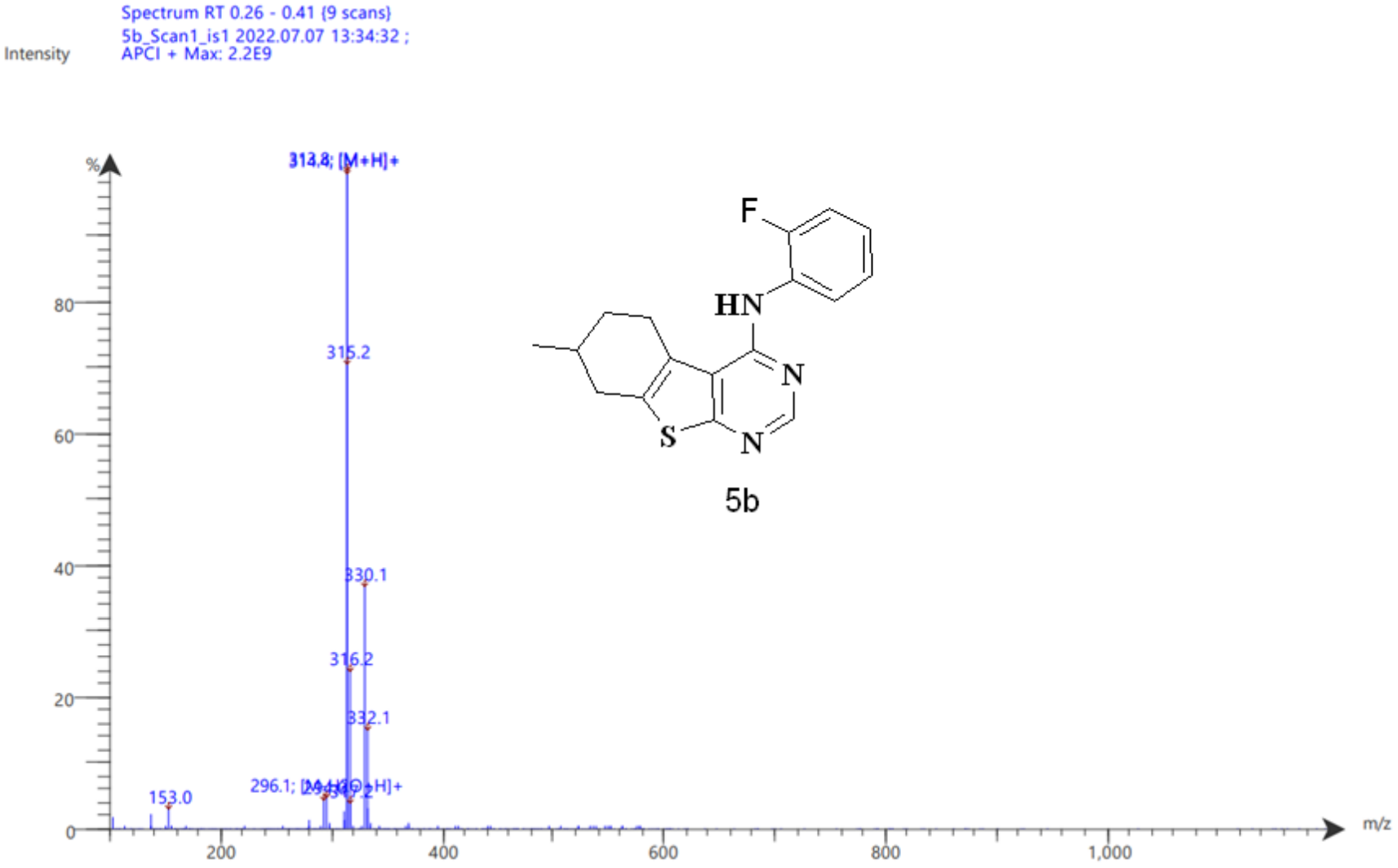
IR spectra of compound 8



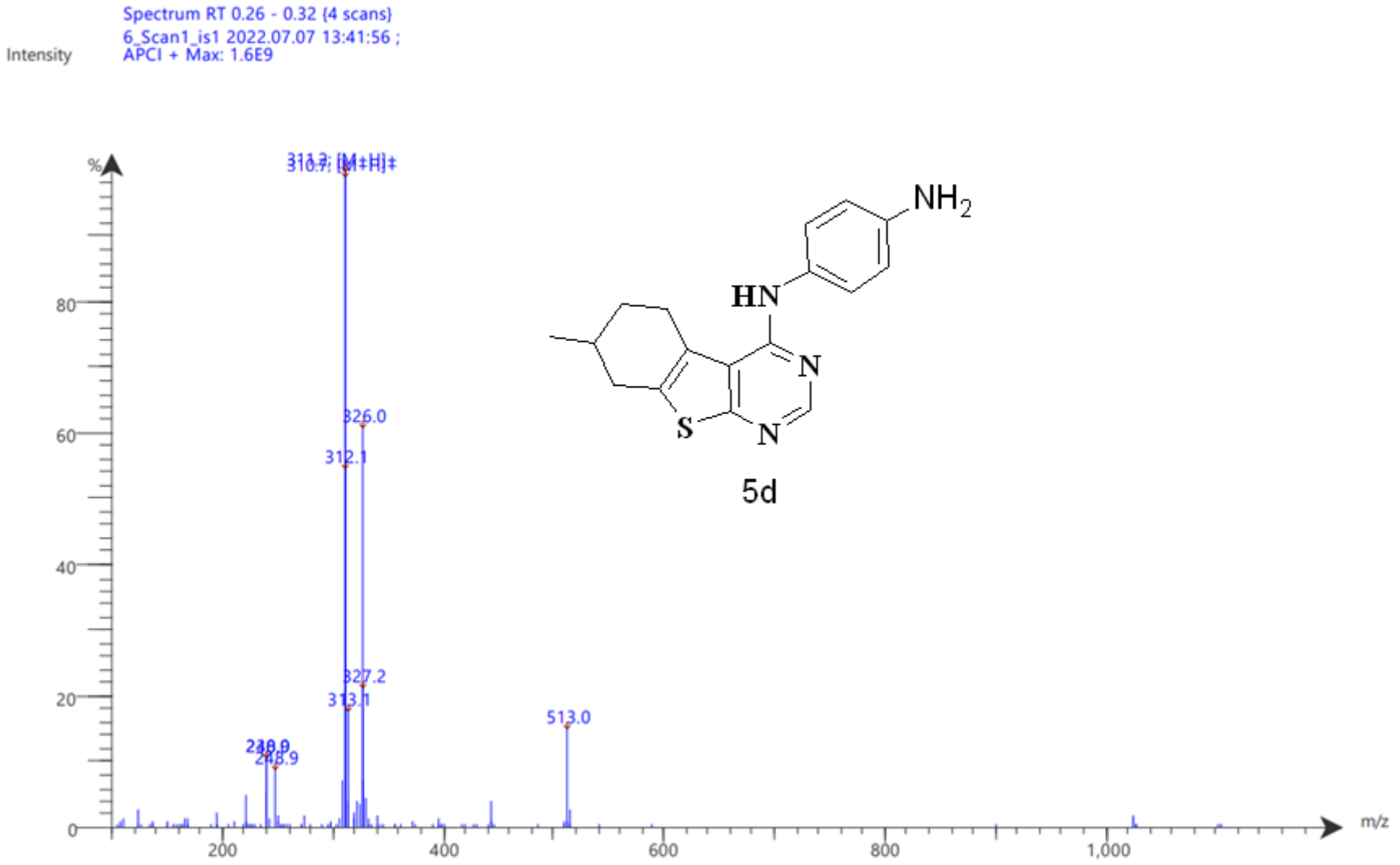
Mass spectra of compound 5a



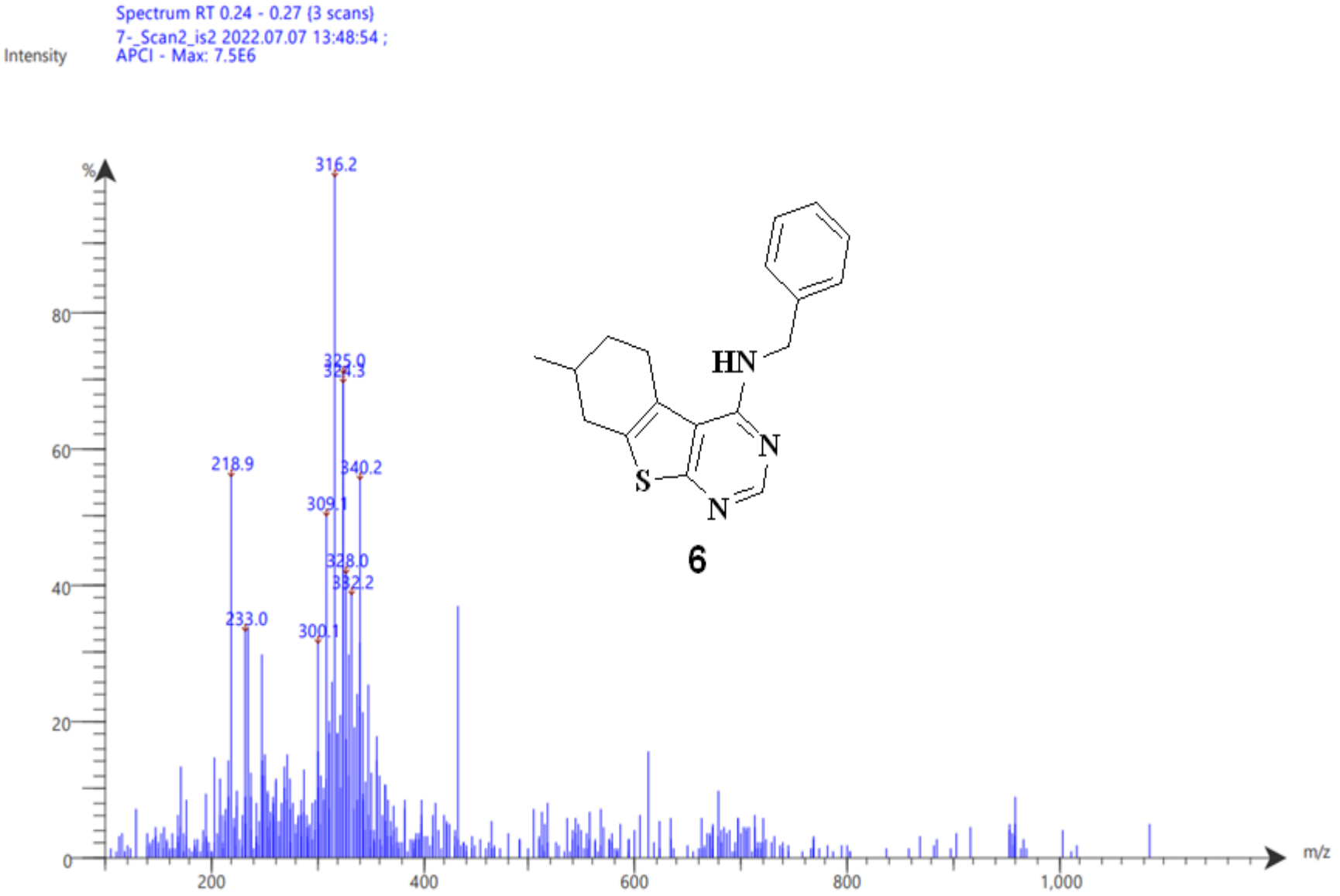
Mass spectra of compound 5b



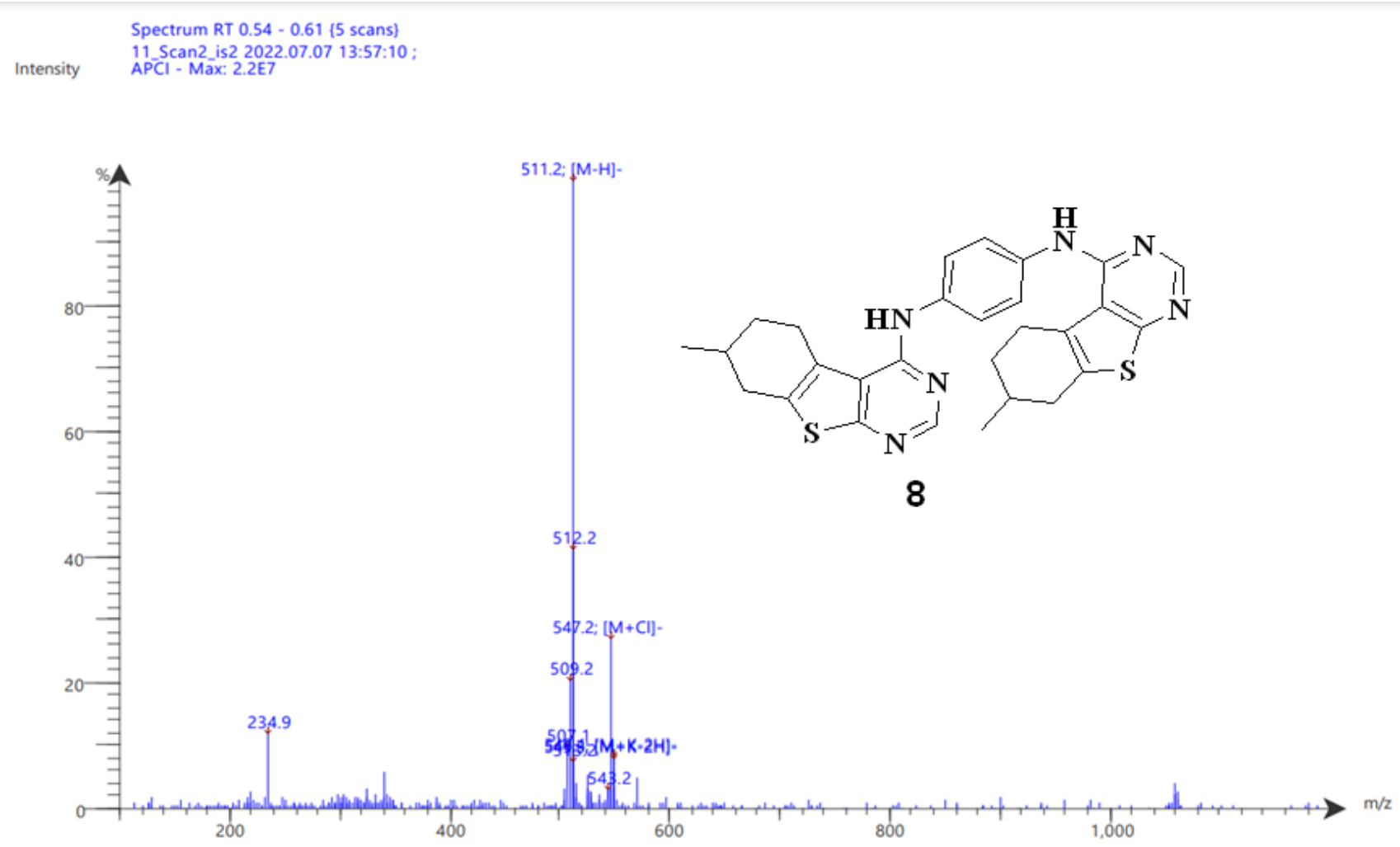
Mass spectra of compound 5d



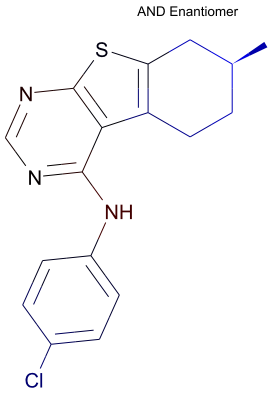
Mass spectra of compound 6



Mass spectra of compound 8



TOPKAT_Ames_Mutagenicity



$C_{17}H_{16}ClN_3S$

Molecular Weight: 329.84704

ALogP: 5.5

Rotatable Bonds: 2

Acceptors: 3

Donors: 1

Model Prediction

Prediction: Non-Mutagen

Probability: 0.612

Enrichment: 1.1

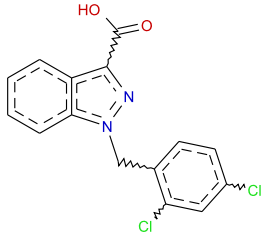
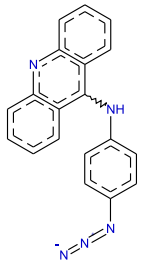
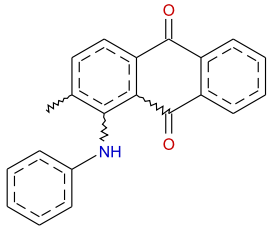
Bayesian Score: -4.69

Mahalanobis Distance: 9.56

Mahalanobis Distance p-value: 0.558

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	50264-69-2	89873-24-5	4947-27-7
Structure			
Actual Endpoint	Non-Mutagen	Mutagen	Mutagen
Predicted Endpoint	Non-Mutagen	Mutagen	Mutagen
Distance	0.555	0.557	0.559
Reference	Kazius et. al., J. Med. Chem. (2005) 48, 312-320	Kazius et. al., J. Med. Chem. (2005) 48, 312-320	Kazius et. al., J. Med. Chem. (2005) 48, 312-320

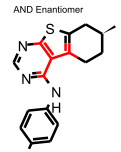
Model Applicability

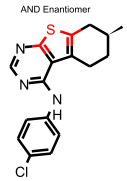
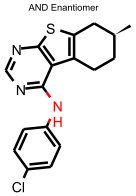
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

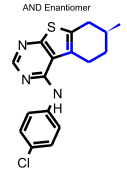
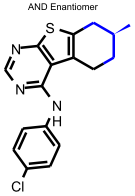
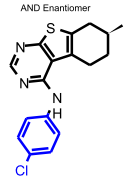
Feature Contribution

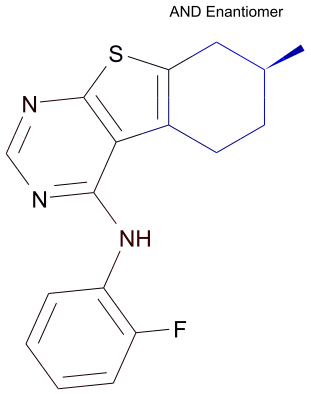
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Mutagen in training set
SCFP_12	112346096	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.36	1035 out of 1263

SCFP_12	1310748454	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.312	126 out of 161
SCFP_12	10	 [*]N[*]	0.306	1774 out of 2287

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Mutagen in training set
SCFP_12	-55982834	 [*:[c]1:[*]C[C@@H](C)CC1	-1.82	0 out of 9
SCFP_12	-1043339860	 [*]CC(C)C[*]	-1.09	76 out of 399
SCFP_12	1905487031	 [*][c]1:[cH]:[cH]:[c](Cl):[cH]:[cH]:1	-0.59	23 out of 74



$C_{17}H_{16}FN_3S$

Molecular Weight: 313.39244

ALogP: 5.041

Rotatable Bonds: 2

Acceptors: 3

Donors: 1

Model Prediction

Prediction: Non-Mutagen

Probability: 0.678

Enrichment: 1.21

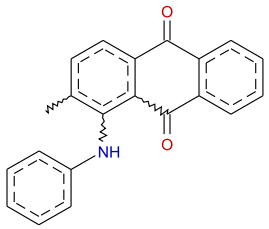
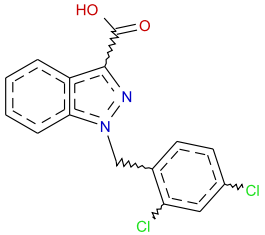
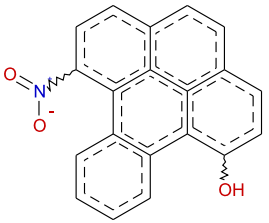
Bayesian Score: -2.6

Mahalanobis Distance: 10.9

Mahalanobis Distance p-value: 0.0403

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	4947-27-7	50264-69-2	115664-51-2
Structure			
Actual Endpoint	Mutagen	Non-Mutagen	Mutagen
Predicted Endpoint	Mutagen	Non-Mutagen	Mutagen
Distance	0.539	0.546	0.546
Reference	Kazius et. al., J. Med. Chem. (2005) 48, 312-320	Kazius et. al., J. Med. Chem. (2005) 48, 312-320	Kazius et. al., J. Med. Chem. (2005) 48, 312-320

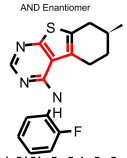
Model Applicability

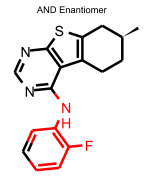
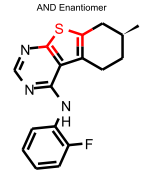
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

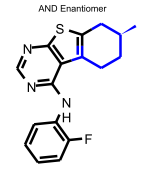
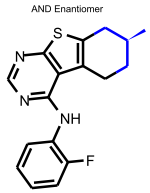
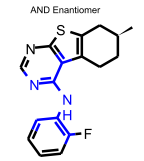
Feature Contribution

Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Mutagen in training set
SCFP_12	112346096	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.36	1035 out of 1263

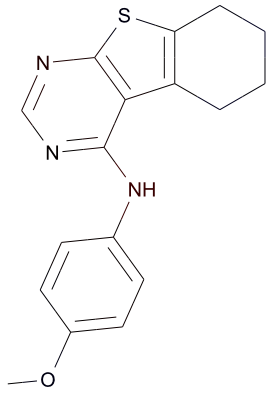
SCFP_12	-1551011249	 [*]N[c]1:[cH]:[*]:[cH]:[cH]:[c]:1F	0.322	13 out of 16
SCFP_12	1310748454	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.312	126 out of 161

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Mutagen in training set
SCFP_12	-55982834	 [*:[c]1:[*]C[C@@H](C)CC1	-1.82	0 out of 9
SCFP_12	-1043339860	 [*]CC(C)C[*]	-1.09	76 out of 399
SCFP_12	1328855840	 [*]:[cH]:[c](N[c](:n:[*]):[c](:[*]):[*]):[cH]:[*]	-0.496	1 out of 4

5c

TOPKAT_Ames_Mutagenicity



$C_{17}H_{17}N_3OS$

Molecular Weight: 311.40138

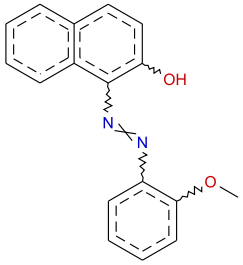
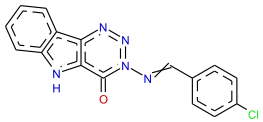
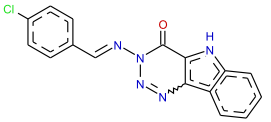
ALogP: 4.568

Rotatable Bonds: 3

Acceptors: 4

Donors: 1

Structural Similar Compounds

Name	1229-55-6	3-(4'-Chlorobenzylidenamino)-5H-1;2;3-triazin-[5;4b]indol-4-one	135086-93-0
Structure			
Actual Endpoint	Mutagen	Mutagen	Mutagen
Predicted Endpoint	Mutagen	Mutagen	Mutagen
Distance	0.539	0.540	0.540
Reference	Kazius et. al., J. Med. Chem. (2005) 48, 312-320	Mutagenesis 7(1):37-39; 1992	Kazius et. al., J. Med. Chem. (2005) 48, 312-320

Model Prediction

Prediction: Mutagen

Probability: 0.76

Enrichment: 1.36

Bayesian Score: 1.2

Mahalanobis Distance: 7.63

Mahalanobis Distance p-value: 0.999

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

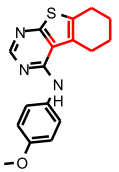
Model Applicability

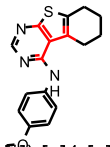
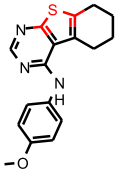
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

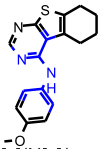
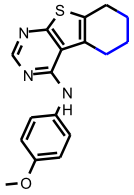
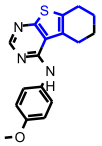
Feature Contribution

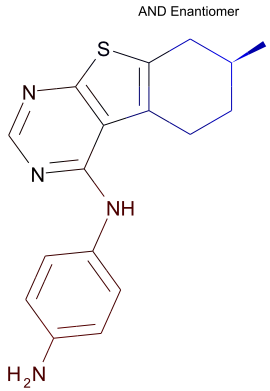
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Mutagen in training set
SCFP_12	-1825024803	 [*]:[c]1:[*]:[*]:[c]2 CCCC[c]:1:2	0.472	18 out of 19

SCFP_12	112346096	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.36	1035 out of 1263
SCFP_12	1310748454	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.312	126 out of 161

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Mutagen in training set
SCFP_12	1328855840	 [*]:[cH]:[c](N[c](:n:[*]):[c](:[*]):[*]):[cH]:[*]	-0.496	1 out of 4
SCFP_12	-1272798659	 [*]CCC([*])[*]	-0.466	439 out of 1225
SCFP_12	815479470	 [*][C@H]1[*]C[c]2:[c](C1):s:[c](:[*]):[c]:2:[*]	-0.452	0 out of 1



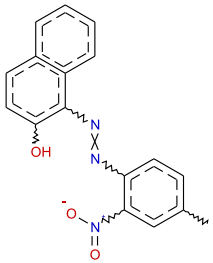
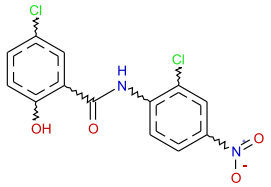
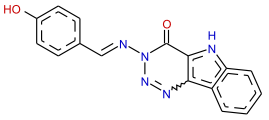
$C_{17}H_{18}N_4S$
Molecular Weight: 310.41662
ALogP: 4.089
Rotatable Bonds: 2
Acceptors: 4
Donors: 2

Model Prediction

Prediction: Non-Mutagen
Probability: 0.725
Enrichment: 1.3
Bayesian Score: -0.687
Mahalanobis Distance: 9.01
Mahalanobis Distance p-value: 0.823

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	2425-85-6	50-65-7	139953-76-7
Structure			
Actual Endpoint	Mutagen	Mutagen	Mutagen
Predicted Endpoint	Mutagen	Mutagen	Mutagen
Distance	0.557	0.557	0.562
Reference	Helma, C., Cramer, T., Kramer, S., and De Raedt, L., J. Chem. Inf. Comput. Sci., 2004, pp. 1402-1411	Kazius et. al., J. Med. Chem. (2005) 48, 312-320	Kazius et. al., J. Med. Chem. (2005) 48, 312-320

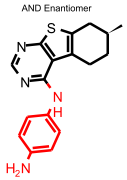
Model Applicability

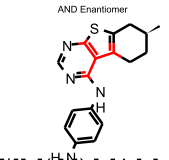
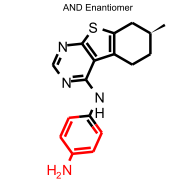
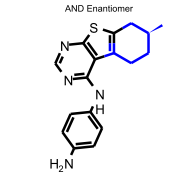
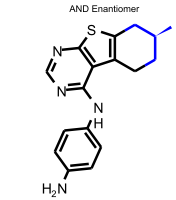
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

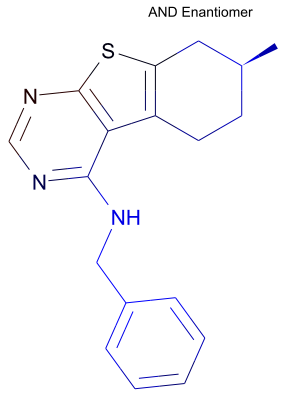
1. All properties and OPS components are within expected ranges.

Feature Contribution

Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Mutagen in training set
SCFP_12	-1728149235	 [*]N[c]1:[cH]:[cH]:[c](N):[cH]:[cH]:1	0.442	21 out of 23

SCFP_12	112346096	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.36	1035 out of 1263
SCFP_12	-192131231	 N[c]1:[cH]:[cH]:[*]:[cH]:[cH]:1	0.318	192 out of 244
Top Features for negative contribution				
Fingerprint	**Bit/Smiles**	**Feature Structure**	**Score**	**Mutagen in training set**
SCFP_12	-55982834	 [*:[c]1:[*]C[C@@H](C)CC1	-1.82	0 out of 9
SCFP_12	-1043339860	 [*]CC(C)C[*]	-1.09	76 out of 399
SCFP_12	1328855840	 [*]:[cH]:[c](N[c](:n:[*]):[c](:[*]):[*]):[cH]:[*]	-0.496	1 out of 4



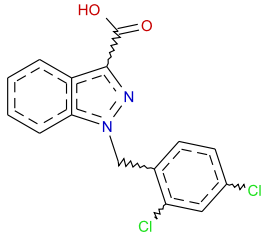
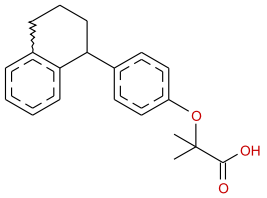
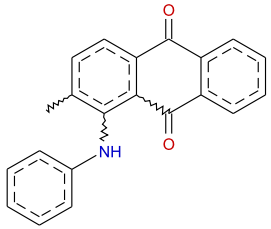
$C_{18}H_{19}N_3S$
Molecular Weight: 309.42856
ALogP: 4.678
Rotatable Bonds: 3
Acceptors: 3
Donors: 1

Model Prediction

Prediction: Non-Mutagen
Probability: 0.473
Enrichment: 0.848
Bayesian Score: -8.11
Mahalanobis Distance: 8.95
Mahalanobis Distance p-value: 0.843

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	50264-69-2	3771-19-5	4947-27-7
Structure			
Actual Endpoint	Non-Mutagen	Non-Mutagen	Mutagen
Predicted Endpoint	Non-Mutagen	Non-Mutagen	Mutagen
Distance	0.501	0.554	0.557
Reference	Kazius et. al., J. Med. Chem. (2005) 48, 312-320	Kazius et. al., J. Med. Chem. (2005) 48, 312-320	Kazius et. al., J. Med. Chem. (2005) 48, 312-320

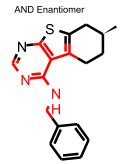
Model Applicability

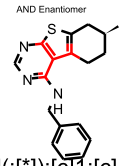
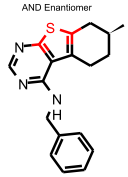
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

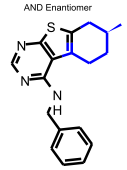
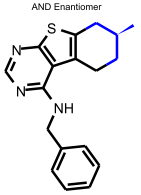
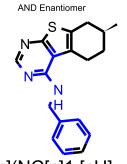
Feature Contribution

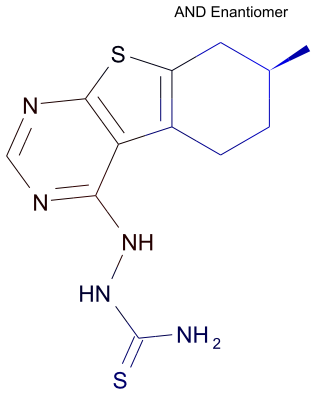
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Mutagen in training set
SCFP_12	-1231050790	 [*]CN[c]1:n:[cH]:[*]:[c]2:[*]:[*]:[c]([*]):[c]:1:2	0.388	3 out of 3

SCFP_12	112346096	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.36	1035 out of 1263
SCFP_12	1310748454	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.312	126 out of 161

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Mutagen in training set
SCFP_12	-55982834	 [*:[c]1:[*]C[C@@H](C)CC1	-1.82	0 out of 9
SCFP_12	-1043339860	 [*]CC(C)C[*]	-1.09	76 out of 399
SCFP_12	227993601	 [*]:n:[c](NC[c]1:[cH]:[cH]:[*]:[cH]:[cH]:1):[c](:[*]):[*]	-0.998	0 out of 3



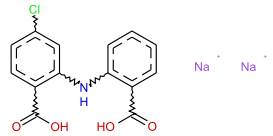
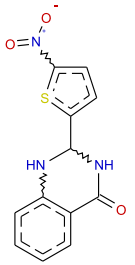
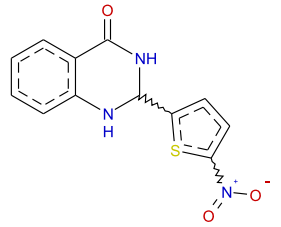
$C_{12}H_{15}N_5S_2$
Molecular Weight: 293.411
ALogP: 3.209
Rotatable Bonds: 3
Acceptors: 4
Donors: 3

Model Prediction

Prediction: Non-Mutagen
Probability: 0.608
Enrichment: 1.09
Bayesian Score: -4.8
Mahalanobis Distance: 13.4
Mahalanobis Distance p-value: 2.93e-007

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	64808-48-6	2;3-DIHYDRO-2-(5-NITRO-2-THIENYL)-4-QUINAZOLINE	33389-33-2
Structure			
Actual Endpoint	Non-Mutagen	Mutagen	Mutagen
Predicted Endpoint	Non-Mutagen	Mutagen	Mutagen
Distance	0.611	0.615	0.616
Reference	Kazius et. al., J. Med. Chem. (2005) 48, 312-320	EMIC	Kazius et. al., J. Med. Chem. (2005) 48, 312-320

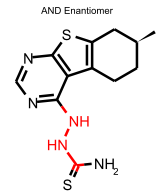
Model Applicability

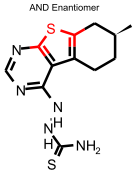
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

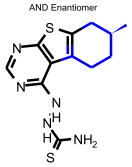
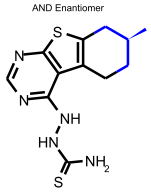
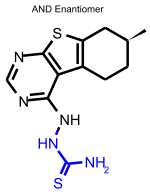
Feature Contribution

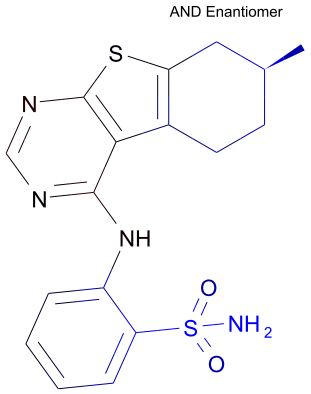
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Mutagen in training set
SCFP_12	-1848869096	 [*]NNC(=[*])[*]	0.38	18 out of 21

SCFP_12	112346096	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.36	1035 out of 1263
SCFP_12	1310748454	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.312	126 out of 161

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Mutagen in training set
SCFP_12	-55982834	 [*:[c]1:[*]C[C@@H](C)CC1	-1.82	0 out of 9
SCFP_12	-1043339860	 [*]CC(C)C[*]	-1.09	76 out of 399
SCFP_12	382734644	 [*]NC(=S)N	-0.811	3 out of 14



$C_{17}H_{18}N_4O_2S_2$

Molecular Weight: 374.48042

ALogP: 3.541

Rotatable Bonds: 3

Acceptors: 5

Donors: 2

Model Prediction

Prediction: Non-Mutagen

Probability: 0.423

Enrichment: 0.757

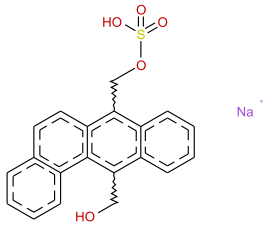
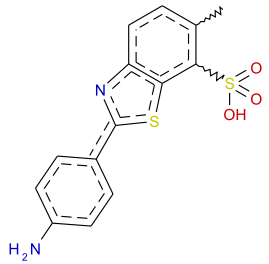
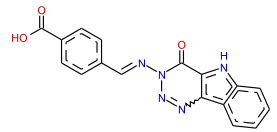
Bayesian Score: -9.21

Mahalanobis Distance: 11.8

Mahalanobis Distance p-value: 0.00178

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	98644-23-6	130-17-6	139953-77-8
Structure			
Actual Endpoint	Mutagen	Mutagen	Mutagen
Predicted Endpoint	Mutagen	Mutagen	Mutagen
Distance	0.534	0.565	0.567
Reference	Kazius et. al., J. Med. Chem. (2005) 48, 312-320	Kazius et. al., J. Med. Chem. (2005) 48, 312-320	Kazius et. al., J. Med. Chem. (2005) 48, 312-320

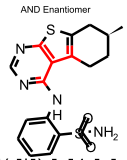
Model Applicability

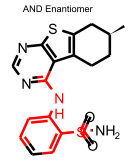
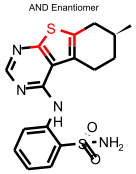
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

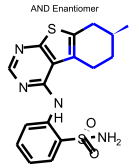
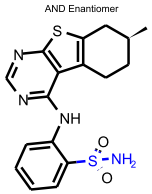
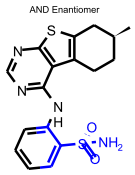
Feature Contribution

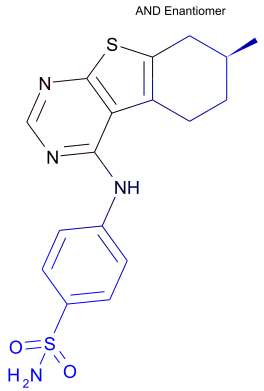
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Mutagen in training set
SCFP_12	112346096	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.36	1035 out of 1263

SCFP_12	896331226	 [*]S(=[*])(=[*])[c]1:[cH]:[*]:[cH]:[cH]:[c]:1N[c](:[*]):[*]	0.337	6 out of 7
SCFP_12	1310748454	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.312	126 out of 161

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Mutagen in training set
SCFP_12	-55982834	 [*:[c]1:[*]C[C@@H](C)CC1	-1.82	0 out of 9
SCFP_12	-1358544872	 [*]S(=[*])(=[*])N	-1.57	1 out of 15
SCFP_12	-1463646519	 [*][c](:[*]):[c](:[cH]:[*])S(=O)(=O)N	-1.29	1 out of 11



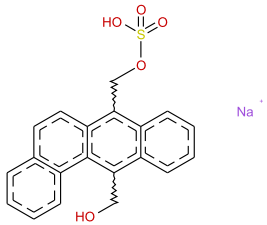
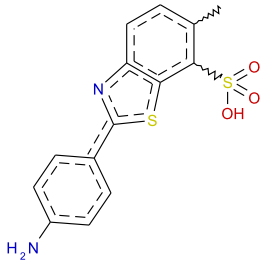
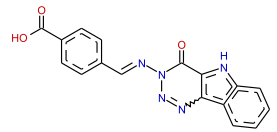
$C_{17}H_{18}N_4O_2S_2$
Molecular Weight: 374.48042
ALogP: 3.541
Rotatable Bonds: 3
Acceptors: 5
Donors: 2

Model Prediction

Prediction: Non-Mutagen
Probability: 0.308
Enrichment: 0.552
Bayesian Score: -11.6
Mahalanobis Distance: 11.8
Mahalanobis Distance p-value: 0.00178

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	98644-23-6	130-17-6	139953-77-8
Structure			
Actual Endpoint	Mutagen	Mutagen	Mutagen
Predicted Endpoint	Mutagen	Mutagen	Mutagen
Distance	0.539	0.567	0.571
Reference	Kazius et. al., J. Med. Chem. (2005) 48, 312-320	Kazius et. al., J. Med. Chem. (2005) 48, 312-320	Kazius et. al., J. Med. Chem. (2005) 48, 312-320

Model Applicability

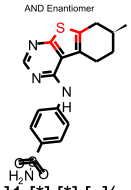
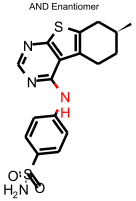
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

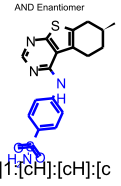
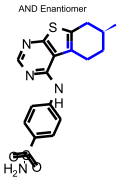
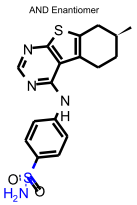
Feature Contribution

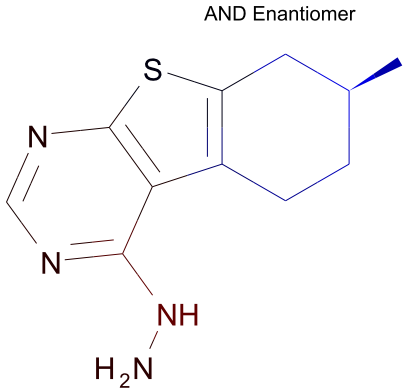
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Mutagen in training set
SCFP_12	112346096	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.36	1035 out of 1263

SCFP_12	1310748454	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.312	126 out of 161
SCFP_12	10	 [*]N[*]	0.306	1774 out of 2287

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Mutagen in training set
SCFP_12	1892918731	 [*]N[c]1:[cH]:[cH]:[c](:[cH]:[cH]:1)S(=O)(=O)N	-2.2	0 out of 14
SCFP_12	-55982834	 [*]:[c]1:[*]C[C@@H](C)CC1	-1.82	0 out of 9
SCFP_12	-1358544872	 [*]S(=[*])(=[*])N	-1.57	1 out of 15



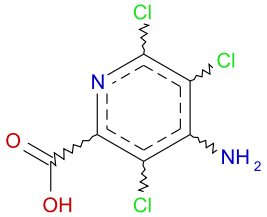
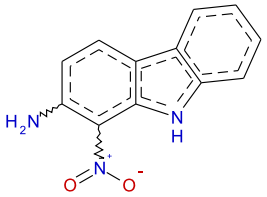
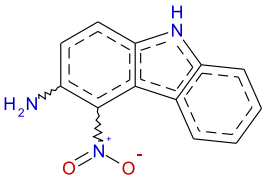
$C_{11}H_{14}N_4S$
Molecular Weight: 234.32065
ALogP: 2.561
Rotatable Bonds: 1
Acceptors: 4
Donors: 2

Model Prediction

Prediction: Non-Mutagen
Probability: 0.712
Enrichment: 1.28
Bayesian Score: -1.25
Mahalanobis Distance: 10.5
Mahalanobis Distance p-value: 0.117

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Picloram	158321-20-1	96014-36-7
Structure			
Actual Endpoint	Non-Mutagen	Mutagen	Mutagen
Predicted Endpoint	Non-Mutagen	Mutagen	Mutagen
Distance	0.522	0.540	0.540
Reference	Mut. Res. 204: 17-115; 1988	Kazius et. al., J. Med. Chem. (2005) 48, 312-320	Kazius et. al., J. Med. Chem. (2005) 48, 312-320

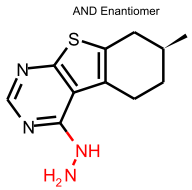
Model Applicability

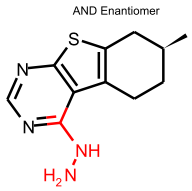
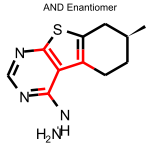
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

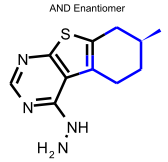
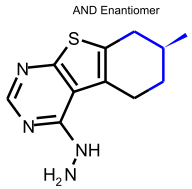
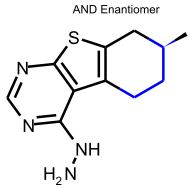
Feature Contribution

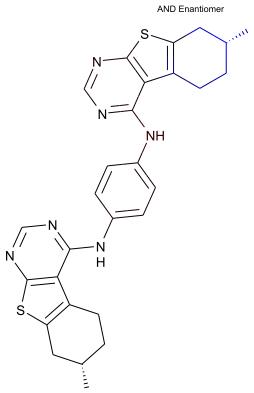
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Mutagen in training set
SCFP_12	260535663	 [*]NN	0.442	13 out of 14

SCFP_12	-915345805	 [*]:[c](:[*])NN	0.442	13 out of 14
SCFP_12	112346096	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.36	1035 out of 1263

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Mutagen in training set
SCFP_12	-55982834	 [*]:[c]1:[*]C[C@@H](C)CC1	-1.82	0 out of 9
SCFP_12	-1043339860	 [*]CC(C)C[*]	-1.09	76 out of 399
SCFP_12	-1272798659	 [*]CCC([*])[*]	-0.466	439 out of 1225



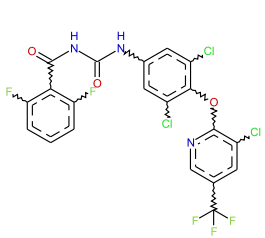
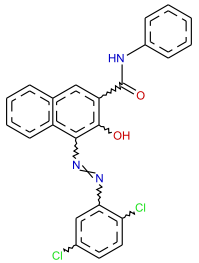
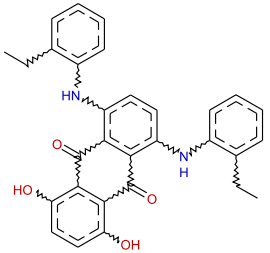
$C_{28}H_{28}N_6S_2$
Molecular Weight: 512.69212
ALogP: 7.842
Rotatable Bonds: 4
Acceptors: 6
Donors: 2

Model Prediction

Prediction: Non-Mutagen
Probability: 0.658
Enrichment: 1.18
Bayesian Score: -3.27
Mahalanobis Distance: 9.58
Mahalanobis Distance p-value: 0.546

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	71422-67-8	Pigment red 2	69657-89-2
Structure			
Actual Endpoint	Non-Mutagen	Mutagen	Mutagen
Predicted Endpoint	Non-Mutagen	Mutagen	Mutagen
Distance	0.693	0.699	0.721
Reference	Kazius et. al., J. Med. Chem. (2005) 48, 312-320	Environ. Mol. Mut. 19(21):1992	Kazius et. al., J. Med. Chem. (2005) 48, 312-320

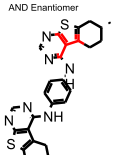
Model Applicability

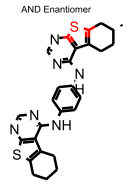
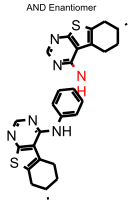
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

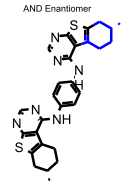
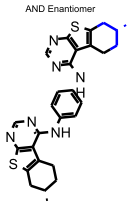
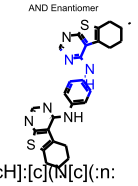
Feature Contribution

Top features for positive contribution

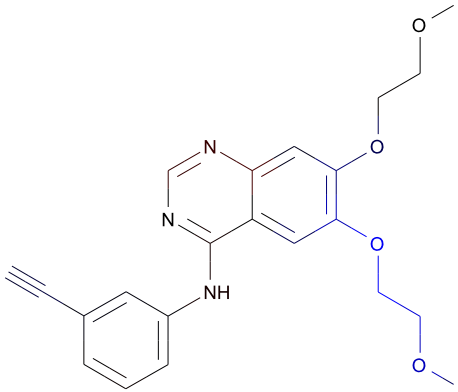
Fingerprint	Bit/Smiles	Feature Structure	Score	Mutagen in training set
SCFP_12	112346096	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.36	1035 out of 1263

SCFP_12	1310748454	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.312	126 out of 161
SCFP_12	10	 [*]N[*]	0.306	1774 out of 2287

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Mutagen in training set
SCFP_12	-55982834	 [*:[c]1:[*]C[C@@H](C)CC1	-1.82	0 out of 9
SCFP_12	-1043339860	 [*]CC(C)C[*]	-1.09	76 out of 399
SCFP_12	1328855840	 [*]:[cH]:[c](N[c](:n:[*]):[c](:[*]):[*]):[cH]:[*]	-0.496	1 out of 4

Erlotinib



$C_{22}H_{23}N_3O_4$

Molecular Weight: 393.43572

ALogP: 4.309

Rotatable Bonds: 10

Acceptors: 7

Donors: 1

Model Prediction

Prediction: Non-Mutagen

Probability: 0.6

Enrichment: 1.07

Bayesian Score: -5.04

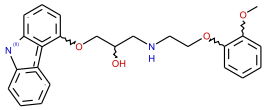
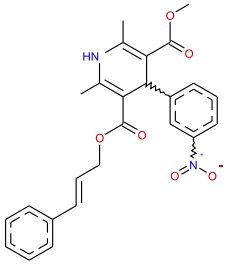
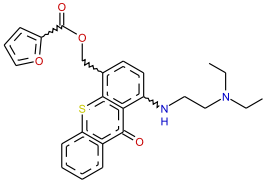
Mahalanobis Distance: 14.6

Mahalanobis Distance p-value: 6.74e-011

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

TOPKAT_Ames_Mutagenicity

Structural Similar Compounds

Name	Carvedilol	99522-79-9	HYCANTHONE FUROATE
Structure			
Actual Endpoint	Non-Mutagen	Non-Mutagen	Mutagen
Predicted Endpoint	Non-Mutagen	Non-Mutagen	Mutagen
Distance	0.594	0.598	0.606
Reference	Contrera, J.F., Matthews, E.J., Kruhlak, N.L., and Benz, R.D., Regulatory Toxicology and Pharmacology 2005, 313-323.	Kazius et. al., J. Med. Chem. (2005) 48, 312-320	EMIC

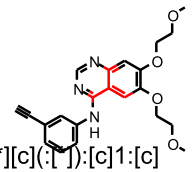
Model Applicability

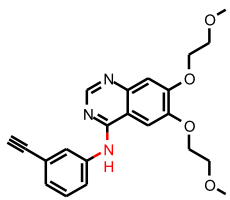
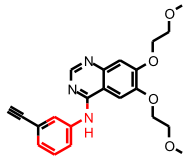
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

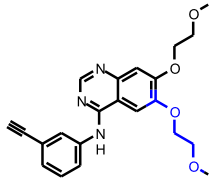
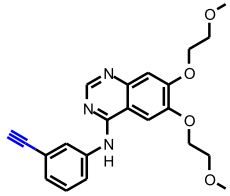
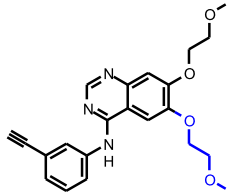
Feature Contribution

Top features for positive contribution

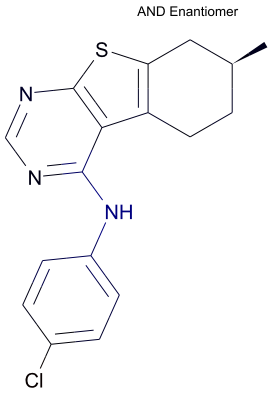
Fingerprint	Bit/Smiles	Feature Structure	Score	Mutagen in training set
SCFP_12	112346096	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.36	1035 out of 1263

SCFP_12	10	 [*]N[*]	0.306	1774 out of 2287
SCFP_12	-1380909229	 [*]N[c]1:[cH]:[*]:[c] ([*]):[cH]:[cH]:1	0.304	957 out of 1235

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Mutagen in training set
SCFP_12	-1099149596	 [*]OCCO[c](:[*]):[*]	-1.12	1 out of 9
SCFP_12	-677502852	 [*]C#C	-0.863	4 out of 19
SCFP_12	-417738003	 [*]OCCOC	-0.782	12 out of 48

TOPKAT_Developmental_Toxicity_Potential



$C_{17}H_{16}ClN_3S$

Molecular Weight: 329.84704

ALogP: 5.5

Rotatable Bonds: 2

Acceptors: 3

Donors: 1

Model Prediction

Prediction: Non-Toxic

Probability: 0.419

Enrichment: 0.797

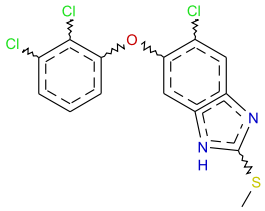
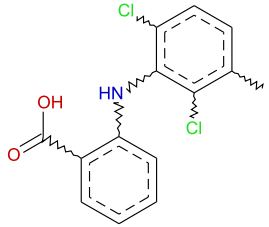
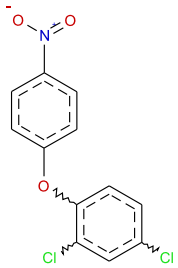
Bayesian Score: -3.75

Mahalanobis Distance: 11.5

Mahalanobis Distance p-value: 0.000182

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Triclabendazole	Meclofenamate Sodium (Free acid form)	Nitrofen
Structure			
Actual Endpoint	Toxic	Non-Toxic	Toxic
Predicted Endpoint	Toxic	Non-Toxic	Toxic
Distance	0.531	0.601	0.613
Reference	Toxicology 43(3):283-287; 1987	Fundam Appl Toxicol 5:665-671; 1985	Environ Health Perspect 70:137-47; 1986

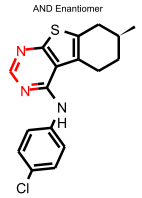
Model Applicability

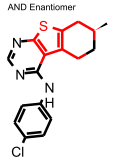
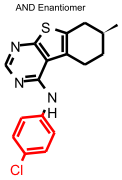
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

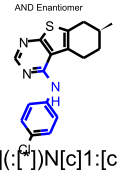
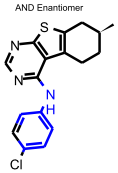
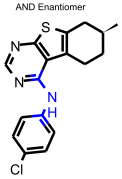
Feature Contribution

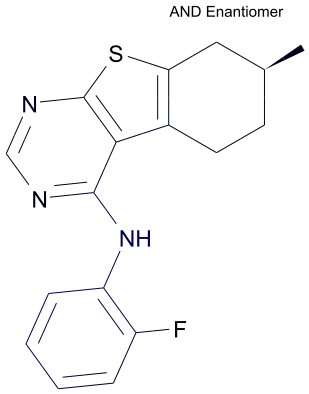
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Toxic in training set
SCFP_6	-1181430618	 [*]:n:[cH]:n:[*]	0.298	6 out of 8

SCFP_6	815479470	 [*][C@H]1[*]C[c]2:[c](C1):s:[c](:[*]):[c]:2:[*]	0.271	1 out of 1
SCFP_6	1905487031	 [*][c]1:[cH]:[cH]:[c](Cl):[cH]:[cH]:1	0.153	2 out of 3

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Toxic in training set
SCFP_6	-300914917	 [*]:[c](:[*])N[c]1:[cH]:[cH]:[*]:[cH]:[cH]:1	-0.718	0 out of 2
SCFP_6	-1380909229	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	-0.449	6 out of 19
SCFP_6	951581613	 [*]:[c](:[*])N[c](:[*]):[*]	-0.438	1 out of 4



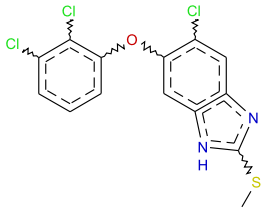
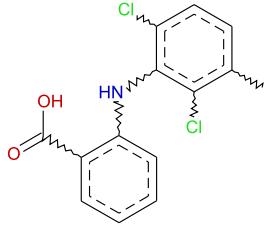
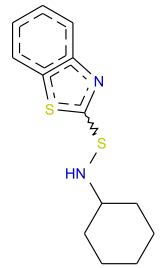
$C_{17}H_{16}FN_3S$
Molecular Weight: 313.39244
ALogP: 5.041
Rotatable Bonds: 2
Acceptors: 3
Donors: 1

Model Prediction

Prediction: Non-Toxic
Probability: 0.435
Enrichment: 0.827
Bayesian Score: -3.23
Mahalanobis Distance: 11.1
Mahalanobis Distance p-value: 0.000905

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Triclabendazole	Meclofenamate Sodium (Free acid form)	N-Cyclohexyl-2-benzothiazylsulfenamide
Structure			
Actual Endpoint	Toxic	Non-Toxic	Non-Toxic
Predicted Endpoint	Toxic	Non-Toxic	Non-Toxic
Distance	0.588	0.602	0.611
Reference	Toxicology 43(3):283-287; 1987	Fundam Appl Toxicol 5:665-671; 1985	J Appl Toxicol 9(3):187-90; 1989

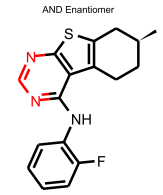
Model Applicability

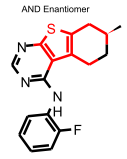
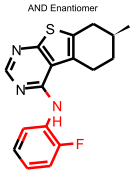
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

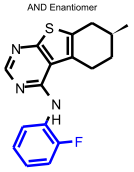
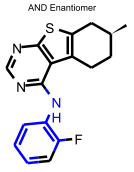
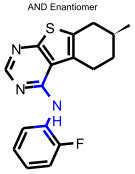
Feature Contribution

Top features for positive contribution

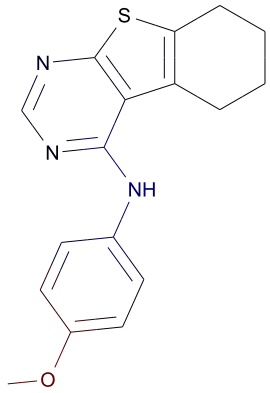
Fingerprint	Bit/Smiles	Feature Structure	Score	Toxic in training set
SCFP_6	-1181430618	 [*]:n:[cH]:n:[*]	0.298	6 out of 8

SCFP_6	815479470	 [*][C@H]1[*]C[c]2:[c](C1):s:[c](:[*]):[c]:2:[*]	0.271	1 out of 1
SCFP_6	-1551011249	 [*]N[c]1:[cH]:[*]:[cH]:[cH]:[c]:1F	0.271	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Toxic in training set
SCFP_6	1655894345	 [*][c]1:[cH]:[cH]:[cH]:[cH]:[c]:1F	-0.718	0 out of 2
SCFP_6	-1380909229	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	-0.449	6 out of 19
SCFP_6	951581613	 [*]:[c](:[*])N[c](:[*]):[*]	-0.438	1 out of 4

TOPKAT_Developmental_Toxicity_Potential



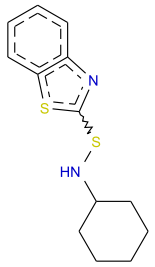
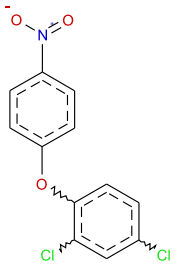
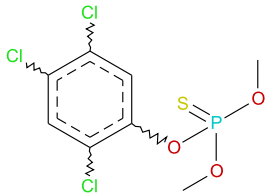
$C_{17}H_{17}N_3OS$
Molecular Weight: 311.40138
ALogP: 4.568
Rotatable Bonds: 3
Acceptors: 4
Donors: 1

Model Prediction

Prediction: Non-Toxic
Probability: 0.495
Enrichment: 0.941
Bayesian Score: -1.44
Mahalanobis Distance: 10.5
Mahalanobis Distance p-value: 0.00495

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	N-Cyclohexyl-2-benzothiazylsulfenamide	Nitrofen	Ronnel
Structure			
Actual Endpoint	Non-Toxic	Toxic	Toxic
Predicted Endpoint	Non-Toxic	Toxic	Toxic
Distance	0.580	0.607	0.608
Reference	J Appl Toxicol 9(3):187-90; 1989	Environ Health Perspect 70:137-47; 1986	J Toxicol Environ Health 10:111-119; 1982

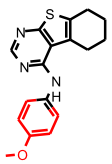
Model Applicability

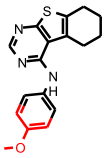
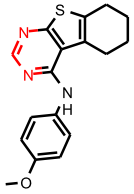
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. OPS PC12 out of range. Value: 3.4923. Training min, max, SD, explained variance: -3.7514, 3.3159, 1.318, 0.0255.

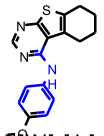
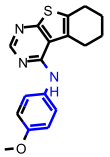
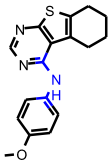
Feature Contribution

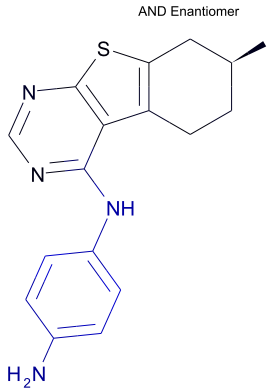
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Toxic in training set
SCFP_6	1237755852	 CO[c]1:[cH]:[cH]:[*]:[cH]:[cH]:1	0.453	8 out of 9

SCFP_6	591469355	 [*]:[cH]:[c](OC):[cH]:[*]	0.411	10 out of 12
SCFP_6	-1181430618	 [*]:n:[cH]:n:[*]	0.298	6 out of 8

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Toxic in training set
SCFP_6	-300914917	 [*]:[c](:[*])N[c]1:[cH]:[cH]:[*]:[cH]:[cH]:1	-0.718	0 out of 2
SCFP_6	-1380909229	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	-0.449	6 out of 19
SCFP_6	951581613	 [*]:[c](:[*])N[c](:[*]):[*]	-0.438	1 out of 4



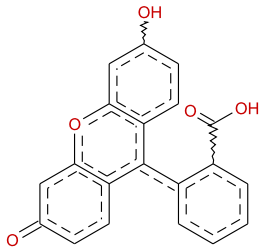
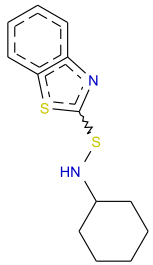
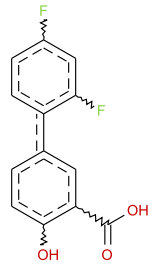
$C_{17}H_{18}N_4S$
Molecular Weight: 310.41662
ALogP: 4.089
Rotatable Bonds: 2
Acceptors: 4
Donors: 2

Model Prediction

Prediction: Non-Toxic
Probability: 0.336
Enrichment: 0.639
Bayesian Score: -6.97
Mahalanobis Distance: 10.9
Mahalanobis Distance p-value: 0.00165

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	D&C Yellow 8	N-Cyclohexyl-2-benzothiazylsulfenamide	Diflunisal
Structure			
Actual Endpoint	Non-Toxic	Non-Toxic	Toxic
Predicted Endpoint	Non-Toxic	Non-Toxic	Toxic
Distance	0.614	0.625	0.642
Reference	Food Chem Toxicol 24:819-823; 1986	J Appl Toxicol 9(3):187-90; 1989	Oyo Yakuri 17(4):551-557; 1979

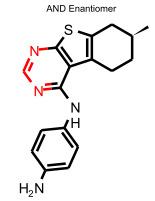
Model Applicability

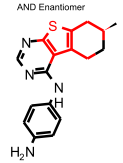
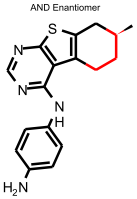
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

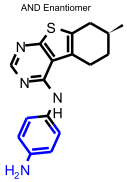
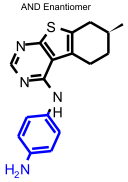
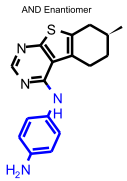
Feature Contribution

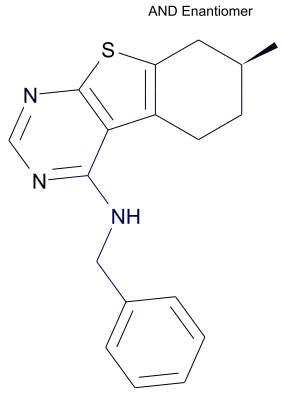
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Toxic in training set
SCFP_6	-1181430618	 [*]:n:[cH]:n:[*]	0.298	6 out of 8

SCFP_6	815479470	 [*][C@H]1[*]C[c]2:[c](C1):s:[c](:[*]):[c]:2:[*]	0.271	1 out of 1
SCFP_6	-1272798659	 [*]CCC([*])[*]	0.0708	44 out of 78

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Toxic in training set
SCFP_6	-192131231	 N[c]1:[cH]:[cH]:[*]:[cH]:[cH]:1	-1.13	0 out of 4
SCFP_6	1181470699	 [*][c]1:[cH]:[cH]:[c](N):[cH]:[cH]:1	-0.718	0 out of 2
SCFP_6	-1728149235	 [*]N[c]1:[cH]:[cH]:[c](N):[cH]:[cH]:1	-0.718	0 out of 2



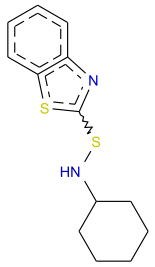
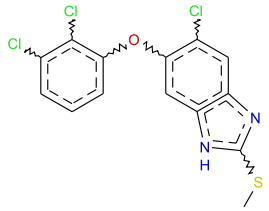
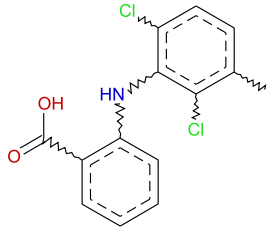
$C_{18}H_{19}N_3S$
Molecular Weight: 309.42856
ALogP: 4.678
Rotatable Bonds: 3
Acceptors: 3
Donors: 1

Model Prediction

Prediction: Non-Toxic
Probability: 0.427
Enrichment: 0.811
Bayesian Score: -3.51
Mahalanobis Distance: 10.6
Mahalanobis Distance p-value: 0.00391

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	N-Cyclohexyl-2-benzothiazylsulfenamide	Triclabendazole	Meclofenamate Sodium (Free acid form)
Structure			
Actual Endpoint	Non-Toxic	Toxic	Non-Toxic
Predicted Endpoint	Non-Toxic	Toxic	Non-Toxic
Distance	0.592	0.601	0.601
Reference	J Appl Toxicol 9(3):187-90; 1989	Toxicology 43(3):283-287; 1987	Fundam Appl Toxicol 5:665-671; 1985

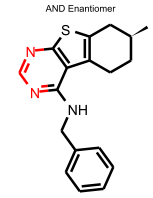
Model Applicability

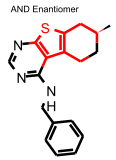
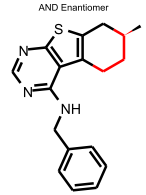
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

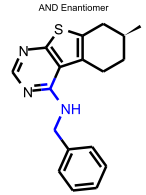
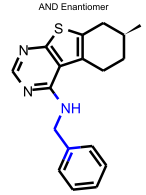
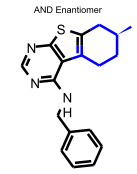
Feature Contribution

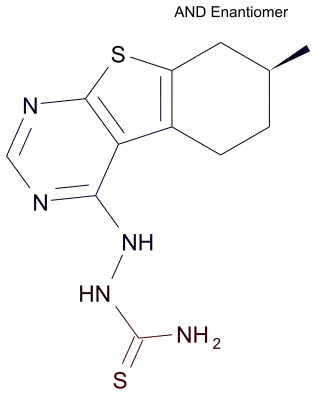
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Toxic in training set
SCFP_6	-1181430618	 [*]:n:[cH]:n:[*]	0.298	6 out of 8

SCFP_6	815479470	 [*][C@H]1[*]C[c]2:[c](C1):s:[c](:[*]):[c]:2:[*]	0.271	1 out of 1
SCFP_6	-1272798659	 [*]CCC([*])[*]	0.0708	44 out of 78

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Toxic in training set
SCFP_6	18117904	 [*]CN[c](:[*]):[*]	-0.945	0 out of 3
SCFP_6	1155330592	 [*]NC[c](:[*]):[*]	-0.422	0 out of 1
SCFP_6	-55982834	 [*:[c]1:[*]C[C@@H](C)CC1	-0.422	0 out of 1



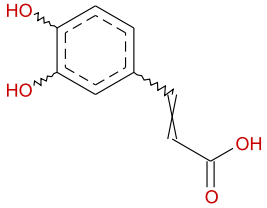
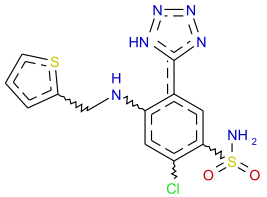
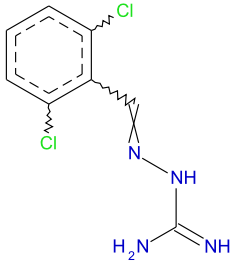
$C_{12}H_{15}N_5S_2$
Molecular Weight: 293.411
ALogP: 3.209
Rotatable Bonds: 3
Acceptors: 4
Donors: 3

Model Prediction

Prediction: Non-Toxic
Probability: 0.529
Enrichment: 1.01
Bayesian Score: -0.498
Mahalanobis Distance: 11.2
Mahalanobis Distance p-value: 0.000502

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Caffeic Acid	Azosemide	Guanabenz
Structure			
Actual Endpoint	Toxic	Non-Toxic	Toxic
Predicted Endpoint	Toxic	Non-Toxic	Toxic
Distance	0.723	0.732	0.741
Reference	Toxicol Appl Pharmacol 36(2):227-37; 1976	Kiso to Rinsho 18:5187-5195; 1984	Journal of Toxic Sciences 11:107-119; 1982

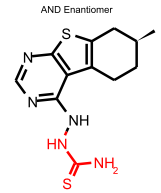
Model Applicability

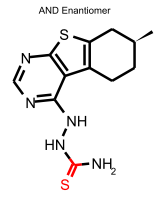
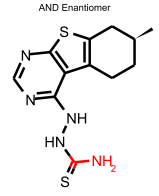
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

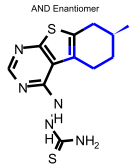
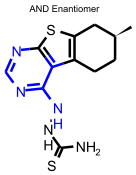
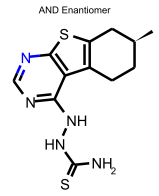
Feature Contribution

Top features for positive contribution

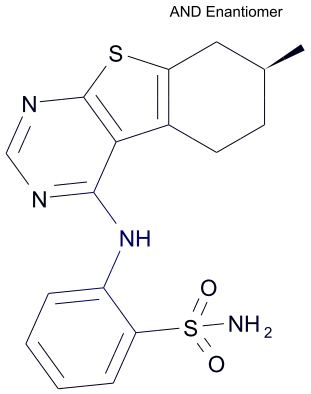
Fingerprint	Bit/Smiles	Feature Structure	Score	Toxic in training set
SCFP_6	382734644	 [*]NC(=S)N	0.478	4 out of 4

SCFP_6	1435188938	 [*]C(=S)[*]	0.478	4 out of 4
SCFP_6	384861283	 [*]C(=[*])N	0.441	3 out of 3

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Toxic in training set
SCFP_6	-55982834	 [*:[c]1:[*]C[C@@H](C)CC1	-0.422	0 out of 1
SCFP_6	-2147171373	 [*]N[c]1:n:[cH]:n:[*]:[c]:1:[*]	-0.422	0 out of 1
SCFP_6	8	 [*]:n:[*]	-0.278	24 out of 61

TOPKAT_Developmental_Toxicity_Potential



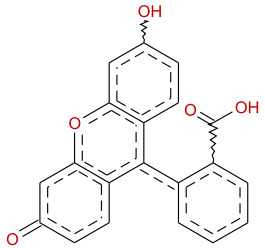
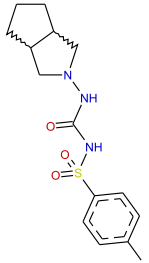
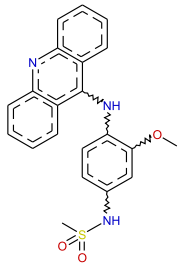
$C_{17}H_{18}N_4O_2S_2$
Molecular Weight: 374.48042
ALogP: 3.541
Rotatable Bonds: 3
Acceptors: 5
Donors: 2

Model Prediction

Prediction: Non-Toxic
Probability: 0.419
Enrichment: 0.797
Bayesian Score: -3.75
Mahalanobis Distance: 12
Mahalanobis Distance p-value: 3.47e-005

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	D&C Yellow 8	Sulfonylurea Gliclazide	Amsacrine
Structure			
Actual Endpoint	Non-Toxic	Toxic	Toxic
Predicted Endpoint	Non-Toxic	Toxic	Toxic
Distance	0.654	0.658	0.664
Reference	Food Chem Toxicol 24:819-823; 1986	Yakuri to Chiryo 9:3551-3571; 1981	Fundam Appl Toxicol 7(2):214-20; 1986

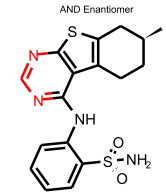
Model Applicability

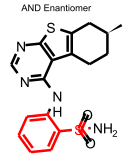
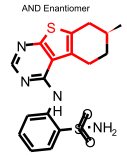
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

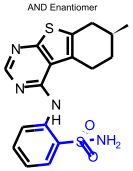
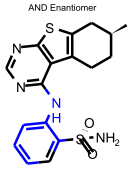
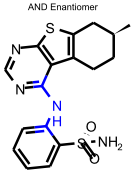
Feature Contribution

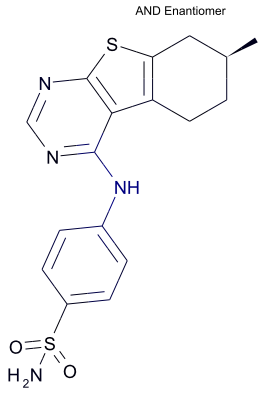
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Toxic in training set
SCFP_6	-1181430618	 [*]:n:[cH]:n:[*]	0.298	6 out of 8

SCFP_6	1655803608	 [*][c]1:[cH]:[cH]:[cH]:[cH]:[c]:1S(=[*])(=[*])[*]	0.271	1 out of 1
SCFP_6	815479470	 [*][C@H]1[*]C[c]2:[c](C1):s:[c](:[*]):[c]:2:[*]	0.271	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Toxic in training set
SCFP_6	-1463646519	 [*][c](:[*]):[c](:[cH]:[*])S(=O)(=O)N	-0.718	0 out of 2
SCFP_6	-1380909229	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	-0.449	6 out of 19
SCFP_6	951581613	 [*]:[c](:[*])N[c](:[*]):[*]	-0.438	1 out of 4



$C_{17}H_{18}N_4O_2S_2$

Molecular Weight: 374.48042

ALogP: 3.541

Rotatable Bonds: 3

Acceptors: 5

Donors: 2

Model Prediction

Prediction: Non-Toxic

Probability: 0.411

Enrichment: 0.781

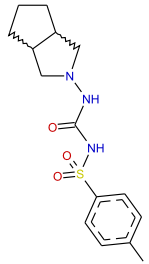
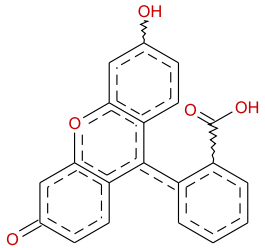
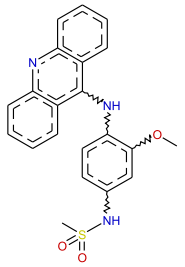
Bayesian Score: -4.03

Mahalanobis Distance: 12.2

Mahalanobis Distance p-value: 1.11e-005

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Sulfonylurea Gliclazide	D&C Yellow 8	Amsacrine
Structure			
Actual Endpoint	Toxic	Non-Toxic	Toxic
Predicted Endpoint	Toxic	Non-Toxic	Toxic
Distance	0.651	0.658	0.668
Reference	Yakuri to Chiryo 9:3551-3571; 1981	Food Chem Toxicol 24:819-823; 1986	Fundam Appl Toxicol 7(2):214-20; 1986

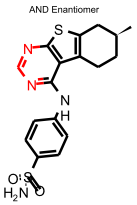
Model Applicability

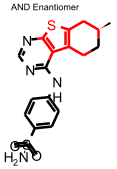
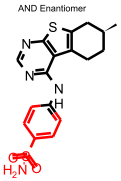
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

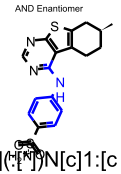
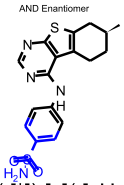
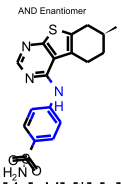
Feature Contribution

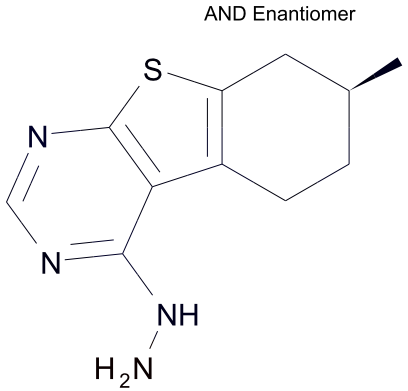
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Toxic in training set
SCFP_6	-1181430618	 [*]:n:[cH]:n:[*]	0.298	6 out of 8

SCFP_6	815479470	 [*][C@H]1[*]C[c]2:[c](C1):s:[c](:[*]):[c]:2:[*]	0.271	1 out of 1
SCFP_6	-1247518081	 NS(=O)(=O)[c]1:[cH]:[cH]:[*]:[cH]:[cH]:1	0.271	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Toxic in training set
SCFP_6	-300914917	 [*]:[c](:[*])N[c]1:[cH]:[cH]:[*]:[cH]:[cH]:1	-0.718	0 out of 2
SCFP_6	-1463646519	 [*][c](:[*]):[c](:[cH]:[*])S(=O)(=O)N	-0.718	0 out of 2
SCFP_6	-1380909229	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	-0.449	6 out of 19



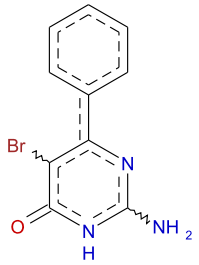
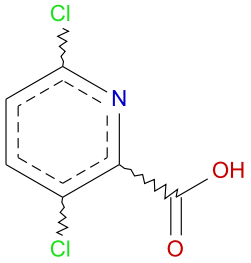
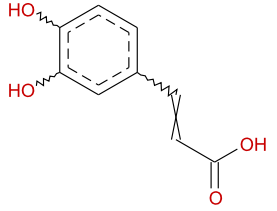
$C_{11}H_{14}N_4S$
Molecular Weight: 234.32065
ALogP: 2.561
Rotatable Bonds: 1
Acceptors: 4
Donors: 2

Model Prediction

Prediction: Non-Toxic
Probability: 0.481
Enrichment: 0.915
Bayesian Score: -1.83
Mahalanobis Distance: 12.1
Mahalanobis Distance p-value: 2.12e-005

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Bropirimine	3;6-Dichloropicolinic Acid	Caffeic Acid
Structure			
Actual Endpoint	Non-Toxic	Non-Toxic	Toxic
Predicted Endpoint	Non-Toxic	Non-Toxic	Toxic
Distance	0.667	0.685	0.687
Reference	Teratology 38(1):7-14; 1988	Fundam Appl Toxicol 4:91-97; 1984	Toxicol Appl Pharmacol 36(2):227-37; 1976

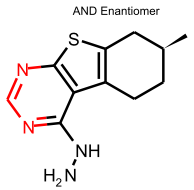
Model Applicability

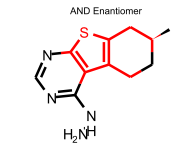
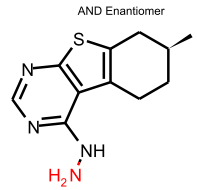
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

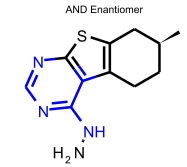
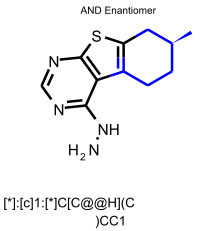
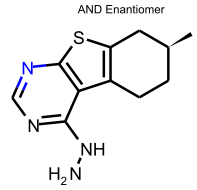
Feature Contribution

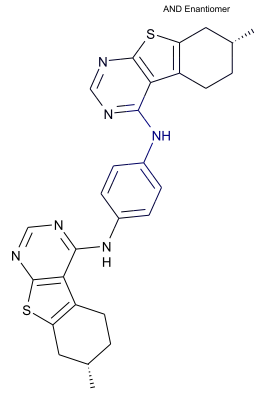
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Toxic in training set
SCFP_6	-1181430618	 [*]:n:[cH]:n:[*]	0.298	6 out of 8

SCFP_6	815479470	 [*][C@H]1[*]C[c]2:[c](C1):s:[c](:[*]):[c]:2:[*]	0.271	1 out of 1
SCFP_6	5	 [*]N	0.228	51 out of 77

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Toxic in training set
SCFP_6	-2147171373	 [*]N[c]1:n:[cH]:n:[*]:[c]:1:[*]	-0.422	0 out of 1
SCFP_6	-55982834	 [*]:[c]1:[*]C[C@@H](C)CC1	-0.422	0 out of 1
SCFP_6	8	 [*]:n:[*]	-0.278	24 out of 61



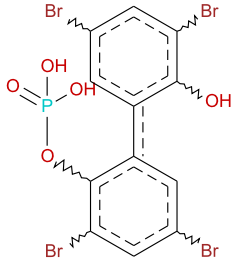
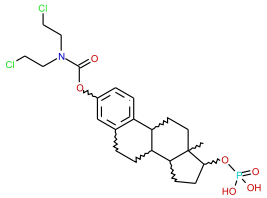
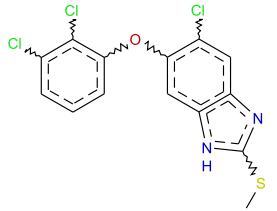
$C_{28}H_{28}N_6S_2$
Molecular Weight: 512.69212
ALogP: 7.842
Rotatable Bonds: 4
Acceptors: 6
Donors: 2

Model Prediction

Prediction: Non-Toxic
Probability: 0.435
Enrichment: 0.827
Bayesian Score: -3.24
Mahalanobis Distance: 11.8
Mahalanobis Distance p-value: 5.91e-005

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Bromofenofos	Estramustine Phosphate Disodium (Free acid form)	Triclabendazole
Structure			
Actual Endpoint	Toxic	Non-Toxic	Toxic
Predicted Endpoint	Toxic	Non-Toxic	Toxic
Distance	0.761	0.793	0.838
Reference	Toxicol Letters 31:243-247; 1986	Oyo Yakuri 20(6):1219-1236; 1980	Toxicology 43(3):283-287; 1987

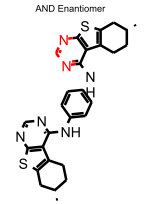
Model Applicability

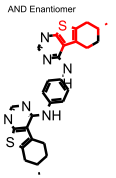
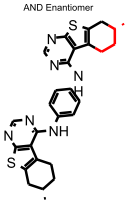
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

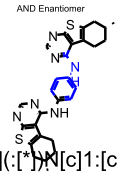
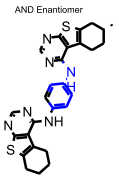
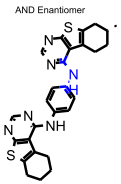
Feature Contribution

Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Toxic in training set
SCFP_6	-1181430618	 [*]:n:[cH]:n:[*]	0.298	6 out of 8

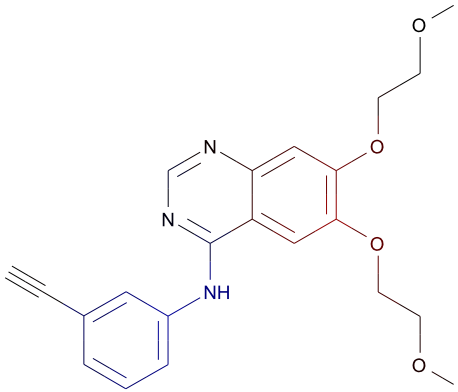
SCFP_6	815479470	 [*][C@H]1[*]C[c]2:[c](C1):s:[c](:[*]):[c]:2:[*]	0.271	1 out of 1
SCFP_6	-1272798659	 [*]CCC([*])[*]	0.0708	44 out of 78

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Toxic in training set
SCFP_6	-300914917	 [*]:[c](:[*]):N[c]1:[cH]:[cH]:[*]:[cH]:[cH]:1	-0.718	0 out of 2
SCFP_6	-1380909229	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	-0.449	6 out of 19
SCFP_6	951581613	 [*]:[c](:[*])N[c](:[*]):[*]	-0.438	1 out of 4

Erlotinib

TOPKAT_Developmental_Toxicity_Potential



$C_{22}H_{23}N_3O_4$

Molecular Weight: 393.43572

ALogP: 4.309

Rotatable Bonds: 10

Acceptors: 7

Donors: 1

Model Prediction

Prediction: Non-Toxic

Probability: 0.504

Enrichment: 0.959

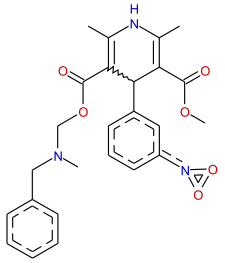
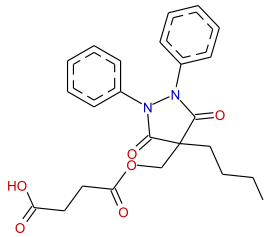
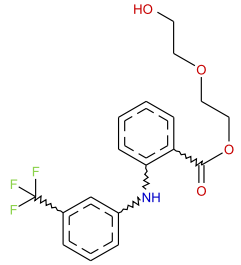
Bayesian Score: -1.17

Mahalanobis Distance: 8.76

Mahalanobis Distance p-value: 0.258

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Nicardipine	Suxibuzone	Etofenamate
Structure			
Actual Endpoint	Non-Toxic	Toxic	Non-Toxic
Predicted Endpoint	Non-Toxic	Toxic	Non-Toxic
Distance	0.608	0.620	0.635
Reference	Kiso to Rinsho 13:1149-1159; 1979	Oyo Yakuri 20:377-386; 1980	Iyakuhin Kenkyu 13(4):896-909; 1982

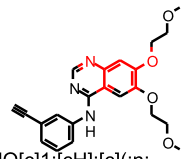
Model Applicability

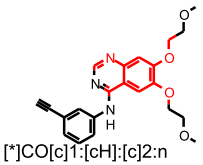
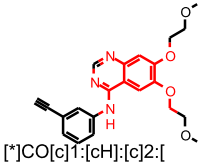
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

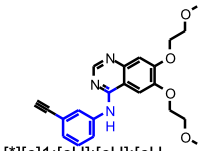
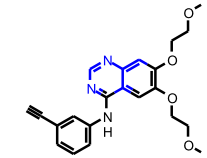
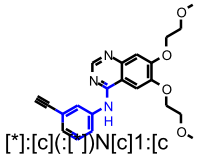
Feature Contribution

Top features for positive contribution

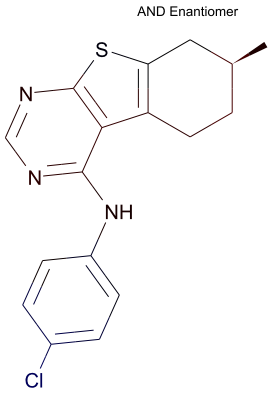
Fingerprint	Bit/Smiles	Feature Structure	Score	Toxic in training set
SCFP_6	123285475	 [*]O[c]1:[cH]:[c](:n:[*]):[c](:[*]):[*]:[c]:1[*]	0.478	4 out of 4

SCFP_6	446954673	 [*]CO[c]1:[cH]:[c]2:n :[cH]:[*]:[c]([*]):[c]:2:[cH]:[c]:1O[*]	0.381	2 out of 2
SCFP_6	-1814968949	 [*]CO[c]1:[cH]:[c]2:[c](N[*]):n:[*]:n:[c] :2:[cH]:[c]:1O[*]	0.381	2 out of 2

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Toxic in training set
SCFP_6	-2020651081	 [*][c]1:[cH]:[cH]:[cH]:[c](N[c](:[*]):[*]):[cH]:1	-0.718	0 out of 2
SCFP_6	2142015375	 [*]:[cH]:[c]1:n:[cH]: n:[*]:[c]:1:[*]	-0.718	0 out of 2
SCFP_6	-300914917	 [*]:[c](:[*])N[c]1:[c H]:[cH]:[*]:[cH]:[cH]:1	-0.718	0 out of 2

TOPKAT_Mouse_Female_FDA_None_vs_Carcinogen



$C_{17}H_{16}ClN_3S$

Molecular Weight: 329.84704

ALogP: 5.5

Rotatable Bonds: 2

Acceptors: 3

Donors: 1

Model Prediction

Prediction: Carcinogen

Probability: 0.274

Enrichment: 0.855

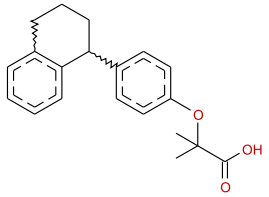
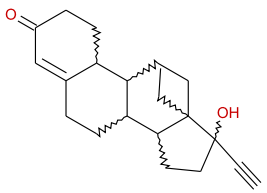
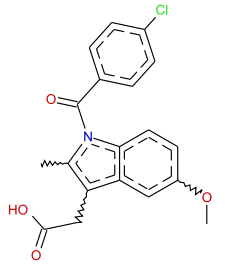
Bayesian Score: 0.526

Mahalanobis Distance: 13.5

Mahalanobis Distance p-value: 8.88e-005

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Nafenopin	Levonorgestrel	Indomethacin
Structure			
Actual Endpoint	Carcinogen	Carcinogen	Non-Carcinogen
Predicted Endpoint	Carcinogen	Carcinogen	Non-Carcinogen
Distance	0.629	0.647	0.652
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

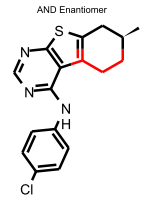
Model Applicability

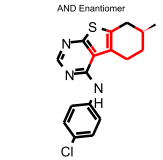
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]

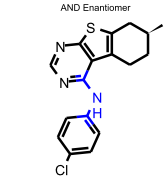
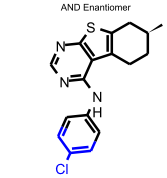
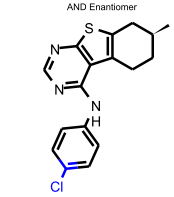
Feature Contribution

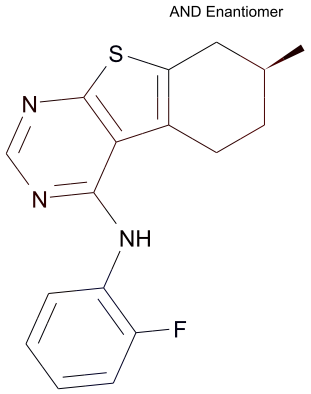
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_6	51876938	 [*]CC[c](:[*]):[*]	0.473	16 out of 31

ECFP_6	-1661653144	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.442	2 out of 3
ECFP_6	553181281	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2CC1	0.424	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_6	-1242906247	 [*]:[c](:[*])N[c](:[*]):[*]	-0.482	0 out of 2
ECFP_6	-176494269	 [*]:[cH]:[c](Cl):[cH]:[*]	-0.476	5 out of 28
ECFP_6	99947387	 [*]:[c](:[*])Cl	-0.461	9 out of 48



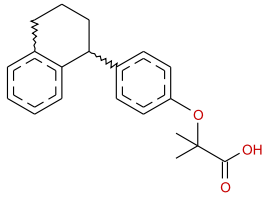
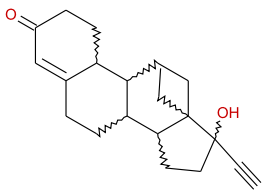
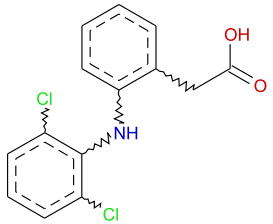
$C_{17}H_{16}FN_3S$
Molecular Weight: 313.39244
ALogP: 5.041
Rotatable Bonds: 2
Acceptors: 3
Donors: 1

Model Prediction

Prediction: Carcinogen
Probability: 0.305
Enrichment: 0.951
Bayesian Score: 1.75
Mahalanobis Distance: 11.3
Mahalanobis Distance p-value: 0.0631

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Nafenopin	Levonorgestrel	Diclofenac
Structure			
Actual Endpoint	Carcinogen	Carcinogen	Non-Carcinogen
Predicted Endpoint	Carcinogen	Carcinogen	Non-Carcinogen
Distance	0.613	0.640	0.654
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

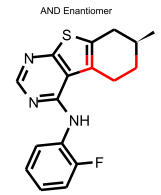
Model Applicability

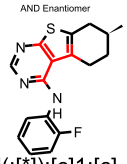
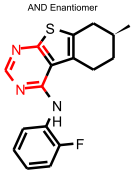
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]

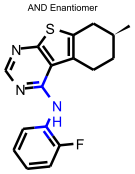
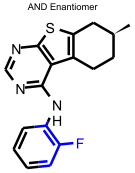
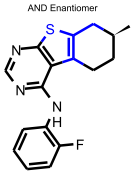
Feature Contribution

Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_6	51876938	 [*]CC[c](:[*]):[*]	0.473	16 out of 31

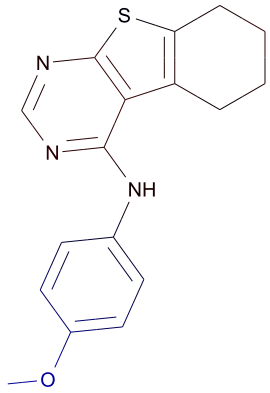
ECFP_6	-1661653144	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.442	2 out of 3
ECFP_6	-1448786963	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.424	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_6	-1242906247	 [*]:[c](:[*])N[c](:[*]):[*]	-0.482	0 out of 2
ECFP_6	-1311285389	 [*][c](:[*]):[c](F):[cH]:[*]	-0.459	1 out of 7
ECFP_6	-1672647522	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	-0.27	0 out of 1

5c

TOPKAT_Mouse_Female_FDA_None_vs_Carcinogen



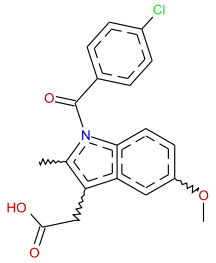
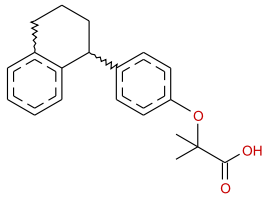
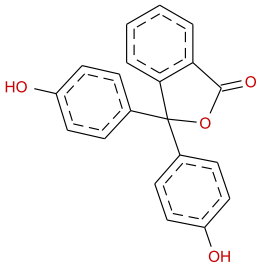
$C_{17}H_{17}N_3OS$
Molecular Weight: 311.40138
ALogP: 4.568
Rotatable Bonds: 3
Acceptors: 4
Donors: 1

Model Prediction

Prediction: Non-Carcinogen
Probability: 0.244
Enrichment: 0.761
Bayesian Score: -1.06
Mahalanobis Distance: 12.6
Mahalanobis Distance p-value: 0.00166

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Indomethacin	Nafenopin	Phenolphthalein
Structure			
Actual Endpoint	Non-Carcinogen	Carcinogen	Carcinogen
Predicted Endpoint	Non-Carcinogen	Carcinogen	Carcinogen
Distance	0.579	0.624	0.649
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

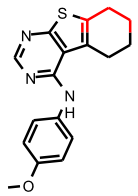
Model Applicability

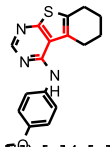
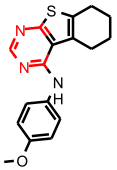
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]

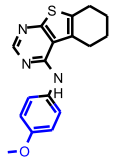
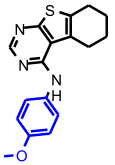
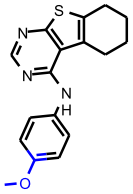
Feature Contribution

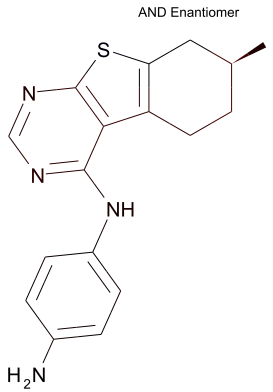
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_6	51876938	 [*]CC[c](:[*]):[*]	0.473	16 out of 31

ECFP_6	-1661653144	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.442	2 out of 3
ECFP_6	-1448786963	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.424	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_6	-1271104377	 CO[c]1:[cH]:[cH]:[*]:[cH]:[cH]:1	-0.805	0 out of 4
ECFP_6	693720869	 [*][c]1:[cH]:[cH]:[c](OC):[cH]:[cH]:1	-0.805	0 out of 4
ECFP_6	1307307440	 [*]:[c](:[*])OC	-0.558	4 out of 25



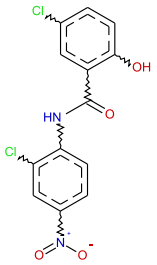
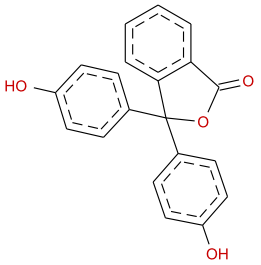
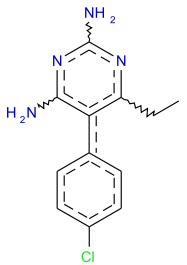
$C_{17}H_{18}N_4S$
Molecular Weight: 310.41662
ALogP: 4.089
Rotatable Bonds: 2
Acceptors: 4
Donors: 2

Model Prediction

Prediction: Carcinogen
Probability: 0.33
Enrichment: 1.03
Bayesian Score: 2.59
Mahalanobis Distance: 11.5
Mahalanobis Distance p-value: 0.035

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Niclosamide	Phenolphthalein	Pyrimethamine
Structure			
Actual Endpoint	Non-Carcinogen	Carcinogen	Non-Carcinogen
Predicted Endpoint	Non-Carcinogen	Carcinogen	Non-Carcinogen
Distance	0.568	0.581	0.626
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

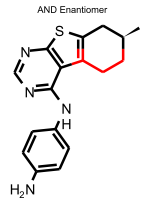
Model Applicability

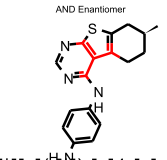
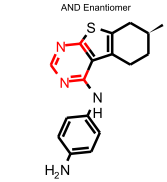
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]

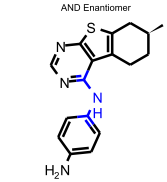
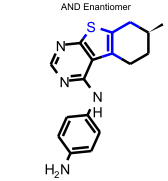
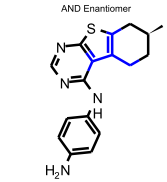
Feature Contribution

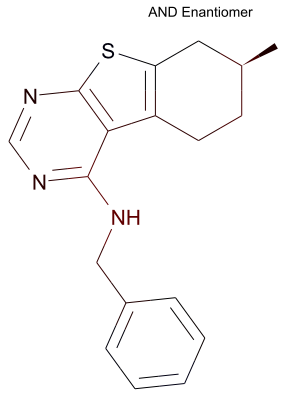
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_6	51876938	 [*]CC[c](:[*]):[*]	0.473	16 out of 31

ECFP_6	-1661653144	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.442	2 out of 3
ECFP_6	-1448786963	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.424	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_6	-1242906247	 [*]:[c](:[*])N[c](:[*]):[*]	-0.482	0 out of 2
ECFP_6	-1672647522	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	-0.27	0 out of 1
ECFP_6	-1660340418	 [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.232	2 out of 9



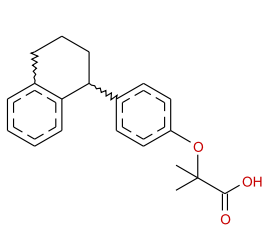
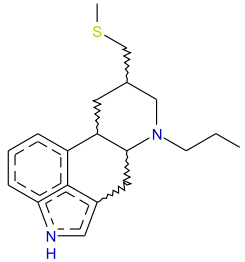
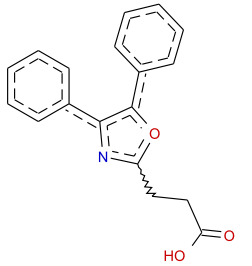
$C_{18}H_{19}N_3S$
Molecular Weight: 309.42856
ALogP: 4.678
Rotatable Bonds: 3
Acceptors: 3
Donors: 1

Model Prediction

Prediction: Carcinogen
Probability: 0.35
Enrichment: 1.09
Bayesian Score: 3.17
Mahalanobis Distance: 12.9
Mahalanobis Distance p-value: 0.000738

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Nafenopin	Pergolide	Oxaprocin
Structure			
Actual Endpoint	Carcinogen	Carcinogen	Non-Carcinogen
Predicted Endpoint	Carcinogen	Carcinogen	Non-Carcinogen
Distance	0.566	0.613	0.617
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

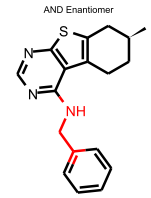
Model Applicability

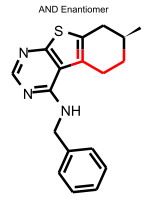
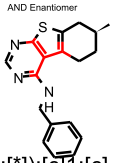
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]

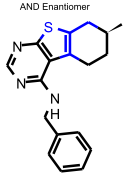
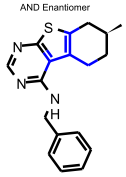
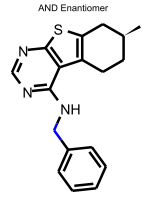
Feature Contribution

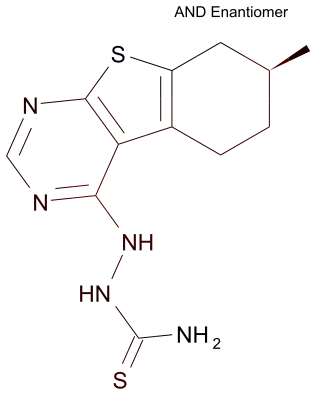
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_6	769925792	 [*]NC[c](:[*]):[*]	0.617	2 out of 2

ECFP_6	51876938	 [*]CC[c](:[*]):[*]	0.473	16 out of 31
ECFP_6	-1661653144	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.442	2 out of 3

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_6	-1672647522	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	-0.27	0 out of 1
ECFP_6	-1660340418	 [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.232	2 out of 9
ECFP_6	1559650422	 [*]C[*]	-0.164	50 out of 191



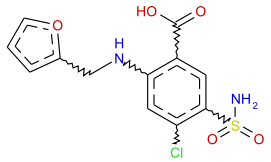
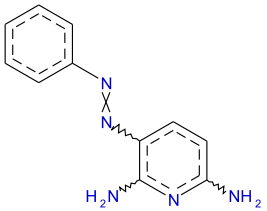
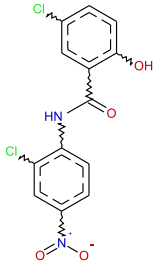
$C_{12}H_{15}N_5S_2$
Molecular Weight: 293.411
ALogP: 3.209
Rotatable Bonds: 3
Acceptors: 4
Donors: 3

Model Prediction

Prediction: Carcinogen
Probability: 0.415
Enrichment: 1.29
Bayesian Score: 4.8
Mahalanobis Distance: 12.2
Mahalanobis Distance p-value: 0.00594

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Furosemide	Phenazopyridine	Niclosamide
Structure			
Actual Endpoint	Carcinogen	Carcinogen	Non-Carcinogen
Predicted Endpoint	Carcinogen	Carcinogen	Non-Carcinogen
Distance	0.715	0.729	0.734
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

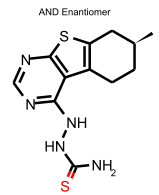
Model Applicability

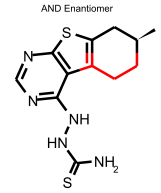
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown ECFP_2 feature: -571028867: [*]NC(=S)N

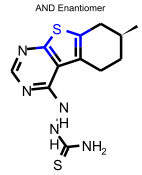
Feature Contribution

Top features for positive contribution

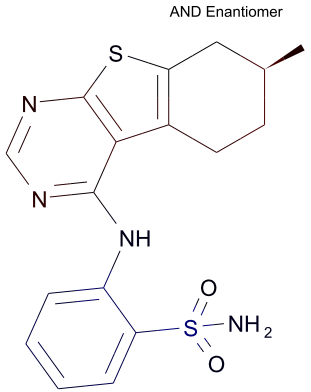
Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_6	-845108448	 [*]=S	0.675	4 out of 5

ECFP_6	51876938	 [*]CC[c](:[*]):[*]	0.473	16 out of 31
ECFP_6	-1661653144	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.442	2 out of 3

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_6	-1672647522	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	-0.27	0 out of 1
ECFP_6	-1660340418	 [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.232	2 out of 9
ECFP_6	85262808	 [*][c]1:[*]:[*]:[c](:[*]):s:1	-0.112	1 out of 4

TOPKAT_Mouse_Female_FDA_None_vs_Carcinogen



$C_{17}H_{18}N_4O_2S_2$

Molecular Weight: 374.48042

ALogP: 3.541

Rotatable Bonds: 3

Acceptors: 5

Donors: 2

Model Prediction

Prediction: Carcinogen

Probability: 0.249

Enrichment: 0.776

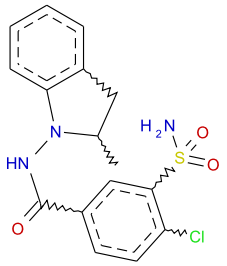
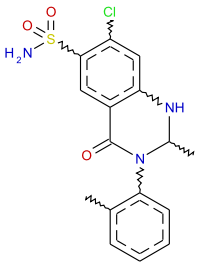
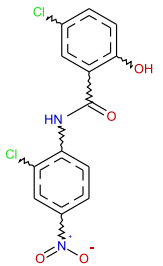
Bayesian Score: -0.764

Mahalanobis Distance: 11.5

Mahalanobis Distance p-value: 0.0367

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Indapamide	Metolazone	Niclosamide
Structure			
Actual Endpoint	Non-Carcinogen	Non-Carcinogen	Non-Carcinogen
Predicted Endpoint	Non-Carcinogen	Non-Carcinogen	Non-Carcinogen
Distance	0.579	0.616	0.616
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

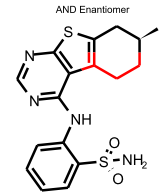
Model Applicability

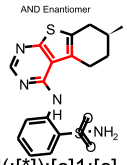
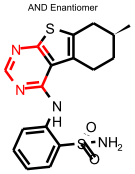
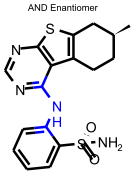
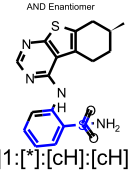
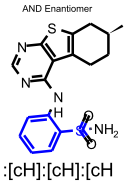
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

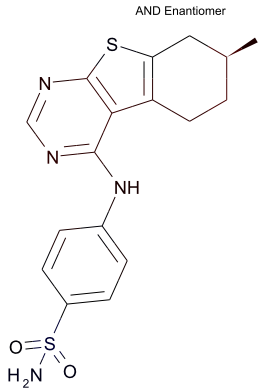
1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]

Feature Contribution

Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_6	51876938	 [*]CC[c](:[*]):[*]	0.473	16 out of 31

ECFP_6	-1661653144	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.442	2 out of 3
ECFP_6	-1448786963	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.424	1 out of 1
Top Features for negative contribution				
Fingerprint	**Bit/Smiles**	**Feature Structure**	**Score**	**Carcinogen in training set**
ECFP_6	-1242906247	 [*]:[c](:[*])N[c](:[*]):[*]	-0.482	0 out of 2
ECFP_6	1634465935	 [*][c]1:[*]:[cH]:[cH]:[cH]:[c]:1S(=[*])(=[*])[*]	-0.27	0 out of 1
ECFP_6	-1114960102	 [*][c]1:[cH]:[cH]:[cH]:[cH]:[c]:1S(=[*])(=[*])[*]	-0.27	0 out of 1



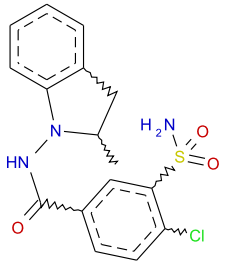
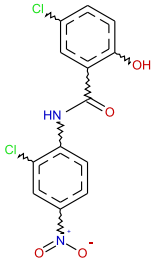
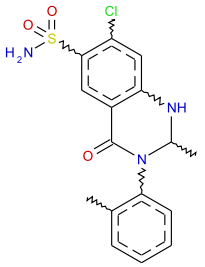
$C_{17}H_{18}N_4O_2S_2$
Molecular Weight: 374.48042
ALogP: 3.541
Rotatable Bonds: 3
Acceptors: 5
Donors: 2

Model Prediction

Prediction: Carcinogen
Probability: 0.286
Enrichment: 0.893
Bayesian Score: 1.05
Mahalanobis Distance: 12.1
Mahalanobis Distance p-value: 0.00933

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Indapamide	Niclosamide	Metolazone
Structure			
Actual Endpoint	Non-Carcinogen	Non-Carcinogen	Non-Carcinogen
Predicted Endpoint	Non-Carcinogen	Non-Carcinogen	Non-Carcinogen
Distance	0.596	0.620	0.633
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

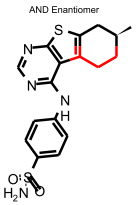
Model Applicability

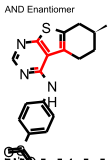
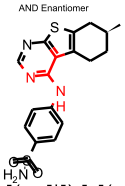
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]

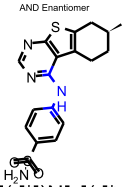
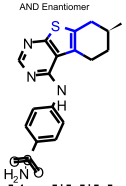
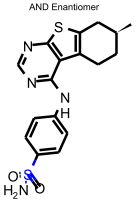
Feature Contribution

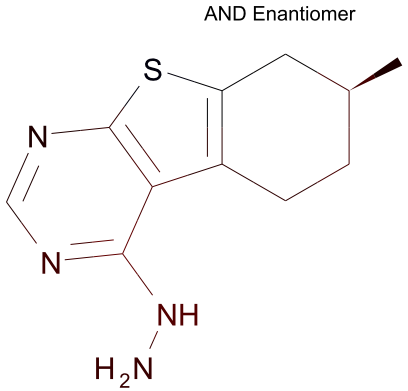
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_6	51876938	 [*]CC[c](:[*]):[*]	0.473	16 out of 31

ECFP_6	-1661653144	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.442	2 out of 3
ECFP_6	1049768340	 [*]N[c](:n:[*]):[c](:[*]):[*]	0.424	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_6	-1242906247	 [*]:[c](:[*])N[c](:[*]):[*]	-0.482	0 out of 2
ECFP_6	-1672647522	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	-0.27	0 out of 1
ECFP_6	-797085356	 [*]S(=[*])(=[*])[*]	-0.263	5 out of 22



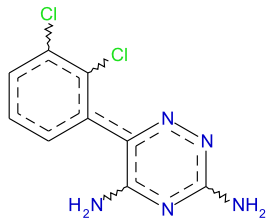
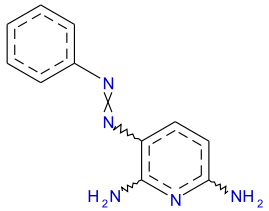
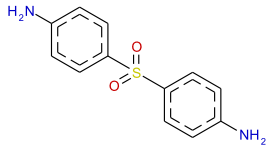
$C_{11}H_{14}N_4S$
Molecular Weight: 234.32065
ALogP: 2.561
Rotatable Bonds: 1
Acceptors: 4
Donors: 2

Model Prediction

Prediction: Carcinogen
Probability: 0.407
Enrichment: 1.27
Bayesian Score: 4.63
Mahalanobis Distance: 11.5
Mahalanobis Distance p-value: 0.0391

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Lamotrigine	Phenazopyridine	Dapsone
Structure			
Actual Endpoint	Non-Carcinogen	Carcinogen	Non-Carcinogen
Predicted Endpoint	Non-Carcinogen	Carcinogen	Non-Carcinogen
Distance	0.571	0.586	0.601
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

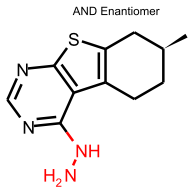
Model Applicability

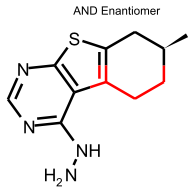
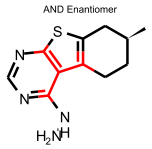
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]

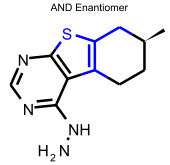
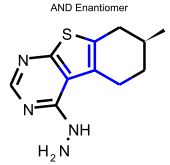
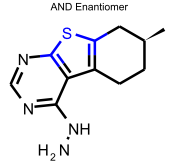
Feature Contribution

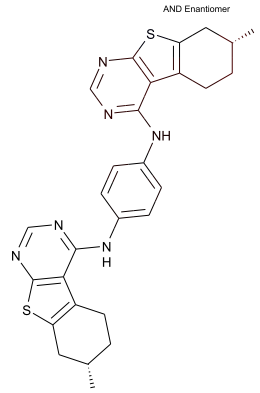
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_6	-934039951	 [*]NN	0.581	3 out of 4

ECFP_6	51876938	 [*]CC[c](:[*]):[*]	0.473	16 out of 31
ECFP_6	-1661653144	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.442	2 out of 3

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_6	-1672647522	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	-0.27	0 out of 1
ECFP_6	-1660340418	 [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.232	2 out of 9
ECFP_6	85262808	 [*][c]1:[*]:[*]:[c](:[*]):s:1	-0.112	1 out of 4



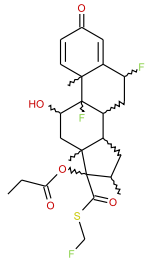
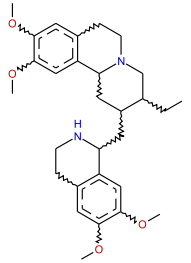
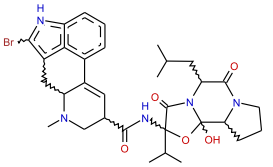
$C_{28}H_{28}N_6S_2$
Molecular Weight: 512.69212
ALogP: 7.842
Rotatable Bonds: 4
Acceptors: 6
Donors: 2

Model Prediction

Prediction: Carcinogen
Probability: 0.318
Enrichment: 0.993
Bayesian Score: 2.21
Mahalanobis Distance: 13.1
Mahalanobis Distance p-value: 0.000434

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Fluticasone	Emetine	Bromocriptine
Structure			
Actual Endpoint	Non-Carcinogen	Non-Carcinogen	Non-Carcinogen
Predicted Endpoint	Non-Carcinogen	Non-Carcinogen	Non-Carcinogen
Distance	0.878	0.893	0.907
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

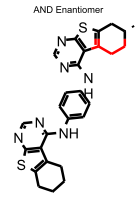
Model Applicability

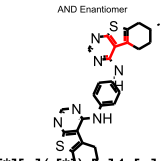
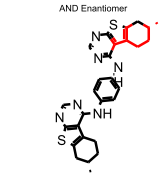
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]

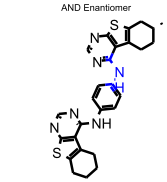
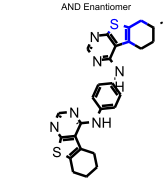
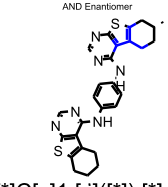
Feature Contribution

Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_6	51876938	 [*]CC[c](:[*]):[*]	0.473	16 out of 31

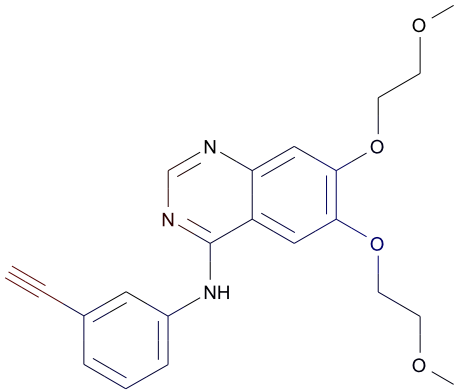
ECFP_6	-1661653144	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.442	2 out of 3
ECFP_6	553181281	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2CC1	0.424	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_6	-1242906247	 [*]:[c](:[*])N[c](:[*]):[*]	-0.482	0 out of 2
ECFP_6	-1672647522	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	-0.27	0 out of 1
ECFP_6	-1660340418	 [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.232	2 out of 9

Erlotinib

TOPKAT_Mouse_Female_FDA_None_vs_Carcinogen



$C_{22}H_{23}N_3O_4$

Molecular Weight: 393.43572

ALogP: 4.309

Rotatable Bonds: 10

Acceptors: 7

Donors: 1

Model Prediction

Prediction: Non-Carcinogen

Probability: 0.235

Enrichment: 0.733

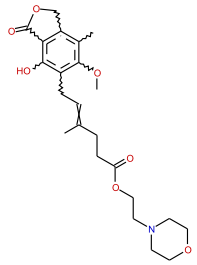
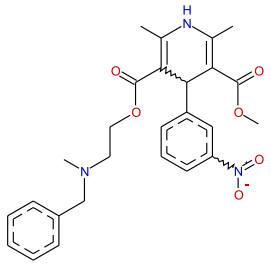
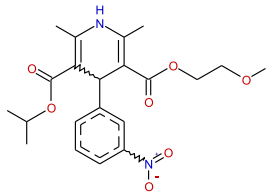
Bayesian Score: -1.68

Mahalanobis Distance: 15.3

Mahalanobis Distance p-value: 7.99e-008

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Mycophenolate	Nicardipine	Nimodipine
Structure			
Actual Endpoint	Non-Carcinogen	Non-Carcinogen	Non-Carcinogen
Predicted Endpoint	Non-Carcinogen	Non-Carcinogen	Non-Carcinogen
Distance	0.632	0.664	0.675
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

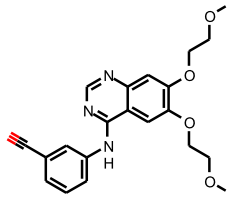
Model Applicability

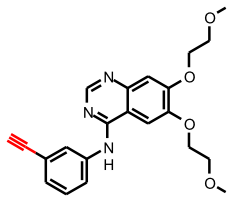
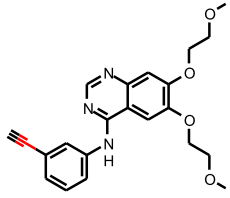
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -182178874: [*]#C[c](:c:[*]):c:[*]
3. Unknown ECFP_2 feature: 1139738044: [*]:[c](:[*])C#C

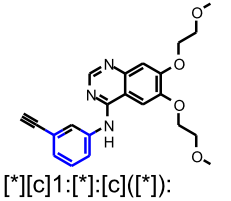
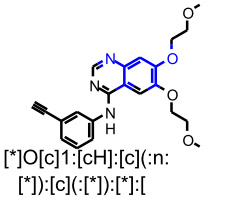
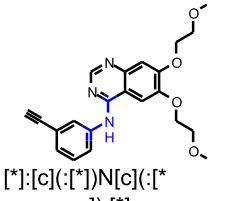
Feature Contribution

Top features for positive contribution

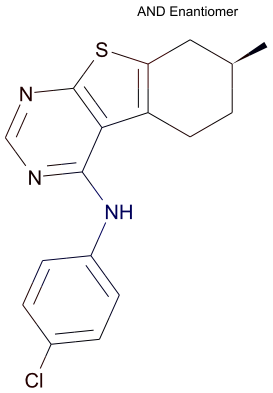
Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_6	-1939823063	 [*]#C	0.866	8 out of 9

ECFP_6	-1545539812	 [*]C#C	0.866	8 out of 9
ECFP_6	-1114776580	 [*]C#[*]	0.755	11 out of 15

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_6	2007300961	 [*][c]1:[*]:[c]([*]):[cH]:[cH]:[cH]:1	-0.652	5 out of 34
ECFP_6	-2063202154	 [*]O[c]1:[cH]:[c](:n:[*]):[c](:[*]):[*]:[c]:1[*]	-0.482	0 out of 2
ECFP_6	-1242906247	 [*]:[c](:[*])N[c](:[*]):[*]	-0.482	0 out of 2

TOPKAT_Mouse_Female_FDA_Single_vs_Multiple



$C_{17}H_{16}ClN_3S$

Molecular Weight: 329.84704

ALogP: 5.5

Rotatable Bonds: 2

Acceptors: 3

Donors: 1

Model Prediction

Prediction: Multiple-Carcinogen

Probability: 0.415

Enrichment: 1.01

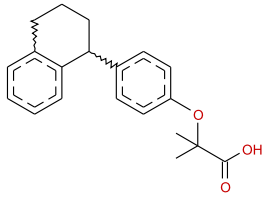
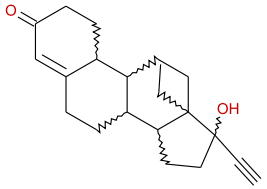
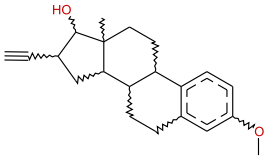
Bayesian Score: 0.333

Mahalanobis Distance: 15.5

Mahalanobis Distance p-value: 3.16e-007

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Nafenopin	Levonorgestrel	Mestranol
Structure			
Actual Endpoint	Single-Carcinogen	Single-Carcinogen	Multiple-Carcinogen
Predicted Endpoint	Single-Carcinogen	Single-Carcinogen	Multiple-Carcinogen
Distance	0.612	0.641	0.655
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

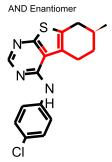
Model Applicability

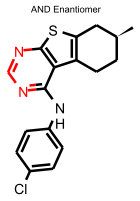
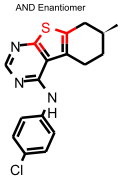
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1672647522: [*]C[c]1:s:[*]:[*]:[c]:1[*]
3. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
4. Unknown ECFP_2 feature: -1242906247: [*]:[c](:[*])N[c](:[*]):[*]

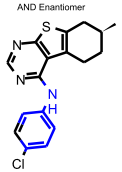
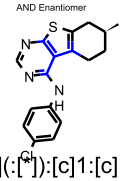
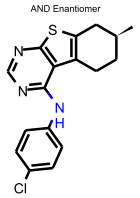
Feature Contribution

Top features for positive contribution

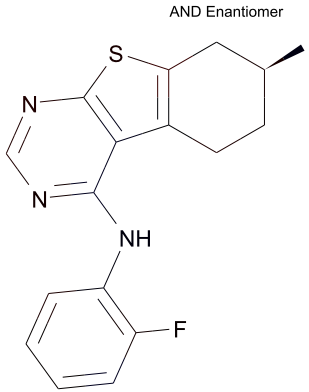
Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
ECFP_4	553181281	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2CC1	0.351	1 out of 1

ECFP_4	-710237522	 [*]:n:[cH]:n:[*]	0.351	1 out of 1
ECFP_4	85262808	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.351	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
ECFP_4	888054369	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	-0.8	0 out of 3
ECFP_4	-1661653144	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.597	0 out of 2
ECFP_4	-1897341097	 [*]N[*]	-0.356	8 out of 29

TOPKAT_Mouse_Female_FDA_Single_vs_Multiple



$C_{17}H_{16}FN_3S$

Molecular Weight: 313.39244

ALogP: 5.041

Rotatable Bonds: 2

Acceptors: 3

Donors: 1

Model Prediction

Prediction: Multiple-Carcinogen

Probability: 0.472

Enrichment: 1.15

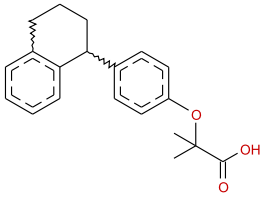
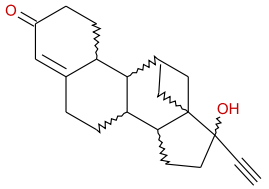
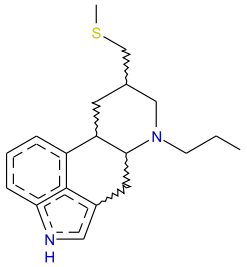
Bayesian Score: 1.6

Mahalanobis Distance: 13.5

Mahalanobis Distance p-value: 1.91e-005

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Nafenopin	Levonorgestrel	Pergolide
Structure			
Actual Endpoint	Single-Carcinogen	Single-Carcinogen	Single-Carcinogen
Predicted Endpoint	Single-Carcinogen	Single-Carcinogen	Single-Carcinogen
Distance	0.593	0.636	0.655
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

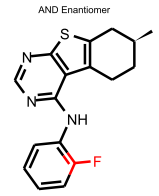
Model Applicability

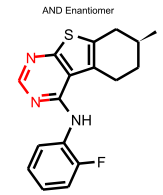
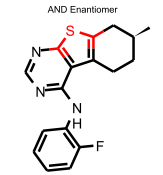
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1672647522: [*]C[c]1:s:[*]:[*]:[c]:1[*]
3. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
4. Unknown ECFP_2 feature: -1242906247: [*]:[c](:[*])N[c](:[*]):[*]

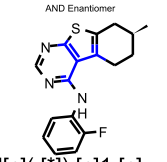
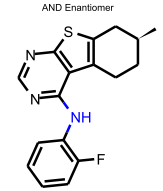
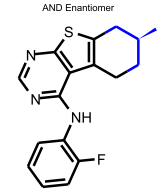
Feature Contribution

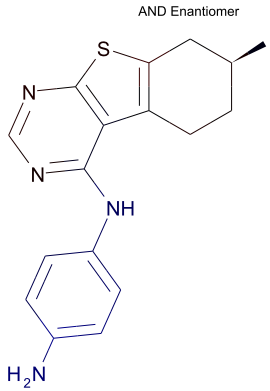
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
ECFP_4	220735655	 [*]:[c](:[*])F	0.497	4 out of 5

ECFP_4	-710237522	 [*]:n:[cH]:n:[*]	0.351	1 out of 1
ECFP_4	85262808	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.351	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
ECFP_4	-1661653144	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.597	0 out of 2
ECFP_4	-1897341097	 [*]N[*]	-0.356	8 out of 29
ECFP_4	292958156	 [*]CC(C)C[*]	-0.342	0 out of 1



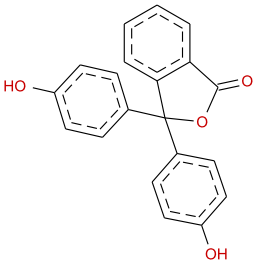
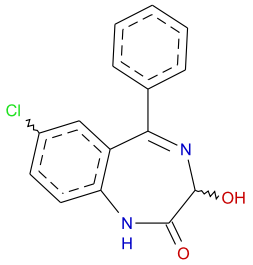
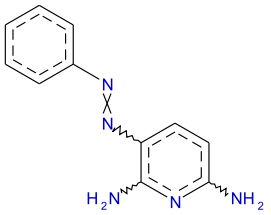
$C_{17}H_{18}N_4S$
Molecular Weight: 310.41662
ALogP: 4.089
Rotatable Bonds: 2
Acceptors: 4
Donors: 2

Model Prediction

Prediction: Single-Carcinogen
Probability: 0.305
Enrichment: 0.744
Bayesian Score: -2.95
Mahalanobis Distance: 15.9
Mahalanobis Distance p-value: 1.43e-007

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Phenolphthalein	Oxazepam	Phenazopyridine
Structure			
Actual Endpoint	Multiple-Carcinogen	Multiple-Carcinogen	Single-Carcinogen
Predicted Endpoint	Multiple-Carcinogen	Multiple-Carcinogen	Single-Carcinogen
Distance	0.578	0.655	0.715
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

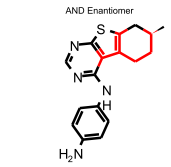
Model Applicability

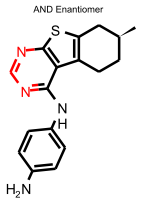
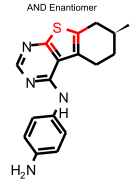
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1672647522: [*]C[c]1:s:[*]:[*]:[c]:1[*]
3. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
4. Unknown ECFP_2 feature: -1242906247: [*]:[c](:[*])N[c](:[*]):[*]

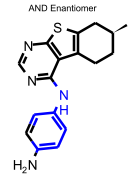
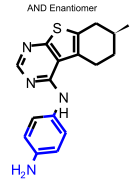
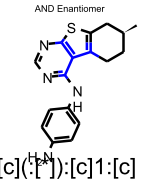
Feature Contribution

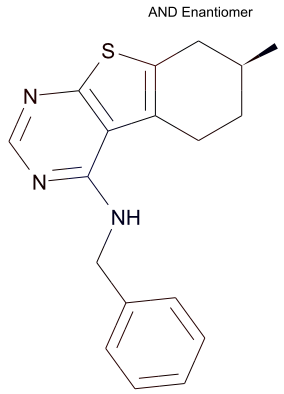
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
ECFP_4	553181281	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2 CC1	0.351	1 out of 1

ECFP_4	-710237522	 [*]:n:[cH]:n:[*]	0.351	1 out of 1
ECFP_4	85262808	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.351	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
ECFP_4	888054369	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	-0.8	0 out of 3
ECFP_4	924664308	 [*][c]1:[*]:[cH]:[c](N):[cH]:[cH]:1	-0.597	0 out of 2
ECFP_4	-1661653144	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.597	0 out of 2



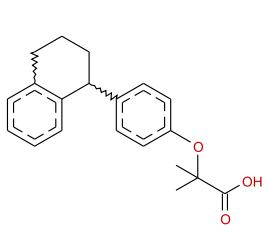
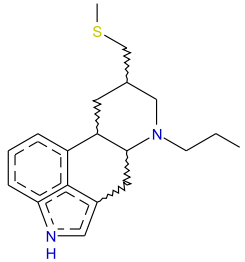
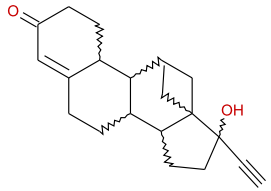
$C_{18}H_{19}N_3S$
Molecular Weight: 309.42856
ALogP: 4.678
Rotatable Bonds: 3
Acceptors: 3
Donors: 1

Model Prediction

Prediction: Multiple-Carcinogen
Probability: 0.439
Enrichment: 1.07
Bayesian Score: 0.904
Mahalanobis Distance: 13.8
Mahalanobis Distance p-value: 1.14e-005

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Nafenopin	Pergolide	Levonorgestrel
Structure			
Actual Endpoint	Single-Carcinogen	Single-Carcinogen	Single-Carcinogen
Predicted Endpoint	Single-Carcinogen	Single-Carcinogen	Single-Carcinogen
Distance	0.547	0.602	0.651
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

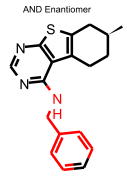
Model Applicability

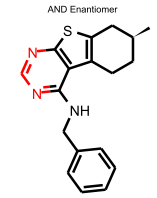
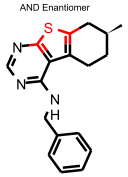
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1672647522: [*]C[c]1:s:[*]:[*]:[c]:1[*]
3. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]

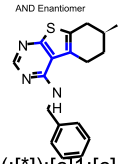
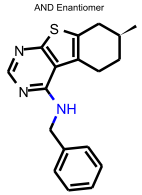
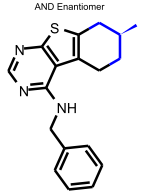
Feature Contribution

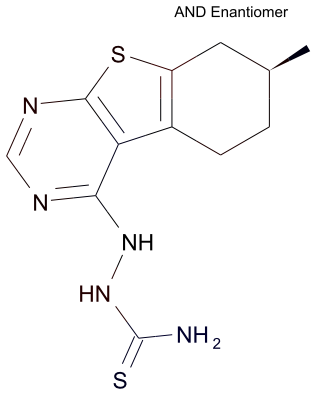
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
ECFP_4	110318898	 [*]NC[c]1:[cH]:[cH]:[*]:[cH]:[cH]:1	0.351	1 out of 1

ECFP_4	-710237522	 [*]:n:[cH]:n:[*]	0.351	1 out of 1
ECFP_4	85262808	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.351	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
ECFP_4	-1661653144	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.597	0 out of 2
ECFP_4	-1897341097	 [*]N[*]	-0.356	8 out of 29
ECFP_4	292958156	 [*]CC(C)C[*]	-0.342	0 out of 1



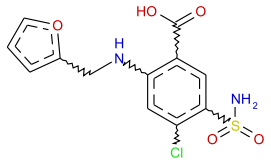
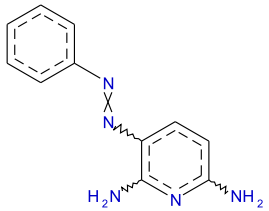
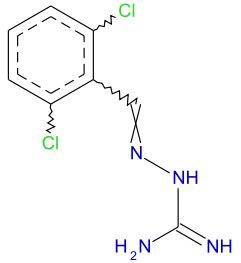
$C_{12}H_{15}N_5S_2$
Molecular Weight: 293.411
ALogP: 3.209
Rotatable Bonds: 3
Acceptors: 4
Donors: 3

Model Prediction

Prediction: Multiple-Carcinogen
Probability: 0.338
Enrichment: 0.825
Bayesian Score: -1.78
Mahalanobis Distance: 14.7
Mahalanobis Distance p-value: 1.82e-006

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Furosemide	Phenazopyridine	Guanabenz
Structure			
Actual Endpoint	Single-Carcinogen	Single-Carcinogen	Single-Carcinogen
Predicted Endpoint	Single-Carcinogen	Single-Carcinogen	Single-Carcinogen
Distance	0.708	0.744	0.758
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

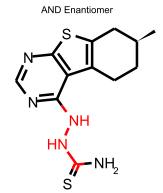
Model Applicability

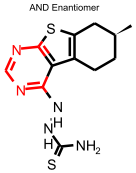
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1672647522: [*]C[c]1:s:[*]:[*]:[c]:1[*]
3. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
4. Unknown ECFP_2 feature: -571028867: [*]NC(=S)N

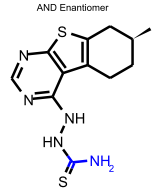
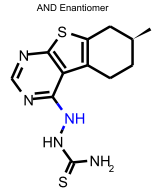
Feature Contribution

Top features for positive contribution

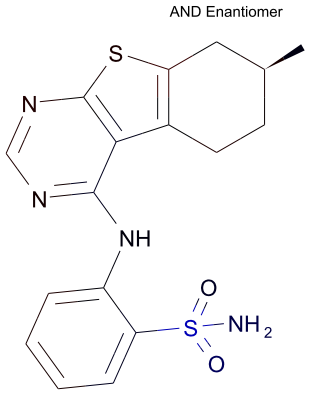
Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
ECFP_4	1635339976	 [*]NNC(=[*])[*]	0.351	1 out of 1

ECFP_4	553181281	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2 CC1	0.351	1 out of 1
ECFP_4	-1448786963	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.351	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
ECFP_4	-1661653144	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.597	0 out of 2
ECFP_4	-932108170	 [*]C(=[*])N	-0.545	1 out of 6
ECFP_4	-1897341097	 [*]N[*]	-0.356	8 out of 29

TOPKAT_Mouse_Female_FDA_Single_vs_Multiple



$C_{17}H_{18}N_4O_2S_2$

Molecular Weight: 374.48042

ALogP: 3.541

Rotatable Bonds: 3

Acceptors: 5

Donors: 2

Model Prediction

Prediction: Single-Carcinogen

Probability: 0.265

Enrichment: 0.646

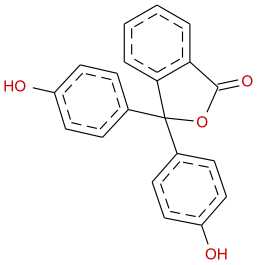
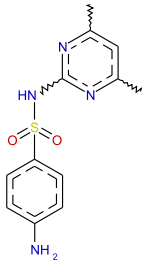
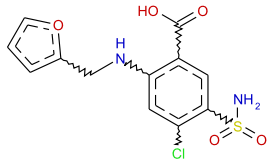
Bayesian Score: -4.84

Mahalanobis Distance: 14.3

Mahalanobis Distance p-value: 3.91e-006

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Phenolphthalein	Sulfamethazine	Furosemide
Structure			
Actual Endpoint	Multiple-Carcinogen	Single-Carcinogen	Single-Carcinogen
Predicted Endpoint	Multiple-Carcinogen	Single-Carcinogen	Single-Carcinogen
Distance	0.719	0.719	0.719
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

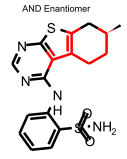
Model Applicability

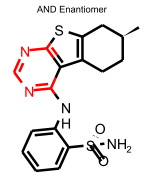
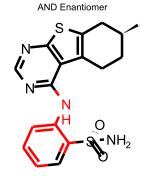
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1672647522: [*]C[c]1:s:[*]:[*]:[c]:1[*]
3. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
4. Unknown ECFP_2 feature: -1242906247: [*]:[c](:[*])N[c](:[*]):[*]

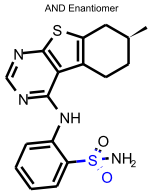
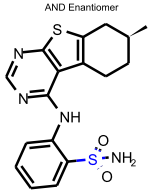
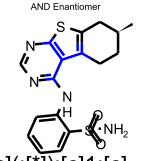
Feature Contribution

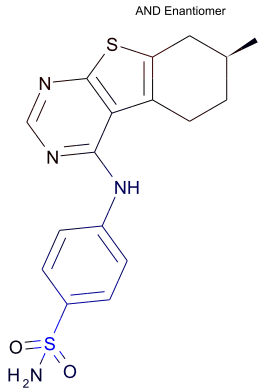
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
ECFP_4	553181281	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2 CC1	0.351	1 out of 1

ECFP_4	-1448786963	 [*][c]1:[*]:[c](:[*]) :n:[cH]:n:1	0.351	1 out of 1
ECFP_4	1635992319	 [*]N[c]1:[cH]:[cH]:[c H]:[*]:[c]:1[*]	0.351	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
ECFP_4	2102150379	 [*]S(=[*])(=O)[*]	-1.11	0 out of 5
ECFP_4	-797085356	 [*]S(=[*])(=[*])[*]	-1.11	0 out of 5
ECFP_4	-1661653144	 [*][c](:[*]):[c]1:[c] ([*]):[*]:[*]:[c]:1: [*]	-0.597	0 out of 2



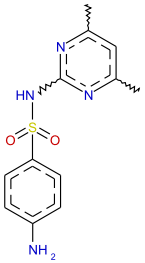
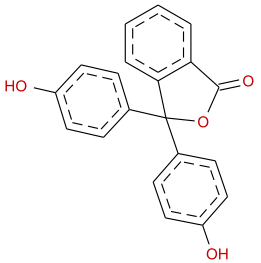
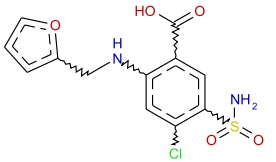
$C_{17}H_{18}N_4O_2S_2$
Molecular Weight: 374.48042
ALogP: 3.541
Rotatable Bonds: 3
Acceptors: 5
Donors: 2

Model Prediction

Prediction: Single-Carcinogen
Probability: 0.229
Enrichment: 0.558
Bayesian Score: -7.71
Mahalanobis Distance: 15.5
Mahalanobis Distance p-value: 3.18e-007

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Sulfamethazine	Phenolphthalein	Furosemide
Structure			
Actual Endpoint	Single-Carcinogen	Multiple-Carcinogen	Single-Carcinogen
Predicted Endpoint	Single-Carcinogen	Multiple-Carcinogen	Single-Carcinogen
Distance	0.700	0.732	0.744
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

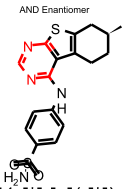
Model Applicability

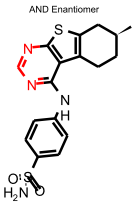
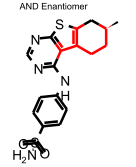
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1672647522: [*]C[c]1:s:[*]:[*]:[c]:1[*]
3. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
4. Unknown ECFP_2 feature: -1242906247: [*]:[c](:[*])N[c](:[*]):[*]

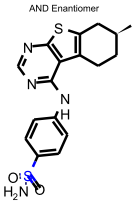
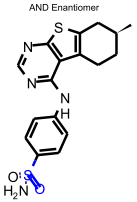
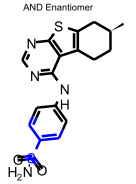
Feature Contribution

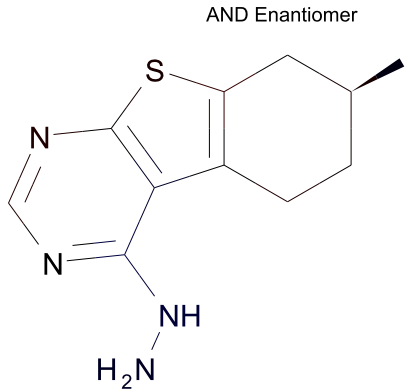
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
ECFP_4	-1448786963	 [*][c]1:[*]:[c](:[*]) :n:[cH]:n:1	0.351	1 out of 1

ECFP_4	-710237522	 [*]:n:[cH]:n:[*]	0.351	1 out of 1
ECFP_4	553181281	 [*][C@@H]1[*][c]2:[*] :[*]:[c](:[*]):[c]:2 CC1	0.351	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
ECFP_4	-797085356	 [*]S(=[*])(=[*])[*]	-1.11	0 out of 5
ECFP_4	2102150379	 [*]S(=[*])(=O)[*]	-1.11	0 out of 5
ECFP_4	-177264675	 [*]S(=[*])(=[*])[c](: [cH]:[*]):[cH]:[*]	-0.968	0 out of 4



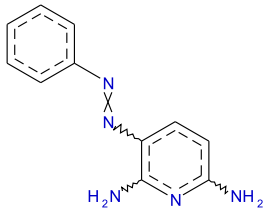
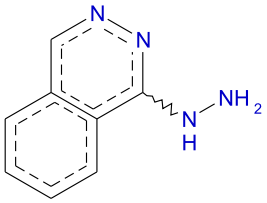
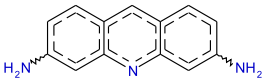
$C_{11}H_{14}N_4S$
Molecular Weight: 234.32065
ALogP: 2.561
Rotatable Bonds: 1
Acceptors: 4
Donors: 2

Model Prediction

Prediction: Single-Carcinogen
Probability: 0.327
Enrichment: 0.798
Bayesian Score: -2.14
Mahalanobis Distance: 15.2
Mahalanobis Distance p-value: 6.92e-007

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Phenazopyridine	Hydralazine	Proflavine
Structure			
Actual Endpoint	Single-Carcinogen	Single-Carcinogen	Single-Carcinogen
Predicted Endpoint	Single-Carcinogen	Single-Carcinogen	Single-Carcinogen
Distance	0.584	0.608	0.638
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

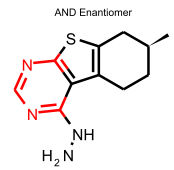
Model Applicability

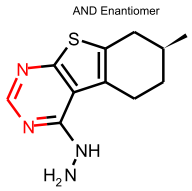
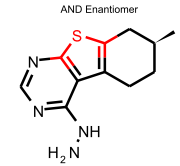
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1672647522: [*]C[c]1:s:[*]:[*]:[c]:1[*]
3. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]

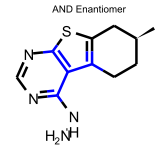
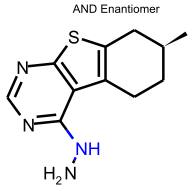
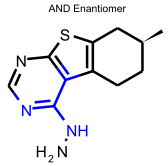
Feature Contribution

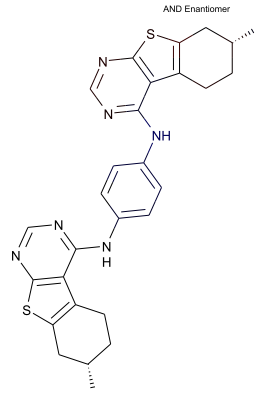
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
ECFP_4	-1448786963	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.351	1 out of 1

ECFP_4	-710237522	 [*]:n:[cH]:n:[*]	0.351	1 out of 1
ECFP_4	85262808	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.351	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
ECFP_4	-1661653144	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.597	0 out of 2
ECFP_4	-1897341097	 [*]N[*]	-0.356	8 out of 29
ECFP_4	1049768340	 [*]N[c](:n:[*]):[c](:[*]):[*]	-0.342	0 out of 1



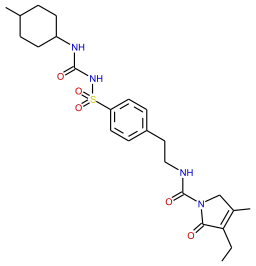
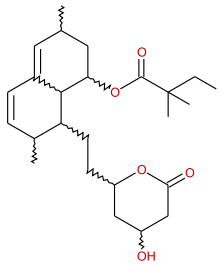
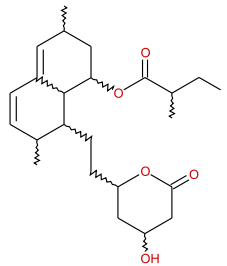
$C_{28}H_{28}N_6S_2$
Molecular Weight: 512.69212
ALogP: 7.842
Rotatable Bonds: 4
Acceptors: 6
Donors: 2

Model Prediction

Prediction: Multiple-Carcinogen
Probability: 0.381
Enrichment: 0.929
Bayesian Score: -0.526
Mahalanobis Distance: 16.4
Mahalanobis Distance p-value: 6e-008

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Glimepride	Simvastatin	Lovastatin
Structure			
Actual Endpoint	Single-Carcinogen	Multiple-Carcinogen	Multiple-Carcinogen
Predicted Endpoint	Single-Carcinogen	Multiple-Carcinogen	Multiple-Carcinogen
Distance	0.899	0.911	0.940
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

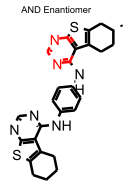
Model Applicability

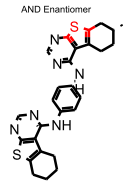
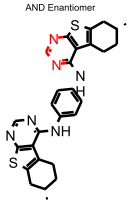
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1672647522: [*]C[c]1:s:[*]:[*]:[c]:1[*]
3. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
4. Unknown ECFP_2 feature: -1242906247: [*]:[c](:[*])N[c](:[*]):[*]

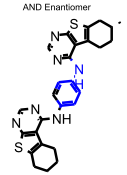
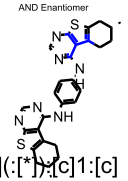
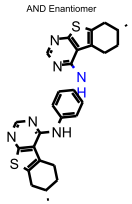
Feature Contribution

Top features for positive contribution

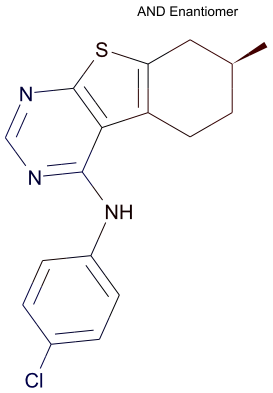
Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
ECFP_4	-1448786963	 [*][c]1:[*]:[c](:[*]) :n:[cH]:n:1	0.351	1 out of 1

ECFP_4	85262808	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.351	1 out of 1
ECFP_4	-710237522	 [*]:n:[cH]:n:[*]	0.351	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
ECFP_4	888054369	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	-0.8	0 out of 3
ECFP_4	-1661653144	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.597	0 out of 2
ECFP_4	-1897341097	 [*]N[*]	-0.356	8 out of 29

TOPKAT_Mouse_Male_FDA_None_vs_Carcinogen



$C_{17}H_{16}ClN_3S$

Molecular Weight: 329.84704

ALogP: 5.5

Rotatable Bonds: 2

Acceptors: 3

Donors: 1

Model Prediction

Prediction: Carcinogen

Probability: 0.266

Enrichment: 0.904

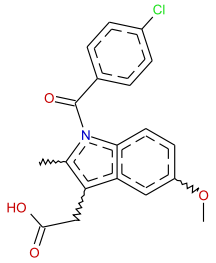
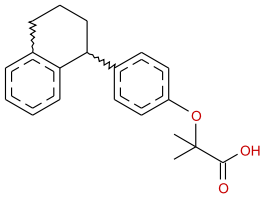
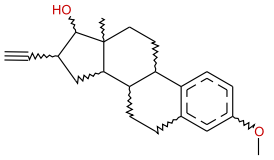
Bayesian Score: -1.58

Mahalanobis Distance: 15.4

Mahalanobis Distance p-value: 1.47e-008

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Indomethacin	Nafenopin	Mestranol
Structure			
Actual Endpoint	Non-Carcinogen	Carcinogen	Carcinogen
Predicted Endpoint	Non-Carcinogen	Carcinogen	Carcinogen
Distance	0.619	0.622	0.639
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

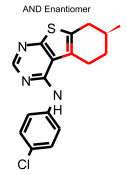
Model Applicability

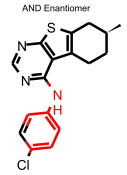
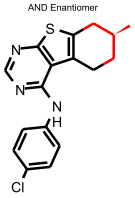
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. OPS PC19 out of range. Value: -3.237. Training min, max, SD, explained variance: -2.8152, 4.6113, 1.185, 0.0147.

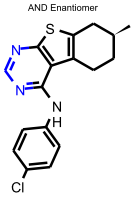
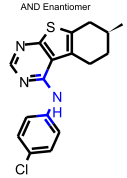
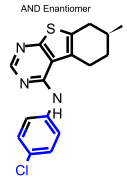
Feature Contribution

Top features for positive contribution

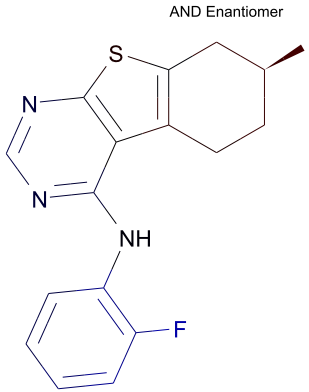
Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
FCFP_6	-1441604640	 [*]:[c]1:[*]C[C@@H](C)CC1	0.77	4 out of 5

FCFP_6	-773983804	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	0.409	10 out of 24
FCFP_6	-1043339860	 [*]CC(C)C[*]	0.383	24 out of 61

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
FCFP_6	-124685461	 [*]:n:[cH]:n:[*]	-0.731	1 out of 12
FCFP_6	1293778554	 [*]:[c](:[*])N[c](:[*]):[*]	-0.719	0 out of 4
FCFP_6	551850122	 [*][c]1:[*]:[cH]:[c](Cl):[cH]:[cH]:1	-0.433	8 out of 49

TOPKAT_Mouse_Male_FDA_None_vs_Carcinogen



$C_{17}H_{16}FN_3S$

Molecular Weight: 313.39244

ALogP: 5.041

Rotatable Bonds: 2

Acceptors: 3

Donors: 1

Model Prediction

Prediction: Carcinogen

Probability: 0.273

Enrichment: 0.926

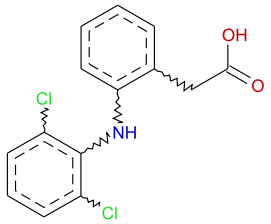
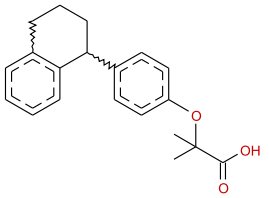
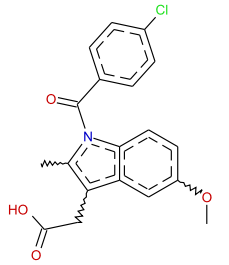
Bayesian Score: -1.3

Mahalanobis Distance: 17.2

Mahalanobis Distance p-value: 2.45e-012

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Diclofenac	Nafenopin	Indomethacin
Structure			
Actual Endpoint	Non-Carcinogen	Carcinogen	Non-Carcinogen
Predicted Endpoint	Non-Carcinogen	Carcinogen	Non-Carcinogen
Distance	0.600	0.610	0.621
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

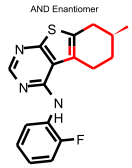
Model Applicability

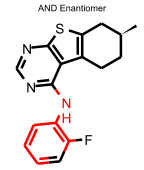
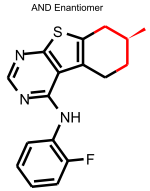
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. OPS PC19 out of range. Value: -2.8919. Training min, max, SD, explained variance: -2.8152, 4.6113, 1.185, 0.0147.

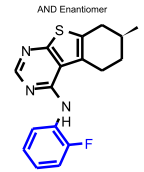
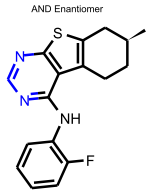
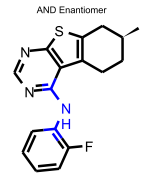
Feature Contribution

Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
FCFP_6	-1441604640	 [*]:[c]1:[*]C[C@@H](C)CC1	0.77	4 out of 5

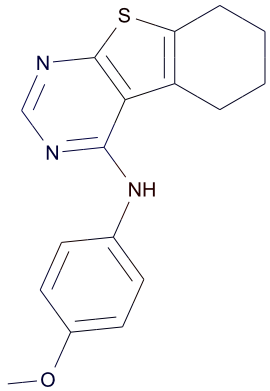
FCFP_6	-773983804	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	0.409	10 out of 24
FCFP_6	-1043339860	 [*]CC(C)C[*]	0.383	24 out of 61

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
FCFP_6	-2095752315	 [*][c]1:[cH]:[cH]:[cH]:[cH]:[c]:1F	-1.13	0 out of 8
FCFP_6	-124685461	 [*]:n:[cH]:n:[*]	-0.731	1 out of 12
FCFP_6	1293778554	 [*]:[c](:[*])N[c](:[*]):[*]	-0.719	0 out of 4

5c

TOPKAT_Mouse_Male_FDA_None_vs_Carcinogen



$C_{17}H_{17}N_3OS$

Molecular Weight: 311.40138

ALogP: 4.568

Rotatable Bonds: 3

Acceptors: 4

Donors: 1

Model Prediction

Prediction: Non-Carcinogen

Probability: 0.232

Enrichment: 0.789

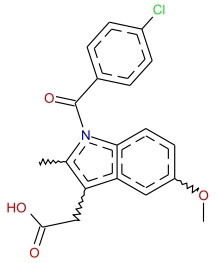
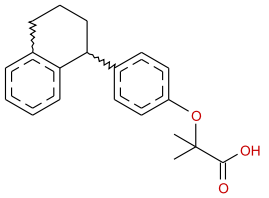
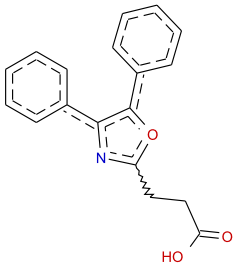
Bayesian Score: -3.15

Mahalanobis Distance: 15.4

Mahalanobis Distance p-value: 1.79e-008

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Indomethacin	Nafenopin	Oxaprocin
Structure			
Actual Endpoint	Non-Carcinogen	Carcinogen	Carcinogen
Predicted Endpoint	Non-Carcinogen	Carcinogen	Carcinogen
Distance	0.540	0.597	0.632
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

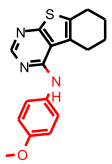
Model Applicability

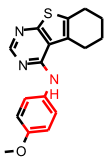
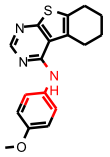
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. OPS PC19 out of range. Value: -3.0431. Training min, max, SD, explained variance: -2.8152, 4.6113, 1.185, 0.0147.

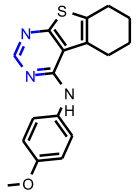
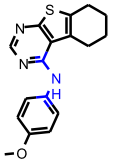
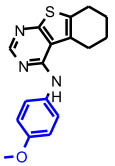
Feature Contribution

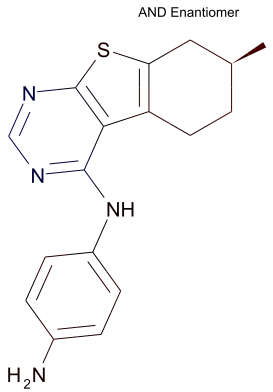
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
FCFP_6	-1060187936	 [*]N[c]1:[cH]:[cH]:[c](OC):[cH]:[cH]:1	0.46	1 out of 1

FCFP_6	-773983804	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	0.409	10 out of 24
FCFP_6	590925877	 [*]N[c](:[cH]:[*]):[cH]:[*]	0.369	13 out of 33

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
FCFP_6	-124685461	 [*]:n:[cH]:n:[*]	-0.731	1 out of 12
FCFP_6	1293778554	 [*]:[c](:[*])N[c](:[*]):[*]	-0.719	0 out of 4
FCFP_6	-9847677	 [*][c]1:[cH]:[cH]:[c](OC):[cH]:[cH]:1	-0.719	0 out of 4



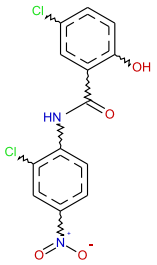
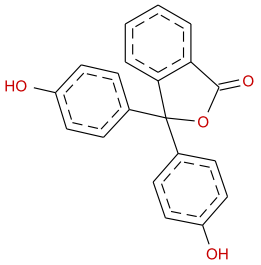
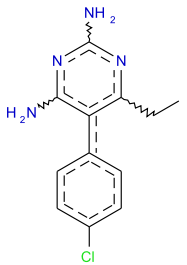
$C_{17}H_{18}N_4S$
Molecular Weight: 310.41662
ALogP: 4.089
Rotatable Bonds: 2
Acceptors: 4
Donors: 2

Model Prediction

Prediction: Carcinogen
Probability: 0.339
Enrichment: 1.15
Bayesian Score: 1.16
Mahalanobis Distance: 13.3
Mahalanobis Distance p-value: 8.27e-005

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Niclosamide	Phenolphthalein	Pyrimethamine
Structure			
Actual Endpoint	Non-Carcinogen	Carcinogen	Non-Carcinogen
Predicted Endpoint	Non-Carcinogen	Carcinogen	Non-Carcinogen
Distance	0.548	0.572	0.594
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

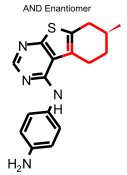
Model Applicability

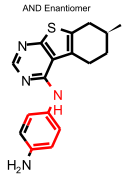
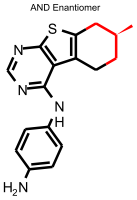
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

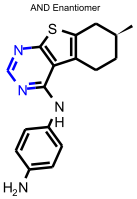
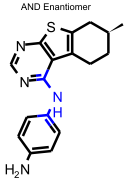
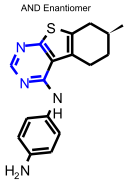
Feature Contribution

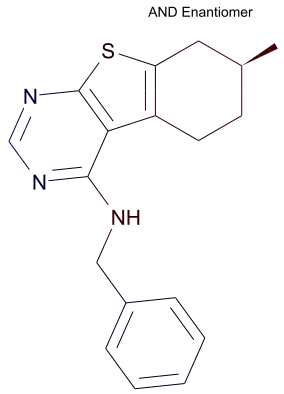
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
FCFP_6	-1441604640	 [*]:[c]1:[*]C[C@@H](C)CC1	0.77	4 out of 5

FCFP_6	-773983804	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	0.409	10 out of 24
FCFP_6	-1043339860	 [*]CC(C)C[*]	0.383	24 out of 61

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
FCFP_6	-124685461	 [*]:n:[cH]:n:[*]	-0.731	1 out of 12
FCFP_6	1293778554	 [*]:[c](:[*])N[c](:[*]):[*]	-0.719	0 out of 4
FCFP_6	-475316933	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	-0.423	0 out of 2



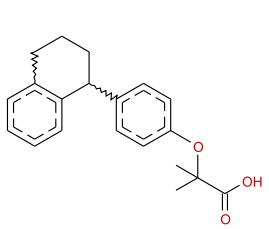
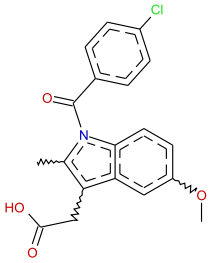
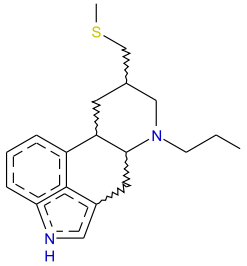
$C_{18}H_{19}N_3S$
Molecular Weight: 309.42856
ALogP: 4.678
Rotatable Bonds: 3
Acceptors: 3
Donors: 1

Model Prediction

Prediction: Carcinogen
Probability: 0.325
Enrichment: 1.1
Bayesian Score: 0.677
Mahalanobis Distance: 14.1
Mahalanobis Distance p-value: 4.11e-006

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Nafenopin	Indomethacin	Pergolide
Structure			
Actual Endpoint	Carcinogen	Non-Carcinogen	Non-Carcinogen
Predicted Endpoint	Carcinogen	Non-Carcinogen	Non-Carcinogen
Distance	0.548	0.591	0.601
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

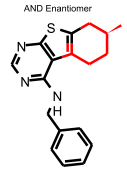
Model Applicability

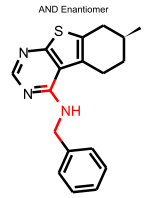
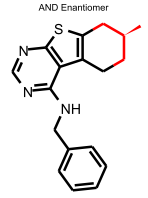
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

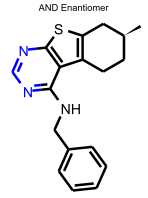
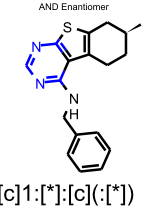
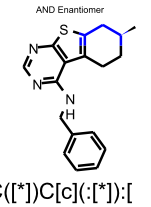
Feature Contribution

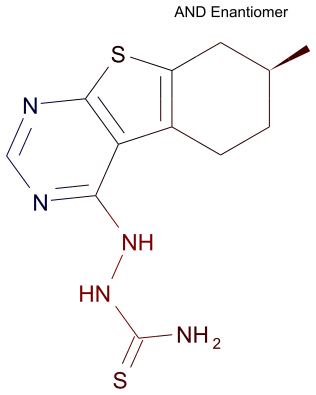
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
FCFP_6	-1441604640	 [*:[c]1:[*]C[C@@H](C)CC1	0.77	4 out of 5

FCFP_6	1294255210	 [*]CN[c](:[*]):[*]	0.441	12 out of 28
FCFP_6	-1043339860	 [*]CC(C)C[*]	0.383	24 out of 61

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
FCFP_6	-124685461	 [*]:n:[cH]:n:[*]	-0.731	1 out of 12
FCFP_6	-475316933	 [*][c]1:[*]:[c](:[*]) :n:[cH]:n:1	-0.423	0 out of 2
FCFP_6	907007053	 [*]C([*])C[c](:[*]):[*]	-0.366	11 out of 62



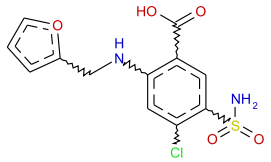
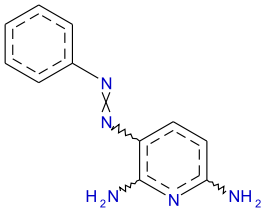
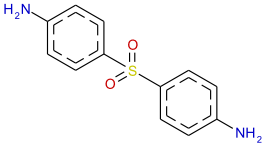
$C_{12}H_{15}N_5S_2$
Molecular Weight: 293.411
ALogP: 3.209
Rotatable Bonds: 3
Acceptors: 4
Donors: 3

Model Prediction

Prediction: Carcinogen
Probability: 0.397
Enrichment: 1.35
Bayesian Score: 2.93
Mahalanobis Distance: 14
Mahalanobis Distance p-value: 7.25e-006

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Furosemide	Phenazopyridine	Dapsone
Structure			
Actual Endpoint	Non-Carcinogen	Non-Carcinogen	Non-Carcinogen
Predicted Endpoint	Non-Carcinogen	Carcinogen	Carcinogen
Distance	0.683	0.712	0.715
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

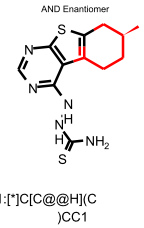
Model Applicability

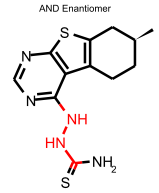
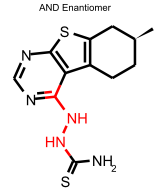
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. OPS PC30 out of range. Value: -2.6109. Training min, max, SD, explained variance: -2.5648, 3.3898, 0.9347, 0.0092.

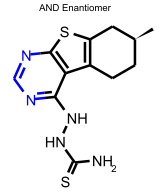
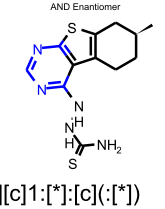
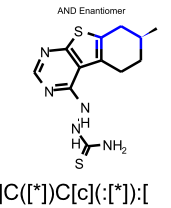
Feature Contribution

Top features for positive contribution

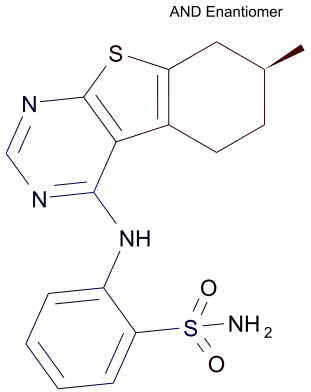
Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
FCFP_6	-1441604640	 [*]:[c]1:[*]C[C@@H](C)CC1	0.77	4 out of 5

FCFP_6	-885461129	 [*]NNC(=[*])[*]	0.547	3 out of 5
FCFP_6	1294344583	 [*]NN[c](:[*]):[*]	0.517	2 out of 3

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
FCFP_6	-124685461	 [*]:n:[cH]:n:[*]	-0.731	1 out of 12
FCFP_6	-475316933	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	-0.423	0 out of 2
FCFP_6	907007053	 [*]C([*])C[c](:[*]):[*]	-0.366	11 out of 62

TOPKAT_Mouse_Male_FDA_None_vs_Carcinogen



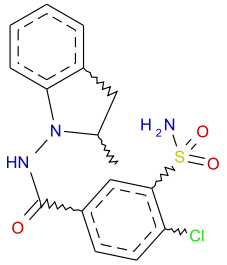
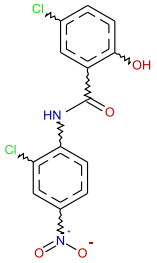
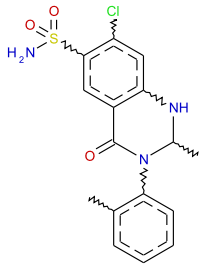
$C_{17}H_{18}N_4O_2S_2$
Molecular Weight: 374.48042
ALogP: 3.541
Rotatable Bonds: 3
Acceptors: 5
Donors: 2

Model Prediction

Prediction: Carcinogen
Probability: 0.286
Enrichment: 0.973
Bayesian Score: -0.74
Mahalanobis Distance: 15.1
Mahalanobis Distance p-value: 6.79e-008

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Indapamide	Niclosamide	Metolazone
Structure			
Actual Endpoint	Non-Carcinogen	Non-Carcinogen	Non-Carcinogen
Predicted Endpoint	Non-Carcinogen	Non-Carcinogen	Non-Carcinogen
Distance	0.584	0.590	0.609
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

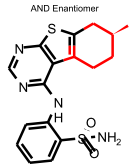
Model Applicability

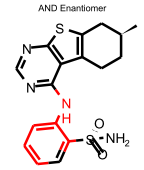
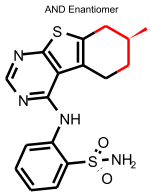
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

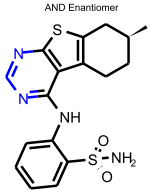
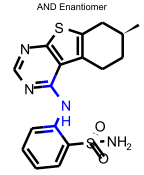
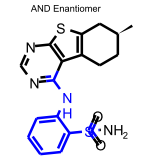
Feature Contribution

Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
FCFP_6	-1441604640	 [*:][c]1:[*]C[C@@H](C)CC1	0.77	4 out of 5

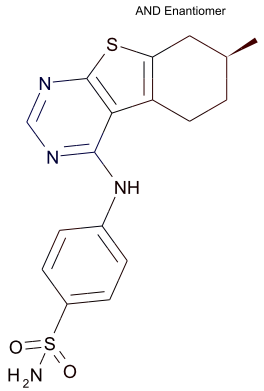
FCFP_6	-773983804	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	0.409	10 out of 24
FCFP_6	-1043339860	 [*]CC(C)C[*]	0.383	24 out of 61

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
FCFP_6	-124685461	 [*]:n:[cH]:n:[*]	-0.731	1 out of 12
FCFP_6	1293778554	 [*]:[c](:[*])N[c](:[*]):[*]	-0.719	0 out of 4
FCFP_6	-103236997	 [*]S(=[*])(=[*])[c]1:[cH]:[cH]:[cH]:[cH]:[c]:1N[c](:[*]):[*]	-0.582	0 out of 3

9b

TOPKAT_Mouse_Male_FDA_None_vs_Carcinogen



$C_{17}H_{18}N_4O_2S_2$

Molecular Weight: 374.48042

ALogP: 3.541

Rotatable Bonds: 3

Acceptors: 5

Donors: 2

Model Prediction

Prediction: Carcinogen

Probability: 0.321

Enrichment: 1.09

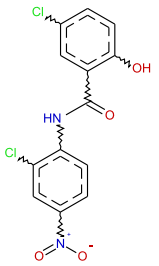
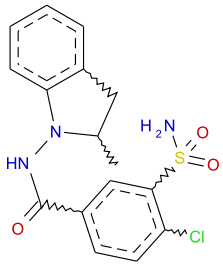
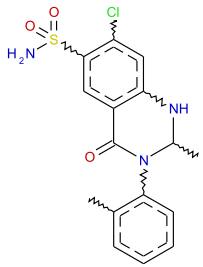
Bayesian Score: 0.528

Mahalanobis Distance: 14.5

Mahalanobis Distance p-value: 7.14e-007

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Niclosamide	Indapamide	Metolazone
Structure			
Actual Endpoint	Non-Carcinogen	Non-Carcinogen	Non-Carcinogen
Predicted Endpoint	Non-Carcinogen	Non-Carcinogen	Non-Carcinogen
Distance	0.588	0.593	0.618
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

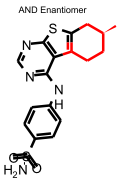
Model Applicability

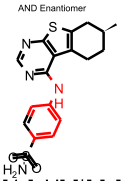
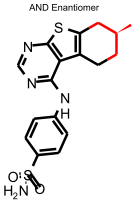
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. OPS PC19 out of range. Value: -2.8409. Training min, max, SD, explained variance: -2.8152, 4.6113, 1.185, 0.0147.
2. OPS PC30 out of range. Value: -2.7012. Training min, max, SD, explained variance: -2.5648, 3.3898, 0.9347, 0.0092.

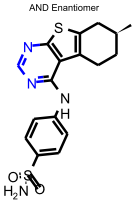
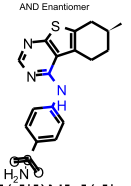
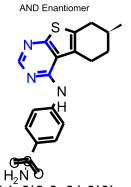
Feature Contribution

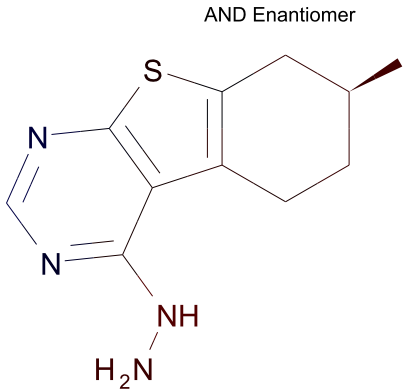
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
FCFP_6	-1441604640	 [*]:[c]1:[*]C[C@@H](C)CC1	0.77	4 out of 5

FCFP_6	-773983804	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	0.409	10 out of 24
FCFP_6	-1043339860	 [*]CC(C)C[*]	0.383	24 out of 61

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
FCFP_6	-124685461	 [*]:n:[cH]:n:[*]	-0.731	1 out of 12
FCFP_6	1293778554	 [*]:[c](:[*])N[c](:[*]):[*]	-0.719	0 out of 4
FCFP_6	-475316933	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	-0.423	0 out of 2



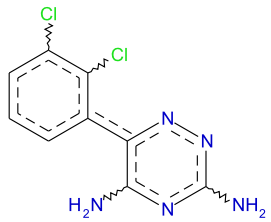
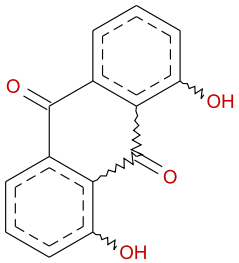
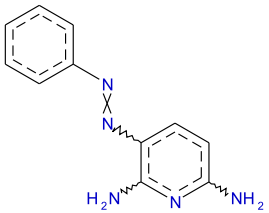
$C_{11}H_{14}N_4S$
Molecular Weight: 234.32065
ALogP: 2.561
Rotatable Bonds: 1
Acceptors: 4
Donors: 2

Model Prediction

Prediction: Carcinogen
Probability: 0.387
Enrichment: 1.32
Bayesian Score: 2.64
Mahalanobis Distance: 14.1
Mahalanobis Distance p-value: 4.16e-006

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Lamotrigine	Danthron	Phenazopyridine
Structure			
Actual Endpoint	Non-Carcinogen	Carcinogen	Non-Carcinogen
Predicted Endpoint	Non-Carcinogen	Carcinogen	Carcinogen
Distance	0.561	0.572	0.574
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

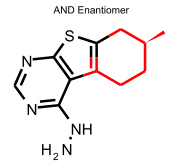
Model Applicability

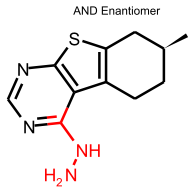
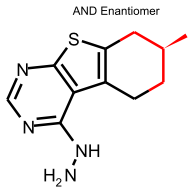
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

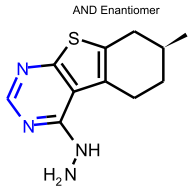
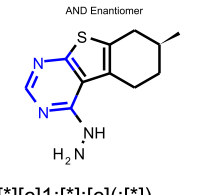
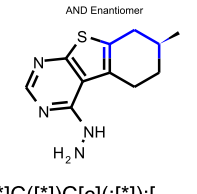
Feature Contribution

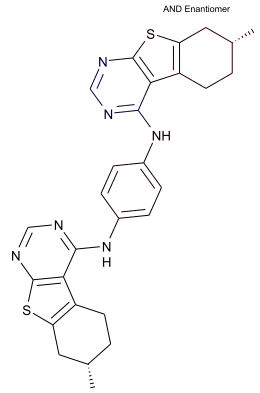
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
FCFP_6	-1441604640	 [*]:[c]1:[*]C[C@@H](C)CC1	0.77	4 out of 5

FCFP_6	1294344583	 [*]NN[c](:[*]):[*]	0.517	2 out of 3
FCFP_6	-1043339860	 [*]CC(C)C[*]	0.383	24 out of 61

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
FCFP_6	-124685461	 [*]:n:[cH]:n:[*]	-0.731	1 out of 12
FCFP_6	-475316933	 [*][c]1:[*]:[c](:[*]) :n:[cH]:n:1	-0.423	0 out of 2
FCFP_6	907007053	 [*]C([*])C[c](:[*]):[*]	-0.366	11 out of 62



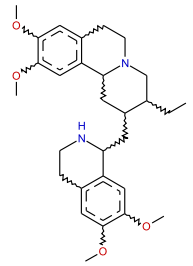
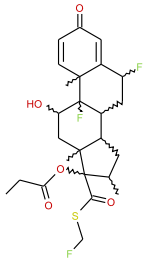
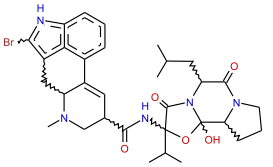
$C_{28}H_{28}N_6S_2$
Molecular Weight: 512.69212
ALogP: 7.842
Rotatable Bonds: 4
Acceptors: 6
Donors: 2

Model Prediction

Prediction: Carcinogen
Probability: 0.286
Enrichment: 0.971
Bayesian Score: -0.759
Mahalanobis Distance: 15.5
Mahalanobis Distance p-value: 1.06e-008

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Emetine	Fluticasone	Bromocriptine
Structure			
Actual Endpoint	Non-Carcinogen	Non-Carcinogen	Non-Carcinogen
Predicted Endpoint	Non-Carcinogen	Carcinogen	Non-Carcinogen
Distance	0.875	0.879	0.906
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

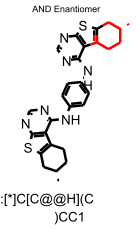
Model Applicability

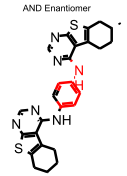
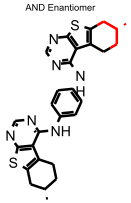
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. OPS PC19 out of range. Value: -3.2042. Training min, max, SD, explained variance: -2.8152, 4.6113, 1.185, 0.0147.

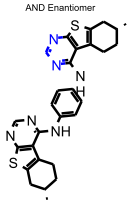
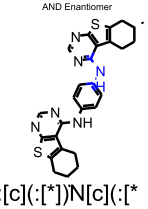
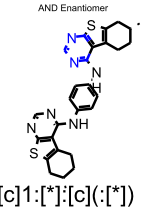
Feature Contribution

Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
FCFP_6	-1441604640	 [*]:[c]1:[*]C[C@@H](C)CC1	0.77	4 out of 5

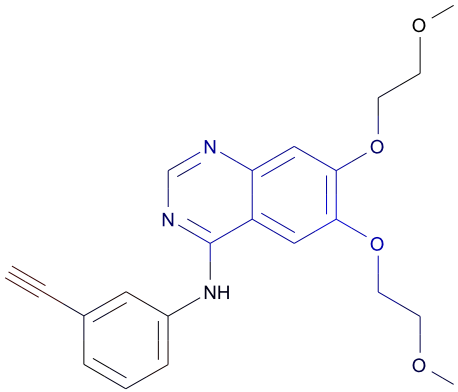
FCFP_6	-773983804	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	0.409	10 out of 24
FCFP_6	-1043339860	 [*]CC(C)C[*]	0.383	24 out of 61

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
FCFP_6	-124685461	 [*]:n:[cH]:n:[*]	-0.731	1 out of 12
FCFP_6	1293778554	 [*]:[c](:[*])N[c](:[*]):[*]	-0.719	0 out of 4
FCFP_6	-475316933	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	-0.423	0 out of 2

Erlotinib

TOPKAT_Mouse_Male_FDA_None_vs_Carcinogen



$C_{22}H_{23}N_3O_4$

Molecular Weight: 393.43572

ALogP: 4.309

Rotatable Bonds: 10

Acceptors: 7

Donors: 1

Model Prediction

Prediction: Non-Carcinogen

Probability: 0.181

Enrichment: 0.614

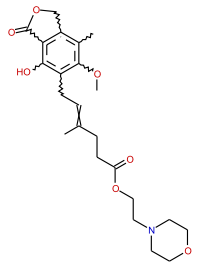
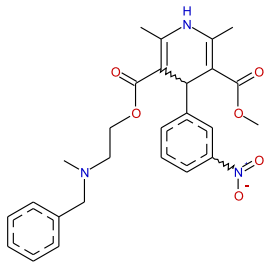
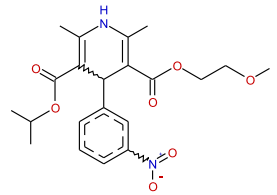
Bayesian Score: -6.29

Mahalanobis Distance: 16

Mahalanobis Distance p-value: 1.07e-009

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Mycophenolate	Nicardipine	Nimodipine
Structure			
Actual Endpoint	Non-Carcinogen	Non-Carcinogen	Non-Carcinogen
Predicted Endpoint	Non-Carcinogen	Non-Carcinogen	Non-Carcinogen
Distance	0.615	0.655	0.668
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

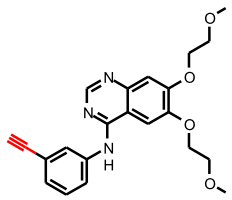
Model Applicability

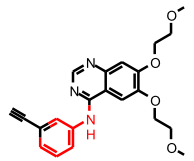
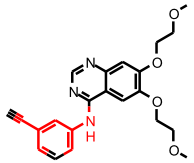
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: 902193919: [*]:[c](:[*])C#C

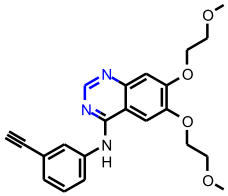
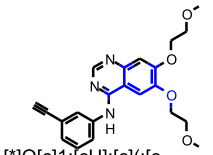
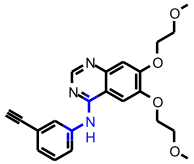
Feature Contribution

Top features for positive contribution

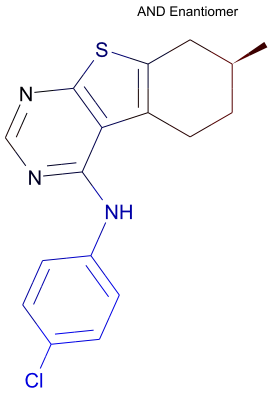
Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
FCFP_6	131784192	 [*]C#C	0.983	8 out of 9

FCFP_6	-773983804	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	0.409	10 out of 24
FCFP_6	-771557733	 [*]N[c]1:[cH]:[*]:[cH]:[c](:[cH]:1)C#[*]	0.38	2 out of 4

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
FCFP_6	-124685461	 [*]:n:[cH]:n:[*]	-0.731	1 out of 12
FCFP_6	1674955425	 [*]O[c]1:[cH]:[c](:[c]([*]):[*]):[c](:[*]):[*]:[c]:1[*]	-0.719	0 out of 4
FCFP_6	1293778554	 [*]:[c](:[*])N[c](:[*]):[*]	-0.719	0 out of 4

TOPKAT_Mouse_Male_FDA_Single_vs_Multiple



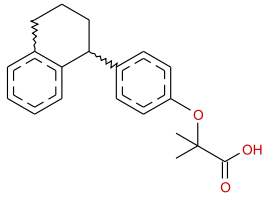
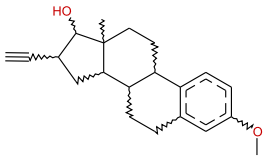
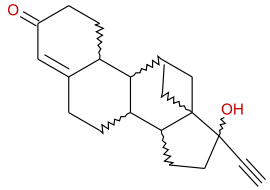
$C_{17}H_{16}ClN_3S$
Molecular Weight: 329.84704
ALogP: 5.5
Rotatable Bonds: 2
Acceptors: 3
Donors: 1

Model Prediction

Prediction: Single-Carcinogen
Probability: 0.146
Enrichment: 0.486
Bayesian Score: -8.59
Mahalanobis Distance: 15.7
Mahalanobis Distance p-value: 7.7e-007

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Nafenopin	Mestranol	Levonorgestrel
Structure			
Actual Endpoint	Single-Carcinogen	Multiple-Carcinogen	Single-Carcinogen
Predicted Endpoint	Single-Carcinogen	Multiple-Carcinogen	Multiple-Carcinogen
Distance	0.638	0.659	0.663
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

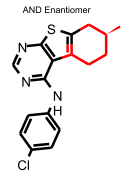
Model Applicability

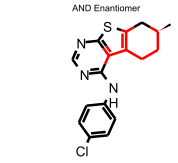
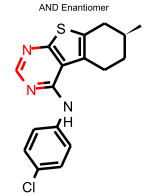
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. OPS PC7 out of range. Value: -5.152. Training min, max, SD, explained variance: -3.9478, 3.0766, 1.527, 0.0435.
2. Unknown FCFP_2 feature: 1293778554: [*]:[c](:[*])N[c](:[*]):[*]

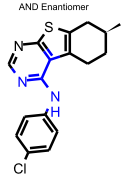
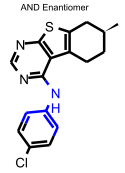
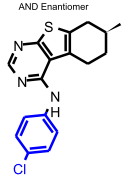
Feature Contribution

Top features for positive contribution

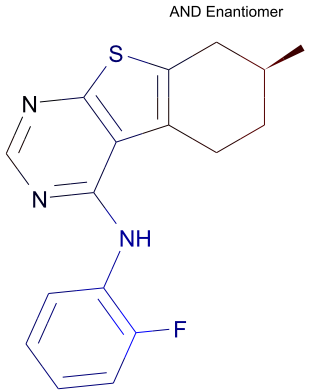
Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
FCFP_12	-1441604640	 [*]:[c]1:[*]C[C@@H](C)CC1	0.75	4 out of 4

FCFP_12	-2002183168	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2 CC1	0.616	4 out of 5
FCFP_12	-124685461	 [*]:n:[cH]:n:[*]	0.4	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
FCFP_12	-1151884458	 [*]N[c](:n:[*]):[c](:[*]):[*]	-1.11	0 out of 6
FCFP_12	590925877	 [*]N[c](:[cH]:[*]):[cH]:[*]	-0.998	1 out of 13
FCFP_12	-1508180856	 [*][c]1:[cH]:[cH]:[c](Cl):[cH]:[cH]:1	-0.859	0 out of 4

TOPKAT_Mouse_Male_FDA_Single_vs_Multiple



$C_{17}H_{16}FN_3S$

Molecular Weight: 313.39244

ALogP: 5.041

Rotatable Bonds: 2

Acceptors: 3

Donors: 1

Model Prediction

Prediction: Single-Carcinogen

Probability: 0.152

Enrichment: 0.505

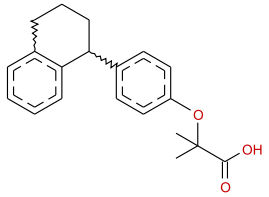
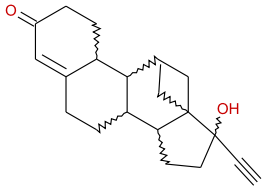
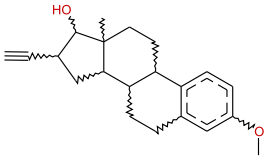
Bayesian Score: -6.97

Mahalanobis Distance: 18.1

Mahalanobis Distance p-value: 9.82e-009

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Nafenopin	Levonorgestrel	Mestranol
Structure			
Actual Endpoint	Single-Carcinogen	Single-Carcinogen	Multiple-Carcinogen
Predicted Endpoint	Single-Carcinogen	Multiple-Carcinogen	Multiple-Carcinogen
Distance	0.627	0.656	0.658
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

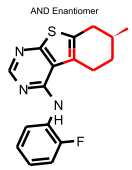
Model Applicability

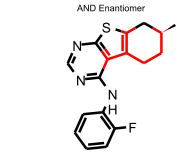
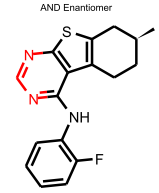
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. OPS PC7 out of range. Value: -4.7493. Training min, max, SD, explained variance: -3.9478, 3.0766, 1.527, 0.0435.
2. Unknown FCFP_2 feature: 1293778554: [*]:[c](:[*])N[c](:[*]):[*]

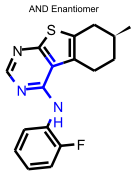
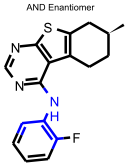
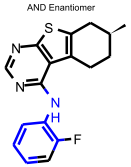
Feature Contribution

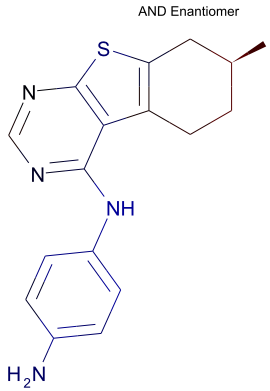
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
FCFP_12	-1441604640	 [*]:[c]1:[*]C[C@@H](C)CC1	0.75	4 out of 4

FCFP_12	-2002183168	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2 CC1	0.616	4 out of 5
FCFP_12	-124685461	 [*]:n:[cH]:n:[*]	0.4	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
FCFP_12	-1151884458	 [*]N[c](:n:[*]):[c](:[*]):[*]	-1.11	0 out of 6
FCFP_12	590925877	 [*]N[c](:[cH]:[*]):[cH]:[*]	-0.998	1 out of 13
FCFP_12	-773983804	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	-0.789	1 out of 10



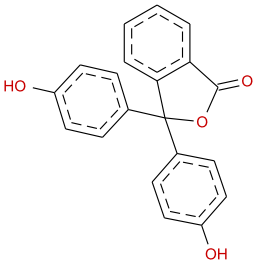
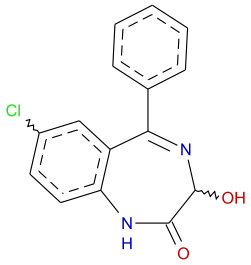
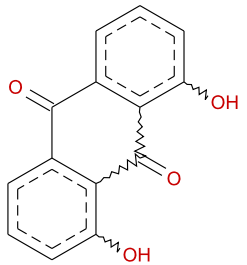
$C_{17}H_{18}N_4S$
Molecular Weight: 310.41662
ALogP: 4.089
Rotatable Bonds: 2
Acceptors: 4
Donors: 2

Model Prediction

Prediction: Single-Carcinogen
Probability: 0.163
Enrichment: 0.54
Bayesian Score: -5.43
Mahalanobis Distance: 12.7
Mahalanobis Distance p-value: 0.000159

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Phenolphthalein	Oxazepam	Danthron
Structure			
Actual Endpoint	Multiple-Carcinogen	Single-Carcinogen	Single-Carcinogen
Predicted Endpoint	Multiple-Carcinogen	Single-Carcinogen	Single-Carcinogen
Distance	0.573	0.658	0.721
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

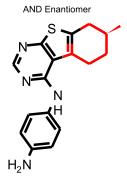
Model Applicability

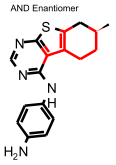
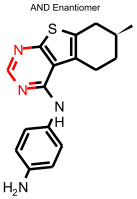
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: 1293778554: [*]:[c](:[*])N[c](:[*]):[*]

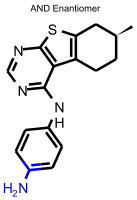
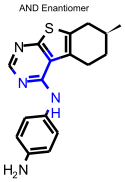
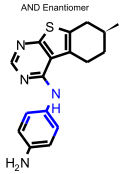
Feature Contribution

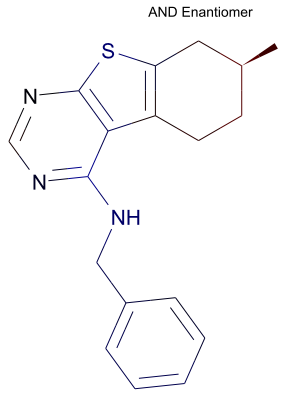
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
FCFP_12	-1441604640	 [*]:[c]1:[*]C[C@@H](C)CC1	0.75	4 out of 4

FCFP_12	-2002183168	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2 CC1	0.616	4 out of 5
FCFP_12	-124685461	 [*]:n:[cH]:n:[*]	0.4	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
FCFP_12	1069584379	 [*]:[c](:[*])N	-1.11	0 out of 6
FCFP_12	-1151884458	 [*]N[c](:n:[*]):[c](:[*]):[*]	-1.11	0 out of 6
FCFP_12	590925877	 [*]N[c](:[cH]:[*]):[cH]:[*]	-0.998	1 out of 13



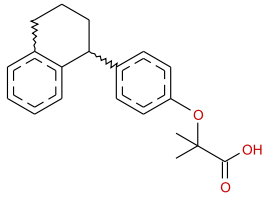
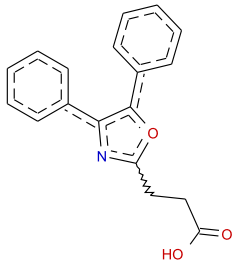
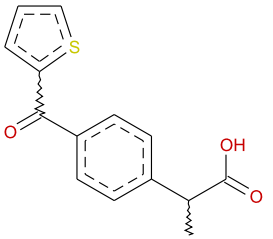
$C_{18}H_{19}N_3S$
Molecular Weight: 309.42856
ALogP: 4.678
Rotatable Bonds: 3
Acceptors: 3
Donors: 1

Model Prediction

Prediction: Multiple-Carcinogen
Probability: 0.169
Enrichment: 0.563
Bayesian Score: -4.74
Mahalanobis Distance: 12.2
Mahalanobis Distance p-value: 0.000442

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Nafenopin	Oxaprocin	Suprofen
Structure			
Actual Endpoint	Single-Carcinogen	Single-Carcinogen	Single-Carcinogen
Predicted Endpoint	Single-Carcinogen	Single-Carcinogen	Single-Carcinogen
Distance	0.566	0.622	0.665
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

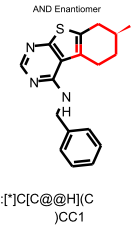
Model Applicability

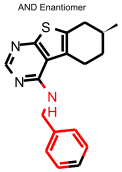
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

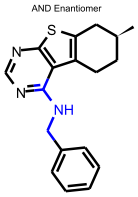
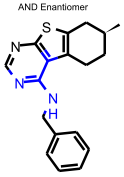
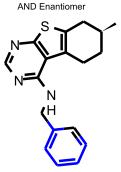
Feature Contribution

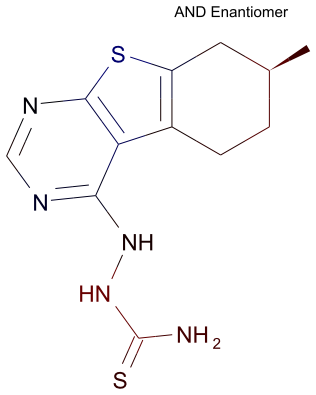
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
FCFP_12	-1441604640	 [*]:[c]1:[*]C[C@@H](C)CC1	0.75	4 out of 4

FCFP_12	-2002183168	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2 CC1	0.616	4 out of 5
FCFP_12	427906732	 [*]NC[c]1:[cH]:[cH]:[*]:[cH]:[cH]:1	0.4	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
FCFP_12	1294255210	 [*]CN[c](:[*]):[*]	-1.63	0 out of 12
FCFP_12	-1151884458	 [*]N[c](:n:[*]):[c](:[*]):[*]	-1.11	0 out of 6
FCFP_12	991735244	 [*][c]1:[*]:[cH]:[cH]:[cH]:[cH]:1	-0.562	5 out of 28



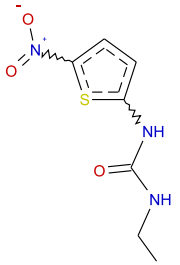
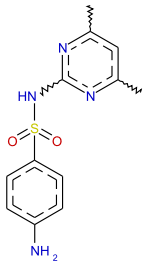
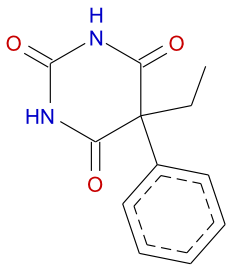
$C_{12}H_{15}N_5S_2$
Molecular Weight: 293.411
ALogP: 3.209
Rotatable Bonds: 3
Acceptors: 4
Donors: 3

Model Prediction

Prediction: Multiple-Carcinogen
Probability: 0.249
Enrichment: 0.828
Bayesian Score: -0.38
Mahalanobis Distance: 13.8
Mahalanobis Distance p-value: 2.12e-005

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Nithiazide	Sulfamethazine	Phenobarbital
Structure			
Actual Endpoint	Single-Carcinogen	Single-Carcinogen	Multiple-Carcinogen
Predicted Endpoint	Single-Carcinogen	Single-Carcinogen	Multiple-Carcinogen
Distance	0.757	0.771	0.799
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

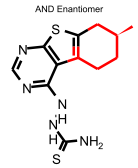
Model Applicability

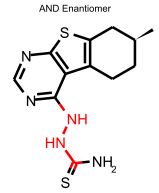
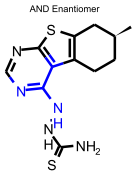
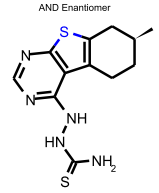
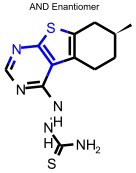
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

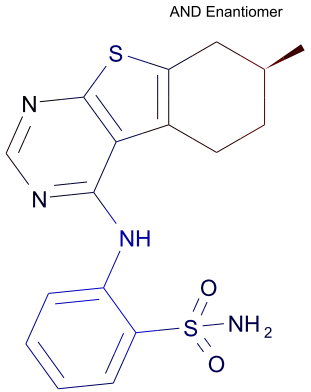
Feature Contribution

Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
FCFP_12	-1441604640	 [*]:[c]1:[*]C[C@@H](C)CC1	0.75	4 out of 4

FCFP_12	-885461129	 [*]NNC(=[*])[*]	0.683	3 out of 3
FCFP_12	-2002183168	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2CC1	0.616	4 out of 5
Top Features for negative contribution				
Fingerprint	**Bit/Smiles**	**Feature Structure**	**Score**	**Multiple-Carcinogen in training set**
FCFP_12	-1151884458	 [*]N[c](:n:[*]):[c](:[*]):[*]	-1.11	0 out of 6
FCFP_12	17	 [*]:s:[*]	-0.53	5 out of 27
FCFP_12	-1564473960	 [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]	-0.519	0 out of 2

TOPKAT_Mouse_Male_FDA_Single_vs_Multiple



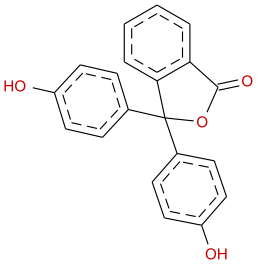
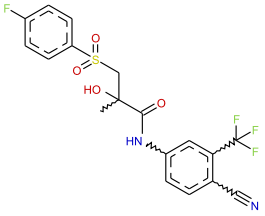
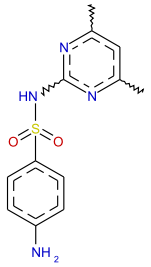
$C_{17}H_{18}N_4O_2S_2$
Molecular Weight: 374.48042
ALogP: 3.541
Rotatable Bonds: 3
Acceptors: 5
Donors: 2

Model Prediction

Prediction: Single-Carcinogen
Probability: 0.146
Enrichment: 0.484
Bayesian Score: -9.03
Mahalanobis Distance: 14
Mahalanobis Distance p-value: 1.58e-005

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Phenolphthalein	Bicalutamide	Sulfamethazine
Structure			
Actual Endpoint	Multiple-Carcinogen	Single-Carcinogen	Single-Carcinogen
Predicted Endpoint	Multiple-Carcinogen	Single-Carcinogen	Single-Carcinogen
Distance	0.712	0.715	0.719
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

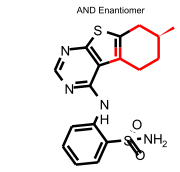
Model Applicability

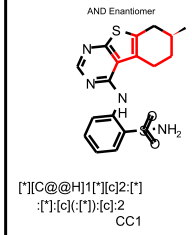
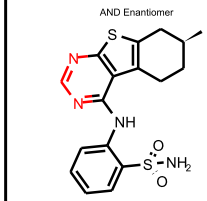
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: 1293778554: [*]:[c](:[*])N[c](:[*]):[*]

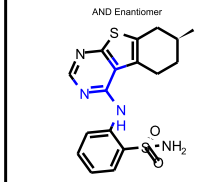
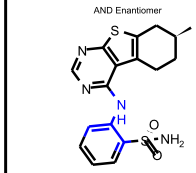
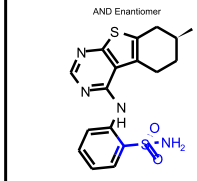
Feature Contribution

Top features for positive contribution

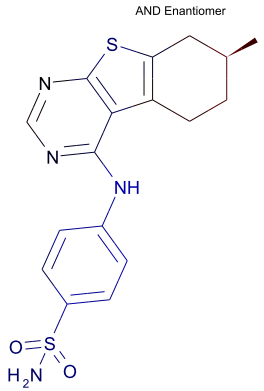
Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
FCFP_12	-1441604640	 [*]:[c]1:[*]C[C@@H](C)CC1	0.75	4 out of 4

FCFP_12	-2002183168	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2CC1	0.616	4 out of 5
FCFP_12	-124685461	 [*]:n:[cH]:n:[*]	0.4	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
FCFP_12	-1151884458	 [*]N[c](:n:[*]):[c](:[*]):[*]	-1.11	0 out of 6
FCFP_12	590925877	 [*]N[c](:[cH]:[*]):[cH]:[*]	-0.998	1 out of 13
FCFP_12	-1096219292	 [*]:[c](:[*])S(=O)(=O)N	-0.859	0 out of 4

TOPKAT_Mouse_Male_FDA_Single_vs_Multiple



$C_{17}H_{18}N_4O_2S_2$

Molecular Weight: 374.48042

ALogP: 3.541

Rotatable Bonds: 3

Acceptors: 5

Donors: 2

Model Prediction

Prediction: Single-Carcinogen

Probability: 0.146

Enrichment: 0.485

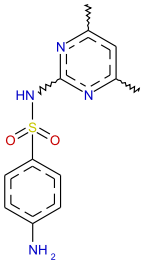
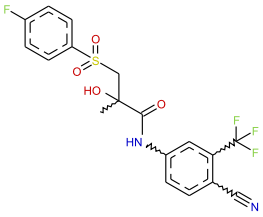
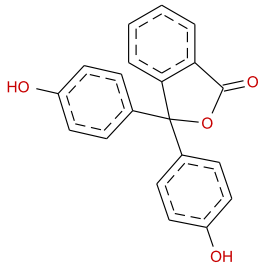
Bayesian Score: -8.75

Mahalanobis Distance: 11.9

Mahalanobis Distance p-value: 0.00077

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Sulfamethazine	Bicalutamide	Phenolphthalein
Structure			
Actual Endpoint	Single-Carcinogen	Single-Carcinogen	Multiple-Carcinogen
Predicted Endpoint	Single-Carcinogen	Single-Carcinogen	Multiple-Carcinogen
Distance	0.711	0.716	0.723
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

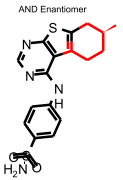
Model Applicability

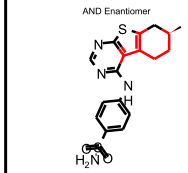
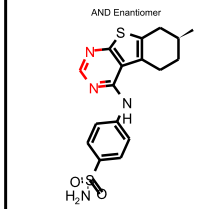
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: 1293778554: [*]:[c](:[*])N[c](:[*]):[*]

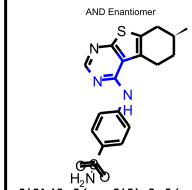
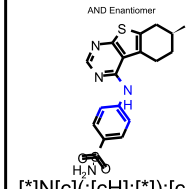
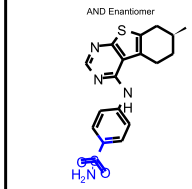
Feature Contribution

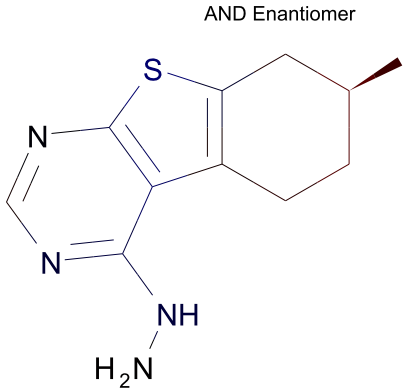
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
FCFP_12	-1441604640	 [*]:[c]1:[*]C[C@@H](C)CC1	0.75	4 out of 4

FCFP_12	-2002183168	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2CC1	0.616	4 out of 5
FCFP_12	-124685461	 [*]:n:[cH]:n:[*]	0.4	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
FCFP_12	-1151884458	 [*]N[c](:n:[*]):[c](:[*]):[*]	-1.11	0 out of 6
FCFP_12	590925877	 [*]N[c](:[cH]:[*]):[cH]:[*]	-0.998	1 out of 13
FCFP_12	-1096219292	 [*]:[c](:[*])S(=O)(=O)N	-0.859	0 out of 4



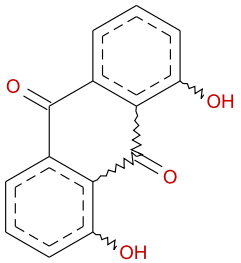
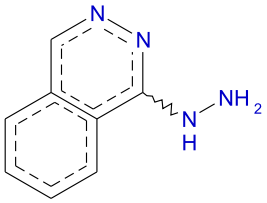
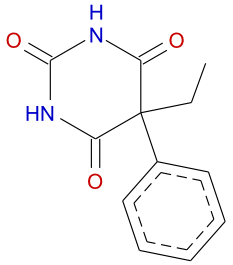
$C_{11}H_{14}N_4S$
Molecular Weight: 234.32065
ALogP: 2.561
Rotatable Bonds: 1
Acceptors: 4
Donors: 2

Model Prediction

Prediction: Multiple-Carcinogen
Probability: 0.201
Enrichment: 0.666
Bayesian Score: -2.53
Mahalanobis Distance: 15.1
Mahalanobis Distance p-value: 2.29e-006

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Danthron	Hydralazine	Phenobarbital
Structure			
Actual Endpoint	Single-Carcinogen	Single-Carcinogen	Multiple-Carcinogen
Predicted Endpoint	Single-Carcinogen	Single-Carcinogen	Multiple-Carcinogen
Distance	0.576	0.636	0.643
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

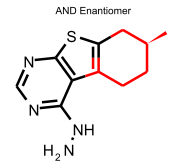
Model Applicability

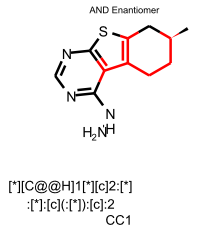
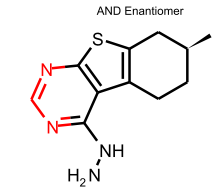
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

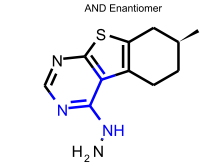
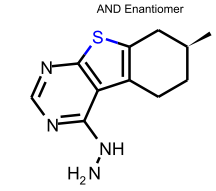
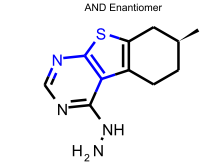
Feature Contribution

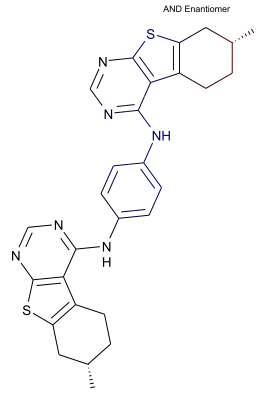
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
FCFP_12	-1441604640	 [*:[c]1:[*]C[C@@H](C)CC1	0.75	4 out of 4

FCFP_12	-2002183168		0.616	4 out of 5
FCFP_12	-124685461		0.4	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
FCFP_12	-1151884458		-1.11	0 out of 6
FCFP_12	17		-0.53	5 out of 27
FCFP_12	-1564473960		-0.519	0 out of 2



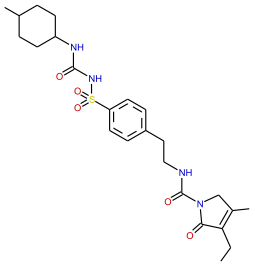
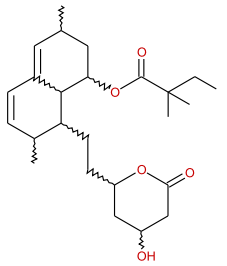
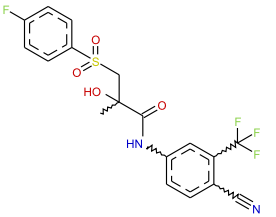
$C_{28}H_{28}N_6S_2$
Molecular Weight: 512.69212
ALogP: 7.842
Rotatable Bonds: 4
Acceptors: 6
Donors: 2

Model Prediction

Prediction: Single-Carcinogen
Probability: 0.159
Enrichment: 0.527
Bayesian Score: -5.92
Mahalanobis Distance: 14.5
Mahalanobis Distance p-value: 5.83e-006

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Glimepride	Simvastatin	Bicalutamide
Structure			
Actual Endpoint	Single-Carcinogen	Multiple-Carcinogen	Single-Carcinogen
Predicted Endpoint	Single-Carcinogen	Multiple-Carcinogen	Single-Carcinogen
Distance	0.924	0.936	0.939
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

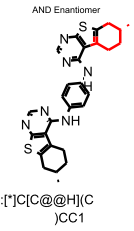
Model Applicability

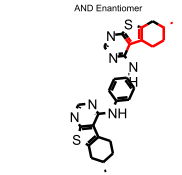
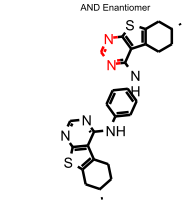
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. OPS PC7 out of range. Value: -4.4901. Training min, max, SD, explained variance: -3.9478, 3.0766, 1.527, 0.0435.
2. Unknown FCFP_2 feature: 1293778554: [*]:[c](:[*])N[c](:[*]):[*]

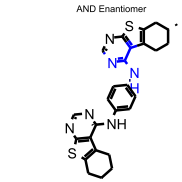
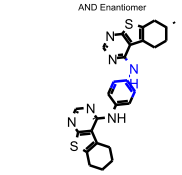
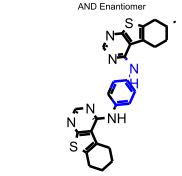
Feature Contribution

Top features for positive contribution

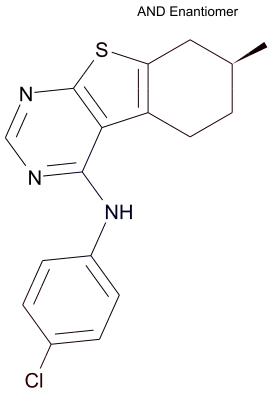
Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
FCFP_12	-1441604640	 [*]:[c]1:[*]C[C@@H](C)CC1	0.75	4 out of 4

FCFP_12	-2002183168	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2 CC1	0.616	4 out of 5
FCFP_12	-124685461	 [*]:n:[cH]:n:[*]	0.4	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
FCFP_12	-1151884458	 [*]N[c](:n:[*]):[c](:[*]):[*]	-1.11	0 out of 6
FCFP_12	590925877	 [*]N[c](:[cH]:[*]):[cH]:[*]	-0.998	1 out of 13
FCFP_12	-773983804	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	-0.789	1 out of 10

TOPKAT_Ocular_Irritancy_Mild_vs_Moderate_Severe



$C_{17}H_{16}ClN_3S$

Molecular Weight: 329.84704

ALogP: 5.5

Rotatable Bonds: 2

Acceptors: 3

Donors: 1

Model Prediction

Prediction: Moderate_Severe

Probability: 0.833

Enrichment: 1.21

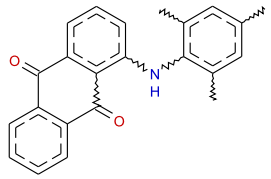
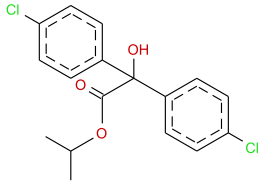
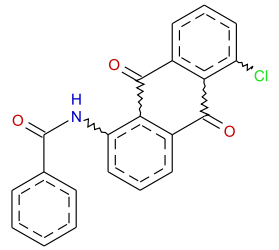
Bayesian Score: 0.771

Mahalanobis Distance: 8.73

Mahalanobis Distance p-value: 0.657

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	ANTHRAQUINONE;1-(2;4;6-TRIMETHYLPHENYLAMINO)-	BENZILIC ACID; 4;4'-DICHLORO-; ISOPROPYL ESTER	BENZAMIDE; N-(5-CHLORO-1-ANTHRAQUINONYL)-
Structure			
Actual Endpoint	Moderate_Severe	Moderate_Severe	Mild
Predicted Endpoint	Mild	Moderate_Severe	Mild
Distance	0.582	0.596	0.597
Reference	28ZPAK-;242;72	CIGET* -;-;77	28ZPAK 89;72

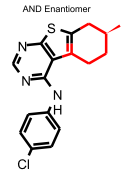
Model Applicability

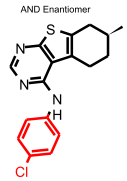
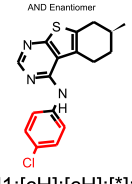
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
4. Unknown FCFP_2 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]

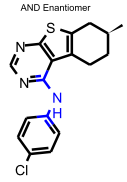
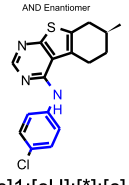
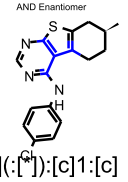
Feature Contribution

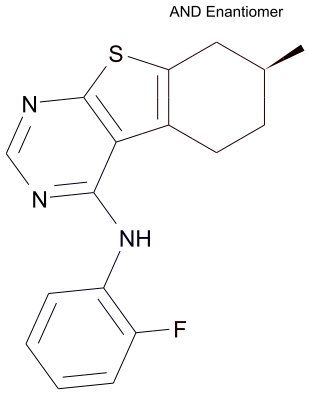
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Moderate_Severe in training set
FCFP_10	-1441604640	 [*]:[c]1:[*]C[C@@H](C)CC1	0.344	6 out of 6

FCFP_10	-1508180856	 [*][c]1:[cH]:[cH]:[c](Cl):[cH]:[cH]:1	0.329	16 out of 17
FCFP_10	-745491832	 Cl[c]1:[cH]:[cH]:[*]:[cH]:[cH]:1	0.304	29 out of 32

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Moderate_Severe in training set
FCFP_10	1293778554	 [*]:[c](:[*])N[c](:[*]):[*]	-0.304	9 out of 19
FCFP_10	-773983804	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	-0.294	50 out of 102
FCFP_10	307419094	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.29	21 out of 43



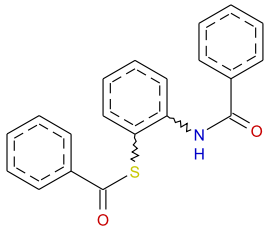
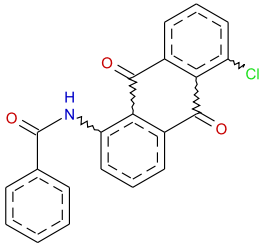
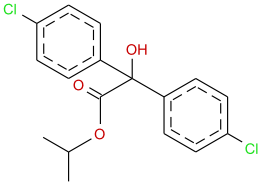
$C_{17}H_{16}FN_3S$
Molecular Weight: 313.39244
ALogP: 5.041
Rotatable Bonds: 2
Acceptors: 3
Donors: 1

Model Prediction

Prediction: Moderate_Severe
Probability: 0.826
Enrichment: 1.2
Bayesian Score: 0.219
Mahalanobis Distance: 8.63
Mahalanobis Distance p-value: 0.708

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	N;S-DIBENZOYL-O-AMINOTHIOPHENOL	BENZAMIDE; N-(5-CHLORO-1-ANTHRAQUINONYL)-	BENZILIC ACID; 4;4'-DICHLORO-; ISOPROPYL ESTER
Structure			
Actual Endpoint	Mild	Mild	Moderate_Severe
Predicted Endpoint	Mild	Mild	Moderate_Severe
Distance	0.566	0.573	0.600
Reference	28ZPAK-;175;72	28ZPAK 89;72	CIGET* -;-;77

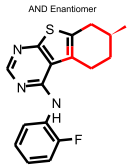
Model Applicability

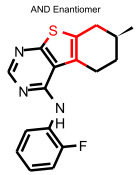
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
4. Unknown FCFP_2 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]

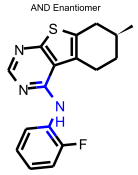
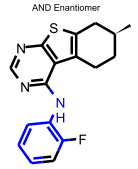
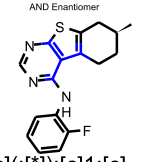
Feature Contribution

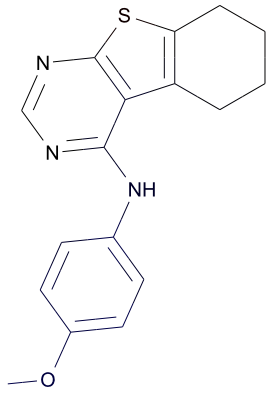
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Moderate_Severe in training set
FCFP_10	-1441604640	 [*]:[c]1:[*]C[C@@H](C)CC1	0.344	6 out of 6

FCFP_10	-1539132615	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	0.224	11 out of 13
FCFP_10	-2002183168	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2CC1	0.207	23 out of 28

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Moderate_Severe in training set
FCFP_10	1293778554	 [*]:[c](:[*])N[c](:[*]):[*]	-0.304	9 out of 19
FCFP_10	-773983804	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	-0.294	50 out of 102
FCFP_10	307419094	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.29	21 out of 43



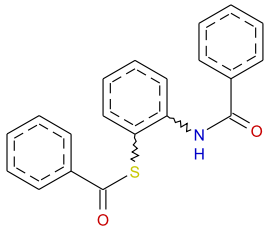
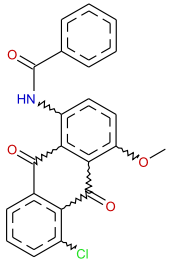
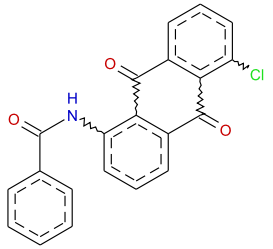
$C_{17}H_{17}N_3OS$
Molecular Weight: 311.40138
ALogP: 4.568
Rotatable Bonds: 3
Acceptors: 4
Donors: 1

Model Prediction

Prediction: Mild
Probability: 0.756
Enrichment: 1.1
Bayesian Score: -2.35
Mahalanobis Distance: 7.33
Mahalanobis Distance p-value: 0.992

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	N;S-DIBENZOYL-O-AMINOTHIOPHENOL	1-BENZOYLAMINO-4-METHOXY-5-CHLORANTHRAQUINONE	BENZAMIDE; N-(5-CHLORO-1-ANTHRAQUINONYL)-
Structure			
Actual Endpoint	Mild	Mild	Mild
Predicted Endpoint	Mild	Mild	Mild
Distance	0.574	0.609	0.622
Reference	28ZPAK-;175;72	28ZPAK-;90;72	28ZPAK 89;72

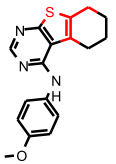
Model Applicability

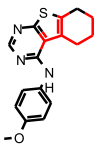
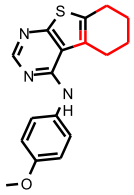
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
4. Unknown FCFP_2 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]

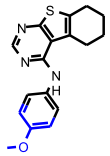
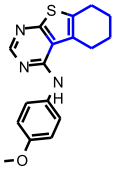
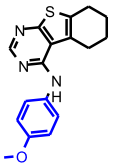
Feature Contribution

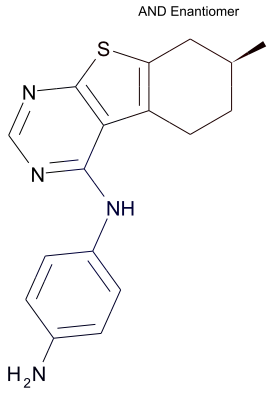
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Moderate_Severe in training set
FCFP_10	-1539132615	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	0.224	11 out of 13

FCFP_10	-2002183168	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2CC1	0.207	23 out of 28
FCFP_10	-1438301350	 [*]:[c]1:[*]CCCC1	0.204	14 out of 17

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Moderate_Severe in training set
FCFP_10	-1977641857	 [*]:[cH]:[c](OC):[cH]:[*]	-0.78	4 out of 15
FCFP_10	-1909820884	 [*]:[c]1:[*]:[*]:[c]2CCCC[c]:1:2	-0.507	0 out of 1
FCFP_10	-9847677	 [*][c]1:[cH]:[cH]:[c](OC):[cH]:[cH]:1	-0.4	1 out of 3



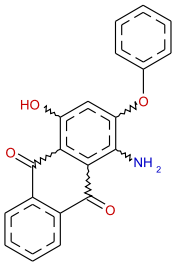
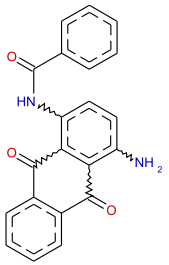
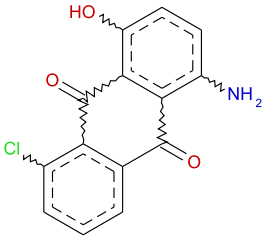
$C_{17}H_{18}N_4S$
Molecular Weight: 310.41662
ALogP: 4.089
Rotatable Bonds: 2
Acceptors: 4
Donors: 2

Model Prediction

Prediction: Mild
Probability: 0.805
Enrichment: 1.17
Bayesian Score: -0.828
Mahalanobis Distance: 7.81
Mahalanobis Distance p-value: 0.956

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	ANTHRAQUINONE; 1-AMINO-4-HYDROXY-2-PHENOXY-	1-AMINO-4-BENZOYLAMINO-ANTHRAQUINONE	1-AMINO-4-HYDROXY-5-CHLORANTHRAQUINONE
Structure			
Actual Endpoint	Mild	Mild	Mild
Predicted Endpoint	Mild	Mild	Mild
Distance	0.596	0.609	0.654
Reference	28ZPAK 239;72	28ZPAK-;124;72	28ZPAK-;83;72

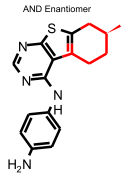
Model Applicability

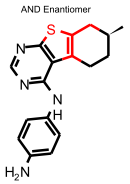
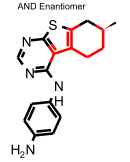
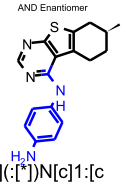
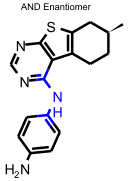
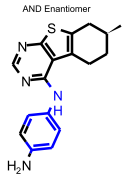
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

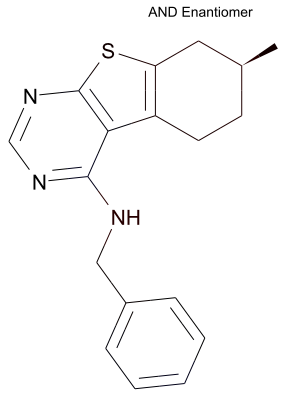
1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
4. Unknown FCFP_2 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]

Feature Contribution

Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Moderate_Severe in training set
FCFP_10	-1441604640	 [*]:[c]1:[*]C[C@@H](C)CC1	0.344	6 out of 6

FCFP_10	-1539132615	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	0.224	11 out of 13
FCFP_10	-2002183168	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2CC1	0.207	23 out of 28
Top Features for negative contribution				
Fingerprint	**Bit/Smiles**	**Feature Structure**	**Score**	**Moderate_Severe in training set**
FCFP_10	-200702388	 [*]:[c](:[*])N[c]1:[cH]:[cH]:[c](N):[cH]:[cH]:1	-0.361	2 out of 5
FCFP_10	1293778554	 [*]:[c](:[*])N[c](:[*]):[*]	-0.304	9 out of 19
FCFP_10	-773983804	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	-0.294	50 out of 102



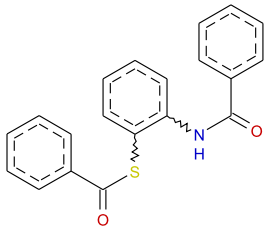
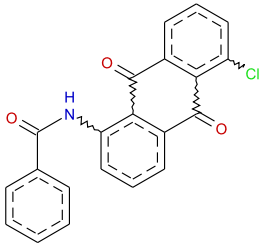
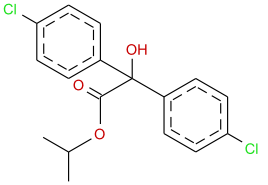
$C_{18}H_{19}N_3S$
Molecular Weight: 309.42856
ALogP: 4.678
Rotatable Bonds: 3
Acceptors: 3
Donors: 1

Model Prediction

Prediction: Moderate_Severe
Probability: 0.833
Enrichment: 1.21
Bayesian Score: 0.713
Mahalanobis Distance: 7.54
Mahalanobis Distance p-value: 0.982

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	N;S-DIBENZOYL-O-AMINOTHIOPHENOL	BENZAMIDE; N-(5-CHLORO-1-ANTHRAQUINONYL)-	BENZILIC ACID; 4;4'-DICHLORO-; ISOPROPYL ESTER
Structure			
Actual Endpoint	Mild	Mild	Moderate_Severe
Predicted Endpoint	Mild	Mild	Moderate_Severe
Distance	0.529	0.568	0.591
Reference	28ZPAK-;175;72	28ZPAK 89;72	CIGET* -;-;77

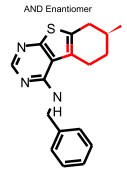
Model Applicability

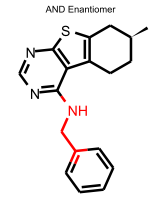
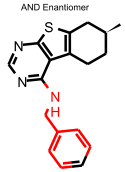
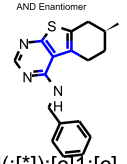
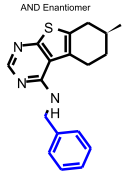
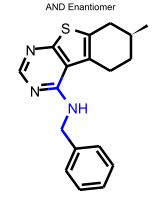
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

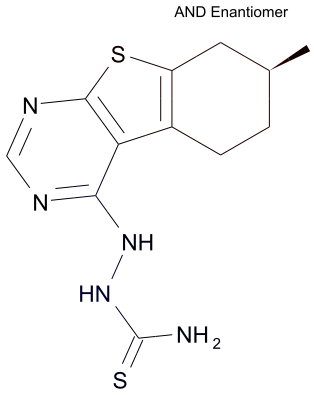
1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
4. Unknown FCFP_2 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]

Feature Contribution

Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Moderate_Severe in training set
FCFP_10	-1441604640	 [*]:[c]1:[*]C[C@@H](C)CC1	0.344	6 out of 6

FCFP_10	907096426	 [*]NC[c](:[*]):[*]	0.332	5 out of 5
FCFP_10	427906732	 [*]NC[c]1:[cH]:[cH]:[*]:[cH]:[cH]:1	0.294	3 out of 3
Top Features for negative contribution				
Fingerprint	**Bit/Smiles**	**Feature Structure**	**Score**	**Moderate_Severe in training set**
FCFP_10	307419094	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.29	21 out of 43
FCFP_10	-1698724694	 [*]C[c]1:[cH]:[cH]:[cH]:[cH]:[cH]:1	-0.284	53 out of 107
FCFP_10	1294255210	 [*]CN[c](:[*]):[*]	-0.218	20 out of 38



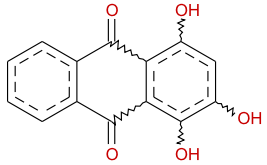
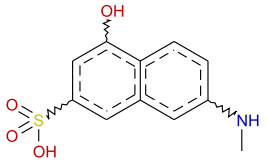
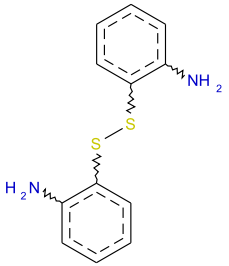
$C_{12}H_{15}N_5S_2$
Molecular Weight: 293.411
ALogP: 3.209
Rotatable Bonds: 3
Acceptors: 4
Donors: 3

Model Prediction

Prediction: Mild
Probability: 0.813
Enrichment: 1.18
Bayesian Score: -0.44
Mahalanobis Distance: 7.72
Mahalanobis Distance p-value: 0.967

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	1;2;4-TRIHYDROXY ANTHRAQUINONE	2-NAPHTHALENESULFONIC ACID; 4-HYDROXY-7-(METHYLAMINO)-	ANILINE;2;2'DITHIOBIS-
Structure			
Actual Endpoint	Mild	Mild	Moderate_Severe
Predicted Endpoint	Mild	Mild	Moderate_Severe
Distance	0.678	0.685	0.740
Reference	28ZPAK-;103;7	28ZPAK 190;72	28ZPAK-;172;72

Model Applicability

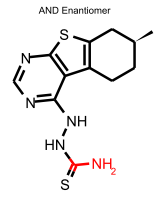
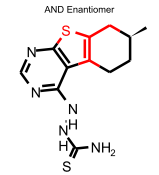
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
4. Unknown FCFP_2 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]
5. Unknown FCFP_2 feature: -885461129: [*]NNC(=[*])[*]

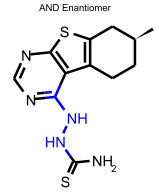
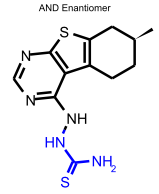
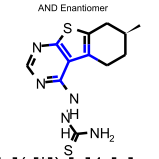
Feature Contribution

Top features for positive contribution

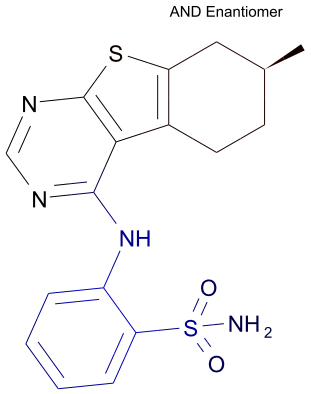
Fingerprint	Bit/Smiles	Feature Structure	Score	Moderate_Severe in training set
FCFP_10	-1441604640	 [*]:[c]1:[*]C[C@@H](C)CC1	0.344	6 out of 6

FCFP_10	1070061035	 [*]C(=[*])N	0.239	284 out of 338
FCFP_10	-1539132615	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	0.224	11 out of 13

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Moderate_Severe in training set
FCFP_10	1294344583	 [*]NN[c](:[*]):[*]	-0.507	0 out of 1
FCFP_10	1499521844	 [*]NC(=S)N	-0.4	1 out of 3
FCFP_10	307419094	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.29	21 out of 43

TOPKAT_Ocular_Irritancy_Mild_vs_Moderate_Severe



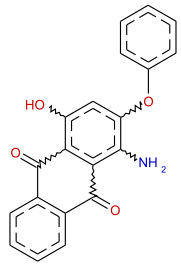
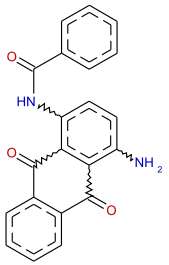
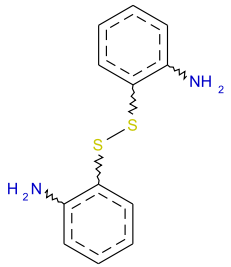
$C_{17}H_{18}N_4O_2S_2$
Molecular Weight: 374.48042
ALogP: 3.541
Rotatable Bonds: 3
Acceptors: 5
Donors: 2

Model Prediction

Prediction: Mild
Probability: 0.706
Enrichment: 1.02
Bayesian Score: -3.42
Mahalanobis Distance: 7.33
Mahalanobis Distance p-value: 0.992

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	ANTHRAQUINONE; 1-AMINO-4-HYDROXY-2-PHENOXY-	1-AMINO-4-BENZOYLAMINO-ANTHRAQUINONE	ANILINE;2;2'DITHIOBIS-
Structure			
Actual Endpoint	Mild	Mild	Moderate_Severe
Predicted Endpoint	Mild	Mild	Moderate_Severe
Distance	0.611	0.651	0.702
Reference	28ZPAK 239;72	28ZPAK-;124;72	28ZPAK-;172;72

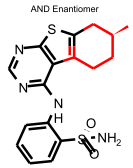
Model Applicability

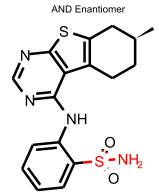
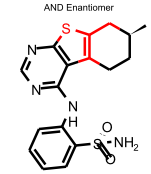
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
4. Unknown FCFP_2 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]

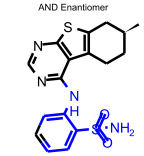
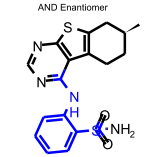
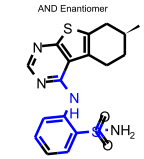
Feature Contribution

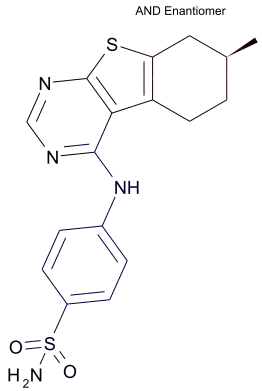
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Moderate_Severe in training set
FCFP_10	-1441604640	 [*]:[c]1:[*]C[C@@H](C)CC1	0.344	6 out of 6

FCFP_10	1070061035	 [*]C(=[*])N	0.239	284 out of 338
FCFP_10	-1539132615	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	0.224	11 out of 13

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Moderate_Severe in training set
FCFP_10	-377913290	 [*]N[c]1:[cH]:[*]:[cH]:[cH]:[c]:1S(=O)(=O)N	-1.03	1 out of 7
FCFP_10	-103236997	 [*]S(=[*])(=[*])[c]1:[cH]:[cH]:[cH]:[cH]:[c]:1N[c](:[*]):[*]	-0.6	1 out of 4
FCFP_10	-605671248	 [*]S(=[*])(=[*])[c]1:[cH]:[*]:[cH]:[cH]:[c]:1N[c](:[*]):[*]	-0.341	3 out of 7



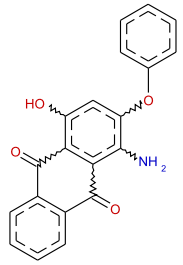
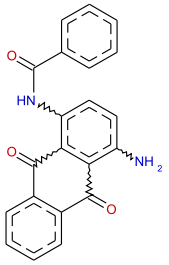
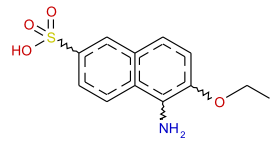
$C_{17}H_{18}N_4O_2S_2$
Molecular Weight: 374.48042
ALogP: 3.541
Rotatable Bonds: 3
Acceptors: 5
Donors: 2

Model Prediction

Prediction: Mild
Probability: 0.792
Enrichment: 1.15
Bayesian Score: -1.29
Mahalanobis Distance: 7.33
Mahalanobis Distance p-value: 0.992

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	ANTHRAQUINONE; 1-AMINO-4-HYDROXY-2-PHENOXY-	1-AMINO-4-BENZOYLAMINO-ANTHRAQUINONE	2-NAPHTHALENESULFONIC ACID;5-AMINO-6-ETHOXY-
Structure			
Actual Endpoint	Mild	Mild	Moderate_Severe
Predicted Endpoint	Mild	Mild	Mild
Distance	0.620	0.660	0.700
Reference	28ZPAK 239;72	28ZPAK-;124;72	28ZPAK-;191;72

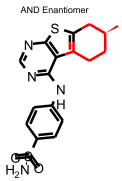
Model Applicability

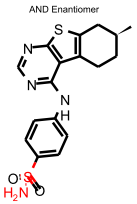
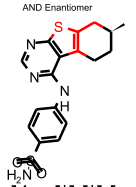
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
4. Unknown FCFP_2 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]

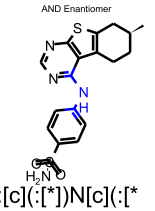
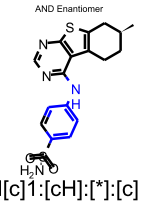
Feature Contribution

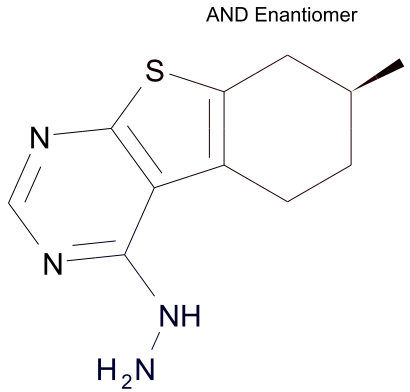
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Moderate_Severe in training set
FCFP_10	-1441604640	 [*]:[c]1:[*]C[C@@H](C)CC1	0.344	6 out of 6

FCFP_10	1070061035	 [*]C(=[*])N	0.239	284 out of 338
FCFP_10	-1539132615	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	0.224	11 out of 13

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Moderate_Severe in training set
FCFP_10	-174657146	 [*]S(=[*])(=[*])[c]1:[cH]:[cH]:[c](N[c](:[*]):[*]):[cH]:[cH]:1	-0.4	1 out of 3
FCFP_10	1293778554	 [*]:[c](:[*])N[c](:[*]):[*]	-0.304	9 out of 19
FCFP_10	-773983804	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	-0.294	50 out of 102



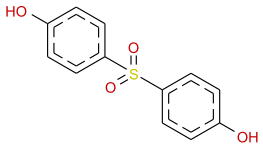
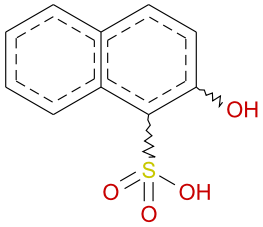
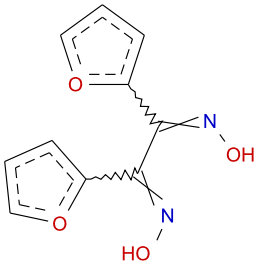
$C_{11}H_{14}N_4S$
Molecular Weight: 234.32065
ALogP: 2.561
Rotatable Bonds: 1
Acceptors: 4
Donors: 2

Model Prediction

Prediction: Mild
Probability: 0.81
Enrichment: 1.18
Bayesian Score: -0.572
Mahalanobis Distance: 7.88
Mahalanobis Distance p-value: 0.946

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	PHENOL; 4;4'-SULFONYLDI-	NAPHTHENESULFONIC ACID;2-HYDROXY-	FURIL;DIOXIME
Structure			
Actual Endpoint	Moderate_Severe	Moderate_Severe	Moderate_Severe
Predicted Endpoint	Moderate_Severe	Moderate_Severe	Moderate_Severe
Distance	0.542	0.551	0.554
Reference	BIOFX* 601-05501;74	28ZPAK-;186;72	28ZPAK

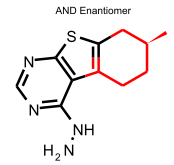
Model Applicability

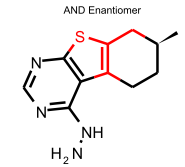
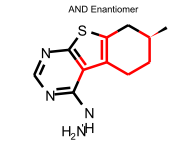
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
4. Unknown FCFP_2 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]

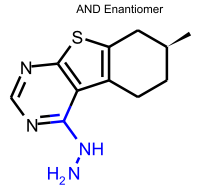
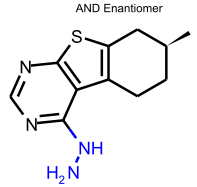
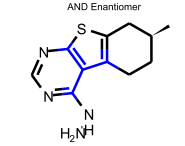
Feature Contribution

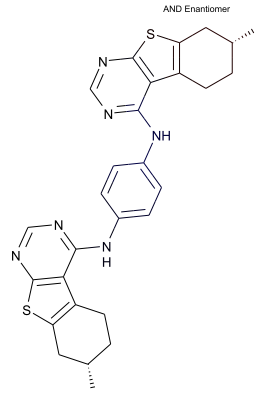
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Moderate_Severe in training set
FCFP_10	-1441604640	 [*]:[c]1:[*]C[C@@H](C)CC1	0.344	6 out of 6

FCFP_10	-1539132615	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	0.224	11 out of 13
FCFP_10	-2002183168	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2CC1	0.207	23 out of 28

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Moderate_Severe in training set
FCFP_10	1294344583	 [*]NN[c](:[*]):[*]	-0.507	0 out of 1
FCFP_10	1070150408	 [*]NN	-0.507	0 out of 1
FCFP_10	307419094	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.29	21 out of 43



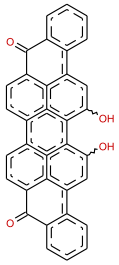
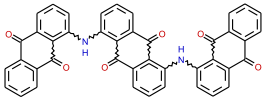
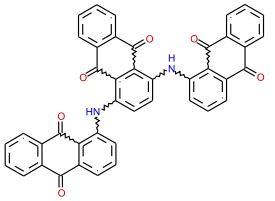
$C_{28}H_{28}N_6S_2$
Molecular Weight: 512.69212
ALogP: 7.842
Rotatable Bonds: 4
Acceptors: 6
Donors: 2

Model Prediction

Prediction: Mild
Probability: 0.808
Enrichment: 1.17
Bayesian Score: -0.679
Mahalanobis Distance: 9.84
Mahalanobis Distance p-value: 0.135

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	DINAPHTHO(1;2;3-CD:3';2';1'-IM)PERYLENE-5;10-DIONE;16;17-DIHYDROXY	Anthraquinone; 1;1'-(anthraquinon-1;5-ylenediimino)di-	Anthraquinone; 1;1'-(anthraquinon-1;4-ylenediimino)di-
Structure			
Actual Endpoint	Mild	Mild	Mild
Predicted Endpoint	Mild	Mild	Mild
Distance	0.767	0.772	0.774
Reference	28ZPAK-;104;72	Prehled Prumyslove Toxikologie; Organicke Latky; Marhold; J. pp 736;86	Prehled Prumyslove Toxikologie; Organicke Latky; Marhold; J. pp 736;86

Model Applicability

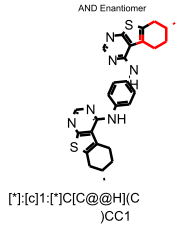
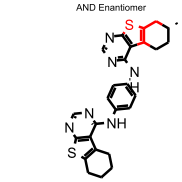
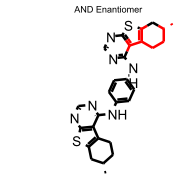
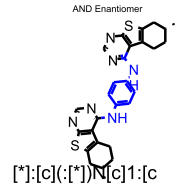
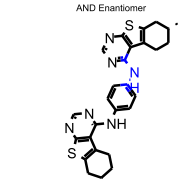
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

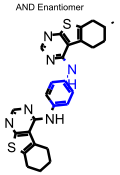
1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
4. Unknown FCFP_2 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]

Feature Contribution

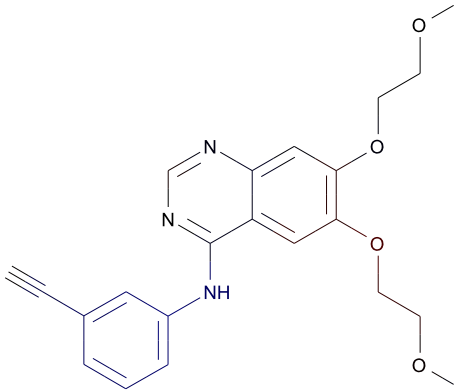
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Moderate_Severe in training set

FCFP_10	-1441604640	 [*:[c]1:[*]C[C@@H](C)CC1	0.344	6 out of 6
FCFP_10	-1539132615	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	0.224	11 out of 13
FCFP_10	-2002183168	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2CC1	0.207	23 out of 28
Top Features for negative contribution				
Fingerprint	**Bit/Smiles**	**Feature Structure**	**Score**	**Moderate_Severe in training set**
FCFP_10	-200702388	 [*:[c](:[*])N[c]1:[cH]:[cH]:[c](N):[cH]:[cH]:1	-0.361	2 out of 5
FCFP_10	1293778554	 [*:[c](:[*])N[c](:[*]):[*]	-0.304	9 out of 19

FCFP_10	-773983804	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	-0.294	50 out of 102

Erlotinib



$C_{22}H_{23}N_3O_4$

Molecular Weight: 393.43572

ALogP: 4.309

Rotatable Bonds: 10

Acceptors: 7

Donors: 1

Model Prediction

Prediction: Mild

Probability: 0.766

Enrichment: 1.11

Bayesian Score: -2.1

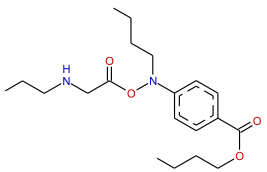
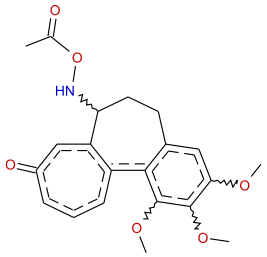
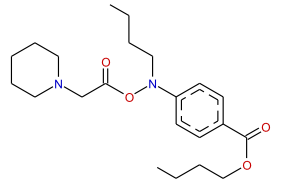
Mahalanobis Distance: 10.4

Mahalanobis Distance p-value: 0.0368

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

TOPKAT_Ocular_Irritancy_Mild_vs_Moderate_Severe

Structural Similar Compounds

Name	Benzoic acid; p-(N-butyl-2-(butylamino)acetamido)-; butyl ester;	COLCHICINE	Benzoic acid; p-(N-butyl-2-(piperidino)acetamido)-; butyl ester;
Structure			
Actual Endpoint	Moderate_Severe	Moderate_Severe	Moderate_Severe
Predicted Endpoint	Moderate_Severe	Moderate_Severe	Moderate_Severe
Distance	0.648	0.707	0.750
Reference	Arzneimittel-Forschung 8;609;58	AJOPAA 31;837;48	Arzneimittel-Forschung 8;609;58

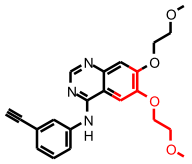
Model Applicability

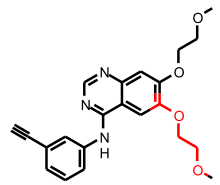
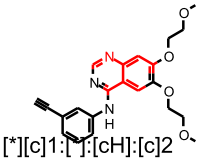
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
3. Unknown FCFP_2 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]
4. Unknown FCFP_2 feature: 902193919: [*]:[c](:[*])C#C

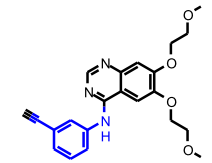
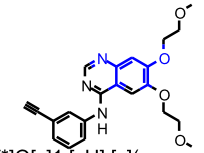
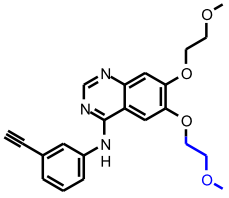
Feature Contribution

Top features for positive contribution

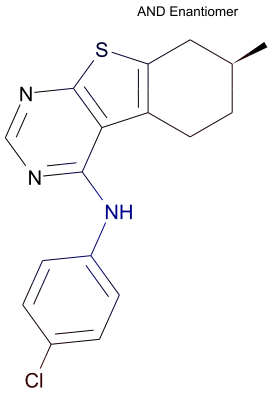
Fingerprint	Bit/Smiles	Feature Structure	Score	Moderate_Severe in training set
FCFP_10	-1059904848	 [*][c](:[*]):[c](OCCOC):[cH]:[*]	0.386	17 out of 17

FCFP_10	365650923	 [*]OCCO[c](:[*]):[*]	0.386	17 out of 17
FCFP_10	-1716224640	 [*][c]1:[*]:[cH]:[c]2 :[c]([*]):[*]:[cH]:n :[c]:2:[cH]:1	0.294	3 out of 3

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Moderate_Severe in training set
FCFP_10	-1699003333	 [*]N[c]1:[cH]:[cH]:[c H]:[c](:[cH]:1)C#[*]	-1.09	2 out of 12
FCFP_10	1679603620	 [*]O[c]1:[cH]:[c](:n: [*]):[c](:[*]):[*]:[c]:1[*]	-0.507	0 out of 1
FCFP_10	341504799	 [*]CCOC	-0.425	7 out of 17

TOPKAT_Ocular_Irritancy_Moderate_vs_Severe



$C_{17}H_{16}ClN_3S$

Molecular Weight: 329.84704

ALogP: 5.5

Rotatable Bonds: 2

Acceptors: 3

Donors: 1

Model Prediction

Prediction: Moderate

Probability: 0.602

Enrichment: 0.971

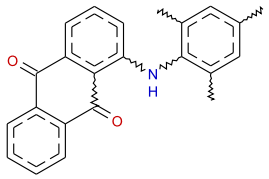
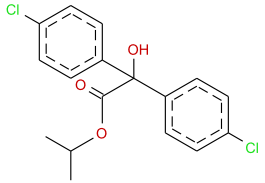
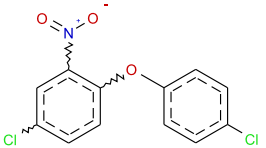
Bayesian Score: -2.21

Mahalanobis Distance: 9.8

Mahalanobis Distance p-value: 0.0717

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	ANTHRAQUINONE;1-(2;4;6-TRIMETHYLPHENYLAMINO)-	BENZILIC ACID; 4;4'-DICHLORO-; ISOPROPYL ESTER	4;4'-DICHLORO-2-NITROBIPHENYL ETHER
Structure			
Actual Endpoint	Moderate	Severe	Moderate
Predicted Endpoint	Moderate	Severe	Moderate
Distance	0.588	0.605	0.722
Reference	28ZPAK-;242;72	CIGET* -;-;77	28ZPAK-;84;72

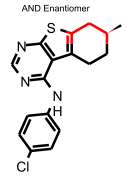
Model Applicability

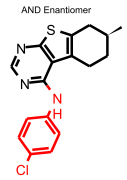
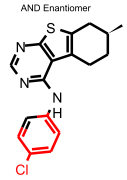
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

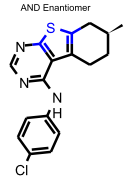
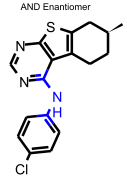
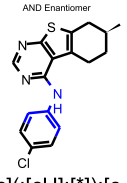
Feature Contribution

Top features for positive contribution

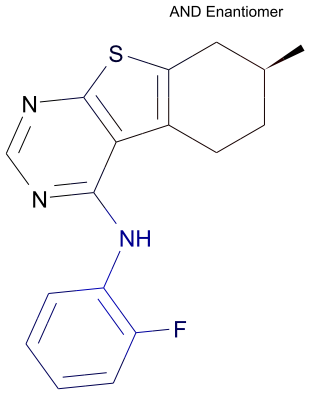
Fingerprint	Bit/Smiles	Feature Structure	Score	Severe in training set
SCFP_12	-1272709286	 [*]C([*])C[c](:[*]):[*]	0.231	24 out of 31

SCFP_12	341480432	 [*]N[c]1:[cH]:[cH]:[c](Cl):[cH]:[cH]:1	0.218	1 out of 1
SCFP_12	-1378360678	 [*][c]1:[*]:[cH]:[c](Cl):[cH]:[cH]:1	0.211	22 out of 29

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Severe in training set
SCFP_12	1310748454	 [*][c]1:[*]:[*]:[c](:[*]):s:1	-1.04	0 out of 3
SCFP_12	951581613	 [*]:[c](:[*])N[c](:[*]):[*]	-0.769	2 out of 9
SCFP_12	1334669481	 [*]N[c](:[cH]:[*]):[cH]:[*]	-0.685	28 out of 93

TOPKAT_Ocular_Irritancy_Moderate_vs_Severe



$C_{17}H_{16}FN_3S$

Molecular Weight: 313.39244

ALogP: 5.041

Rotatable Bonds: 2

Acceptors: 3

Donors: 1

Model Prediction

Prediction: Moderate

Probability: 0.452

Enrichment: 0.729

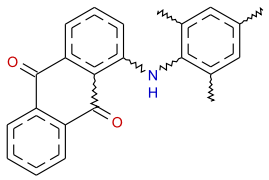
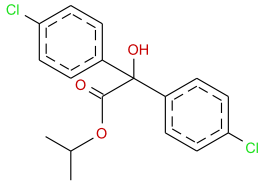
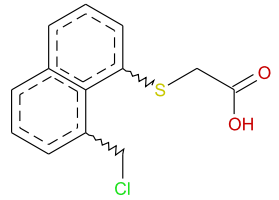
Bayesian Score: -4.89

Mahalanobis Distance: 9.1

Mahalanobis Distance p-value: 0.287

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	ANTHRAQUINONE;1-(2;4;6-TRIMETHYLPHENYLAMINO)-	BENZILIC ACID; 4;4'-DICHLORO-; ISOPROPYL ESTER	ACETIC ACID; 2-(-CHLOROMETHY-1-NAPHTHYLTHIO)-
Structure			
Actual Endpoint	Moderate	Severe	Severe
Predicted Endpoint	Moderate	Severe	Severe
Distance	0.621	0.626	0.679
Reference	28ZPAK-;242;72	CIGET* -;-;77	28ZPAK-;173;72

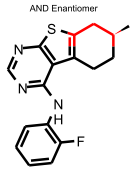
Model Applicability

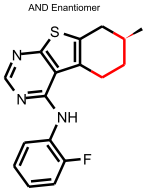
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

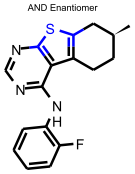
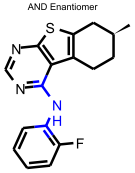
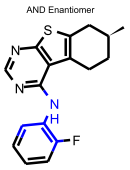
Feature Contribution

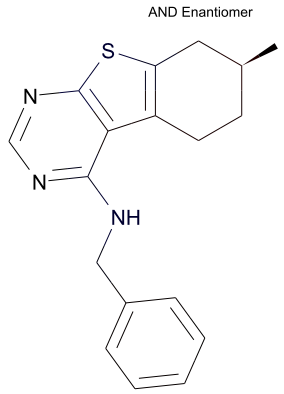
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Severe in training set
SCFP_12	-1272709286	 [*]C([*])C[c](:[*]):[*]	0.231	24 out of 31

SCFP_12	-1849867720	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2CC1	0.168	16 out of 22
SCFP_12	-1272798659	 [*]CCC([*])[*]	0.139	216 out of 309

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Severe in training set
SCFP_12	1310748454	 [*][c]1:[*]:[*]:[c](:[*]):s:1	-1.04	0 out of 3
SCFP_12	951581613	 [*]:[c](:[*])N[c](:[*]):[*]	-0.769	2 out of 9
SCFP_12	1334669481	 [*]N[c](:[cH]:[*]):[cH]:[*]	-0.685	28 out of 93



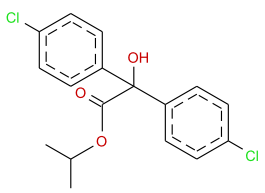
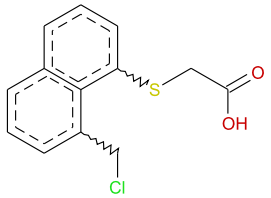
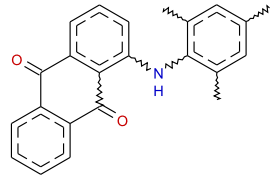
$C_{18}H_{19}N_3S$
Molecular Weight: 309.42856
ALogP: 4.678
Rotatable Bonds: 3
Acceptors: 3
Donors: 1

Model Prediction

Prediction: Moderate
Probability: 0.641
Enrichment: 1.03
Bayesian Score: -1.34
Mahalanobis Distance: 8.92
Mahalanobis Distance p-value: 0.375

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	BENZILIC ACID; 4;4'-DICHLORO-; ISOPROPYL ESTER	ACETIC ACID; 2-(-CHLOROMETHY-1-NAPHTHYLTHIO)-	ANTHRAQUINONE;1-(2;4;6-TRIMETHYLPHENYLAMINO)-
Structure			
Actual Endpoint	Severe	Severe	Moderate
Predicted Endpoint	Severe	Severe	Moderate
Distance	0.598	0.635	0.655
Reference	CIGET* -;-;77	28ZPAK-;173;72	28ZPAK-;242;72

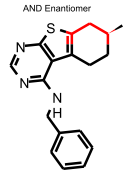
Model Applicability

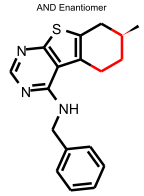
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

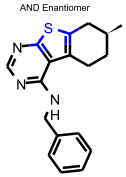
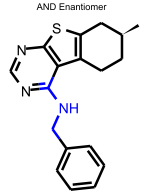
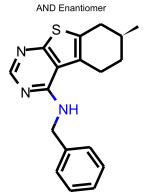
Feature Contribution

Top features for positive contribution

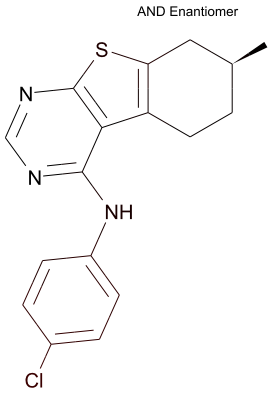
Fingerprint	Bit/Smiles	Feature Structure	Score	Severe in training set
SCFP_12	-1272709286	 [*]C([*])C[c](:[*]):[*]	0.231	24 out of 31

SCFP_12	-1849867720	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2CC1	0.168	16 out of 22
SCFP_12	-1272798659	 [*]CCC([*])[*]	0.139	216 out of 309

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Severe in training set
SCFP_12	1310748454	 [*][c]1:[*]:[*]:[c](:[*]):s:1	-1.04	0 out of 3
SCFP_12	18117904	 [*]CN[c](:[*]):[*]	-0.481	3 out of 9
SCFP_12	10	 [*]N[*]	-0.451	43 out of 112

TOPKAT_Ocular_Irritancy_None_vs_Irritant



$C_{17}H_{16}ClN_3S$

Molecular Weight: 329.84704

ALogP: 5.5

Rotatable Bonds: 2

Acceptors: 3

Donors: 1

Model Prediction

Prediction: Irritant

Probability: 1

Enrichment: 1.18

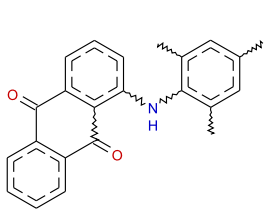
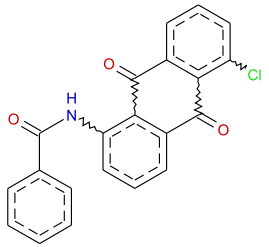
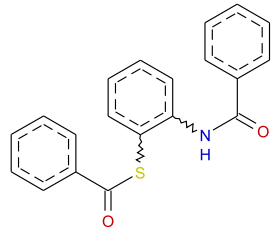
Bayesian Score: 1.98

Mahalanobis Distance: 7.8

Mahalanobis Distance p-value: 0.958

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	ANTHRAQUINONE;1-(2;4;6-TRIMETHYLPHENYLAMINO)-	BENZAMIDE; N-(5-CHLORO-1-ANTHRAQUINONYL)-	N;S-DIBENZOYL-O-AMINOTHIOPHENOL
Structure			
Actual Endpoint	Irritant	Irritant	Irritant
Predicted Endpoint	Irritant	Irritant	Irritant
Distance	0.584	0.584	0.585
Reference	28ZPAK-;242;72	28ZPAK 89;72	28ZPAK-;175;72

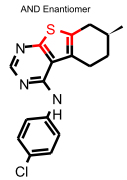
Model Applicability

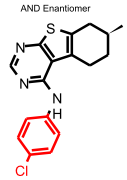
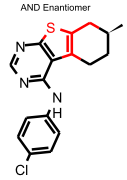
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
4. Unknown FCFP_2 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]

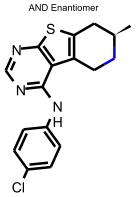
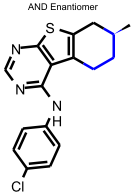
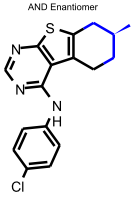
Feature Contribution

Top features for positive contribution

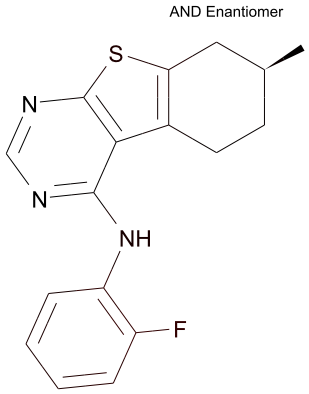
Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set
FCFP_12	1747237384	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.208	44 out of 44

FCFP_12	-1508180856	 [*][c]1:[cH]:[cH]:[c](Cl):[cH]:[cH]:1	0.2	17 out of 17
FCFP_12	-1539132615	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	0.197	13 out of 13

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set
FCFP_12	0	 [*]C[*]	0	1184 out of 1397
FCFP_12	-1272798659	 [*]CCC([*])[*]	0	517 out of 643
FCFP_12	-1043339860	 [*]CC(C)C[*]	0	146 out of 186

TOPKAT_Ocular_Irritancy_None_vs_Irritant



$C_{17}H_{16}FN_3S$

Molecular Weight: 313.39244

ALogP: 5.041

Rotatable Bonds: 2

Acceptors: 3

Donors: 1

Model Prediction

Prediction: Irritant

Probability: 1

Enrichment: 1.18

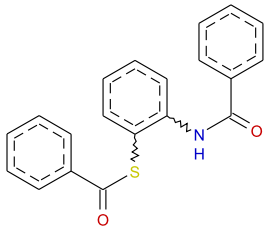
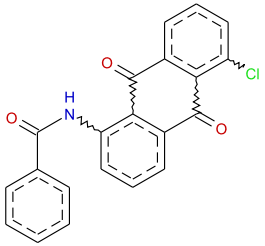
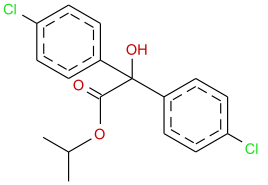
Bayesian Score: 1.75

Mahalanobis Distance: 7.67

Mahalanobis Distance p-value: 0.972

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	N;S-DIBENZOYL-O-AMINOTHIOPHENOL	BENZAMIDE; N-(5-CHLORO-1-ANTHRAQUINONYL)-	BENZILIC ACID; 4;4'-DICHLORO-; ISOPROPYL ESTER
Structure			
Actual Endpoint	Irritant	Irritant	Irritant
Predicted Endpoint	Irritant	Irritant	Irritant
Distance	0.557	0.566	0.595
Reference	28ZPAK-;175;72	28ZPAK 89;72	CIGET* -;-;77

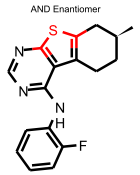
Model Applicability

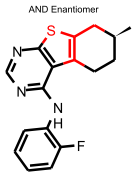
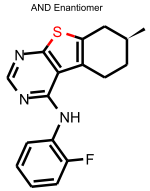
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
4. Unknown FCFP_2 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]

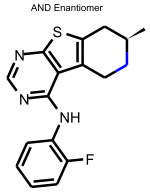
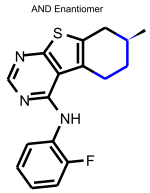
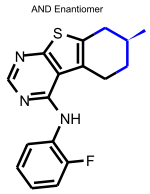
Feature Contribution

Top features for positive contribution

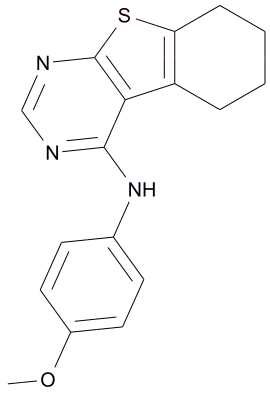
Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set
FCFP_12	1747237384	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.208	44 out of 44

FCFP_12	-1539132615	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	0.197	13 out of 13
FCFP_12	17	 [*]:s:[*]	0.189	48 out of 49

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set
FCFP_12	0	 [*]C[*]	0	1184 out of 1397
FCFP_12	-1272798659	 [*]CCC([*])[*]	0	517 out of 643
FCFP_12	-1043339860	 [*]CC(C)C[*]	0	146 out of 186

TOPKAT_Ocular_Irritancy_None_vs_Irritant



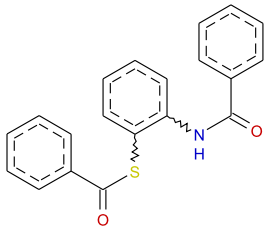
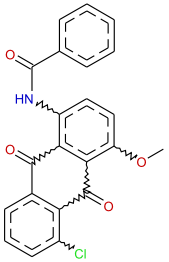
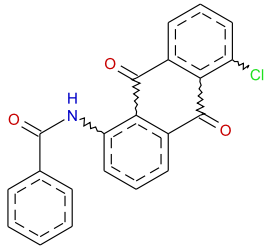
$C_{17}H_{17}N_3OS$
Molecular Weight: 311.40138
ALogP: 4.568
Rotatable Bonds: 3
Acceptors: 4
Donors: 1

Model Prediction

Prediction: Irritant
Probability: 1
Enrichment: 1.18
Bayesian Score: 0.616
Mahalanobis Distance: 7.11
Mahalanobis Distance p-value: 0.997

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	N;S-DIBENZOYL-O-AMINOTHIOPHENOL	1-BENZOYLAMINO-4-METHOXY-5-CHLORANTHRAQUINONE	BENZAMIDE; N-(5-CHLORO-1-ANTHRAQUINONYL)-
Structure			
Actual Endpoint	Irritant	Irritant	Irritant
Predicted Endpoint	Irritant	Irritant	Irritant
Distance	0.572	0.604	0.618
Reference	28ZPAK-;175;72	28ZPAK-;90;72	28ZPAK 89;72

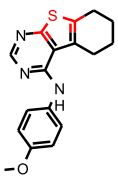
Model Applicability

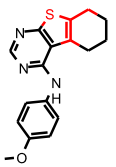
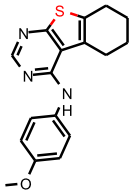
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
4. Unknown FCFP_2 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]

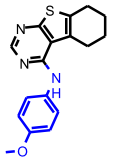
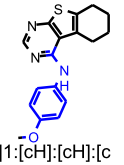
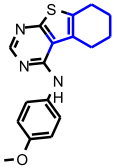
Feature Contribution

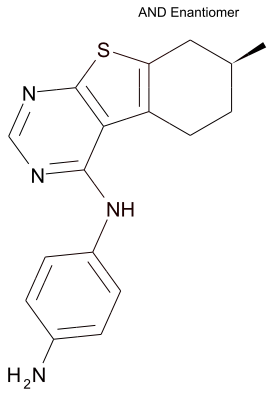
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set
FCFP_12	1747237384	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.208	44 out of 44

FCFP_12	-1539132615	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	0.197	13 out of 13
FCFP_12	17	 [*]:s:[*]	0.189	48 out of 49

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set
FCFP_12	-1060187936	 [*]N[c]1:[cH]:[cH]:[c](OC):[cH]:[cH]:1	-0.344	2 out of 4
FCFP_12	414792462	 [*]O[c]1:[cH]:[cH]:[c](N[c](:[*]):[*]):[cH]:[cH]:1	-0.268	1 out of 2
FCFP_12	-1909820884	 [*]:[c]1:[*]:[*]:[c]2CCCC[c]:1:2	-0.268	1 out of 2



$C_{17}H_{18}N_4S$

Molecular Weight: 310.41662

ALogP: 4.089

Rotatable Bonds: 2

Acceptors: 4

Donors: 2

Model Prediction

Prediction: Irritant

Probability: 1

Enrichment: 1.18

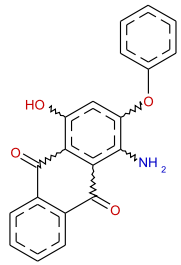
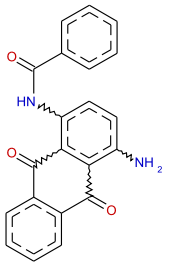
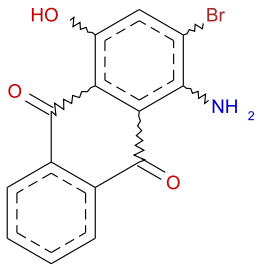
Bayesian Score: 1.13

Mahalanobis Distance: 7.73

Mahalanobis Distance p-value: 0.966

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	ANTHRAQUINONE; 1-AMINO-4-HYDROXY-2-PHENOXY-	1-AMINO-4-BENZOYLAMINO-ANTHRAQUINONE	Anthraquinone; 1-amino-2-bromo-4-hydroxy-
Structure			
Actual Endpoint	Irritant	Irritant	Non-Irritant
Predicted Endpoint	Irritant	Irritant	Non-Irritant
Distance	0.590	0.595	0.618
Reference	28ZPAK 239;72	28ZPAK-;124;72	Prehled Prumyslove Toxikologie; Organicke Latky; Marhold; J. pp 535;86

Model Applicability

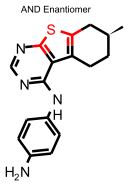
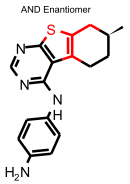
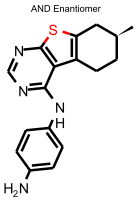
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
4. Unknown FCFP_2 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]

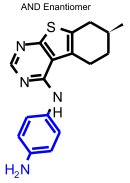
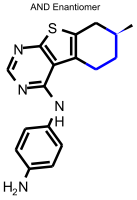
Feature Contribution

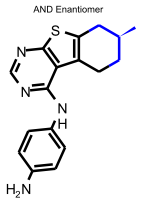
Top features for positive contribution

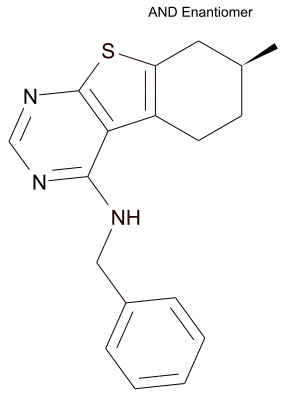
Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set

FCFP_12	1747237384	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.208	44 out of 44
FCFP_12	-1539132615	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	0.197	13 out of 13
FCFP_12	17	 [*]:s:[*]	0.189	48 out of 49

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set
FCFP_12	880832703	 [*][c]1:[cH]:[cH]:[c](N):[cH]:[cH]:1	-0.0697	15 out of 20
FCFP_12	-1272798659	 [*]CCC([*])[*]	0	517 out of 643

FCFP_12	-1043339860	 [*]CC(C)C[*]	0	146 out of 186



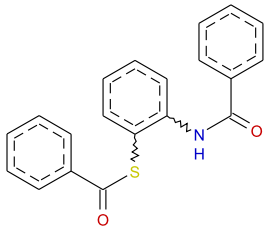
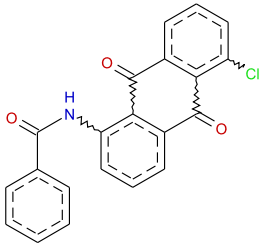
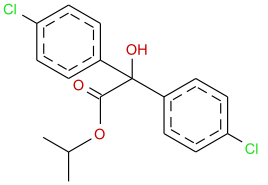
$C_{18}H_{19}N_3S$
Molecular Weight: 309.42856
ALogP: 4.678
Rotatable Bonds: 3
Acceptors: 3
Donors: 1

Model Prediction

Prediction: Irritant
Probability: 1
Enrichment: 1.18
Bayesian Score: 1.35
Mahalanobis Distance: 7.49
Mahalanobis Distance p-value: 0.986

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	N;S-DIBENZOYL-O-AMINOTHIOPHENOL	BENZAMIDE; N-(5-CHLORO-1-ANTHRAQUINONYL)-	BENZILIC ACID; 4;4'-DICHLORO-; ISOPROPYL ESTER
Structure			
Actual Endpoint	Irritant	Irritant	Irritant
Predicted Endpoint	Irritant	Irritant	Irritant
Distance	0.526	0.564	0.590
Reference	28ZPAK-;175;72	28ZPAK 89;72	CIGET* -;-;77

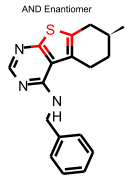
Model Applicability

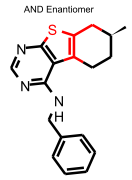
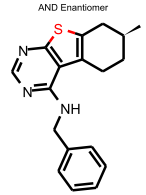
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
4. Unknown FCFP_2 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]

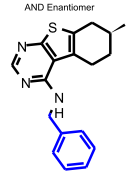
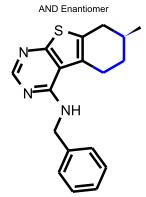
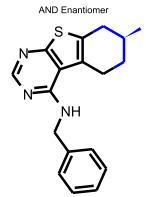
Feature Contribution

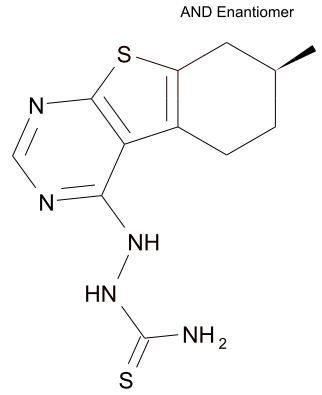
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set
FCFP_12	1747237384	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.208	44 out of 44

FCFP_12	-1539132615	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	0.197	13 out of 13
FCFP_12	17	 [*]:s:[*]	0.189	48 out of 49

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set
FCFP_12	-1698724694	 [*]C[c]1:[cH]:[cH]:[cH]:[cH]:[cH]:1	-0.0964	107 out of 146
FCFP_12	-1272798659	 [*]CCC([*])[*]	0	517 out of 643
FCFP_12	-1043339860	 [*]CC(C)C[*]	0	146 out of 186



$C_{12}H_{15}N_5S_2$

Molecular Weight: 293.411

ALogP: 3.209

Rotatable Bonds: 3

Acceptors: 4

Donors: 3

Model Prediction

Prediction: Irritant

Probability: 1

Enrichment: 1.18

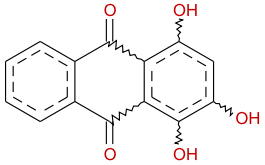
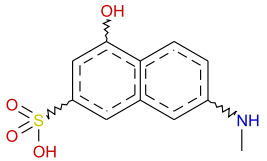
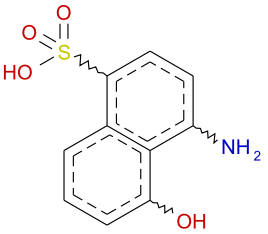
Bayesian Score: 1.04

Mahalanobis Distance: 7.39

Mahalanobis Distance p-value: 0.99

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	1;2;4-TRIHYDROXY ANTHRAQUINONE	2-NAPHTHALENESULFONIC ACID; 4-HYDROXY-7-(METHYLAMINO)-	1-Naphthalenesulfonic acid; 4-amino-5-hydroxy-
Structure			
Actual Endpoint	Irritant	Irritant	Non-Irritant
Predicted Endpoint	Irritant	Irritant	Non-Irritant
Distance	0.664	0.669	0.695
Reference	28ZPAK-;103;7	28ZPAK 190;72	Prehled Prumyslove Toxikologie; Organicke Latky; Marhold; J. pp 1057;86

Model Applicability

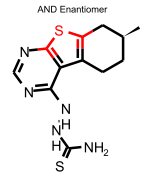
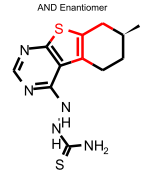
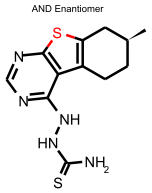
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
4. Unknown FCFP_2 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]
5. Unknown FCFP_2 feature: -885461129: [*]NNC(=[*])[*]

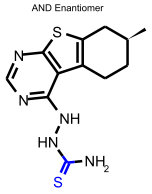
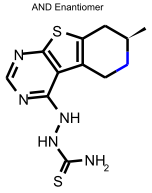
Feature Contribution

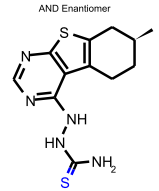
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set

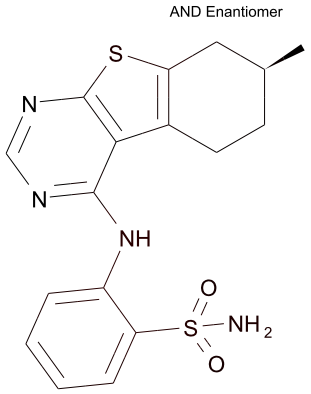
FCFP_12	1747237384	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.208	44 out of 44
FCFP_12	-1539132615	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	0.197	13 out of 13
FCFP_12	17	 [*]:s:[*]	0.189	48 out of 49

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set
FCFP_12	1872154524	 [*]C(=S)[*]	0	563 out of 690
FCFP_12	0	 [*]C[*]	0	1184 out of 1397

FCFP_12	1	AND Enantiomer  [*]O[*]	0	872 out of 1051

TOPKAT_Ocular_Irritancy_None_vs_Irritant



$C_{17}H_{18}N_4O_2S_2$

Molecular Weight: 374.48042

ALogP: 3.541

Rotatable Bonds: 3

Acceptors: 5

Donors: 2

Model Prediction

Prediction: Irritant

Probability: 1

Enrichment: 1.18

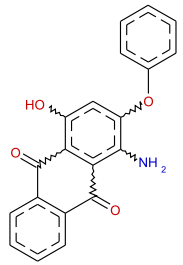
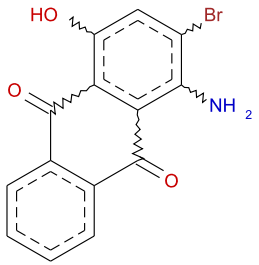
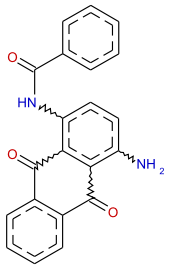
Bayesian Score: 1.68

Mahalanobis Distance: 7.29

Mahalanobis Distance p-value: 0.993

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	ANTHRAQUINONE; 1-AMINO-4-HYDROXY-2-PHENOXY-	Anthraquinone; 1-amino-2-bromo-4-hydroxy-	1-AMINO-4-BENZOYLAMINO-ANTHRAQUINONE
Structure			
Actual Endpoint	Irritant	Non-Irritant	Irritant
Predicted Endpoint	Irritant	Non-Irritant	Irritant
Distance	0.612	0.646	0.649
Reference	28ZPAK 239;72	Prehled Prumyslove Toxikologie; Organicke Latky; Marhold; J. pp 535;86	28ZPAK-;124;72

Model Applicability

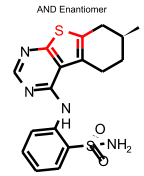
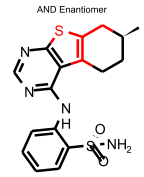
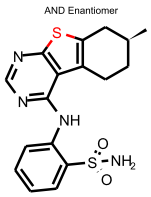
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
4. Unknown FCFP_2 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]

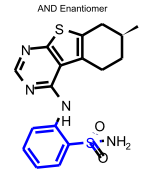
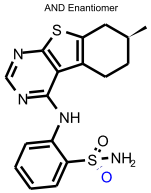
Feature Contribution

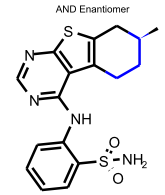
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set

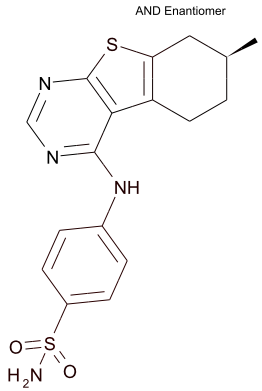
FCFP_12	1747237384	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.208	44 out of 44
FCFP_12	-1539132615	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	0.197	13 out of 13
FCFP_12	17	 [*]:s:[*]	0.189	48 out of 49

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set
FCFP_12	-1698724694	 [*]C[c]1:[cH]:[cH]:[cH]:[cH]:[cH]:1	-0.0964	107 out of 146
FCFP_12	1	 [*]O[*]	0	872 out of 1051

FCFP_12	-1272798659	 [*]CCC([*])[*]	0	517 out of 643

TOPKAT_Ocular_Irritancy_None_vs_Irritant



$C_{17}H_{18}N_4O_2S_2$

Molecular Weight: 374.48042

ALogP: 3.541

Rotatable Bonds: 3

Acceptors: 5

Donors: 2

Model Prediction

Prediction: Irritant

Probability: 1

Enrichment: 1.18

Bayesian Score: 1.9

Mahalanobis Distance: 7.29

Mahalanobis Distance p-value: 0.993

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
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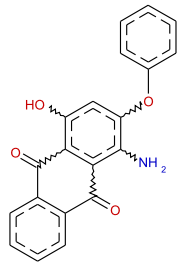
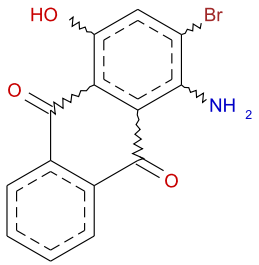
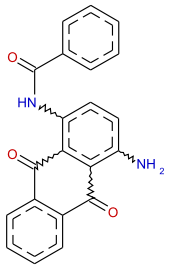
Structural Similar Compounds

Name	ANTHRAQUINONE; 1-AMINO-4-HYDROXY-2-PHENOXY-	Anthraquinone; 1-amino-2-bromo-4-hydroxy-	1-AMINO-4-BENZOYLAMINO-ANTHRAQUINONE
Structure			
Actual Endpoint	Irritant	Non-Irritant	Irritant
Predicted Endpoint	Irritant	Non-Irritant	Irritant
Distance	0.621	0.657	0.659
Reference	28ZPAK 239;72	Prehled Prumyslove Toxikologie; Organicke Latky; Marhold; J. pp 535;86	28ZPAK-;124;72

Model Applicability

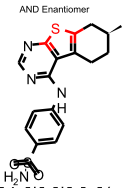
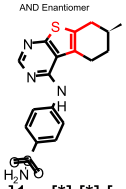
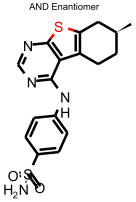
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
4. Unknown FCFP_2 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]

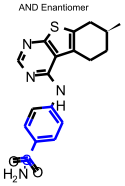
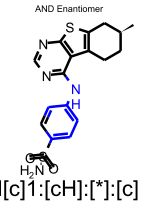
Feature Contribution

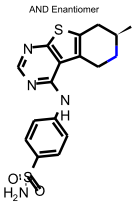
Top features for positive contribution

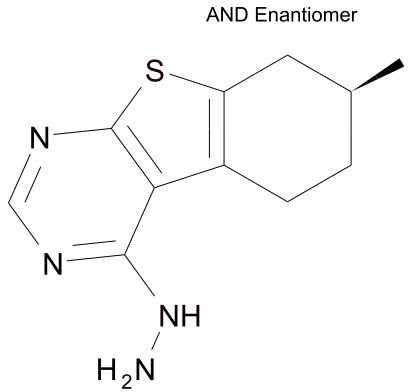
Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set

FCFP_12	1747237384	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.208	44 out of 44
FCFP_12	-1539132615	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	0.197	13 out of 13
FCFP_12	17	 [*]:s:[*]	0.189	48 out of 49

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set
FCFP_12	-453677277	 [*]C[c]1:[cH]:[*]:[cH]:[cH]:[cH]:1	0	264 out of 323
FCFP_12	-773983804	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	0	102 out of 121

FCFP_12	0	 [*]C[*]	0	1184 out of 1397



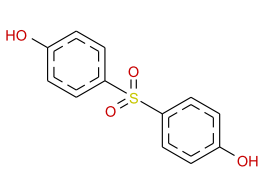
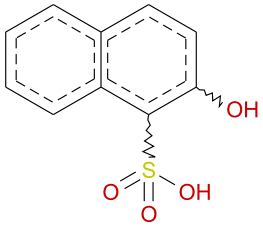
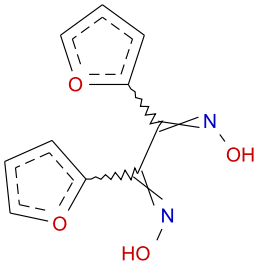
$C_{11}H_{14}N_4S$
Molecular Weight: 234.32065
ALogP: 2.561
Rotatable Bonds: 1
Acceptors: 4
Donors: 2

Model Prediction

Prediction: Irritant
Probability: 1
Enrichment: 1.18
Bayesian Score: 1
Mahalanobis Distance: 7.79
Mahalanobis Distance p-value: 0.96

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	PHENOL; 4;4'-SULFONYLDI-	NAPHTHENESULFONIC ACID;2-HYDROXY-	FURIL;DIOXIME
Structure			
Actual Endpoint	Irritant	Irritant	Irritant
Predicted Endpoint	Irritant	Irritant	Irritant
Distance	0.540	0.542	0.547
Reference	BIOFX* 601-05501;74	28ZPAK-;186;72	28ZPAK

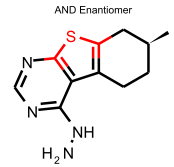
Model Applicability

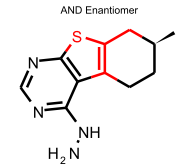
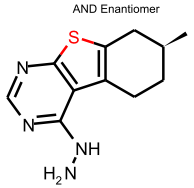
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
4. Unknown FCFP_2 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]

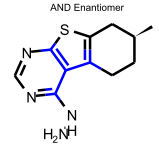
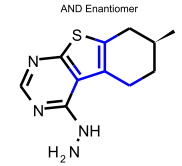
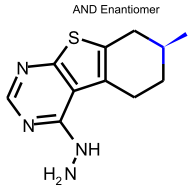
Feature Contribution

Top features for positive contribution

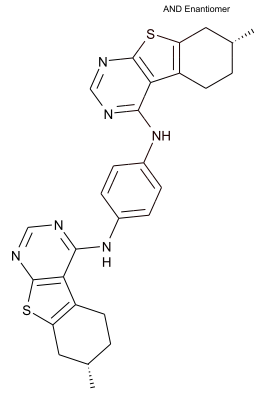
Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set
FCFP_12	1747237384	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.208	44 out of 44

FCFP_12	-1539132615	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	0.197	13 out of 13
FCFP_12	17	 [*]:s:[*]	0.189	48 out of 49

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set
FCFP_12	307419094	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0	43 out of 52
FCFP_12	203677720	 [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0	319 out of 382
FCFP_12	136597326	 [*]C([*])C	0	612 out of 753

TOPKAT_Ocular_Irritancy_None_vs_Irritant



$C_{28}H_{28}N_6S_2$

Molecular Weight: 512.69212

ALogP: 7.842

Rotatable Bonds: 4

Acceptors: 6

Donors: 2

Model Prediction

Prediction: Irritant

Probability: 1

Enrichment: 1.18

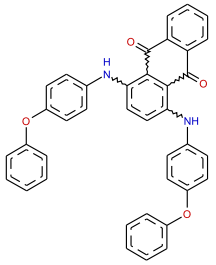
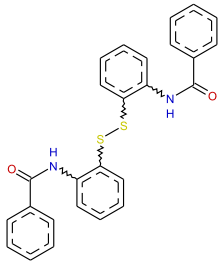
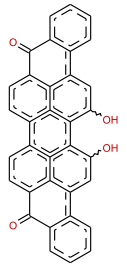
Bayesian Score: 0.917

Mahalanobis Distance: 9.37

Mahalanobis Distance p-value: 0.315

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	ANILINE;N;N'-1;4-ANTHRAQUINONYLENEBIS(4-PHENOXY-	BENZANILIDE;2';2"'-DITHIOBIS-	DINAPHTHO(1;2;3-CD:3';2';1'-IM)PERYLENE-5;10-DIONE;16;17-DIHYDROXY
Structure			
Actual Endpoint	Non-Irritant	Non-Irritant	Irritant
Predicted Endpoint	Non-Irritant	Non-Irritant	Irritant
Distance	0.719	0.737	0.753
Reference	28ZPAK-;114;72	28ZPAK-;173;72	28ZPAK-;104;72

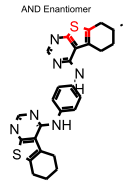
Model Applicability

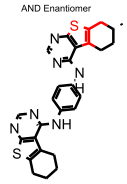
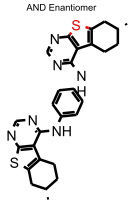
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
4. Unknown FCFP_2 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]

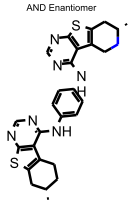
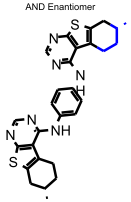
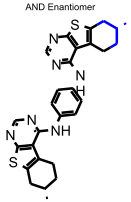
Feature Contribution

Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set
FCFP_12	1747237384	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.208	44 out of 44

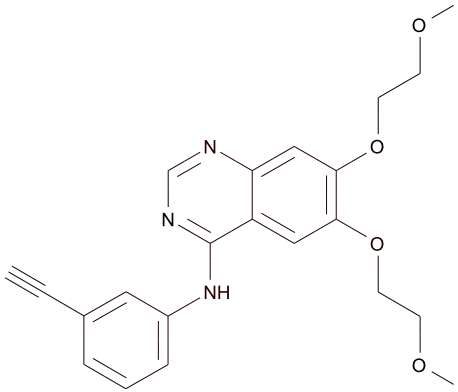
FCFP_12	-1539132615	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	0.197	13 out of 13
FCFP_12	17	 [*]:s:[*]	0.189	48 out of 49

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set
FCFP_12	0	 [*]C[*]	0	1184 out of 1397
FCFP_12	-1272798659	 [*]CCC([*])[*]	0	517 out of 643
FCFP_12	-1043339860	 [*]CC(C)C[*]	0	146 out of 186

Erlotinib

TOPKAT_Ocular_Irritancy_None_vs_Irritant



$C_{22}H_{23}N_3O_4$

Molecular Weight: 393.43572

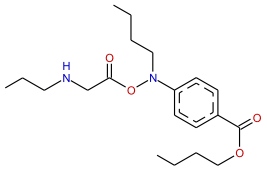
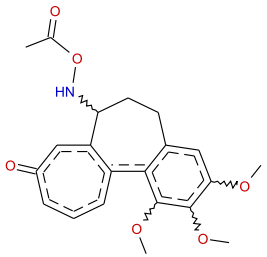
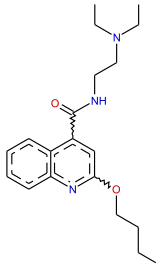
ALogP: 4.309

Rotatable Bonds: 10

Acceptors: 7

Donors: 1

Structural Similar Compounds

Name	Benzoic acid; p-(N-butyl-2-(butylamino)acetamido)-; butyl ester;	COLCHICINE	Cinchoninamide; 2-butoxy-N-(2-(diethylamino)ethyl)-; monohydrochloride
Structure			
Actual Endpoint	Irritant	Irritant	Irritant
Predicted Endpoint	Non-Irritant	Irritant	Irritant
Distance	0.637	0.682	0.747
Reference	Arzneimittel-Forschung 8;609;58	AJOPAA 31;837;48	Arzneimittel-Forschung 8;181;58

Model Prediction

Prediction: Irritant

Probability: 1

Enrichment: 1.18

Bayesian Score: 2.13

Mahalanobis Distance: 9.75

Mahalanobis Distance p-value: 0.161

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

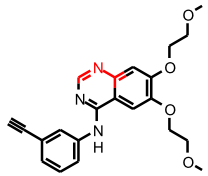
Model Applicability

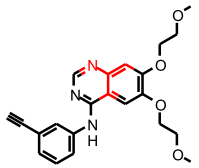
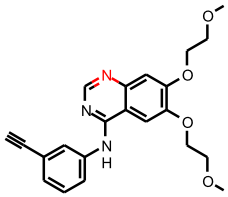
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
3. Unknown FCFP_2 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]
4. Unknown FCFP_2 feature: 902193919: [*]:[c](:[*])C#C

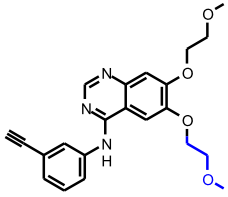
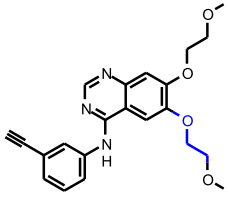
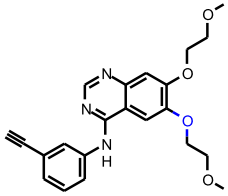
Feature Contribution

Top features for positive contribution

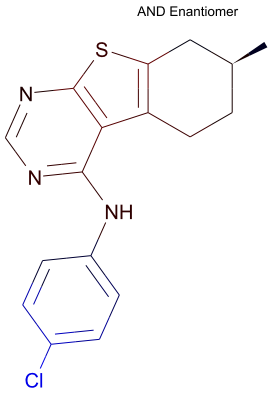
Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set
FCFP_12	1747237384	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.208	44 out of 44

FCFP_12	178336375	 [*]:[cH]:[c](:n:[*]):[c](:[*]):[*]	0.202	19 out of 19
FCFP_12	17	 [*]:s:[*]	0.189	48 out of 49

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set
FCFP_12	341504799	 [*]CCOC	0	17 out of 22
FCFP_12	-1272768868	 [*]CCO[*]	0	396 out of 514
FCFP_12	1	 [*]O[*]	0	872 out of 1051

TOPKAT_Rat_Female_FDA_None_vs_Carcinogen



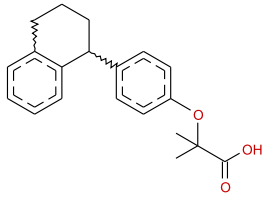
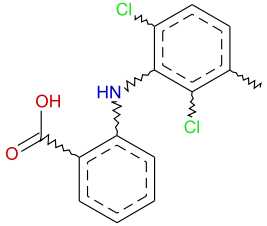
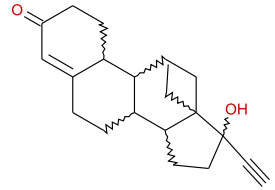
$C_{17}H_{16}ClN_3S$
Molecular Weight: 329.84704
ALogP: 5.5
Rotatable Bonds: 2
Acceptors: 3
Donors: 1

Model Prediction

Prediction: Carcinogen
Probability: 0.288
Enrichment: 0.893
Bayesian Score: -0.553
Mahalanobis Distance: 11.8
Mahalanobis Distance p-value: 0.00845

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Nafenopin	Meclofenamate	Levonorgestrel
Structure			
Actual Endpoint	Non-Carcinogen	Non-Carcinogen	Non-Carcinogen
Predicted Endpoint	Non-Carcinogen	Non-Carcinogen	Carcinogen
Distance	0.638	0.651	0.656
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

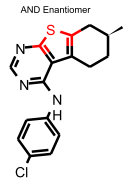
Model Applicability

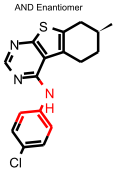
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]

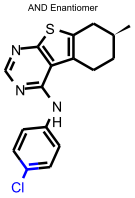
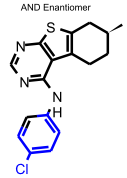
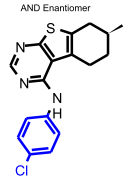
Feature Contribution

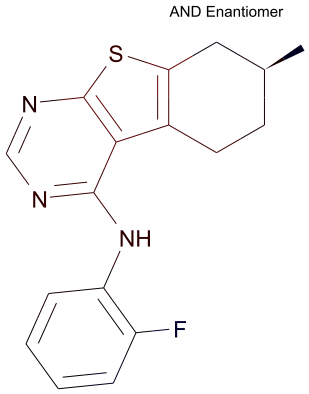
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_12	85262808	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.851	5 out of 5

ECFP_12	553181281	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2CC1	0.613	2 out of 2
ECFP_12	-177077903	 [*]N[c](:[cH]:[*]):[cH]:[*]	0.529	6 out of 10

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_12	99947387	 [*]:[c](:[*])Cl	-0.817	8 out of 62
ECFP_12	1854732111	 [*][c]1:[*]:[cH]:[c](Cl):[cH]:[cH]:1	-0.816	4 out of 33
ECFP_12	-769655848	 [*][c]1:[cH]:[cH]:[c](Cl):[cH]:[cH]:1	-0.797	1 out of 11



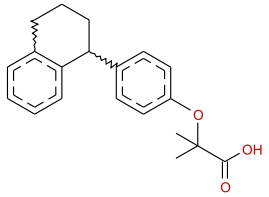
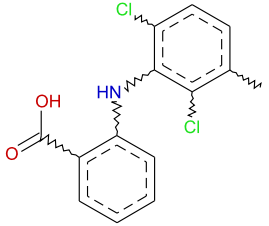
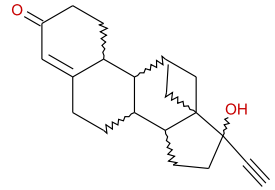
$C_{17}H_{16}FN_3S$
Molecular Weight: 313.39244
ALogP: 5.041
Rotatable Bonds: 2
Acceptors: 3
Donors: 1

Model Prediction

Prediction: Carcinogen
Probability: 0.371
Enrichment: 1.15
Bayesian Score: 3.05
Mahalanobis Distance: 10.5
Mahalanobis Distance p-value: 0.169

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Nafenopin	Meclofenamate	Levonorgestrel
Structure			
Actual Endpoint	Non-Carcinogen	Non-Carcinogen	Non-Carcinogen
Predicted Endpoint	Non-Carcinogen	Non-Carcinogen	Carcinogen
Distance	0.622	0.622	0.648
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

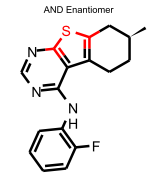
Model Applicability

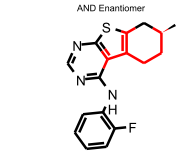
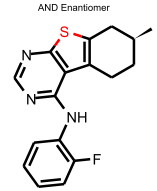
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]

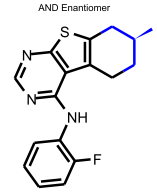
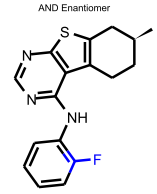
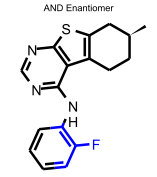
Feature Contribution

Top features for positive contribution

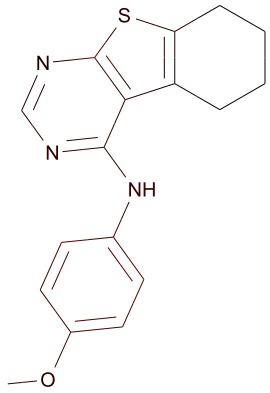
Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_12	85262808	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.851	5 out of 5

ECFP_12	553181281	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2CC1	0.613	2 out of 2
ECFP_12	914325265	 [*]:s:[*]	0.516	8 out of 14

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_12	292958156	 [*]CC(C)C[*]	-0.485	0 out of 2
ECFP_12	220735655	 [*]:[c](:[*])F	-0.327	4 out of 19
ECFP_12	-1311285389	 [*][c](:[*]):[c](F):[cH]:[*]	-0.318	2 out of 10

TOPKAT_Rat_Female_FDA_None_vs_Carcinogen



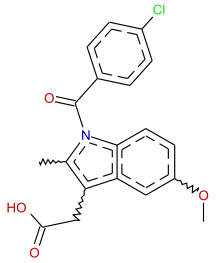
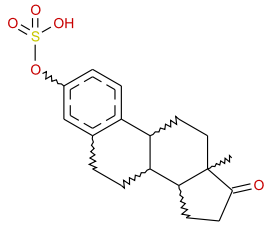
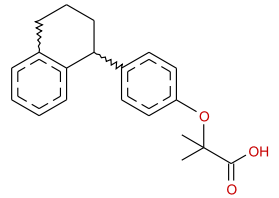
$C_{17}H_{17}N_3OS$
Molecular Weight: 311.40138
ALogP: 4.568
Rotatable Bonds: 3
Acceptors: 4
Donors: 1

Model Prediction

Prediction: Carcinogen
Probability: 0.432
Enrichment: 1.34
Bayesian Score: 5.15
Mahalanobis Distance: 12.4
Mahalanobis Distance p-value: 0.00124

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Indomethacin	Estrogens; conjug.	Nafenopin
Structure			
Actual Endpoint	Non-Carcinogen	Carcinogen	Non-Carcinogen
Predicted Endpoint	Non-Carcinogen	Carcinogen	Non-Carcinogen
Distance	0.592	0.637	0.638
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

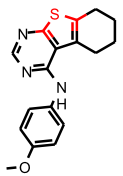
Model Applicability

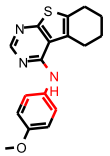
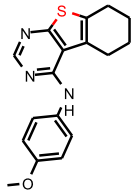
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]

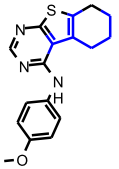
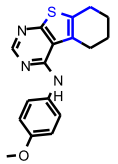
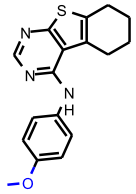
Feature Contribution

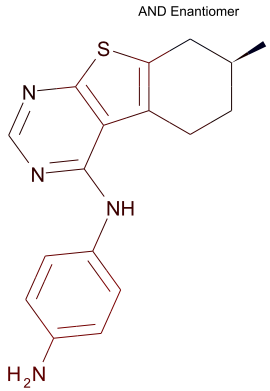
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_12	85262808	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.851	5 out of 5

ECFP_12	-177077903	 [*]N[c](:[cH]:[*]):[cH]:[*]	0.529	6 out of 10
ECFP_12	914325265	 [*]:s:[*]	0.516	8 out of 14

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_12	552088469	 [*]:[c]1:[*]:[*]:[c]2[*]CCC[c]:1:2	-0.272	0 out of 1
ECFP_12	-1672647522	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	-0.272	0 out of 1
ECFP_12	864909220	 [*]OC	-0.147	12 out of 45



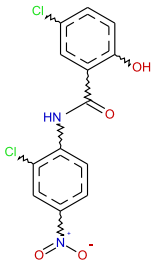
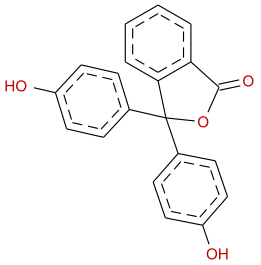
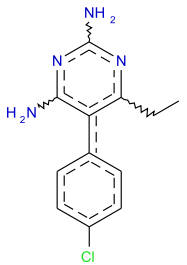
$C_{17}H_{18}N_4S$
Molecular Weight: 310.41662
ALogP: 4.089
Rotatable Bonds: 2
Acceptors: 4
Donors: 2

Model Prediction

Prediction: Carcinogen
Probability: 0.474
Enrichment: 1.47
Bayesian Score: 6.43
Mahalanobis Distance: 12.1
Mahalanobis Distance p-value: 0.00357

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Niclosamide	Phenolphthalein	Pyrimethamine
Structure			
Actual Endpoint	Non-Carcinogen	Carcinogen	Non-Carcinogen
Predicted Endpoint	Non-Carcinogen	Carcinogen	Non-Carcinogen
Distance	0.573	0.584	0.638
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

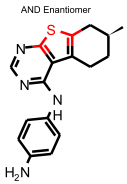
Model Applicability

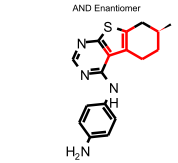
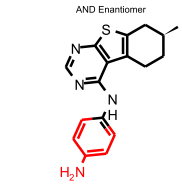
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]

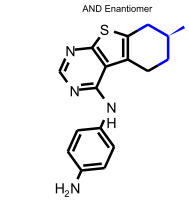
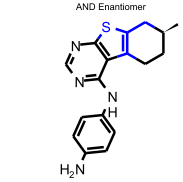
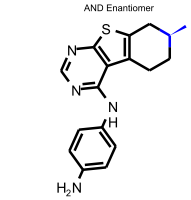
Feature Contribution

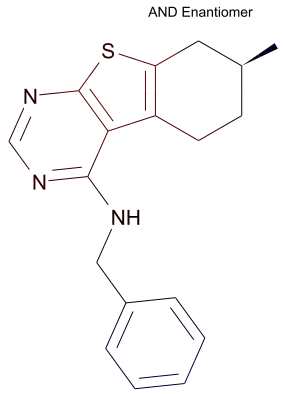
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_12	85262808	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.851	5 out of 5

ECFP_12	553181281	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2CC1	0.613	2 out of 2
ECFP_12	773910207	 N[c]1:[cH]:[cH]:[*]:[cH]:[cH]:1	0.553	4 out of 6

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_12	292958156	 [*]CC(C)C[*]	-0.485	0 out of 2
ECFP_12	-1672647522	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	-0.272	0 out of 1
ECFP_12	865482986	 [*]C([*])C	-0.233	4 out of 17



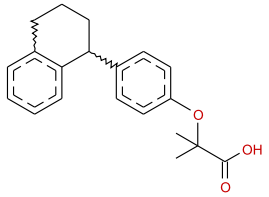
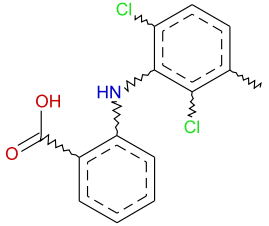
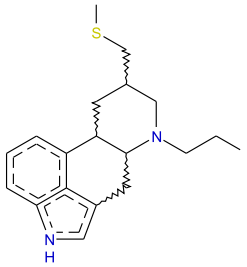
$C_{18}H_{19}N_3S$
Molecular Weight: 309.42856
ALogP: 4.678
Rotatable Bonds: 3
Acceptors: 3
Donors: 1

Model Prediction

Prediction: Carcinogen
Probability: 0.362
Enrichment: 1.13
Bayesian Score: 2.75
Mahalanobis Distance: 13.1
Mahalanobis Distance p-value: 9.36e-005

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Nafenopin	Meclofenamate	Pergolide
Structure			
Actual Endpoint	Non-Carcinogen	Non-Carcinogen	Carcinogen
Predicted Endpoint	Non-Carcinogen	Non-Carcinogen	Carcinogen
Distance	0.577	0.624	0.627
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

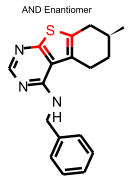
Model Applicability

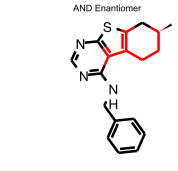
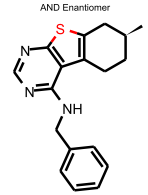
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]

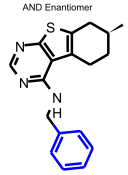
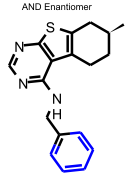
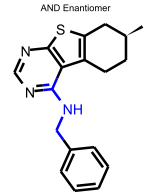
Feature Contribution

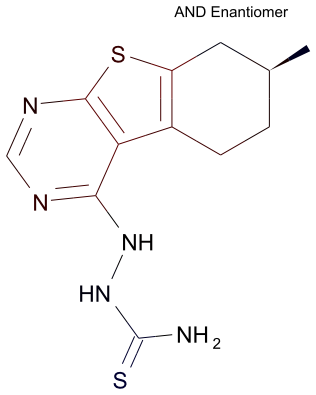
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_12	85262808	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.851	5 out of 5

ECFP_12	553181281	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2 CC1	0.613	2 out of 2
ECFP_12	914325265	 [*]:s:[*]	0.516	8 out of 14

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_12	-281505363	 [*][c]1:[cH]:[cH]:[cH]:[cH]:[cH]:1	-0.56	11 out of 64
ECFP_12	1571214559	 [*]1:[cH]:[cH]:[cH]:[cH]:[cH]:1	-0.56	11 out of 64
ECFP_12	491100606	 [*]CN[c](:[*]):[*]	-0.485	0 out of 2



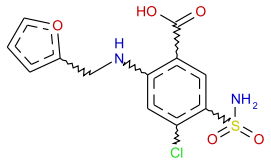
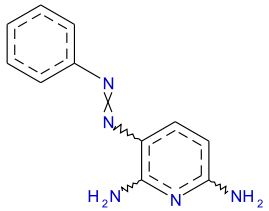
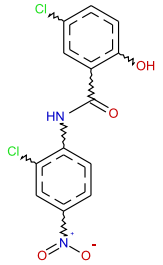
$C_{12}H_{15}N_5S_2$
Molecular Weight: 293.411
ALogP: 3.209
Rotatable Bonds: 3
Acceptors: 4
Donors: 3

Model Prediction

Prediction: Carcinogen
Probability: 0.328
Enrichment: 1.02
Bayesian Score: 1.35
Mahalanobis Distance: 11.9
Mahalanobis Distance p-value: 0.00572

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Furosemide	Phenazopyridine	Niclosamide
Structure			
Actual Endpoint	Non-Carcinogen	Carcinogen	Non-Carcinogen
Predicted Endpoint	Non-Carcinogen	Carcinogen	Non-Carcinogen
Distance	0.724	0.738	0.738
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

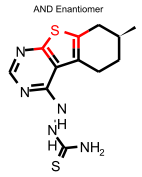
Model Applicability

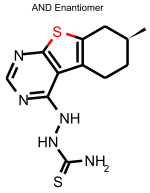
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown ECFP_2 feature: -1238415266: [*]NN[c](:[*]):[*]
4. Unknown ECFP_2 feature: -571028867: [*]NC(=S)N

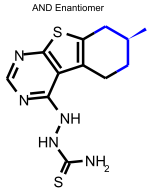
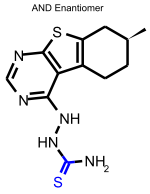
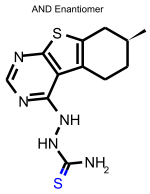
Feature Contribution

Top features for positive contribution

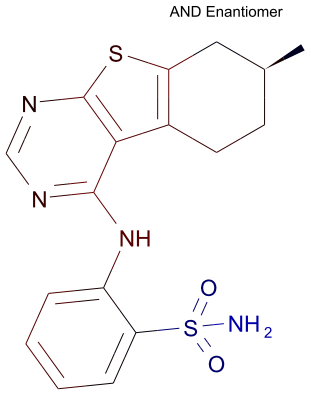
Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_12	85262808	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.851	5 out of 5

ECFP_12	553181281	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2CC1	0.613	2 out of 2
ECFP_12	914325265	 [*]:s:[*]	0.516	8 out of 14

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_12	292958156	 [*]CC(C)C[*]	-0.485	0 out of 2
ECFP_12	1979182050	 [*]C(=S)[*]	-0.485	0 out of 2
ECFP_12	-845108448	 [*]=S	-0.485	0 out of 2

TOPKAT_Rat_Female_FDA_None_vs_Carcinogen



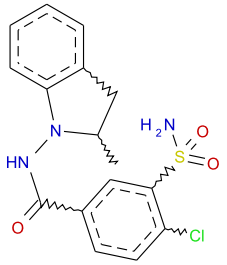
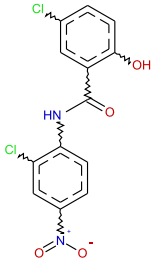
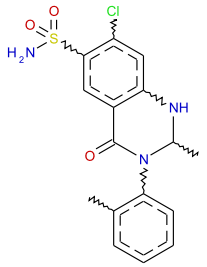
$C_{17}H_{18}N_4O_2S_2$
Molecular Weight: 374.48042
ALogP: 3.541
Rotatable Bonds: 3
Acceptors: 5
Donors: 2

Model Prediction

Prediction: Carcinogen
Probability: 0.332
Enrichment: 1.03
Bayesian Score: 1.53
Mahalanobis Distance: 12.2
Mahalanobis Distance p-value: 0.00246

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Indapamide	Niclosamide	Metolazone
Structure			
Actual Endpoint	Non-Carcinogen	Non-Carcinogen	Non-Carcinogen
Predicted Endpoint	Non-Carcinogen	Non-Carcinogen	Non-Carcinogen
Distance	0.598	0.625	0.635
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

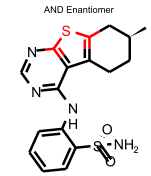
Model Applicability

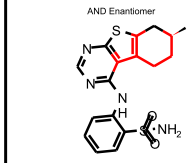
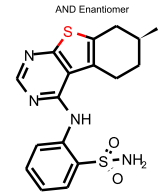
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]

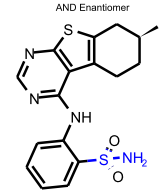
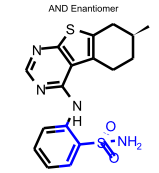
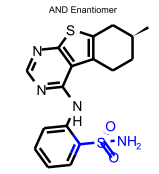
Feature Contribution

Top features for positive contribution

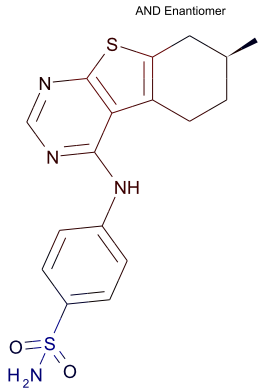
Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_12	85262808	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.851	5 out of 5

ECFP_12	553181281	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2CC1	0.613	2 out of 2
ECFP_12	914325265	 [*]:s:[*]	0.516	8 out of 14

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_12	-934226723	 [*]S(=[*])(=[*])N	-1.16	0 out of 7
ECFP_12	-450780499	 [*][c](:[*]):[c](:[cH]:[*])S(=O)(=O)N	-1.06	0 out of 6
ECFP_12	-2121766239	 [*]:[c](:[*])S(=O)(=O)N	-1.06	0 out of 6

TOPKAT_Rat_Female_FDA_None_vs_Carcinogen



$C_{17}H_{18}N_4O_2S_2$

Molecular Weight: 374.48042

ALogP: 3.541

Rotatable Bonds: 3

Acceptors: 5

Donors: 2

Model Prediction

Prediction: Carcinogen

Probability: 0.341

Enrichment: 1.06

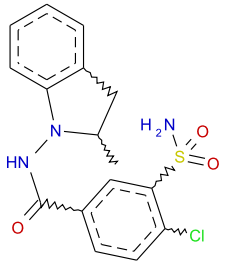
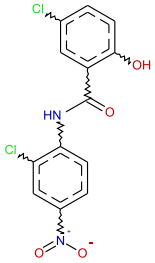
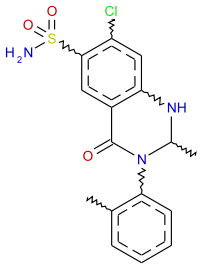
Bayesian Score: 1.92

Mahalanobis Distance: 12.8

Mahalanobis Distance p-value: 0.000276

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Indapamide	Niclosamide	Metolazone
Structure			
Actual Endpoint	Non-Carcinogen	Non-Carcinogen	Non-Carcinogen
Predicted Endpoint	Non-Carcinogen	Non-Carcinogen	Non-Carcinogen
Distance	0.614	0.629	0.650
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

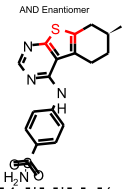
Model Applicability

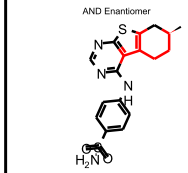
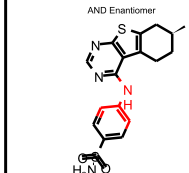
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]

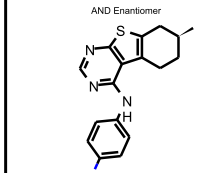
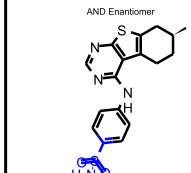
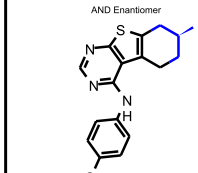
Feature Contribution

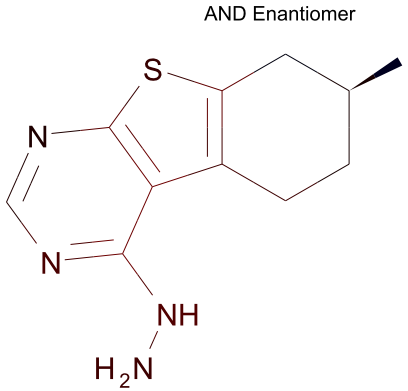
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_12	85262808	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.851	5 out of 5

ECFP_12	553181281	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2CC1	0.613	2 out of 2
ECFP_12	-177077903	 [*]N[c](:[cH]:[*]):[cH]:[*]	0.529	6 out of 10

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_12	-934226723	 [*]S(=[*])(=[*])N	-1.16	0 out of 7
ECFP_12	-2121766239	 [*]:[c](:[*])S(=O)(=O)N	-1.06	0 out of 6
ECFP_12	292958156	 [*]CC(C)C[*]	-0.485	0 out of 2



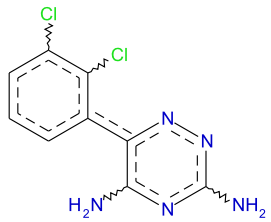
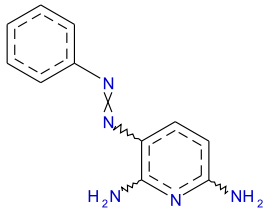
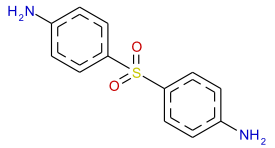
$C_{11}H_{14}N_4S$
Molecular Weight: 234.32065
ALogP: 2.561
Rotatable Bonds: 1
Acceptors: 4
Donors: 2

Model Prediction

Prediction: Carcinogen
Probability: 0.43
Enrichment: 1.34
Bayesian Score: 5.09
Mahalanobis Distance: 11.9
Mahalanobis Distance p-value: 0.00578

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Lamotrigine	Phenazopyridine	Dapsone
Structure			
Actual Endpoint	Non-Carcinogen	Carcinogen	Carcinogen
Predicted Endpoint	Non-Carcinogen	Carcinogen	Carcinogen
Distance	0.578	0.594	0.606
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

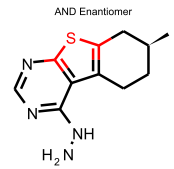
Model Applicability

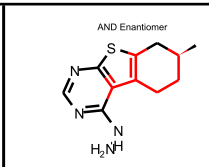
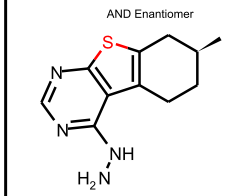
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]

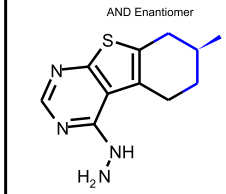
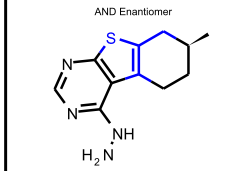
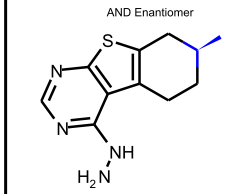
Feature Contribution

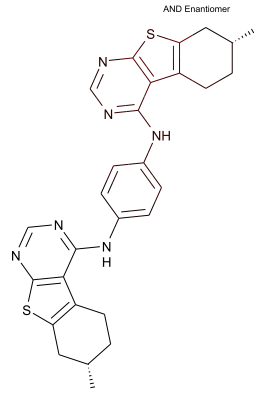
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_12	85262808	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.851	5 out of 5

ECFP_12	553181281	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2CC1	0.613	2 out of 2
ECFP_12	914325265	 [*]:s:[*]	0.516	8 out of 14

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_12	292958156	 [*]CC(C)C[*]	-0.485	0 out of 2
ECFP_12	-1672647522	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	-0.272	0 out of 1
ECFP_12	865482986	 [*]C([*])C	-0.233	4 out of 17



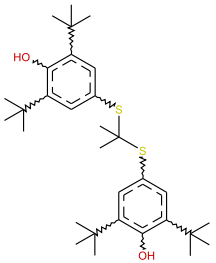
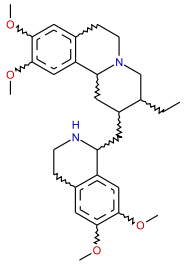
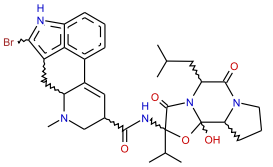
$C_{28}H_{28}N_6S_2$
Molecular Weight: 512.69212
ALogP: 7.842
Rotatable Bonds: 4
Acceptors: 6
Donors: 2

Model Prediction

Prediction: Carcinogen
Probability: 0.401
Enrichment: 1.25
Bayesian Score: 4.13
Mahalanobis Distance: 13.2
Mahalanobis Distance p-value: 7.35e-005

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Probucol	Emetine	Bromocriptine
Structure			
Actual Endpoint	Non-Carcinogen	Non-Carcinogen	Carcinogen
Predicted Endpoint	Non-Carcinogen	Non-Carcinogen	Carcinogen
Distance	0.878	0.906	0.927
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

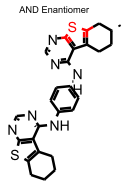
Model Applicability

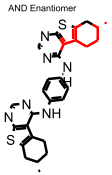
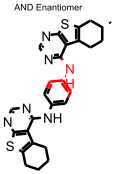
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]

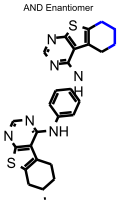
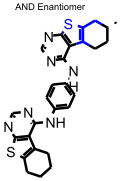
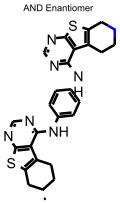
Feature Contribution

Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_12	85262808	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.851	5 out of 5

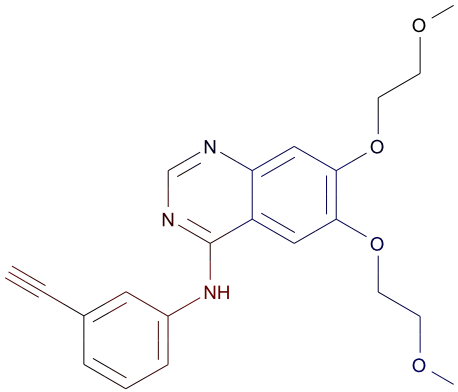
ECFP_12	553181281	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2CC1	0.613	2 out of 2
ECFP_12	-177077903	 [*]N[c](:[cH]:[*]):[cH]:[*]	0.529	6 out of 10

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_12	292958156	 [*]CC(C)C[*]	-0.485	0 out of 2
ECFP_12	-1672647522	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	-0.272	0 out of 1
ECFP_12	865482986	 [*]C([*])C	-0.233	4 out of 17

Erlotinib

TOPKAT_Rat_Female_FDA_None_vs_Carcinogen



$C_{22}H_{23}N_3O_4$

Molecular Weight: 393.43572

ALogP: 4.309

Rotatable Bonds: 10

Acceptors: 7

Donors: 1

Model Prediction

Prediction: Carcinogen

Probability: 0.285

Enrichment: 0.885

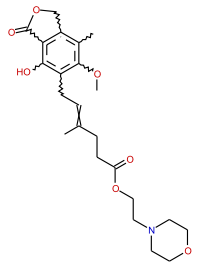
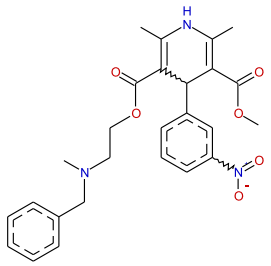
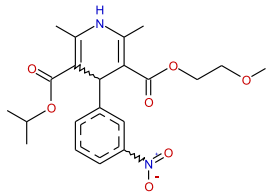
Bayesian Score: -0.692

Mahalanobis Distance: 16.3

Mahalanobis Distance p-value: 1.65e-011

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Mycophenolate	Nicardipine	Nimodipine
Structure			
Actual Endpoint	Non-Carcinogen	Carcinogen	Non-Carcinogen
Predicted Endpoint	Non-Carcinogen	Carcinogen	Non-Carcinogen
Distance	0.644	0.660	0.675
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

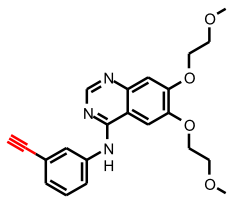
Model Applicability

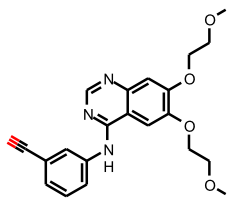
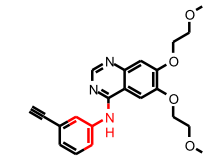
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. OPS PC28 out of range. Value: 3.6564. Training min, max, SD, explained variance: -2.8936, 3.5771, 1.028, 0.0111.
2. Unknown ECFP_2 feature: 1139738044: [*]:[c](:[*])C#C

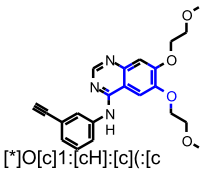
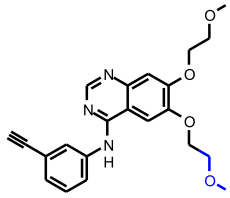
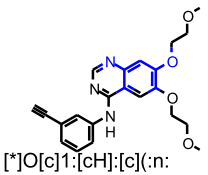
Feature Contribution

Top features for positive contribution

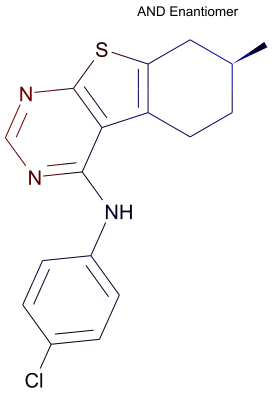
Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_12	-1545539812	 [*]C#C	0.78	8 out of 10

ECFP_12	-1939823063	 [*]#C	0.78	8 out of 10
ECFP_12	-177077903	 [*]N[c](:[cH]:[*]):[cH]:[*]	0.529	6 out of 10

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
ECFP_12	-2063600634	 [*]O[c]1:[cH]:[c](:[c]([*]):[*]):[c](:[*]):[*]:[c]:1[*]	-0.661	0 out of 3
ECFP_12	-1253653003	 [*]COC	-0.661	0 out of 3
ECFP_12	-2063202154	 [*]O[c]1:[cH]:[c](:n:[*]):[c](:[*]):[*]:[c]:1[*]	-0.661	0 out of 3

TOPKAT_Rat_Female_FDA_Single_vs_Multiple



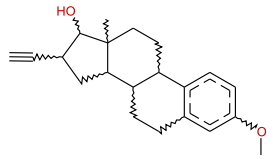
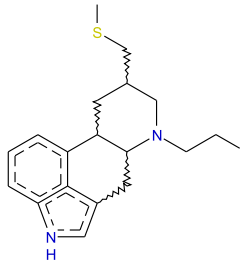
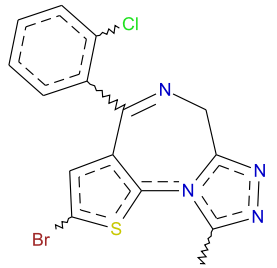
$C_{17}H_{16}ClN_3S$
Molecular Weight: 329.84704
ALogP: 5.5
Rotatable Bonds: 2
Acceptors: 3
Donors: 1

Model Prediction

Prediction: Single-Carcinogen
Probability: 0.441
Enrichment: 1.18
Bayesian Score: -2.22
Mahalanobis Distance: 10.5
Mahalanobis Distance p-value: 0.029

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Mestranol	Pergolide	Brotizolam
Structure			
Actual Endpoint	Single-Carcinogen	Single-Carcinogen	Multiple-Carcinogen
Predicted Endpoint	Single-Carcinogen	Single-Carcinogen	Multiple-Carcinogen
Distance	0.622	0.637	0.694
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

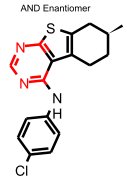
Model Applicability

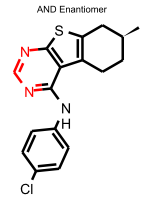
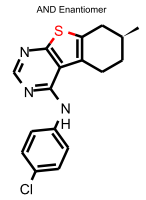
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

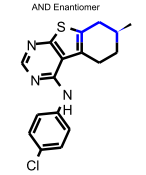
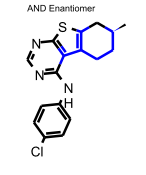
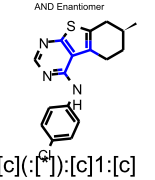
Feature Contribution

Top features for positive contribution

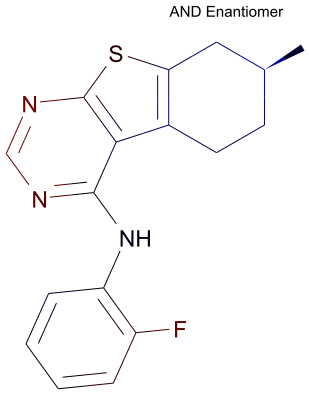
Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_4	-1065373877	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.721	3 out of 3

SCFP_4	-1181430618	 [*]:n:[cH]:n:[*]	0.663	4 out of 5
SCFP_4	17	 [*]:s:[*]	0.548	10 out of 17

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_4	-1272709286	 [*]C([*])C[c](:[*]):[*]	-1.16	1 out of 17
SCFP_4	-1849867720	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2CC1	-0.73	1 out of 10
SCFP_4	112346096	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.73	1 out of 10

TOPKAT_Rat_Female_FDA_Single_vs_Multiple



$C_{17}H_{16}FN_3S$

Molecular Weight: 313.39244

ALogP: 5.041

Rotatable Bonds: 2

Acceptors: 3

Donors: 1

Model Prediction

Prediction: Single-Carcinogen

Probability: 0.496

Enrichment: 1.33

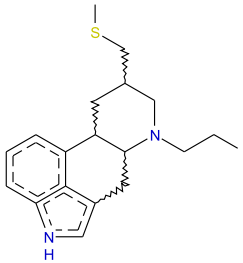
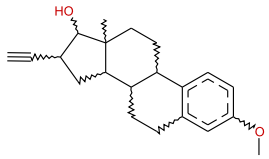
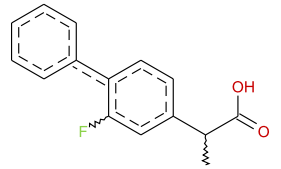
Bayesian Score: -0.556

Mahalanobis Distance: 11.8

Mahalanobis Distance p-value: 0.00242

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Pergolide	Mestranol	Flurbiprofen
Structure			
Actual Endpoint	Single-Carcinogen	Single-Carcinogen	Multiple-Carcinogen
Predicted Endpoint	Single-Carcinogen	Single-Carcinogen	Multiple-Carcinogen
Distance	0.612	0.621	0.647
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

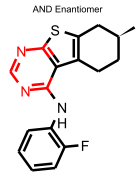
Model Applicability

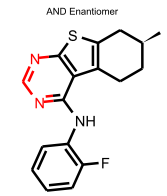
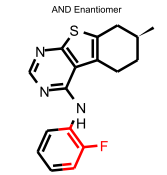
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

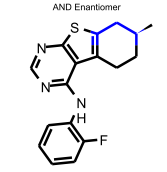
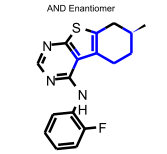
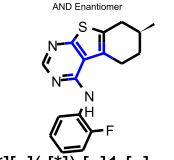
Feature Contribution

Top features for positive contribution

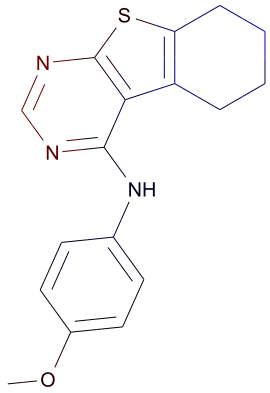
Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_4	-1065373877	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.721	3 out of 3

SCFP_4	-1181430618	 [*]:n:[cH]:n:[*]	0.663	4 out of 5
SCFP_4	-730654023	 [*][c](:[*]):[c](F):[cH]:[*]	0.571	3 out of 4

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_4	-1272709286	 [*]C([*])C[c](:[*]):[*]	-1.16	1 out of 17
SCFP_4	-1849867720	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2CC1	-0.73	1 out of 10
SCFP_4	112346096	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.73	1 out of 10

TOPKAT_Rat_Female_FDA_Single_vs_Multiple



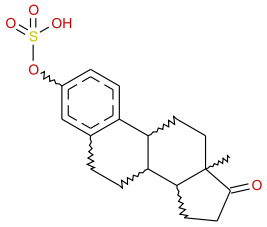
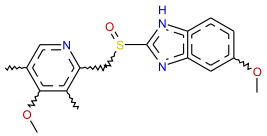
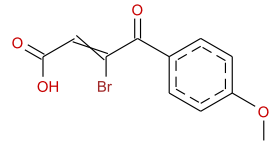
$C_{17}H_{17}N_3OS$
Molecular Weight: 311.40138
ALogP: 4.568
Rotatable Bonds: 3
Acceptors: 4
Donors: 1

Model Prediction

Prediction: Single-Carcinogen
Probability: 0.467
Enrichment: 1.25
Bayesian Score: -1.5
Mahalanobis Distance: 14.1
Mahalanobis Distance p-value: 2.16e-005

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Estrogens; conjug.	Omeprazole	Cytembena
Structure			
Actual Endpoint	Single-Carcinogen	Multiple-Carcinogen	Multiple-Carcinogen
Predicted Endpoint	Single-Carcinogen	Multiple-Carcinogen	Multiple-Carcinogen
Distance	0.598	0.622	0.636
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

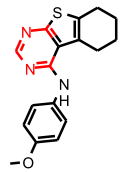
Model Applicability

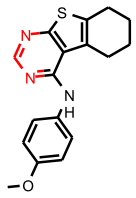
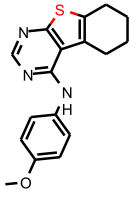
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

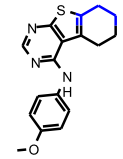
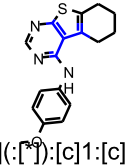
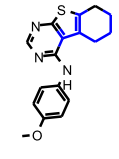
Feature Contribution

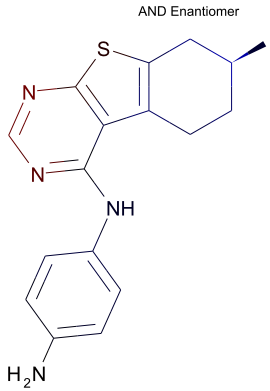
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_4	-1065373877	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.721	3 out of 3

SCFP_4	-1181430618	 [*]:n:[cH]:n:[*]	0.663	4 out of 5
SCFP_4	17	 [*]:s:[*]	0.548	10 out of 17

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_4	-1272709286	 [*]C([*])C[c](:[*]):[*]	-1.16	1 out of 17
SCFP_4	112346096	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.73	1 out of 10
SCFP_4	-1849867720	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2CC1	-0.73	1 out of 10



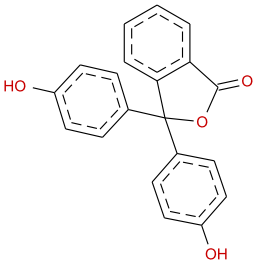
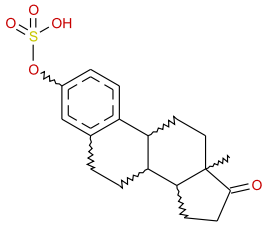
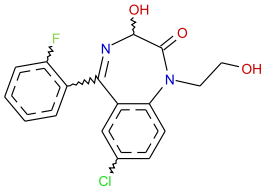
$C_{17}H_{18}N_4S$
Molecular Weight: 310.41662
ALogP: 4.089
Rotatable Bonds: 2
Acceptors: 4
Donors: 2

Model Prediction

Prediction: Single-Carcinogen
Probability: 0.436
Enrichment: 1.17
Bayesian Score: -2.32
Mahalanobis Distance: 10.7
Mahalanobis Distance p-value: 0.0214

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Phenolphthalein	Estrogens; conjug.	Doxefazepam
Structure			
Actual Endpoint	Single-Carcinogen	Single-Carcinogen	Multiple-Carcinogen
Predicted Endpoint	Single-Carcinogen	Single-Carcinogen	Multiple-Carcinogen
Distance	0.556	0.651	0.661
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

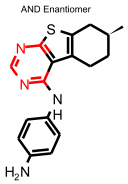
Model Applicability

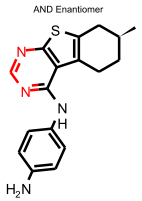
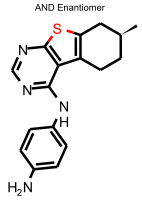
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

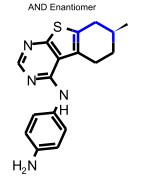
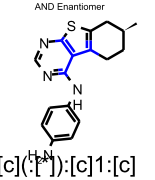
Feature Contribution

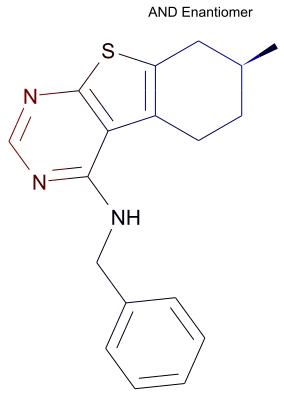
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_4	-1065373877	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.721	3 out of 3

SCFP_4	-1181430618	 [*]:n:[cH]:n:[*]	0.663	4 out of 5
SCFP_4	17	 [*]:s:[*]	0.548	10 out of 17

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_4	-1272709286	 [*]C([*])C[c](:[*]):[*]	-1.16	1 out of 17
SCFP_4	-1849867720	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2CC1	-0.73	1 out of 10
SCFP_4	112346096	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.73	1 out of 10



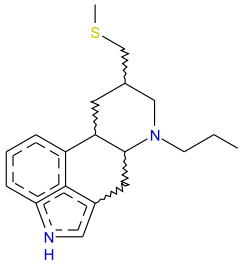
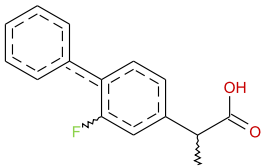
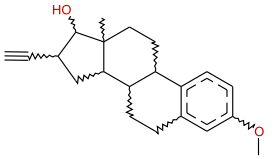
$C_{18}H_{19}N_3S$
Molecular Weight: 309.42856
ALogP: 4.678
Rotatable Bonds: 3
Acceptors: 3
Donors: 1

Model Prediction

Prediction: Single-Carcinogen
Probability: 0.45
Enrichment: 1.2
Bayesian Score: -1.97
Mahalanobis Distance: 8.82
Mahalanobis Distance p-value: 0.283

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Pergolide	Flurbiprofen	Mestranol
Structure			
Actual Endpoint	Single-Carcinogen	Multiple-Carcinogen	Single-Carcinogen
Predicted Endpoint	Single-Carcinogen	Multiple-Carcinogen	Single-Carcinogen
Distance	0.552	0.630	0.632
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

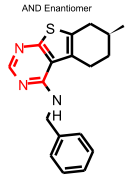
Model Applicability

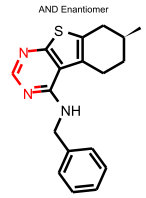
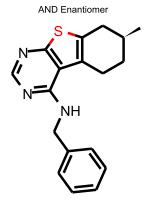
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

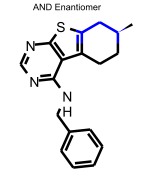
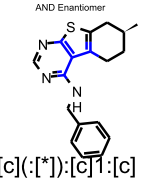
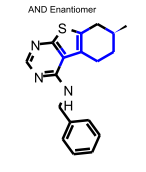
Feature Contribution

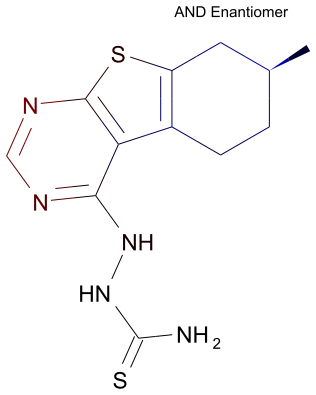
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_4	-1065373877	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.721	3 out of 3

SCFP_4	-1181430618	 [*]:n:[cH]:n:[*]	0.663	4 out of 5
SCFP_4	17	 [*]:s:[*]	0.548	10 out of 17

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_4	-1272709286	 [*]C([*])C[c](:[*]):[*]	-1.16	1 out of 17
SCFP_4	112346096	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.73	1 out of 10
SCFP_4	-1849867720	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2CC1	-0.73	1 out of 10



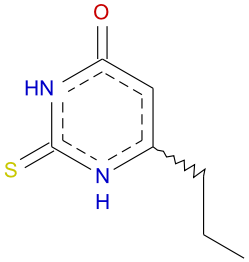
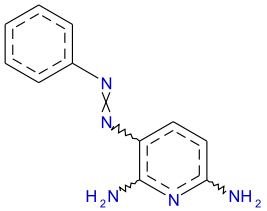
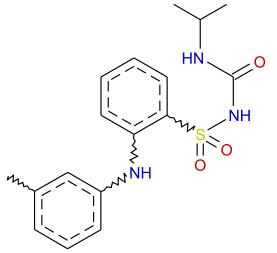
$C_{12}H_{15}N_5S_2$
Molecular Weight: 293.411
ALogP: 3.209
Rotatable Bonds: 3
Acceptors: 4
Donors: 3

Model Prediction

Prediction: Single-Carcinogen
Probability: 0.496
Enrichment: 1.33
Bayesian Score: -0.532
Mahalanobis Distance: 14.7
Mahalanobis Distance p-value: 5.9e-006

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Propylthiouracil	Phenazopyridine	Torsemide
Structure			
Actual Endpoint	Single-Carcinogen	Single-Carcinogen	Single-Carcinogen
Predicted Endpoint	Single-Carcinogen	Single-Carcinogen	Single-Carcinogen
Distance	0.718	0.731	0.748
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

Model Applicability

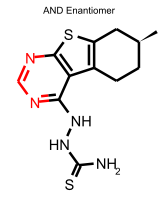
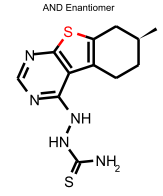
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

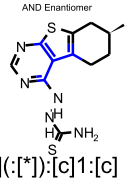
Feature Contribution

Top features for positive contribution

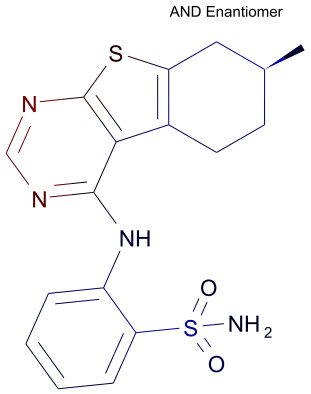
Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_4	-1065373877	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.721	3 out of 3

SCFP_4	-1181430618	 [*]:n:[cH]:n:[*]	0.663	4 out of 5
SCFP_4	17	 [*]:s:[*]	0.548	10 out of 17

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_4	-1272709286	 [*]C([*])C[c](:[*]):[*]	-1.16	1 out of 17
SCFP_4	112346096	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.73	1 out of 10
SCFP_4	-1849867720	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2CC1	-0.73	1 out of 10

TOPKAT_Rat_Female_FDA_Single_vs_Multiple



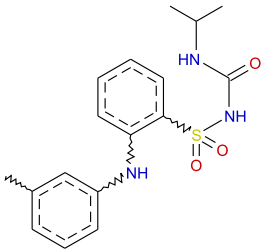
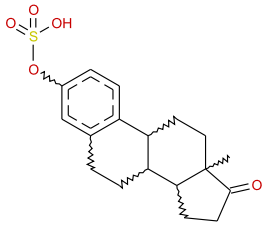
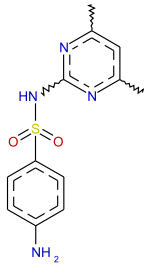
$C_{17}H_{18}N_4O_2S_2$
Molecular Weight: 374.48042
ALogP: 3.541
Rotatable Bonds: 3
Acceptors: 5
Donors: 2

Model Prediction

Prediction: Single-Carcinogen
Probability: 0.312
Enrichment: 0.834
Bayesian Score: -4.89
Mahalanobis Distance: 13
Mahalanobis Distance p-value: 0.000225

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Torsemide	Estrogens; conjug.	Sulfamethazine
Structure			
Actual Endpoint	Single-Carcinogen	Single-Carcinogen	Single-Carcinogen
Predicted Endpoint	Single-Carcinogen	Single-Carcinogen	Single-Carcinogen
Distance	0.631	0.646	0.668
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

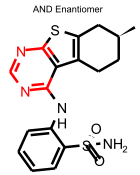
Model Applicability

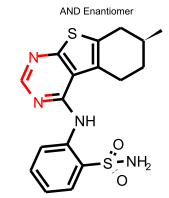
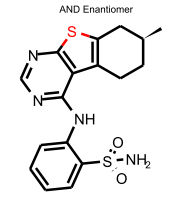
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

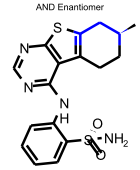
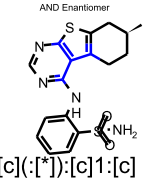
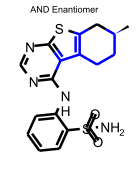
Feature Contribution

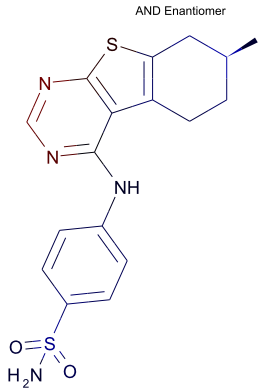
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_4	-1065373877	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.721	3 out of 3

SCFP_4	-1181430618	 [*]:n:[cH]:n:[*]	0.663	4 out of 5
SCFP_4	17	 [*]:s:[*]	0.548	10 out of 17

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_4	-1272709286	 [*]C([*])C[c](:[*]):[*]	-1.16	1 out of 17
SCFP_4	112346096	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.73	1 out of 10
SCFP_4	-1849867720	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2CC1	-0.73	1 out of 10



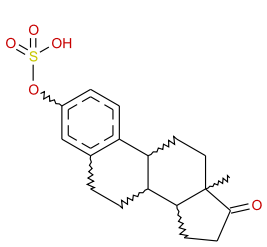
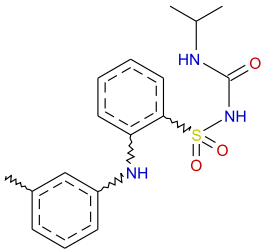
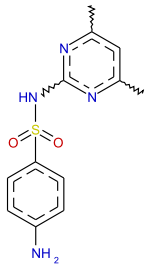
$C_{17}H_{18}N_4O_2S_2$
Molecular Weight: 374.48042
ALogP: 3.541
Rotatable Bonds: 3
Acceptors: 5
Donors: 2

Model Prediction

Prediction: Single-Carcinogen
Probability: 0.305
Enrichment: 0.816
Bayesian Score: -5.01
Mahalanobis Distance: 11.6
Mahalanobis Distance p-value: 0.00379

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Estrogens; conjug.	Torsemide	Sulfamethazine
Structure			
Actual Endpoint	Single-Carcinogen	Single-Carcinogen	Single-Carcinogen
Predicted Endpoint	Single-Carcinogen	Single-Carcinogen	Single-Carcinogen
Distance	0.644	0.649	0.655
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

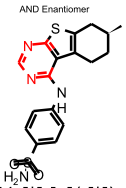
Model Applicability

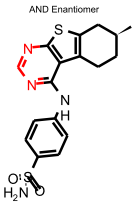
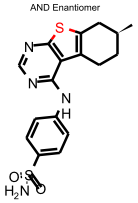
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

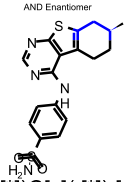
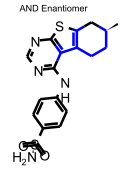
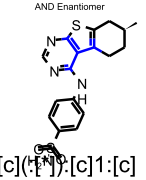
Feature Contribution

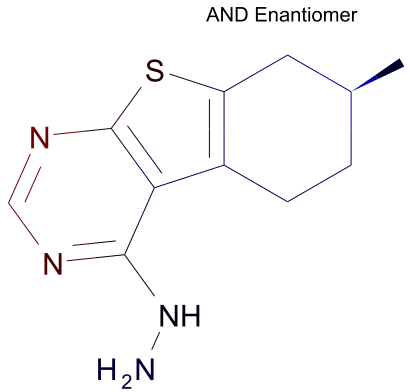
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_4	-1065373877	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.721	3 out of 3

SCFP_4	-1181430618	 [*]:n:[cH]:n:[*]	0.663	4 out of 5
SCFP_4	17	 [*]:s:[*]	0.548	10 out of 17

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_4	-1272709286	 [*]C([*])C[c](:[*]):[*]	-1.16	1 out of 17
SCFP_4	-1849867720	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2CC1	-0.73	1 out of 10
SCFP_4	112346096	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.73	1 out of 10



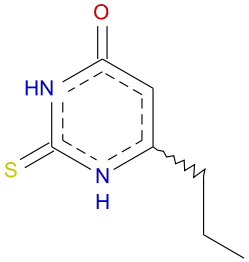
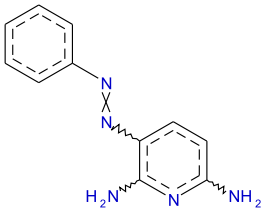
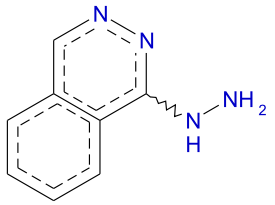
$C_{11}H_{14}N_4S$
Molecular Weight: 234.32065
ALogP: 2.561
Rotatable Bonds: 1
Acceptors: 4
Donors: 2

Model Prediction

Prediction: Single-Carcinogen
Probability: 0.427
Enrichment: 1.14
Bayesian Score: -2.54
Mahalanobis Distance: 13.4
Mahalanobis Distance p-value: 0.000104

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Propylthiouracil	Phenazopyridine	Hydralazine
Structure			
Actual Endpoint	Single-Carcinogen	Single-Carcinogen	Single-Carcinogen
Predicted Endpoint	Single-Carcinogen	Single-Carcinogen	Single-Carcinogen
Distance	0.560	0.570	0.595
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

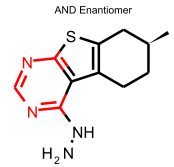
Model Applicability

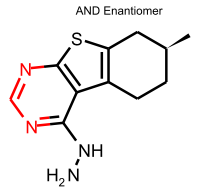
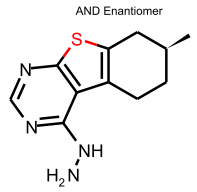
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

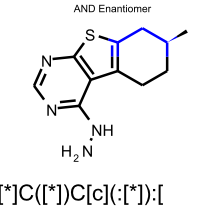
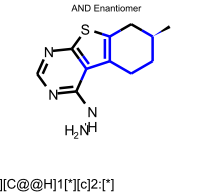
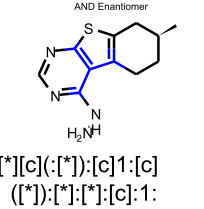
Feature Contribution

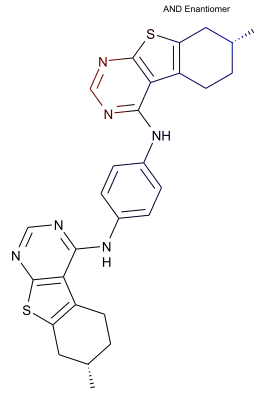
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_4	-1065373877	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.721	3 out of 3

SCFP_4	-1181430618	 [*]:n:[cH]:n:[*]	0.663	4 out of 5
SCFP_4	17	 [*]:s:[*]	0.548	10 out of 17

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_4	-1272709286	 [*]C([*])C[c](:[*]):[*]	-1.16	1 out of 17
SCFP_4	-1849867720	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2CC1	-0.73	1 out of 10
SCFP_4	112346096	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.73	1 out of 10



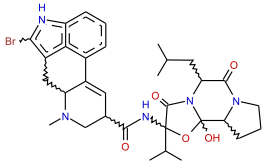
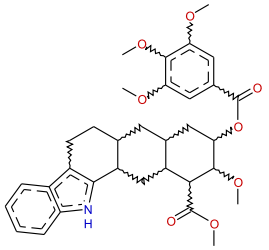
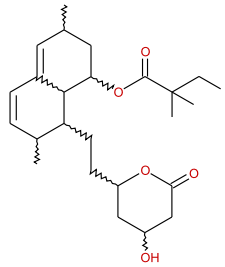
$C_{28}H_{28}N_6S_2$
Molecular Weight: 512.69212
ALogP: 7.842
Rotatable Bonds: 4
Acceptors: 6
Donors: 2

Model Prediction

Prediction: Single-Carcinogen
Probability: 0.387
Enrichment: 1.04
Bayesian Score: -3.43
Mahalanobis Distance: 11.9
Mahalanobis Distance p-value: 0.00213

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Bromocriptine	Deserpidine	Simvastatin
Structure			
Actual Endpoint	Single-Carcinogen	Single-Carcinogen	Multiple-Carcinogen
Predicted Endpoint	Single-Carcinogen	Single-Carcinogen	Multiple-Carcinogen
Distance	0.893	0.903	0.922
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

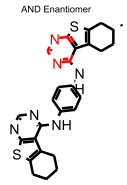
Model Applicability

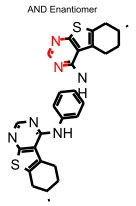
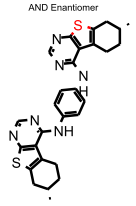
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

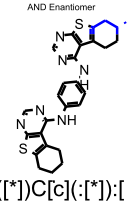
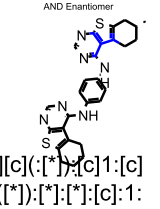
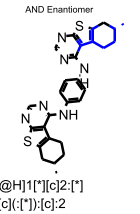
Feature Contribution

Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_4	-1065373877	 [*][c]1:[*]:[c](:[*]) :n:[cH]:n:1	0.721	3 out of 3

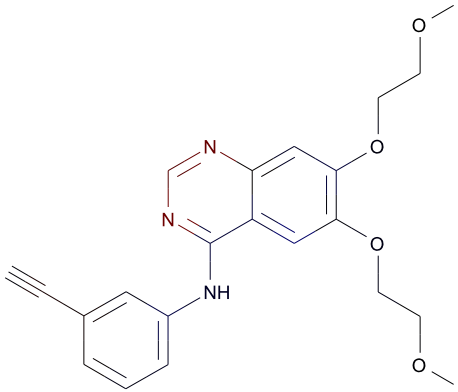
SCFP_4	-1181430618	 [*]:n:[cH]:n:[*]	0.663	4 out of 5
SCFP_4	17	 [*]:s:[*]	0.548	10 out of 17

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_4	-1272709286	 [*]C([*])C[c](:[*]):[*]	-1.16	1 out of 17
SCFP_4	112346096	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.73	1 out of 10
SCFP_4	-1849867720	 [*][C@@H]1[*][c]2:[*]:[*]:[c](:[*]):[c]:2CC1	-0.73	1 out of 10

Erlotinib

TOPKAT_Rat_Female_FDA_Single_vs_Multiple



$C_{22}H_{23}N_3O_4$

Molecular Weight: 393.43572

ALogP: 4.309

Rotatable Bonds: 10

Acceptors: 7

Donors: 1

Model Prediction

Prediction: Single-Carcinogen

Probability: 0.423

Enrichment: 1.13

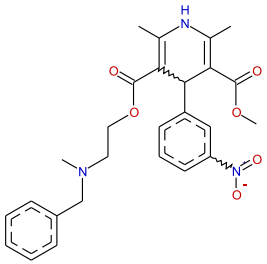
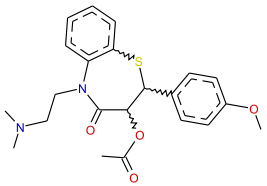
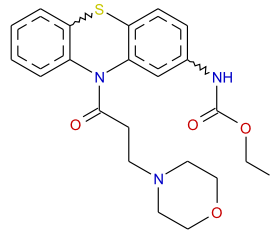
Bayesian Score: -2.63

Mahalanobis Distance: 15.2

Mahalanobis Distance p-value: 2.08e-006

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Nicardipine	Diltiazem	Moricizine
Structure			
Actual Endpoint	Single-Carcinogen	Multiple-Carcinogen	Single-Carcinogen
Predicted Endpoint	Single-Carcinogen	Multiple-Carcinogen	Single-Carcinogen
Distance	0.632	0.748	0.749
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

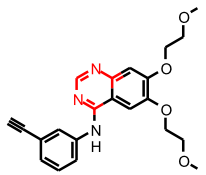
Model Applicability

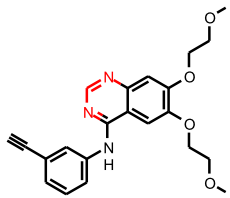
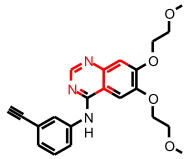
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

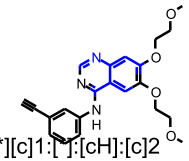
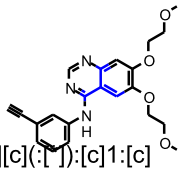
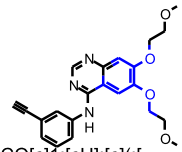
Feature Contribution

Top features for positive contribution

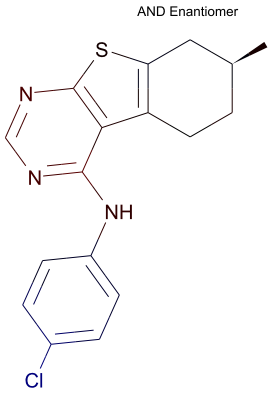
Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_4	-1065373877	 [*][c]1:[*]:[c](:[*]) :n:[cH]:n:1	0.721	3 out of 3

SCFP_4	-1181430618	 [*]:n:[cH]:n:[*]	0.663	4 out of 5
SCFP_4	2142015375	 [*]:[cH]:[c]1:n:[cH]: n:[*]:[c]:1:[*]	0.433	2 out of 3

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_4	622342378	 [*][c]1:[*]:[cH]:[c]2 :[c]([*]):[*]:[cH]:n :[c]:2:[cH]:1	-0.816	0 out of 4
SCFP_4	112346096	 [*][c](:[*]):[c]1:[c] ([*]):[*]:[*]:[c]:1: [*]	-0.73	1 out of 10
SCFP_4	1242547645	 [*]CO[c]1:[cH]:[c](:[*]):[*]:[cH]:[c]:1O[*]	-0.489	0 out of 2

TOPKAT_Rat_Male_FDA_None_vs_Carcinogen



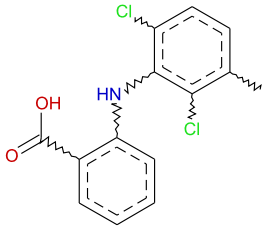
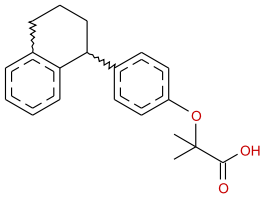
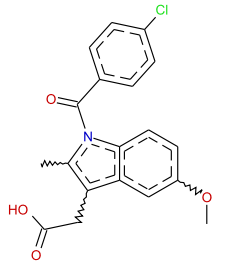
$C_{17}H_{16}ClN_3S$
Molecular Weight: 329.84704
ALogP: 5.5
Rotatable Bonds: 2
Acceptors: 3
Donors: 1

Model Prediction

Prediction: Carcinogen
Probability: 0.373
Enrichment: 1.11
Bayesian Score: 0.553
Mahalanobis Distance: 17.3
Mahalanobis Distance p-value: 5.48e-012

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Meclofenamate	Nafenopin	Indomethacin
Structure			
Actual Endpoint	Non-Carcinogen	Carcinogen	Non-Carcinogen
Predicted Endpoint	Non-Carcinogen	Carcinogen	Non-Carcinogen
Distance	0.614	0.623	0.641
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

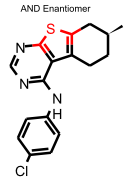
Model Applicability

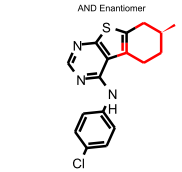
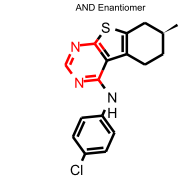
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

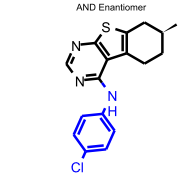
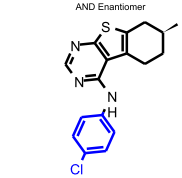
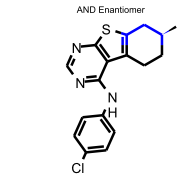
Feature Contribution

Top features for positive contribution

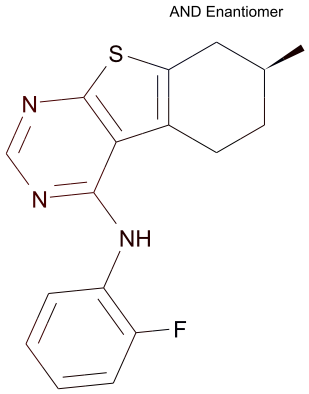
Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
SCFP_6	1310748454	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.437	7 out of 13

SCFP_6	-55982834	 [*]:[c]1:[*]C[C@@H](C)CC1	0.432	4 out of 7
SCFP_6	-1065373877	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.429	3 out of 5

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
SCFP_6	341480432	 [*]N[c]1:[cH]:[cH]:[c](Cl):[cH]:[cH]:1	-0.674	0 out of 3
SCFP_6	1905487031	 [*][c]1:[cH]:[cH]:[c](Cl):[cH]:[cH]:1	-0.48	2 out of 12
SCFP_6	-1272709286	 [*]C([*])C[c](:[*]):[*]	-0.459	12 out of 61

TOPKAT_Rat_Male_FDA_None_vs_Carcinogen



$C_{17}H_{16}FN_3S$

Molecular Weight: 313.39244

ALogP: 5.041

Rotatable Bonds: 2

Acceptors: 3

Donors: 1

Model Prediction

Prediction: Carcinogen

Probability: 0.463

Enrichment: 1.39

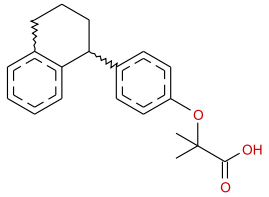
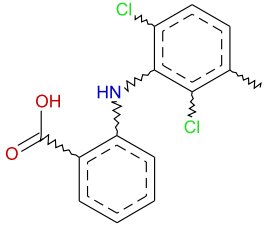
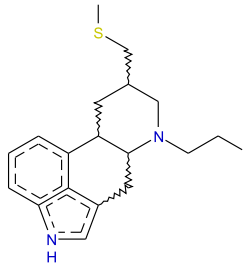
Bayesian Score: 3.32

Mahalanobis Distance: 17.6

Mahalanobis Distance p-value: 1.34e-012

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Nafenopin	Meclofenamate	Pergolide
Structure			
Actual Endpoint	Carcinogen	Non-Carcinogen	Non-Carcinogen
Predicted Endpoint	Carcinogen	Non-Carcinogen	Non-Carcinogen
Distance	0.610	0.612	0.643
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

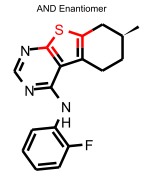
Model Applicability

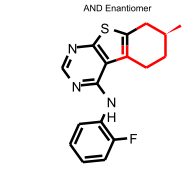
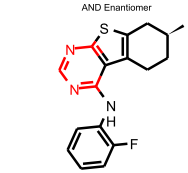
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

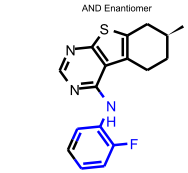
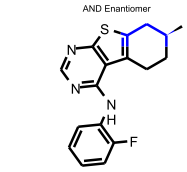
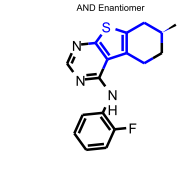
Feature Contribution

Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
SCFP_6	1310748454	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.437	7 out of 13

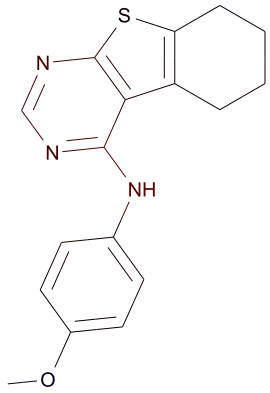
SCFP_6	-55982834	 [*:[c]1:[*]C[C@@H](C)CC1	0.432	4 out of 7
SCFP_6	-1065373877	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.429	3 out of 5

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
SCFP_6	-1551011249	 [*]N[c]1:[cH]:[*]:[cH]:[cH]:[c]:1F	-0.674	0 out of 3
SCFP_6	-1272709286	 [*]C([*])C[c](:[*]):[*]	-0.459	12 out of 61
SCFP_6	815479470	 [*][C@H]1[*]C[c]2:[c](C1):s:[c](:[*]):[c]:2:[*]	-0.278	0 out of 1

5c

TOPKAT_Rat_Male_FDA_None_vs_Carcinogen



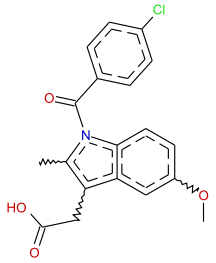
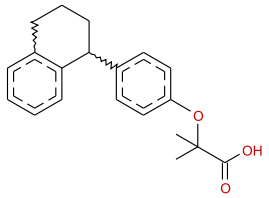
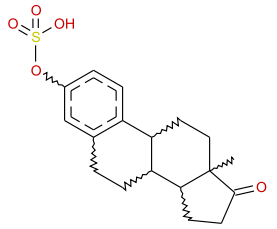
$C_{17}H_{17}N_3OS$
Molecular Weight: 311.40138
ALogP: 4.568
Rotatable Bonds: 3
Acceptors: 4
Donors: 1

Model Prediction

Prediction: Carcinogen
Probability: 0.454
Enrichment: 1.36
Bayesian Score: 3.05
Mahalanobis Distance: 17.5
Mahalanobis Distance p-value: 1.5e-012

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Indomethacin	Nafenopin	Estrogens; conjug.
Structure			
Actual Endpoint	Non-Carcinogen	Carcinogen	Non-Carcinogen
Predicted Endpoint	Non-Carcinogen	Carcinogen	Non-Carcinogen
Distance	0.561	0.600	0.618
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

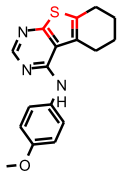
Model Applicability

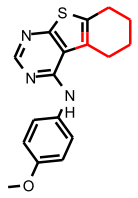
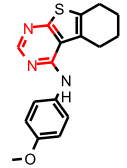
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

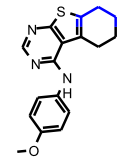
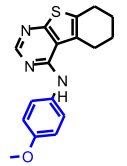
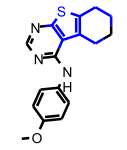
Feature Contribution

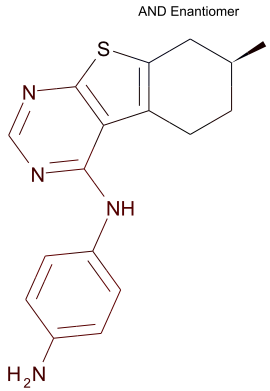
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
SCFP_6	1310748454	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.437	7 out of 13

SCFP_6	494226440	 [*]:[c]1:[*]CCCC1	0.432	4 out of 7
SCFP_6	-1065373877	 [*][c]1:[*]:[c](:[*]) :n:[cH]:n:1	0.429	3 out of 5

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
SCFP_6	-1272709286	 [*]C([*])C[c](:[*]):[*]	-0.459	12 out of 61
SCFP_6	1287669168	 [*][c]1:[cH]:[cH]:[c] (OC):[cH]:[cH]:1	-0.38	1 out of 6
SCFP_6	815479470	 [*][C@H]1[*]C[c]2:[c] (C1):s:[c](:[*]):[c] :2:[*]	-0.278	0 out of 1



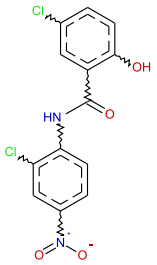
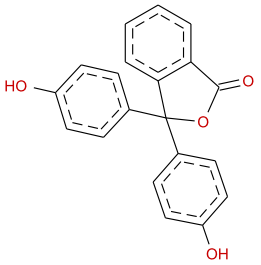
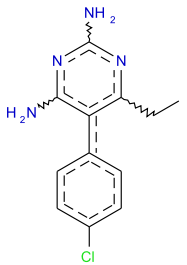
$C_{17}H_{18}N_4S$
Molecular Weight: 310.41662
ALogP: 4.089
Rotatable Bonds: 2
Acceptors: 4
Donors: 2

Model Prediction

Prediction: Carcinogen
Probability: 0.497
Enrichment: 1.49
Bayesian Score: 4.26
Mahalanobis Distance: 16
Mahalanobis Distance p-value: 4.48e-009

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Niclosamide	Phenolphthalein	Pyrimethamine
Structure			
Actual Endpoint	Non-Carcinogen	Carcinogen	Non-Carcinogen
Predicted Endpoint	Non-Carcinogen	Carcinogen	Non-Carcinogen
Distance	0.561	0.573	0.606
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

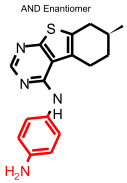
Model Applicability

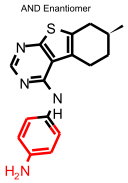
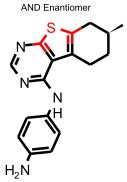
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

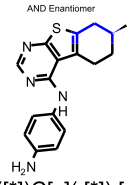
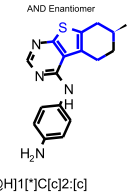
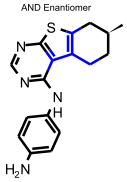
Feature Contribution

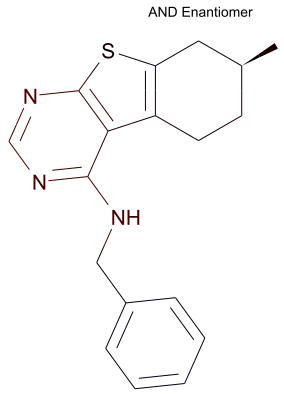
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
SCFP_6	1181470699	 [*][c]1:[cH]:[cH]:[c](N):[cH]:[cH]:1	0.536	4 out of 6

SCFP_6	-192131231	 N[c]1:[cH]:[cH]:[*]:[cH]:[cH]:1	0.52	5 out of 8
SCFP_6	1310748454	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.437	7 out of 13

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
SCFP_6	-1272709286	 [*]C([*])C[c](:[*]):[*]	-0.459	12 out of 61
SCFP_6	815479470	 [*][C@H]1[*]C[c]2:[c](C1):s:[c](:[*]):[c]:2:[*]	-0.278	0 out of 1
SCFP_6	2109165795	 [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.226	42 out of 165



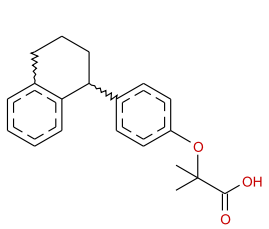
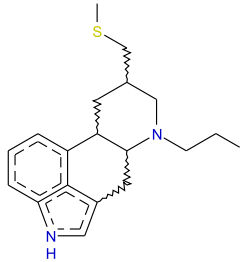
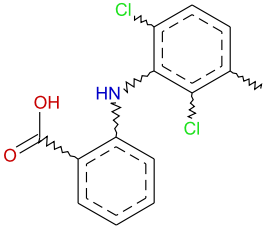
$C_{18}H_{19}N_3S$
Molecular Weight: 309.42856
ALogP: 4.678
Rotatable Bonds: 3
Acceptors: 3
Donors: 1

Model Prediction

Prediction: Carcinogen
Probability: 0.438
Enrichment: 1.31
Bayesian Score: 2.59
Mahalanobis Distance: 16.2
Mahalanobis Distance p-value: 2.02e-009

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Nafenopin	Pergolide	Meclofenamate
Structure			
Actual Endpoint	Carcinogen	Non-Carcinogen	Non-Carcinogen
Predicted Endpoint	Carcinogen	Non-Carcinogen	Non-Carcinogen
Distance	0.550	0.587	0.612
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

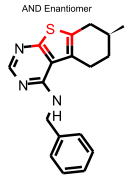
Model Applicability

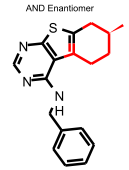
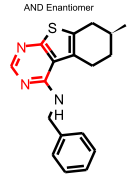
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

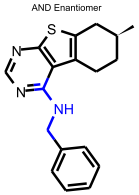
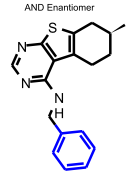
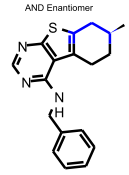
Feature Contribution

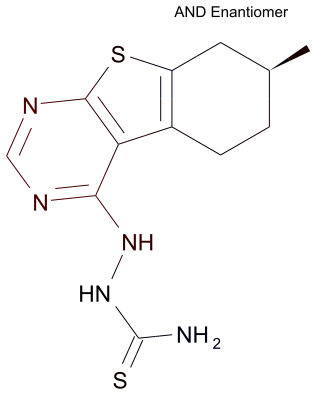
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
SCFP_6	1310748454	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.437	7 out of 13

SCFP_6	-55982834	 [*:[c]1:[*]C[C@@H](C)CC1	0.432	4 out of 7
SCFP_6	-1065373877	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.429	3 out of 5

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
SCFP_6	18117904	 [*]CN[c](:[*]):[*]	-0.578	1 out of 8
SCFP_6	1653911926	 [*][c]1:[cH]:[cH]:[cH]:[cH]:[cH]:1	-0.504	12 out of 64
SCFP_6	-1272709286	 [*]C([*])C[c](:[*]):[*]	-0.459	12 out of 61



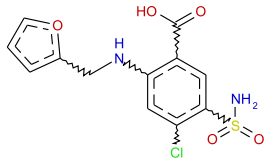
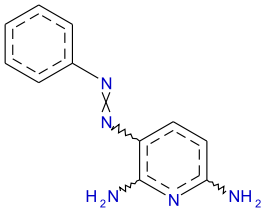
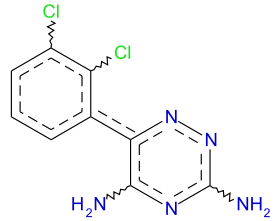
$C_{12}H_{15}N_5S_2$
Molecular Weight: 293.411
ALogP: 3.209
Rotatable Bonds: 3
Acceptors: 4
Donors: 3

Model Prediction

Prediction: Carcinogen
Probability: 0.427
Enrichment: 1.28
Bayesian Score: 2.28
Mahalanobis Distance: 16.8
Mahalanobis Distance p-value: 1.02e-010

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Furosemide	Phenazopyridine	Lamotrigine
Structure			
Actual Endpoint	Carcinogen	Carcinogen	Non-Carcinogen
Predicted Endpoint	Carcinogen	Carcinogen	Non-Carcinogen
Distance	0.722	0.722	0.729
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

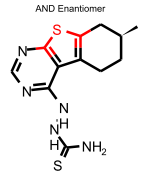
Model Applicability

Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

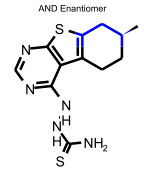
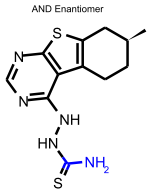
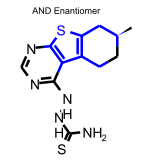
Feature Contribution

Top features for positive contribution

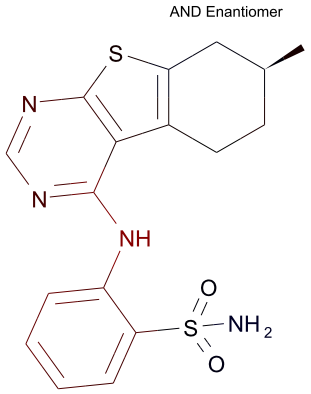
Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
SCFP_6	1310748454	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.437	7 out of 13

SCFP_6	-55982834	 [*:[c]1:[*]C[C@@H](C)CC1	0.432	4 out of 7
SCFP_6	-1065373877	 [*][c]1:[*]:[c](:[*]) :n:[cH]:n:1	0.429	3 out of 5

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
SCFP_6	-1272709286	 [*]C([*])C[c](:[*]):[*]	-0.459	12 out of 61
SCFP_6	384861283	 [*]C(=[*])N	-0.38	1 out of 6
SCFP_6	815479470	 [*][C@H]1[*]C[c]2:[c] (C1):s:[c](:[*]):[c] :2:[*]	-0.278	0 out of 1

TOPKAT_Rat_Male_FDA_None_vs_Carcinogen



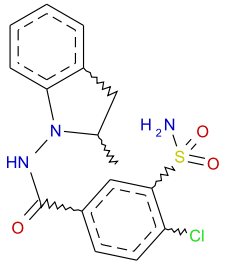
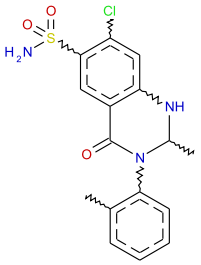
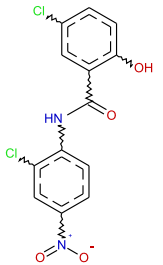
$C_{17}H_{18}N_4O_2S_2$
Molecular Weight: 374.48042
ALogP: 3.541
Rotatable Bonds: 3
Acceptors: 5
Donors: 2

Model Prediction

Prediction: Carcinogen
Probability: 0.434
Enrichment: 1.3
Bayesian Score: 2.49
Mahalanobis Distance: 17.6
Mahalanobis Distance p-value: 1.37e-012

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Indapamide	Metolazone	Niclosamide
Structure			
Actual Endpoint	Non-Carcinogen	Non-Carcinogen	Non-Carcinogen
Predicted Endpoint	Non-Carcinogen	Non-Carcinogen	Non-Carcinogen
Distance	0.572	0.612	0.613
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

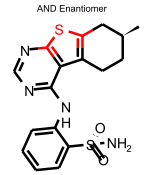
Model Applicability

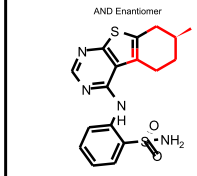
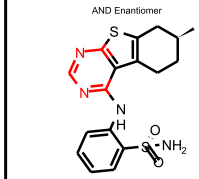
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

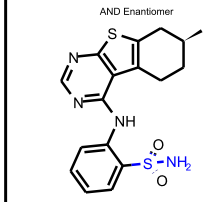
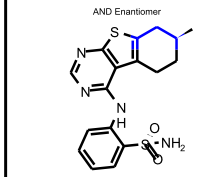
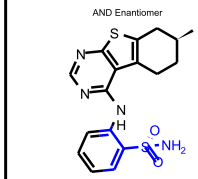
Feature Contribution

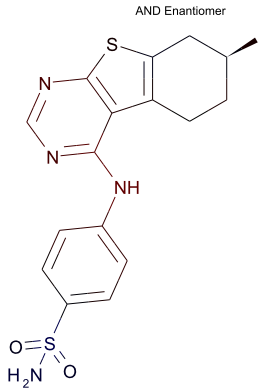
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
SCFP_6	1310748454	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.437	7 out of 13

SCFP_6	-55982834	 [*:[c]1:[*]C[C@@H](C)CC1	0.432	4 out of 7
SCFP_6	-1065373877	 [*][c]1:[*]:[c](:[*]) :n:[cH]:n:1	0.429	3 out of 5

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
SCFP_6	-1358544872	 [*]S(=[*])(=[*])N	-0.484	1 out of 7
SCFP_6	-1272709286	 [*]C([*])C[c](:[*]):[*]	-0.459	12 out of 61
SCFP_6	-1463646519	 [*][c](:[*]):[c](:[cH]:[*])S(=O)(=O)N	-0.38	1 out of 6



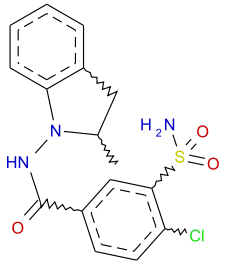
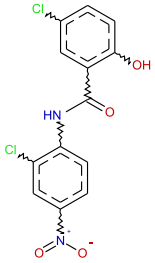
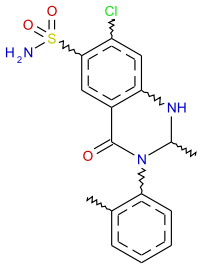
$C_{17}H_{18}N_4O_2S_2$
Molecular Weight: 374.48042
ALogP: 3.541
Rotatable Bonds: 3
Acceptors: 5
Donors: 2

Model Prediction

Prediction: Carcinogen
Probability: 0.397
Enrichment: 1.19
Bayesian Score: 1.36
Mahalanobis Distance: 17.4
Mahalanobis Distance p-value: 3.69e-012

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Indapamide	Niclosamide	Metolazone
Structure			
Actual Endpoint	Non-Carcinogen	Non-Carcinogen	Non-Carcinogen
Predicted Endpoint	Non-Carcinogen	Non-Carcinogen	Non-Carcinogen
Distance	0.581	0.612	0.616
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

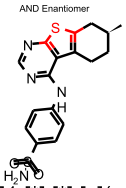
Model Applicability

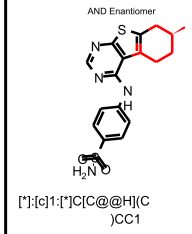
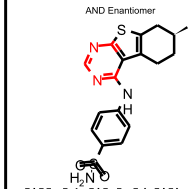
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

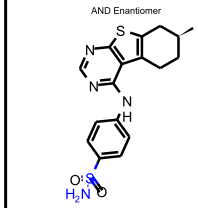
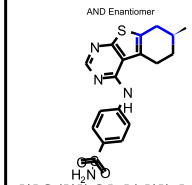
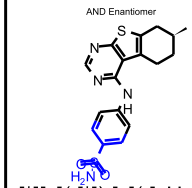
Feature Contribution

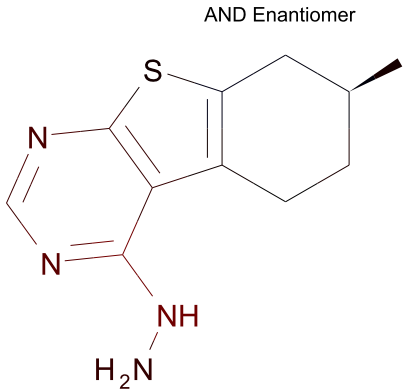
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
SCFP_6	1310748454	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.437	7 out of 13

SCFP_6	-55982834	 [*:[c]1:[*]C[C@@H](C)CC1	0.432	4 out of 7
SCFP_6	-1065373877	 [*][c]1:[*]:[c](:[*]) :n:[cH]:n:1	0.429	3 out of 5

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
SCFP_6	-1358544872	 [*]S(=[*])(=[*])N	-0.484	1 out of 7
SCFP_6	-1272709286	 [*]C([*])C[c](:[*]):[*]	-0.459	12 out of 61
SCFP_6	-1463646519	 [*][c](:[*]):[c](:[cH]:[*])S(=O)(=O)N	-0.38	1 out of 6



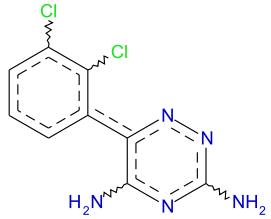
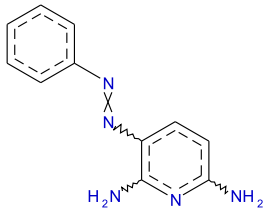
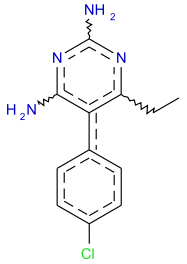
$C_{11}H_{14}N_4S$
Molecular Weight: 234.32065
ALogP: 2.561
Rotatable Bonds: 1
Acceptors: 4
Donors: 2

Model Prediction

Prediction: Carcinogen
Probability: 0.485
Enrichment: 1.45
Bayesian Score: 3.95
Mahalanobis Distance: 18
Mahalanobis Distance p-value: 1.27e-013

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Lamotrigine	Phenazopyridine	Pyrimethamine
Structure			
Actual Endpoint	Non-Carcinogen	Carcinogen	Non-Carcinogen
Predicted Endpoint	Non-Carcinogen	Carcinogen	Non-Carcinogen
Distance	0.566	0.578	0.585
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

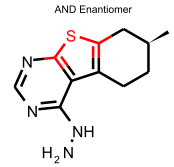
Model Applicability

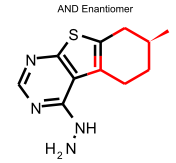
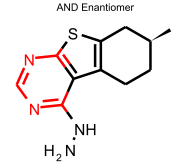
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

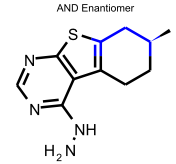
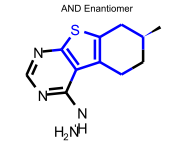
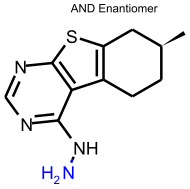
Feature Contribution

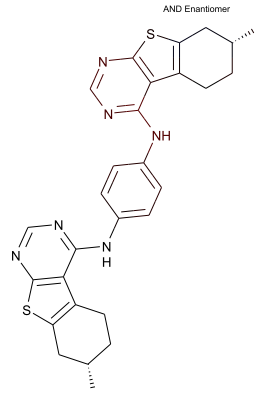
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
SCFP_6	1310748454	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.437	7 out of 13

SCFP_6	-55982834	 [*]:[c]1:[*]C[C@@H](C)CC1	0.432	4 out of 7
SCFP_6	-1065373877	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.429	3 out of 5

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
SCFP_6	-1272709286	 [*]C([*])C[c](:[*]):[*]	-0.459	12 out of 61
SCFP_6	815479470	 [*][C@H]1[*]C[c]2:[c](C1):s:[c](:[*]):[c]:2:[*]	-0.278	0 out of 1
SCFP_6	5	 [*]N	-0.232	41 out of 162



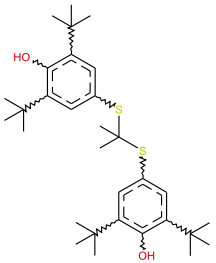
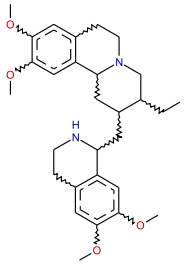
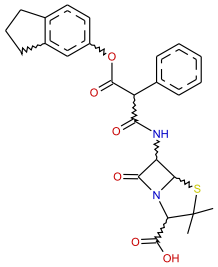
$C_{28}H_{28}N_6S_2$
Molecular Weight: 512.69212
ALogP: 7.842
Rotatable Bonds: 4
Acceptors: 6
Donors: 2

Model Prediction

Prediction: Carcinogen
Probability: 0.418
Enrichment: 1.25
Bayesian Score: 1.99
Mahalanobis Distance: 17.3
Mahalanobis Distance p-value: 5.38e-012

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Probucol	Emetine	Carbenicillin
Structure			
Actual Endpoint	Non-Carcinogen	Non-Carcinogen	Non-Carcinogen
Predicted Endpoint	Non-Carcinogen	Non-Carcinogen	Non-Carcinogen
Distance	0.846	0.878	0.909
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

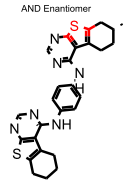
Model Applicability

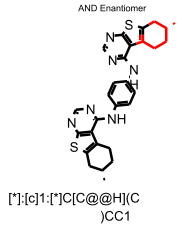
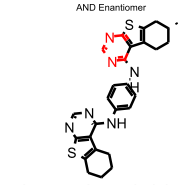
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

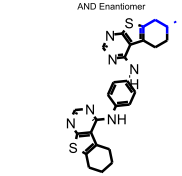
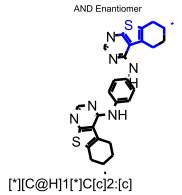
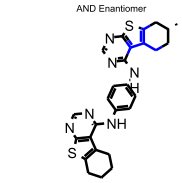
Feature Contribution

Top features for positive contribution

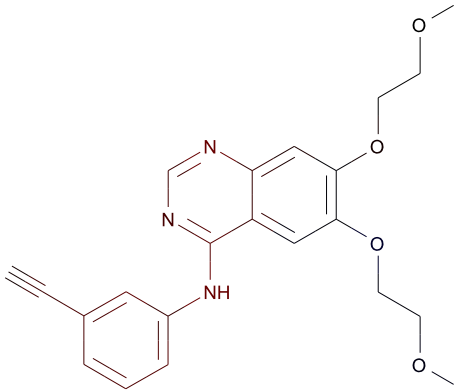
Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
SCFP_6	1310748454	 [*][c]1:[*]:[*]:[c](:[*]):s:1	0.437	7 out of 13

SCFP_6	-55982834	 [*:[c]1:[*]C[C@@H](C)CC1	0.432	4 out of 7
SCFP_6	-1065373877	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.429	3 out of 5

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
SCFP_6	-1272709286	 [*]C([*])C[c](:[*]):[*]	-0.459	12 out of 61
SCFP_6	815479470	 [*][C@H]1[*]C[c]2:[c](C1):s:[c](:[*]):[c]:2:[*]	-0.278	0 out of 1
SCFP_6	2109165795	 [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.226	42 out of 165

Erlotinib



$C_{22}H_{23}N_3O_4$

Molecular Weight: 393.43572

ALogP: 4.309

Rotatable Bonds: 10

Acceptors: 7

Donors: 1

Model Prediction

Prediction: Carcinogen

Probability: 0.52

Enrichment: 1.56

Bayesian Score: 4.91

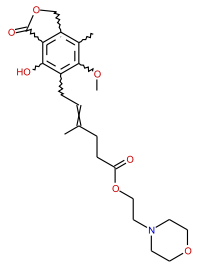
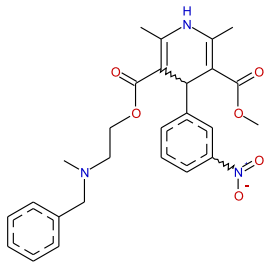
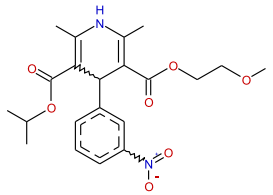
Mahalanobis Distance: 17.4

Mahalanobis Distance p-value: 2.91e-012

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

TOPKAT_Rat_Male_FDA_None_vs_Carcinogen

Structural Similar Compounds

Name	Mycophenolate	Nicardipine	Nimodipine
Structure			
Actual Endpoint	Non-Carcinogen	Carcinogen	Carcinogen
Predicted Endpoint	Non-Carcinogen	Carcinogen	Carcinogen
Distance	0.624	0.667	0.676
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

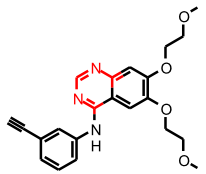
Model Applicability

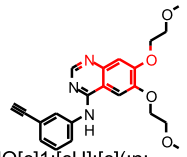
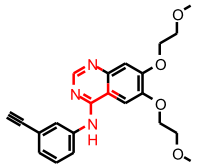
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

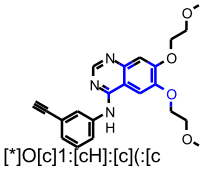
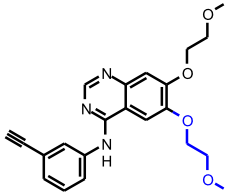
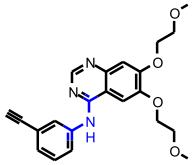
Feature Contribution

Top features for positive contribution

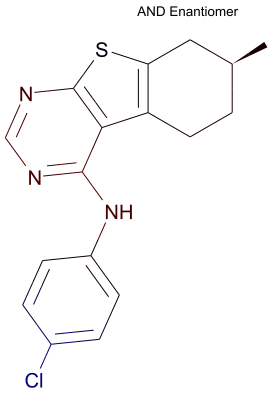
Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
SCFP_6	-1065373877	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.429	3 out of 5

SCFP_6	123285475	 [*]O[c]1:[cH]:[c](:n:[*]):[c](:[*]):[*]:[c]:1[*]	0.429	3 out of 5
SCFP_6	-2147171373	 [*]N[c]1:n:[cH]:n:[*]:[c]:1:[*]	0.415	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Carcinogen in training set
SCFP_6	125474664	 [*]O[c]1:[cH]:[c](:[c]([*]):[*]):[c](:[*]):[*]:[c]:1[*]	-0.484	1 out of 7
SCFP_6	-417738003	 [*]OCCOC	-0.264	1 out of 5
SCFP_6	951581613	 [*]:[c](:[*])N[c](:[*]):[*]	-0.132	1 out of 4

TOPKAT_Rat_Male_FDA_Single_vs_Multiple



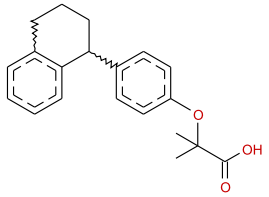
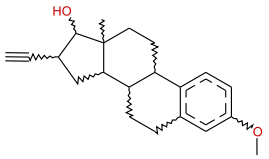
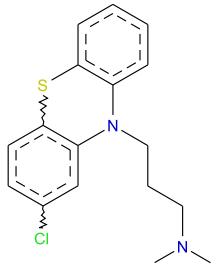
$C_{17}H_{16}ClN_3S$
Molecular Weight: 329.84704
ALogP: 5.5
Rotatable Bonds: 2
Acceptors: 3
Donors: 1

Model Prediction

Prediction: Single-Carcinogen
Probability: 0.562
Enrichment: 1.36
Bayesian Score: -0.202
Mahalanobis Distance: 24.2
Mahalanobis Distance p-value: 7.52e-014

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Nafenopin	Mestranol	Chlorpromazine
Structure			
Actual Endpoint	Multiple-Carcinogen	Single-Carcinogen	Single-Carcinogen
Predicted Endpoint	Multiple-Carcinogen	Multiple-Carcinogen	Single-Carcinogen
Distance	0.637	0.656	0.720
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

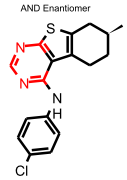
Model Applicability

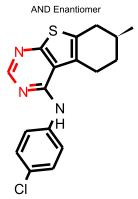
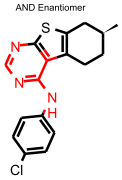
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

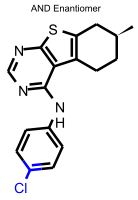
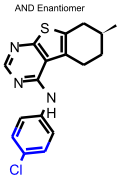
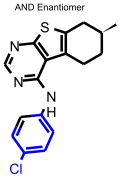
Feature Contribution

Top features for positive contribution

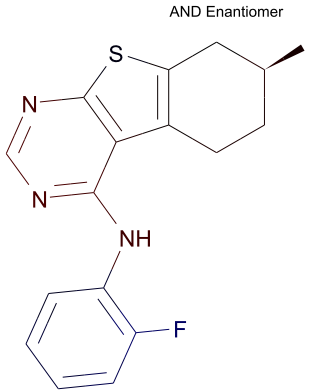
Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_8	-1065373877	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.649	3 out of 3

SCFP_8	-1181430618	 [*]:n:[cH]:n:[*]	0.453	4 out of 6
SCFP_8	-2147171373	 [*]N[c]1:n:[cH]:n:[*] :[c]:1:[*]	0.383	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_8	-52074512	 [*]:[c](:[*])Cl	-0.707	2 out of 14
SCFP_8	-601571304	 [*]:[cH]:[c](Cl):[cH] :[*]	-0.707	2 out of 14
SCFP_8	-1378360678	 [*][c]1:[*]:[cH]:[c](Cl):[cH]:[cH]:1	-0.58	2 out of 12

TOPKAT_Rat_Male_FDA_Single_vs_Multiple



$C_{17}H_{16}FN_3S$

Molecular Weight: 313.39244

ALogP: 5.041

Rotatable Bonds: 2

Acceptors: 3

Donors: 1

Model Prediction

Prediction: Single-Carcinogen

Probability: 0.566

Enrichment: 1.37

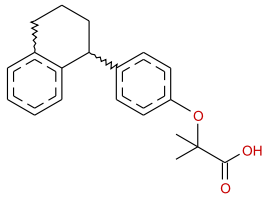
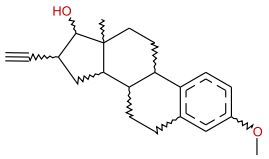
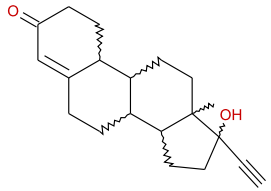
Bayesian Score: 0.263

Mahalanobis Distance: 23.6

Mahalanobis Distance p-value: 2.79e-013

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Nafenopin	Mestranol	Norethindrone
Structure			
Actual Endpoint	Multiple-Carcinogen	Single-Carcinogen	Multiple-Carcinogen
Predicted Endpoint	Multiple-Carcinogen	Multiple-Carcinogen	Multiple-Carcinogen
Distance	0.622	0.653	0.698
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

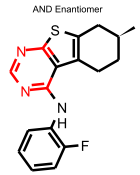
Model Applicability

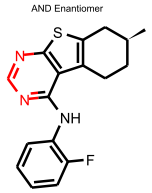
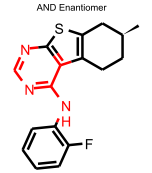
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

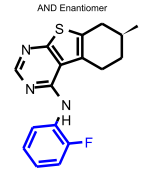
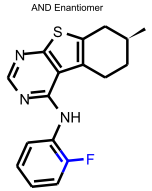
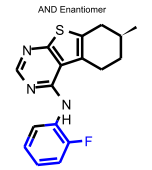
Feature Contribution

Top features for positive contribution

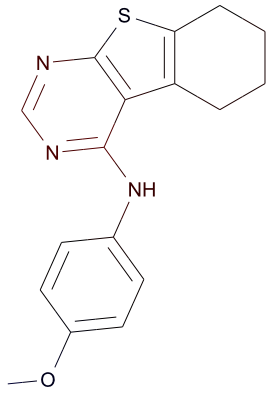
Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_8	-1065373877	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.649	3 out of 3

SCFP_8	-1181430618	 [*]:n:[cH]:n:[*]	0.453	4 out of 6
SCFP_8	-2147171373	 [*]N[c]1:n:[cH]:n:[*]:[c]:1:[*]	0.383	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_8	1655894345	 [*][c]1:[cH]:[cH]:[cH]:[cH]:[c]:1F	-0.546	0 out of 2
SCFP_8	-1794884847	 [*]:[c](:[*])F	-0.463	1 out of 6
SCFP_8	-1381307546	 [*][c]1:[*]:[cH]:[cH]:[cH]:[c]:1F	-0.463	1 out of 6

TOPKAT_Rat_Male_FDA_Single_vs_Multiple



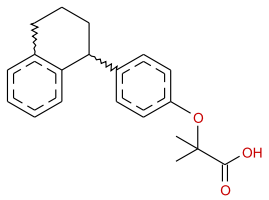
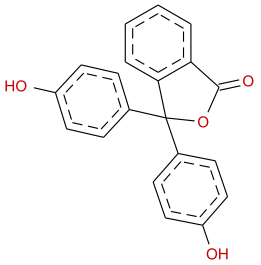
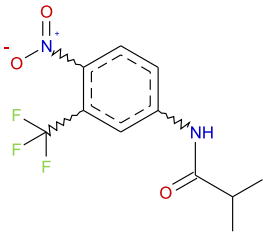
$C_{17}H_{17}N_3OS$
Molecular Weight: 311.40138
ALogP: 4.568
Rotatable Bonds: 3
Acceptors: 4
Donors: 1

Model Prediction

Prediction: Multiple-Carcinogen
Probability: 0.569
Enrichment: 1.37
Bayesian Score: 1.66
Mahalanobis Distance: 22.3
Mahalanobis Distance p-value: 3.23e-012

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Nafenopin	Phenolphthalein	Flutamide
Structure			
Actual Endpoint	Multiple-Carcinogen	Multiple-Carcinogen	Multiple-Carcinogen
Predicted Endpoint	Multiple-Carcinogen	Multiple-Carcinogen	Multiple-Carcinogen
Distance	0.613	0.671	0.683
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

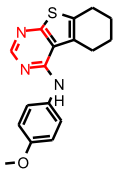
Model Applicability

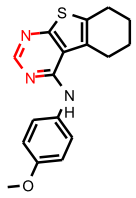
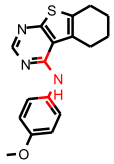
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

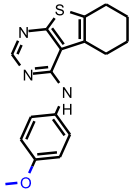
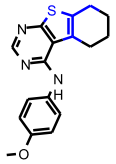
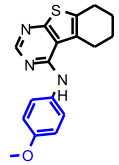
Feature Contribution

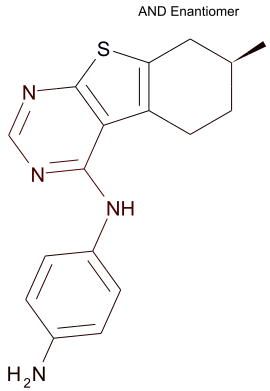
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_8	-1065373877	 [*][c]1:[*]:[c](:[*]) :n:[cH]:n:1	0.649	3 out of 3

SCFP_8	-1181430618	 [*]:n:[cH]:n:[*]	0.453	4 out of 6
SCFP_8	951581613	 [*]:[c](:[*])N[c](:[*]):[*]	0.383	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_8	136239834	 [*]OC	-0.358	3 out of 13
SCFP_8	803350837	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	-0.31	0 out of 1
SCFP_8	1287669168	 [*][c]1:[cH]:[cH]:[c](OC):[cH]:[cH]:1	-0.31	0 out of 1



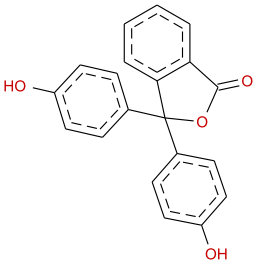
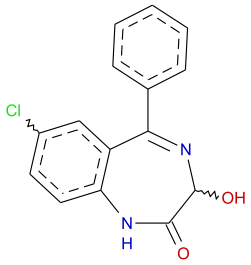
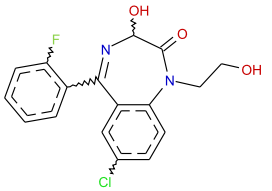
$C_{17}H_{18}N_4S$
Molecular Weight: 310.41662
ALogP: 4.089
Rotatable Bonds: 2
Acceptors: 4
Donors: 2

Model Prediction

Prediction: Multiple-Carcinogen
Probability: 0.558
Enrichment: 1.35
Bayesian Score: 3.3
Mahalanobis Distance: 22.1
Mahalanobis Distance p-value: 4.4e-012

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Phenolphthalein	Oxazepam	Doxefazepam
Structure			
Actual Endpoint	Multiple-Carcinogen	Single-Carcinogen	Single-Carcinogen
Predicted Endpoint	Multiple-Carcinogen	Single-Carcinogen	Single-Carcinogen
Distance	0.572	0.683	0.684
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

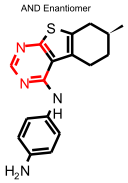
Model Applicability

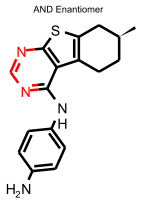
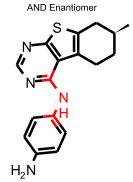
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

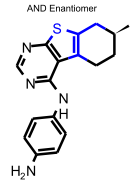
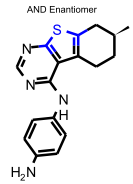
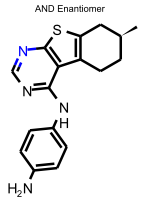
Feature Contribution

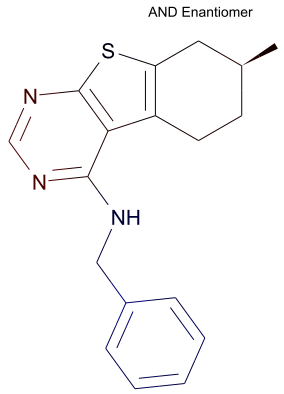
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_8	-1065373877	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.649	3 out of 3

SCFP_8	-1181430618	 [*]:n:[cH]:n:[*]	0.453	4 out of 6
SCFP_8	951581613	 [*]:[c](:[*])N[c](:[*]):[*]	0.383	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_8	803350837	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	-0.31	0 out of 1
SCFP_8	1310748454	 [*][c]1:[*]:[*]:[c](:[*]):s:1	-0.166	2 out of 7
SCFP_8	8	 [*]:n:[*]	-0.154	12 out of 39



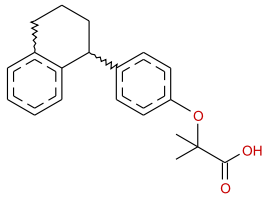
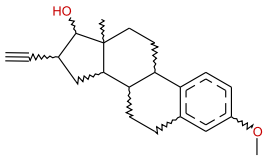
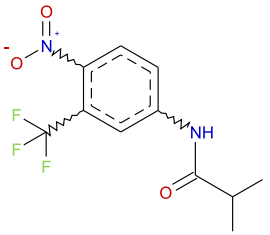
$C_{18}H_{19}N_3S$
Molecular Weight: 309.42856
ALogP: 4.678
Rotatable Bonds: 3
Acceptors: 3
Donors: 1

Model Prediction

Prediction: Single-Carcinogen
Probability: 0.554
Enrichment: 1.34
Bayesian Score: -0.906
Mahalanobis Distance: 19.9
Mahalanobis Distance p-value: 3.76e-010

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Nafenopin	Mestranol	Flutamide
Structure			
Actual Endpoint	Multiple-Carcinogen	Single-Carcinogen	Multiple-Carcinogen
Predicted Endpoint	Multiple-Carcinogen	Multiple-Carcinogen	Multiple-Carcinogen
Distance	0.560	0.677	0.685
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

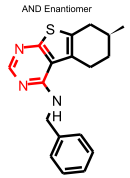
Model Applicability

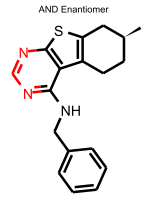
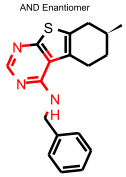
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. OPS PC20 out of range. Value: 3.0614. Training min, max, SD, explained variance: -2.6601, 2.9766, 1.03, 0.0144.

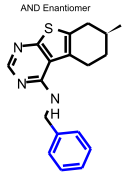
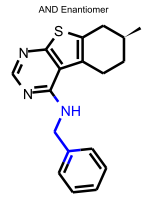
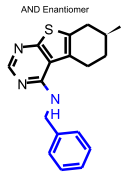
Feature Contribution

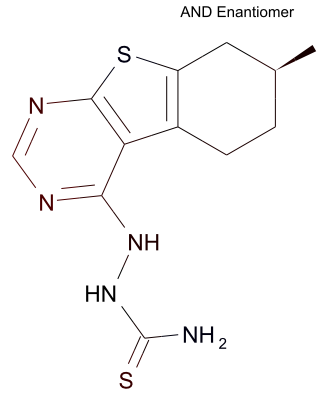
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_8	-1065373877	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.649	3 out of 3

SCFP_8	-1181430618	 [*]:n:[cH]:n:[*]	0.453	4 out of 6
SCFP_8	-2147171373	 [*]N[c]1:n:[cH]:n:[*] :[c]:1:[*]	0.383	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_8	1653911926	 [*][c]1:[cH]:[cH]:[cH]:[cH]:[cH]:1	-0.985	1 out of 12
SCFP_8	1155330592	 [*]NC[c](:[*]):[*]	-0.737	0 out of 3
SCFP_8	1271460694	 [*]NC[c]1:[cH]:[cH]:[cH]:[cH]:[cH]:1	-0.31	0 out of 1



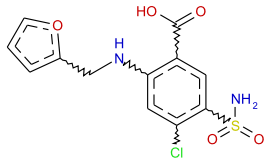
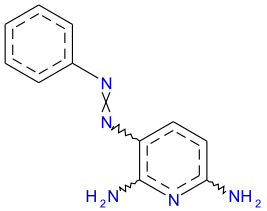
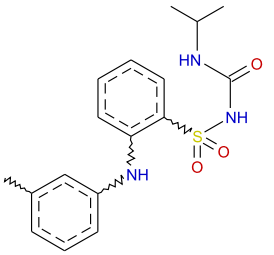
$C_{12}H_{15}N_5S_2$
Molecular Weight: 293.411
ALogP: 3.209
Rotatable Bonds: 3
Acceptors: 4
Donors: 3

Model Prediction

Prediction: Multiple-Carcinogen
Probability: 0.559
Enrichment: 1.35
Bayesian Score: 3.26
Mahalanobis Distance: 23.3
Mahalanobis Distance p-value: 4.48e-013

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Furosemide	Phenazopyridine	Torsemide
Structure			
Actual Endpoint	Single-Carcinogen	Single-Carcinogen	Multiple-Carcinogen
Predicted Endpoint	Single-Carcinogen	Single-Carcinogen	Multiple-Carcinogen
Distance	0.742	0.758	0.774
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

Model Applicability

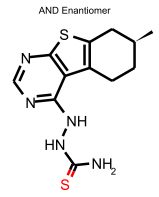
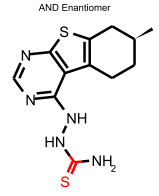
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. OPS PC20 out of range. Value: 3.0652. Training min, max, SD, explained variance: -2.6601, 2.9766, 1.03, 0.0144.

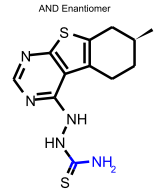
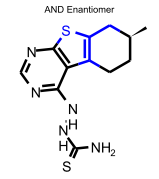
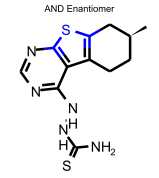
Feature Contribution

Top features for positive contribution

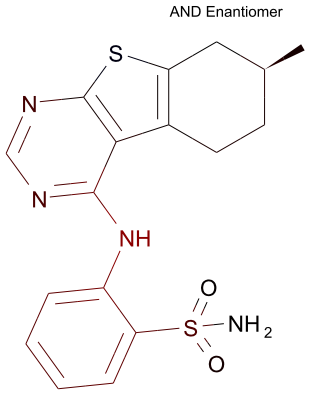
Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_8	-1065373877	 [*][c]1:[*]:[c](:[*]) :n:[cH]:n:1	0.649	3 out of 3

SCFP_8	18	 [*]=S	0.553	2 out of 2
SCFP_8	1435188938	 [*]C(=S)[*]	0.553	2 out of 2

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_8	384861283	 [*]C(=[*])N	-0.31	0 out of 1
SCFP_8	803350837	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	-0.31	0 out of 1
SCFP_8	1310748454	 [*][c]1:[*]:[*]:[c](:[*]):s:1	-0.166	2 out of 7

TOPKAT_Rat_Male_FDA_Single_vs_Multiple



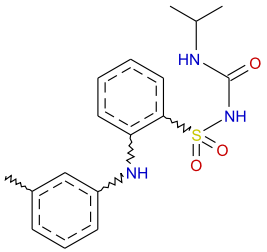
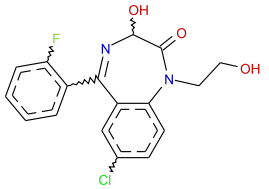
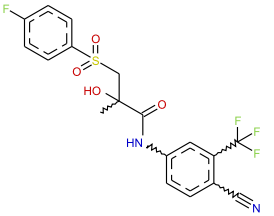
$C_{17}H_{18}N_4O_2S_2$
Molecular Weight: 374.48042
ALogP: 3.541
Rotatable Bonds: 3
Acceptors: 5
Donors: 2

Model Prediction

Prediction: Multiple-Carcinogen
Probability: 0.558
Enrichment: 1.35
Bayesian Score: 3.32
Mahalanobis Distance: 24.5
Mahalanobis Distance p-value: 5.12e-014

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Torsemide	Doxefazepam	Bicalutamide
Structure			
Actual Endpoint	Multiple-Carcinogen	Single-Carcinogen	Multiple-Carcinogen
Predicted Endpoint	Multiple-Carcinogen	Single-Carcinogen	Multiple-Carcinogen
Distance	0.684	0.719	0.722
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

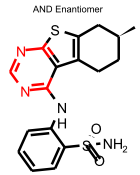
Model Applicability

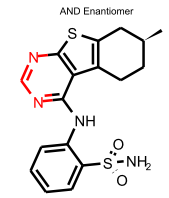
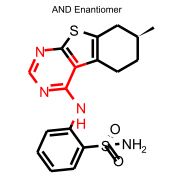
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

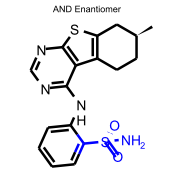
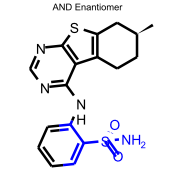
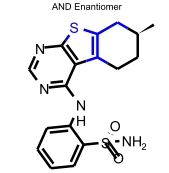
Feature Contribution

Top features for positive contribution

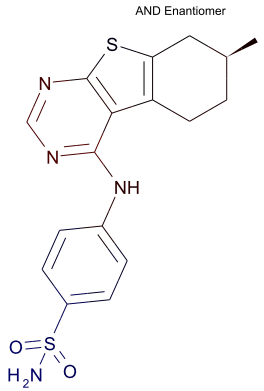
Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_8	-1065373877	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.649	3 out of 3

SCFP_8	-1181430618	 [*]:n:[cH]:n:[*]	0.453	4 out of 6
SCFP_8	-2147171373	 [*]N[c]1:n:[cH]:n:[*]:[c]:1:[*]	0.383	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_8	182991870	 [*]:[c](:[*])S(=O)(=O)N	-0.342	1 out of 5
SCFP_8	-1463646519	 [*][c](:[*]):[c](:[cH]:[*])S(=O)(=O)N	-0.31	0 out of 1
SCFP_8	803350837	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	-0.31	0 out of 1

TOPKAT_Rat_Male_FDA_Single_vs_Multiple



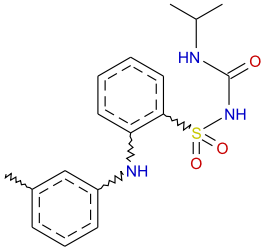
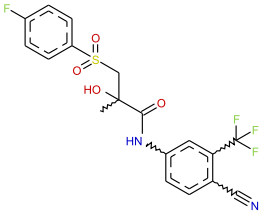
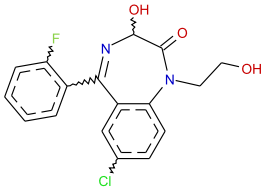
$C_{17}H_{18}N_4O_2S_2$
Molecular Weight: 374.48042
ALogP: 3.541
Rotatable Bonds: 3
Acceptors: 5
Donors: 2

Model Prediction

Prediction: Single-Carcinogen
Probability: 0.567
Enrichment: 1.37
Bayesian Score: 0.552
Mahalanobis Distance: 23.8
Mahalanobis Distance p-value: 1.59e-013

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Torsemide	Bicalutamide	Doxefazepam
Structure			
Actual Endpoint	Multiple-Carcinogen	Multiple-Carcinogen	Single-Carcinogen
Predicted Endpoint	Multiple-Carcinogen	Multiple-Carcinogen	Single-Carcinogen
Distance	0.714	0.721	0.723
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

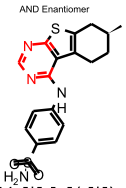
Model Applicability

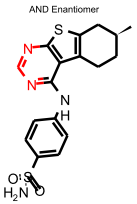
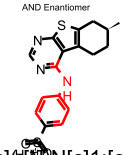
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

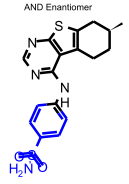
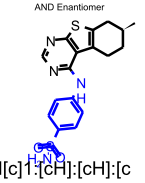
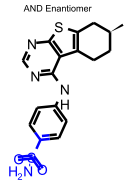
Feature Contribution

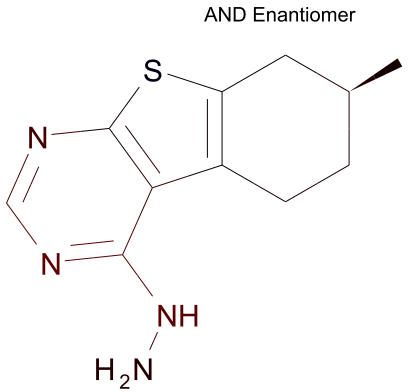
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_8	-1065373877	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.649	3 out of 3

SCFP_8	-1181430618	 [*]:n:[cH]:n:[*]	0.453	4 out of 6
SCFP_8	-300914917	 [*]:[c](:[*])N[c]1:[cH]:[cH]:[*]:[cH]:[cH]:1	0.383	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_8	-1247518081	 NS(=O)(=O)[c]1:[cH]:[cH]:[*]:[cH]:[cH]:1	-0.737	0 out of 3
SCFP_8	1892918731	 [*]N[c]1:[cH]:[cH]:[c](:[cH]:[cH]:1)S(=O)(=O)N	-0.546	0 out of 2
SCFP_8	182991870	 [*]:[c](:[*])S(=O)(=O)N	-0.342	1 out of 5



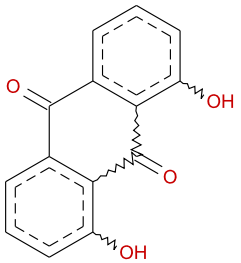
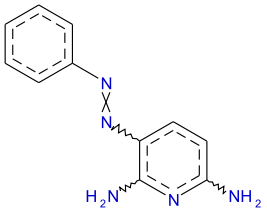
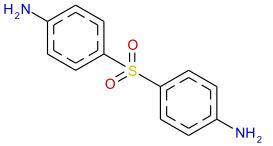
$C_{11}H_{14}N_4S$
Molecular Weight: 234.32065
ALogP: 2.561
Rotatable Bonds: 1
Acceptors: 4
Donors: 2

Model Prediction

Prediction: Multiple-Carcinogen
Probability: 0.568
Enrichment: 1.37
Bayesian Score: 2.08
Mahalanobis Distance: 23.2
Mahalanobis Distance p-value: 5.29e-013

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Danthron	Phenazopyridine	Dapsone
Structure			
Actual Endpoint	Single-Carcinogen	Single-Carcinogen	Multiple-Carcinogen
Predicted Endpoint	Single-Carcinogen	Single-Carcinogen	Multiple-Carcinogen
Distance	0.589	0.591	0.621
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

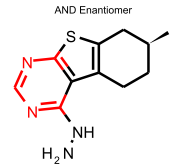
Model Applicability

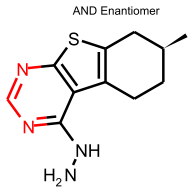
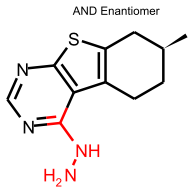
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

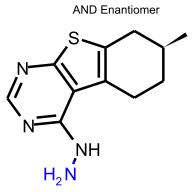
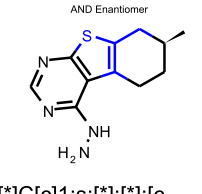
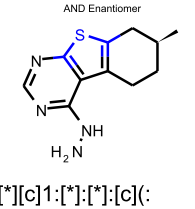
Feature Contribution

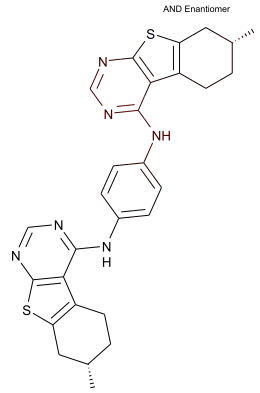
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_8	-1065373877	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.649	3 out of 3

SCFP_8	-1181430618	 [*]:n:[cH]:n:[*]	0.453	4 out of 6
SCFP_8	-915345805	 [*]:[c](:[*])NN	0.383	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_8	5	 [*]N	-0.463	9 out of 41
SCFP_8	803350837	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	-0.31	0 out of 1
SCFP_8	1310748454	 [*][c]1:[*]:[*]:[c](:[*]):s:1	-0.166	2 out of 7



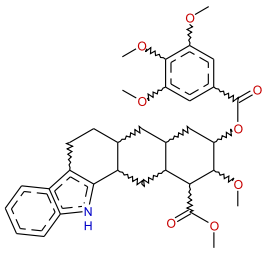
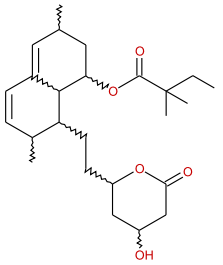
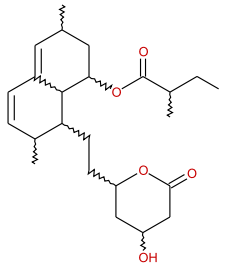
$C_{28}H_{28}N_6S_2$
Molecular Weight: 512.69212
ALogP: 7.842
Rotatable Bonds: 4
Acceptors: 6
Donors: 2

Model Prediction

Prediction: Multiple-Carcinogen
Probability: 0.567
Enrichment: 1.37
Bayesian Score: 2.33
Mahalanobis Distance: 23.1
Mahalanobis Distance p-value: 6.96e-013

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Deserpidine	Simvastatin	Lovastatin
Structure			
Actual Endpoint	Single-Carcinogen	Multiple-Carcinogen	Single-Carcinogen
Predicted Endpoint	Multiple-Carcinogen	Multiple-Carcinogen	Single-Carcinogen
Distance	0.968	0.971	1.006
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

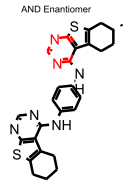
Model Applicability

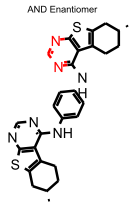
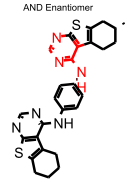
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. ALogP out of range. Value: 7.842. Training min, max, mean, SD: -3.329, 7.238, 2.2886, 2.006.

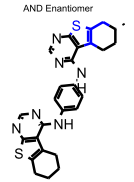
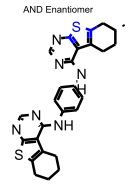
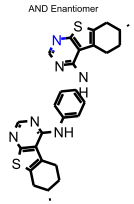
Feature Contribution

Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_8	-1065373877	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.649	3 out of 3

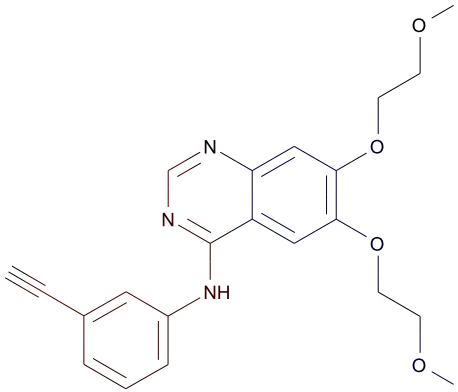
SCFP_8	-1181430618	 [*]:n:[cH]:n:[*]	0.453	4 out of 6
SCFP_8	-2147171373	 [*]N[c]1:n:[cH]:n:[*]:[c]:1:[*]	0.383	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_8	803350837	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	-0.31	0 out of 1
SCFP_8	1310748454	 [*][c]1:[*]:[*]:[c](:[*]):s:1	-0.166	2 out of 7
SCFP_8	8	 [*]:n:[*]	-0.154	12 out of 39

Erlotinib

TOPKAT_Rat_Male_FDA_Single_vs_Multiple



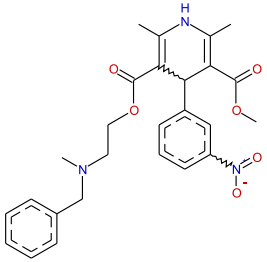
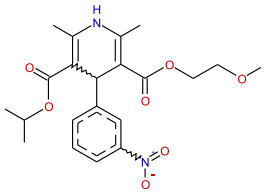
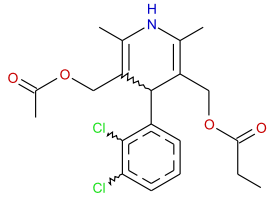
$C_{22}H_{23}N_3O_4$
Molecular Weight: 393.43572
ALogP: 4.309
Rotatable Bonds: 10
Acceptors: 7
Donors: 1

Model Prediction

Prediction: Multiple-Carcinogen
Probability: 0.568
Enrichment: 1.37
Bayesian Score: 0.821
Mahalanobis Distance: 16.5
Mahalanobis Distance p-value: 4.64e-007

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Nicardipine	Nimodipine	Felodipine
Structure			
Actual Endpoint	Single-Carcinogen	Single-Carcinogen	Single-Carcinogen
Predicted Endpoint	Single-Carcinogen	Single-Carcinogen	Single-Carcinogen
Distance	0.685	0.700	0.721
Reference	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997	US FDA (Centre for Drug Eval.& Res./Off. Testing & Res.) Sept. 1997

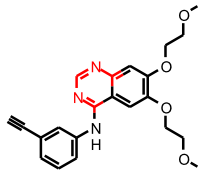
Model Applicability

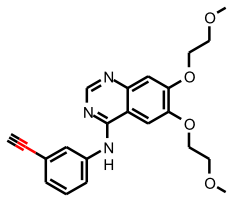
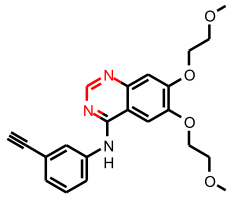
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

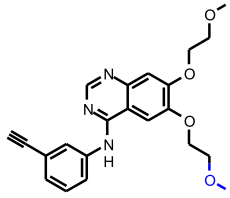
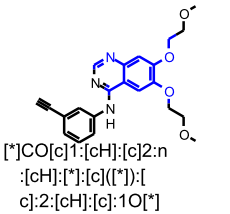
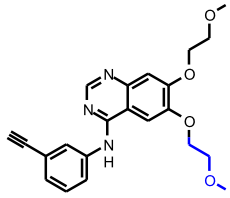
Feature Contribution

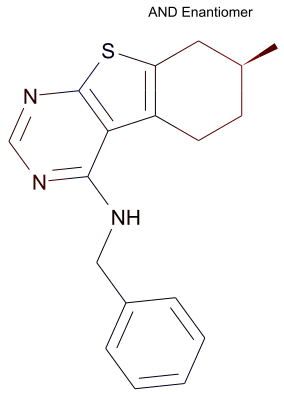
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_8	-1065373877	 [*][c]1:[*]:[c](:[*]) :n:[cH]:n:1	0.649	3 out of 3

SCFP_8	2	 [*]C#[*]	0.584	6 out of 8
SCFP_8	-1181430618	 [*]:n:[cH]:n:[*]	0.453	4 out of 6

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Multiple-Carcinogen in training set
SCFP_8	136239834	 [*]OC	-0.358	3 out of 13
SCFP_8	446954673	 [*]CO[c]1:[cH]:[c]2:n :[cH]:[*]:[c]([*]):[c]:2:[cH]:[c]:1O[*]	-0.31	0 out of 1
SCFP_8	949482168	 [*]CCOC	-0.31	0 out of 1



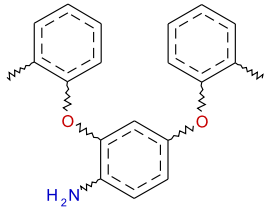
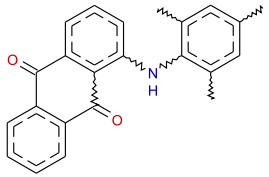
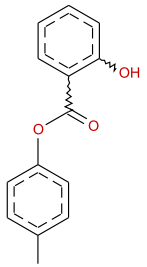
$C_{18}H_{19}N_3S$
Molecular Weight: 309.42856
ALogP: 4.678
Rotatable Bonds: 3
Acceptors: 3
Donors: 1

Model Prediction

Prediction: Mild
Probability: 0.382
Enrichment: 1.04
Bayesian Score: -0.773
Mahalanobis Distance: 7.93
Mahalanobis Distance p-value: 0.808

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Aniline, 2,4-bis(o-methylphenoxy)-	Anthraquinone, 1-(2,4,6-trimethylphenylamino)-	Salicylic acid, p-tolyl ester
Structure			
Actual Endpoint	Mild	Mild	Moderate_Severe
Predicted Endpoint	Mild	Mild	Moderate_Severe
Distance	0.627	0.664	0.687
Reference	85JCAE "Prehled Prumyslove Toxikologie; Organicke Latky," Marhold, J., Prague , Czechoslovakia, Avicenum, 1986 Volume(issue)/page/year: -,725,1986	28ZPAK "Sbornik Vysledku Toxixologickeho Vysetreni Latek A Pripravku," Marhol d, J.V., Institut Pro Vychovu Vedoucicn Pracovniku Chemickeho Prumyclu Praha, Cz echoslovakia, 1972 Volume(issue)/page/year: -,242,1	FCTOD7 Food and Chemical Toxicology. (Pergamon Press Inc., Maxwell House, Fa irview Park, Elmsford, NY 10523) V.20- 1982- Volume(issue)/page/year: 21,835 ,1983

Model Applicability

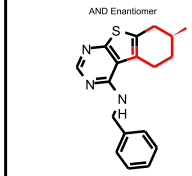
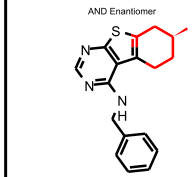
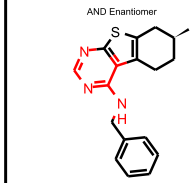
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]

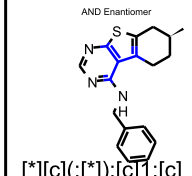
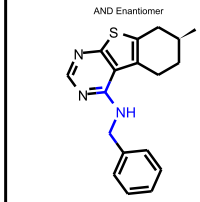
Feature Contribution

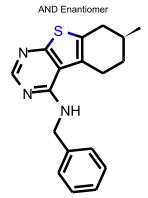
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Moderate_Severe in training set

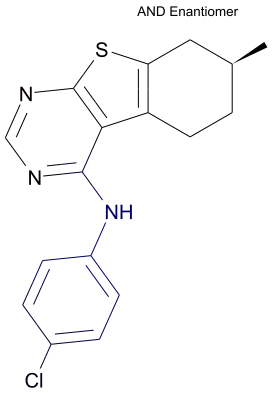
FCFP_12	-1441604640	 [*]:[c]1:[*]C[C@@H](C)CC1	0.385	1 out of 1
FCFP_12	-1731231884	 [*]:[c]1:[*]CC[C@H](C)C1	0.385	1 out of 1
FCFP_12	76292238	 [*]N[c]1:n:[cH]:n:[*]:[c]:1:[*]	0.385	1 out of 1

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Moderate_Severe in training set
FCFP_12	307419094	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.915	2 out of 18
FCFP_12	1294255210	 [*]CN[c](:[*]):[*]	-0.504	2 out of 11

FCFP_12	17	AND Enantiomer  [*]:s:[*]	-0.332	8 out of 32

TOPKAT_Skin_Irritancy_None_vs_Irritant



$C_{17}H_{16}ClN_3S$

Molecular Weight: 329.84704

ALogP: 5.5

Rotatable Bonds: 2

Acceptors: 3

Donors: 1

Model Prediction

Prediction: Non-Irritant

Probability: 0.918

Enrichment: 0.997

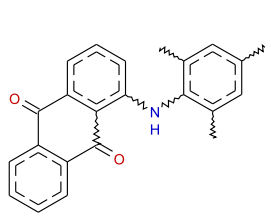
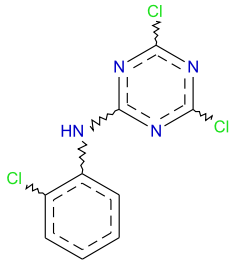
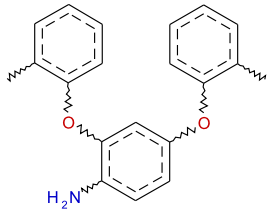
Bayesian Score: -2.53

Mahalanobis Distance: 8.77

Mahalanobis Distance p-value: 0.546

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Anthraquinone, 1-(2,4,6-trimethylphenylamino)-	s-Triazine, 2,4-dichloro-6-(o-chloroanilino)-	Aniline, 2,4-bis(o-methylphenoxy)-
Structure			
Actual Endpoint	Irritant	Irritant	Irritant
Predicted Endpoint	Non-Irritant	Non-Irritant	Non-Irritant
Distance	0.622	0.640	0.655
Reference	28ZPAK "Sbornik Vysledku Toxixologickeho Vysetreni Latek A Pripravku," Marhol d, J.V., Institut Pro Vychovu Vedoucicn Pracovniku Chemickeho Prumyclu Praha, Cz echoslovakia, 1972 Volume(issue)/page/year: -,242,1	34ZIAG* -,235,69	85JCAE "Prehled Prumyslove Toxikologie; Organicke Latky," Marhold, J., Prague , Czechoslovakia, Avicenum, 1986 Volume(issue)/page/year: -,725,1986

Model Applicability

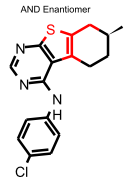
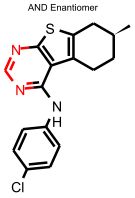
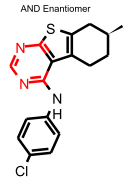
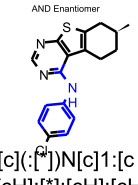
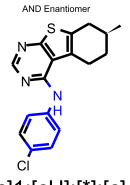
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

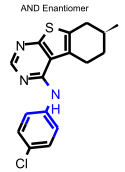
1. All properties and OPS components are within expected ranges.

Feature Contribution

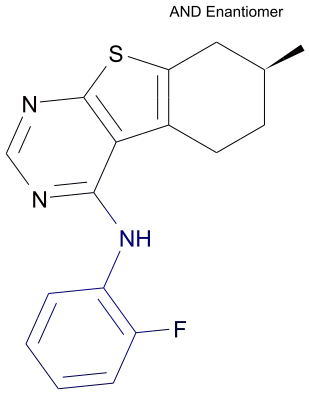
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set

FCFP_12	-1539132615	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	0.0795	9 out of 9
FCFP_12	-124685461	 [*]:n:[cH]:n:[*]	0.0734	5 out of 5
FCFP_12	-475316933	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.0703	4 out of 4
Top Features for negative contribution				
Fingerprint	**Bit/Smiles**	**Feature Structure**	**Score**	**Irritant in training set**
FCFP_12	839741273	 [*]:[c](:[*])N[c]1:[cH]:[cH]:[*]:[cH]:[cH]:1	-0.708	4 out of 10
FCFP_12	-773983804	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	-0.444	46 out of 79

FCFP_12	590925877	 [*]N[c](:[cH]:[*]):[cH]:[*]	-0.434	56 out of 95

TOPKAT_Skin_Irritancy_None_vs_Irritant



$C_{17}H_{16}FN_3S$

Molecular Weight: 313.39244

ALogP: 5.041

Rotatable Bonds: 2

Acceptors: 3

Donors: 1

Model Prediction

Prediction: Non-Irritant

Probability: 0.895

Enrichment: 0.971

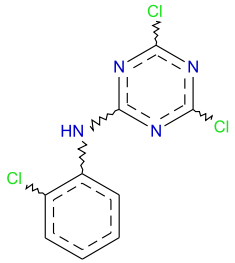
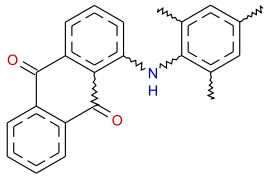
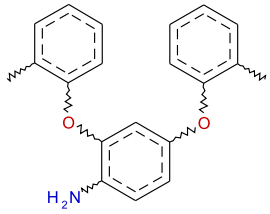
Bayesian Score: -2.82

Mahalanobis Distance: 8.71

Mahalanobis Distance p-value: 0.58

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	s-Triazine, 2,4-dichloro-6-(o-chloroanilino)-	Anthraquinone, 1-(2,4,6-trimethylphenylamino)-	Aniline, 2,4-bis(o-methylphenoxy)-
Structure			
Actual Endpoint	Irritant	Irritant	Irritant
Predicted Endpoint	Non-Irritant	Non-Irritant	Non-Irritant
Distance	0.560	0.644	0.646
Reference	34ZIAG* -,235,69	28ZPAK "Sbornik Vysledku Toxixologickeho Vysetreni Latek A Pripravku," Marhol d, J.V., Institut Pro Vychovu Vedoucicn Pracovniku Chemickeho Prumyclu Praha, Cz echoslovakia, 1972 Volume(issue)/page/year: -,242,1	85JCAE "Prehled Prumyslove Toxikologie; Organicke Latky," Marhold, J., Prague , Czechoslovakia, Avicenum, 1986 Volume(issue)/page/year: -,725,1986

Model Applicability

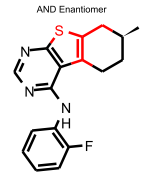
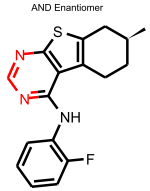
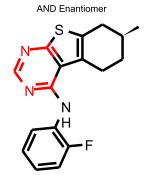
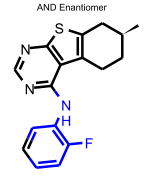
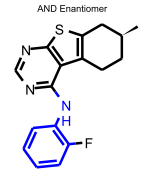
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

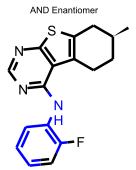
1. All properties and OPS components are within expected ranges.

Feature Contribution

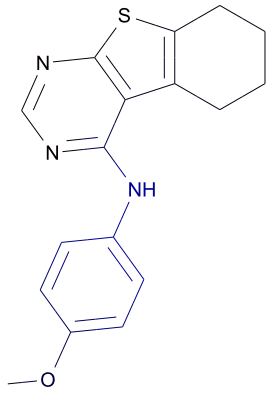
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set

FCFP_12	-1539132615	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	0.0795	9 out of 9
FCFP_12	-124685461	 [*]:n:[cH]:n:[*]	0.0734	5 out of 5
FCFP_12	-475316933	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.0703	4 out of 4
Top Features for negative contribution				
Fingerprint	**Bit/Smiles**	**Feature Structure**	**Score**	**Irritant in training set**
FCFP_12	1783756416	 [*]N[c]1:[cH]:[*]:[cH]:[cH]:[c]:1F	-0.509	4 out of 8
FCFP_12	-1724769936	 [*]N[c]1:[cH]:[cH]:[cH]:[cH]:[c]:1[*]	-0.475	11 out of 20

FCFP_12	-773983804	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	-0.444	46 out of 79

TOPKAT_Skin_Irritancy_None_vs_Irritant



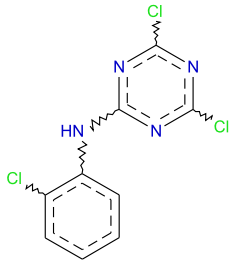
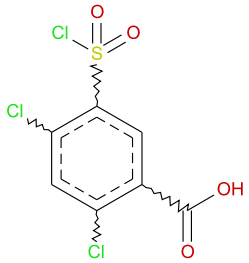
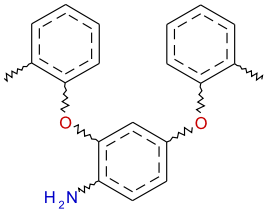
$C_{17}H_{17}N_3OS$
Molecular Weight: 311.40138
ALogP: 4.568
Rotatable Bonds: 3
Acceptors: 4
Donors: 1

Model Prediction

Prediction: Non-Irritant
Probability: 0.709
Enrichment: 0.769
Bayesian Score: -3.91
Mahalanobis Distance: 7.41
Mahalanobis Distance p-value: 0.98

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	s-Triazine, 2,4-dichloro-6-(o-chloroanilino)-	Benzoic acid, 5-(chlorosulfonyl)-2,4-dichloro-	Aniline, 2,4-bis(o-methylphenoxy)-
Structure			
Actual Endpoint	Irritant	Irritant	Irritant
Predicted Endpoint	Non-Irritant	Non-Irritant	Non-Irritant
Distance	0.627	0.701	0.705
Reference	34ZIAG* -,235,69	FCTOD7 Food and Chemical Toxicology. (Pergamon Press Inc., Maxwell House, Fa irview Park, Elmsford, NY 10523) V.20- 1982- Volume(issue)/page/year: 20,563 ,1982	85JCAE "Prehled Prumyslove Toxikologie; Organicke Latky," Marhold, J., Prague , Czechoslovakia, Avicenum, 1986 Volume(issue)/page/year: -,725,1986

Model Applicability

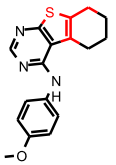
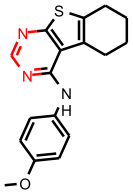
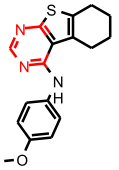
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

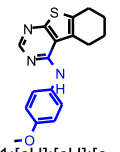
Feature Contribution

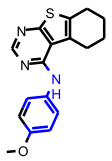
Top features for positive contribution

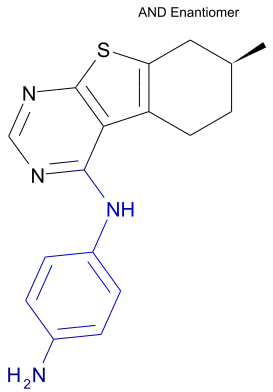
Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set

FCFP_12	-1539132615	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	0.0795	9 out of 9
FCFP_12	-124685461	 [*]:n:[cH]:n:[*]	0.0734	5 out of 5
FCFP_12	-475316933	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.0703	4 out of 4

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set
FCFP_12	839741273	 [*]:[c](:[*])N[c]1:[cH]:[cH]:[*]:[cH]:[cH]:1	-0.708	4 out of 10
FCFP_12	414792462	 [*]O[c]1:[cH]:[cH]:[c](N[c](:[*]):[*]):[cH]:[cH]:1	-0.65	0 out of 1

FCFP_12	-773983804	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	-0.444	46 out of 79



$C_{17}H_{18}N_4S$

Molecular Weight: 310.41662

ALogP: 4.089

Rotatable Bonds: 2

Acceptors: 4

Donors: 2

Model Prediction

Prediction: Non-Irritant

Probability: 0.183

Enrichment: 0.199

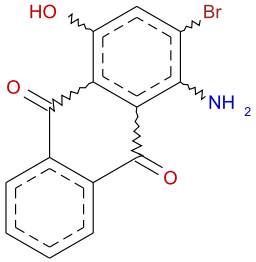
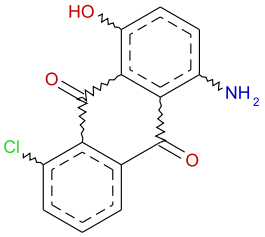
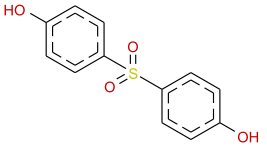
Bayesian Score: -5.47

Mahalanobis Distance: 8.06

Mahalanobis Distance p-value: 0.867

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	1-Amino-2-bromo-4-hydroxyanthraquinone	1-Amino-4-hydroxy-5-chloroanthraquinone	Phenol, 4,4'-sulfonyldi-
Structure			
Actual Endpoint	Non-Irritant	Non-Irritant	Irritant
Predicted Endpoint	Non-Irritant	Non-Irritant	Non-Irritant
Distance	0.650	0.669	0.696
Reference	28ZPAK -,83,72	28ZPAK -,83,72	BIOFX* BIOFAX Industrial Bio-Test Laboratories, Inc., Data Sheets. (1810 Fro ntage Rd., Northbrook, IL 60062) Volume(issue)/page/year: 601-05501,1974

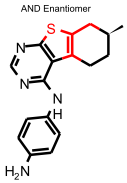
Model Applicability

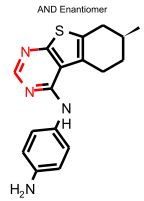
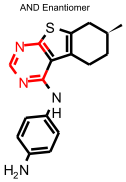
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

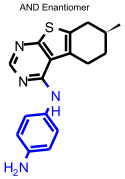
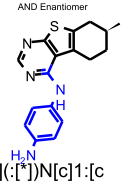
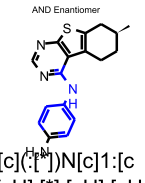
Feature Contribution

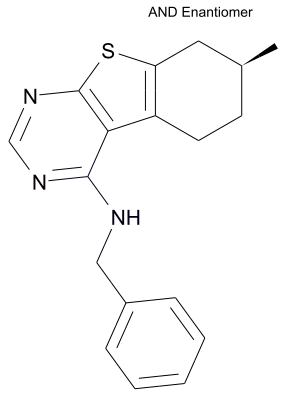
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set
FCFP_12	-1539132615	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	0.0795	9 out of 9

FCFP_12	-124685461	 [*]:n:[cH]:n:[*]	0.0734	5 out of 5
FCFP_12	-475316933	 [*][c]1:[*]:[c](:[*]) :n:[cH]:n:1	0.0703	4 out of 4

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set
FCFP_12	-970693500	 [*]N[c]1:[cH]:[cH]:[c](N):[cH]:[cH]:1	-1.04	0 out of 2
FCFP_12	-200702388	 [*]:[c](:[*])N[c]1:[c H]:[cH]:[c](N):[cH]: [cH]:1	-0.846	1 out of 4
FCFP_12	839741273	 [*]:[c](:[*])N[c]1:[c H]:[cH]:[*]:[cH]:[cH]:1	-0.708	4 out of 10



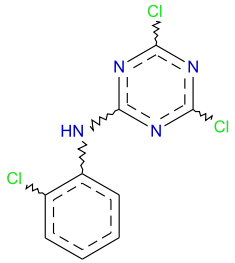
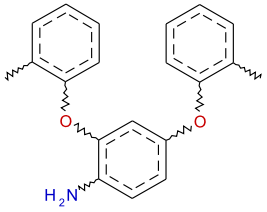
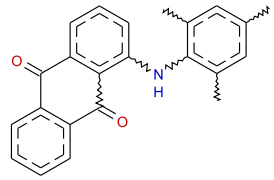
$C_{18}H_{19}N_3S$
Molecular Weight: 309.42856
ALogP: 4.678
Rotatable Bonds: 3
Acceptors: 3
Donors: 1

Model Prediction

Prediction: Irritant
Probability: 0.974
Enrichment: 1.06
Bayesian Score: -0.706
Mahalanobis Distance: 7.74
Mahalanobis Distance p-value: 0.942

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	s-Triazine, 2,4-dichloro-6-(o-chloroanilino)-	Aniline, 2,4-bis(o-methylphenoxy)-	Anthraquinone, 1-(2,4,6-trimethylphenylamino)-
Structure			
Actual Endpoint	Irritant	Irritant	Irritant
Predicted Endpoint	Non-Irritant	Non-Irritant	Non-Irritant
Distance	0.626	0.630	0.668
Reference	34ZIAG* -,235,69	85JCAE "Prehled Prumyslove Toxikologie; Organicke Latky," Marhold, J., Prague , Czechoslovakia, Avicenum, 1986 Volume(issue)/page/year: -,725,1986	28ZPAK "Sbornik Vysledku Toxixologickeho Vysetreni Latek A Pripravku," Marhol d, J.V., Institut Pro Vychovu Vedoucicn Pracovniku Chemickeho Prumyclu Praha, Cz echoslovakia, 1972 Volume(issue)/page/year: -,242,1

Model Applicability

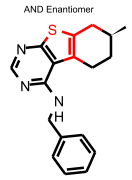
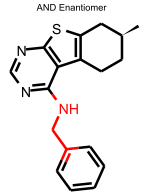
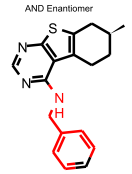
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

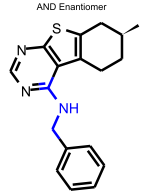
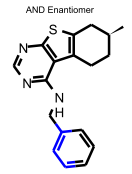
Feature Contribution

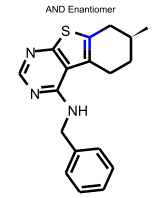
Top features for positive contribution

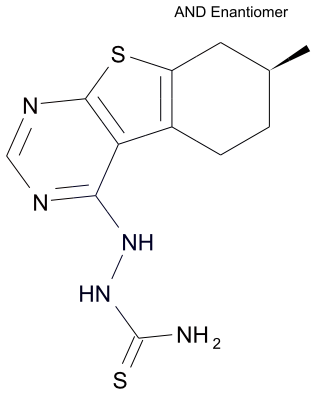
Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set

FCFP_12	-1539132615	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	0.0795	9 out of 9
FCFP_12	907096426	 [*]NC[c](:[*]):[*]	0.0772	7 out of 7
FCFP_12	427906732	 [*]NC[c]1:[cH]:[cH]:[*]:[cH]:[cH]:1	0.0756	6 out of 6

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set
FCFP_12	1294255210	 [*]CN[c](:[*]):[*]	-0.486	12 out of 22
FCFP_12	1618154665	 [*][c](:[*]):[cH]:[cH]:[*]	-0.0845	412 out of 490

FCFP_12	16	AND Enantiomer  [*][c](:[*]):[*]	-0.0843	423 out of 503



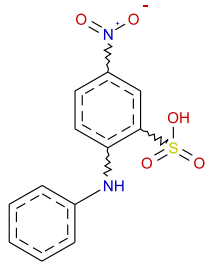
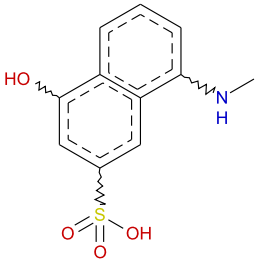
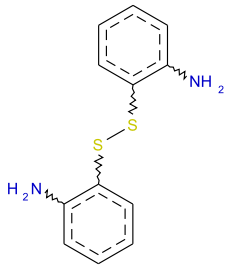
$C_{12}H_{15}N_5S_2$
Molecular Weight: 293.411
ALogP: 3.209
Rotatable Bonds: 3
Acceptors: 4
Donors: 3

Model Prediction

Prediction: Non-Irritant
Probability: 0.966
Enrichment: 1.05
Bayesian Score: -1.27
Mahalanobis Distance: 8.34
Mahalanobis Distance p-value: 0.763

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Benzenesulfonic acid, 2-anilino-5-nitro-	8-Methylamino-4-hydroxy-2-naphthalene sulfonic acid	Aniline, 2,2-dithiobis-
Structure			
Actual Endpoint	Irritant	Non-Irritant	Non-Irritant
Predicted Endpoint	Non-Irritant	Non-Irritant	Non-Irritant
Distance	0.770	0.772	0.781
Reference	85JCAE "Prehled Prumyslove Toxikologie; Organicke Latky," Marhold, J., Prague , Czechoslovakia, Avicenum, 1986 Volume(issue)/page/year: -,1061,1986	28ZPAK -,190,72	28ZPAK -,512,72

Model Applicability

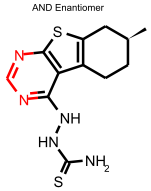
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

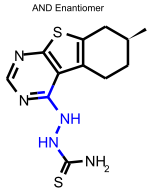
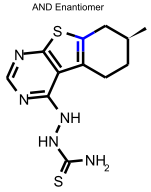
Feature Contribution

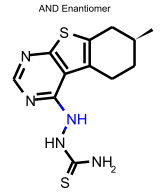
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set

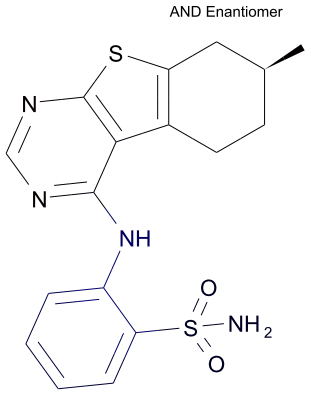
FCFP_12	-1539132615	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	0.0795	9 out of 9
FCFP_12	-124685461	 [*]:n:[cH]:n:[*]	0.0734	5 out of 5
FCFP_12	-475316933	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.0703	4 out of 4

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set
FCFP_12	1294344583	 [*]NN[c](:[*]):[*]	-0.65	0 out of 1
FCFP_12	16	 [*][c](:[*]):[*]	-0.0843	423 out of 503

FCFP_12	3	AND Enantiomer  [*]N[*]	-0.0812	291 out of 345

TOPKAT_Skin_Irritancy_None_vs_Irritant



$C_{17}H_{18}N_4O_2S_2$

Molecular Weight: 374.48042

ALogP: 3.541

Rotatable Bonds: 3

Acceptors: 5

Donors: 2

Model Prediction

Prediction: Non-Irritant

Probability: 0.866

Enrichment: 0.94

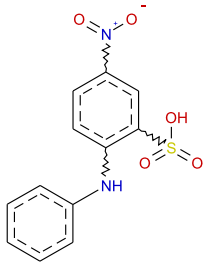
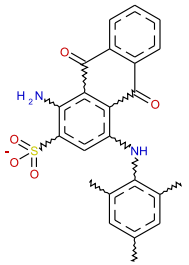
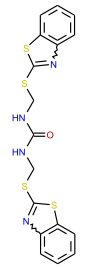
Bayesian Score: -3.08

Mahalanobis Distance: 7.74

Mahalanobis Distance p-value: 0.942

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Benzenesulfonic acid, 2-anilino-5-nitro-	2-Anthracenesulfonic acid, 1-amino-9,10-dihydro-9,10-dioxo-4-(2,4,6 -trimethylanilino)-, monosodium salt	Urea, 1,3-bis(2-benzothiazolylthiomethyl)-
Structure			
Actual Endpoint	Irritant	Irritant	Irritant
Predicted Endpoint	Non-Irritant	Non-Irritant	Irritant
Distance	0.657	0.728	0.769
Reference	85JCAE "Prehled Prumyslove Toxikologie; Organicke Latky," Marhold, J., Prague , Czechoslovakia, Avicenum, 1986 Volume(issue)/page/year: -,1061,1986	85JCAE "Prehled Prumyslove Toxikologie; Organicke Latky," Marhold, J., Prague , Czechoslovakia, Avicenum, 1986 Volume(issue)/page/year: -,1327,1986	AMIHBC AMA Archives of Industrial Hygiene and Occupational Medicine. (Chicago , IL) V.2-10, 1950-54. For publisher information, see AEHLAU. Volume(issue)/pag e/year: 5,311,1952

Model Applicability

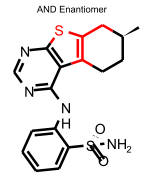
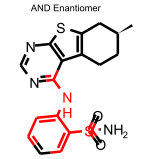
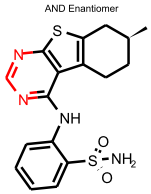
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

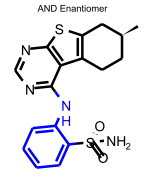
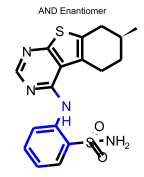
Feature Contribution

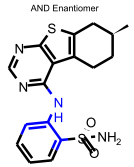
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set

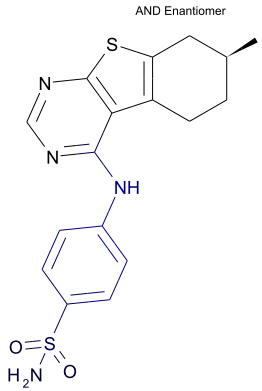
FCFP_12	-1539132615	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	0.0795	9 out of 9
FCFP_12	-605671248	 [*]S(=[*])(=[*])[c]1:[cH]:[*]:[cH]:[cH]:[c]:1N[c](:[*]):[*]	0.0772	7 out of 7
FCFP_12	-124685461	 [*]:n:[cH]:n:[*]	0.0734	5 out of 5

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set
FCFP_12	-1724769936	 [*]N[c]1:[cH]:[cH]:[cH]:[cH]:[c]:1[*]	-0.475	11 out of 20
FCFP_12	-773983804	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	-0.444	46 out of 79

FCFP_12	590925877	 [*]N[c](:[cH]:[*]):[cH]:[*]	-0.434	56 out of 95

TOPKAT_Skin_Irritancy_None_vs_Irritant



$C_{17}H_{18}N_4O_2S_2$

Molecular Weight: 374.48042

ALogP: 3.541

Rotatable Bonds: 3

Acceptors: 5

Donors: 2

Model Prediction

Prediction: Non-Irritant

Probability: 0.663

Enrichment: 0.719

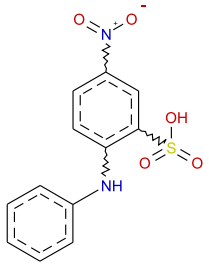
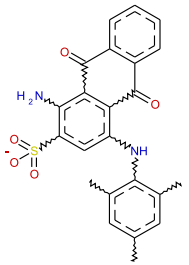
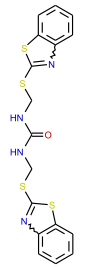
Bayesian Score: -4.07

Mahalanobis Distance: 7.74

Mahalanobis Distance p-value: 0.942

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Benzenesulfonic acid, 2-anilino-5-nitro-	2-Anthracenesulfonic acid, 1-amino-9,10-dihydro-9,10-dioxo-4-(2,4,6 -trimethylanilino)-, monosodium salt	Urea, 1,3-bis(2-benzothiazolylthiomethyl)-
Structure			
Actual Endpoint	Irritant	Irritant	Irritant
Predicted Endpoint	Non-Irritant	Non-Irritant	Irritant
Distance	0.676	0.741	0.774
Reference	85JCAE "Prehled Prumyslove Toxikologie; Organicke Latky," Marhold, J., Prague , Czechoslovakia, Avicenum, 1986 Volume(issue)/page/year: -,1061,1986	85JCAE "Prehled Prumyslove Toxikologie; Organicke Latky," Marhold, J., Prague , Czechoslovakia, Avicenum, 1986 Volume(issue)/page/year: -,1327,1986	AMIHBC AMA Archives of Industrial Hygiene and Occupational Medicine. (Chicago , IL) V.2-10, 1950-54. For publisher information, see AEHLAU. Volume(issue)/pag e/year: 5,311,1952

Model Applicability

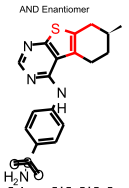
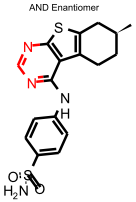
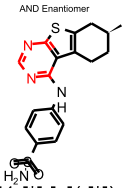
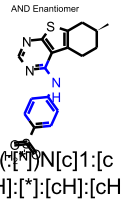
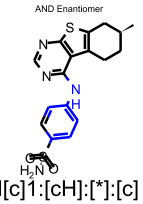
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

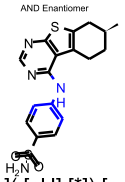
1. All properties and OPS components are within expected ranges.

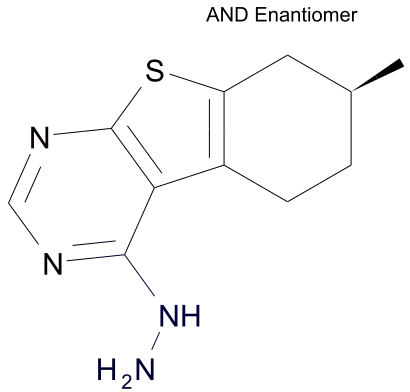
Feature Contribution

Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set

FCFP_12	-1539132615	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	0.0795	9 out of 9
FCFP_12	-124685461	 [*]:n:[cH]:n:[*]	0.0734	5 out of 5
FCFP_12	-475316933	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.0703	4 out of 4
Top Features for negative contribution				
Fingerprint	**Bit/Smiles**	**Feature Structure**	**Score**	**Irritant in training set**
FCFP_12	839741273	 [*]:[c](:[*])N[c]1:[cH]:[cH]:[*]:[cH]:[cH]:1	-0.708	4 out of 10
FCFP_12	-773983804	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	-0.444	46 out of 79

FCFP_12	590925877	 [*]N[c](:[cH]:[*]):[cH]:[*]	-0.434	56 out of 95



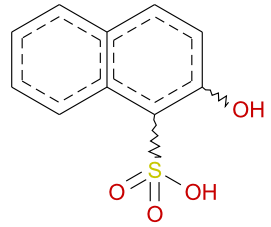
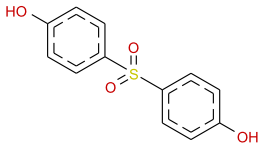
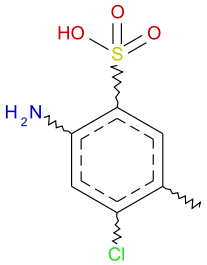
$C_{11}H_{14}N_4S$
Molecular Weight: 234.32065
ALogP: 2.561
Rotatable Bonds: 1
Acceptors: 4
Donors: 2

Model Prediction

Prediction: Non-Irritant
Probability: 0.95
Enrichment: 1.03
Bayesian Score: -1.89
Mahalanobis Distance: 8.12
Mahalanobis Distance p-value: 0.846

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	1-Naphthalenesulfonic acid, 2-hydroxy-	Phenol, 4,4'-sulfonyldi-	m-Toluene sulfonic acid, 6-amino-4-chloro-
Structure			
Actual Endpoint	Irritant	Irritant	Non-Irritant
Predicted Endpoint	Non-Irritant	Non-Irritant	Non-Irritant
Distance	0.559	0.566	0.585
Reference	85JCAE "Prehled Prumyslove Toxikologie; Organicke Latky," Marhold, J., Prague , Czechoslovakia, Avicenum, 1986 Volume(issue)/page/year: -,1059,1986	BIOFX* BIOFAX Industrial Bio-Test Laboratories, Inc., Data Sheets. (1810 Fro ntage Rd., Northbrook, IL 60062) Volume(issue)/page/year: 601-05501,1974	28ZPAK -,526,72

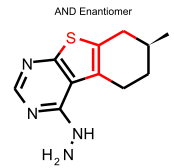
Model Applicability

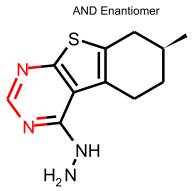
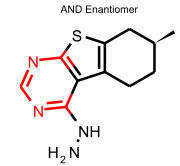
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

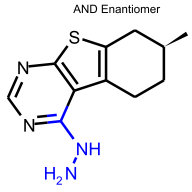
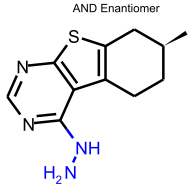
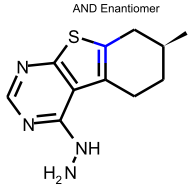
Feature Contribution

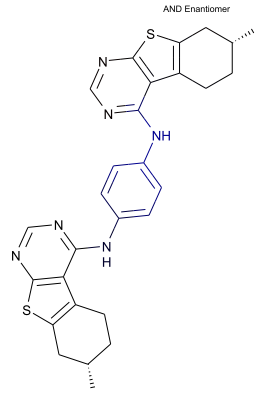
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set
FCFP_12	-1539132615	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	0.0795	9 out of 9

FCFP_12	-124685461	 [*]:n:[cH]:n:[*]	0.0734	5 out of 5
FCFP_12	-475316933	 [*][c]1:[*]:[c](:[*]) :n:[cH]:n:1	0.0703	4 out of 4

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set
FCFP_12	1294344583	 [*]NN[c](:[*]):[*]	-0.65	0 out of 1
FCFP_12	1070150408	 [*]NN	-0.347	1 out of 2
FCFP_12	16	 [*][c](:[*]):[*]	-0.0843	423 out of 503



$C_{28}H_{28}N_6S_2$

Molecular Weight: 512.69212

ALogP: 7.842

Rotatable Bonds: 4

Acceptors: 6

Donors: 2

Model Prediction

Prediction: Non-Irritant

Probability: 0.844

Enrichment: 0.916

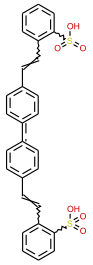
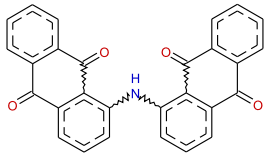
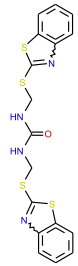
Bayesian Score: -3.25

Mahalanobis Distance: 10

Mahalanobis Distance p-value: 0.0563

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Benzenesulfonic acid, 2,2'-(4,4'-biphenylylenedivinylene)di-, disod ium salt	Anthraquinone, 1,1'-iminodi-	Urea, 1,3-bis(2-benzothiazolylthiomethyl)-
Structure			
Actual Endpoint	Irritant	Irritant	Irritant
Predicted Endpoint	Non-Irritant	Non-Irritant	Irritant
Distance	0.699	0.938	0.953
Reference	MVCRB3 MVC-Report. (Stockholm, Sweden) No.1-2, 1972-73. Discontinued. Volu me(issue)/page/year: 2,193,1973	85JCAE "Prehled Prumyslove Toxikologie; Organicke Latky," Marhold, J., Prague , Czechoslovakia, Avicenum, 1986 Volume(issue)/page/year: -,735,1986	AMIHBC AMA Archives of Industrial Hygiene and Occupational Medicine. (Chicago , IL) V.2-10, 1950-54. For publisher information, see AEHLAU. Volume(issue)/pag e/year: 5,311,1952

Model Applicability

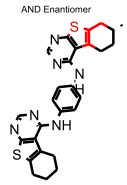
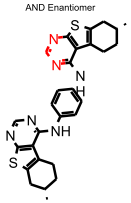
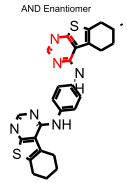
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

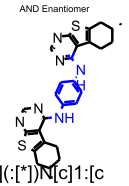
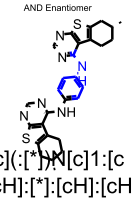
Feature Contribution

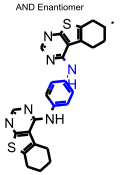
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set

FCFP_12	-1539132615	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	0.0795	9 out of 9
FCFP_12	-124685461	 [*]:n:[cH]:n:[*]	0.0734	5 out of 5
FCFP_12	-475316933	 [*][c]1:[*]:[c](:[*]):n:[cH]:n:1	0.0703	4 out of 4

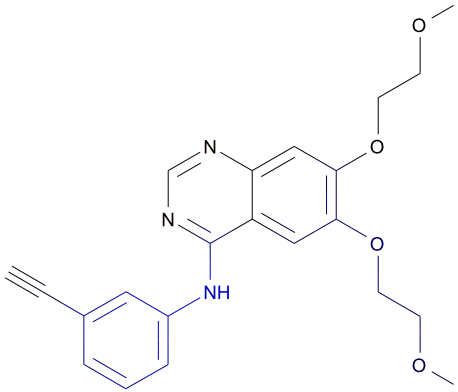
Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set
FCFP_12	-200702388	 [*]:[c](:[*])N[c]1:[cH]:[cH]:[c](N):[cH]:[cH]:1	-0.846	1 out of 4
FCFP_12	839741273	 [*]:[c](:[*])N[c]1:[cH]:[cH]:[*]:[cH]:[cH]:1	-0.708	4 out of 10

FCFP_12	-773983804	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	-0.444	46 out of 79

Erlotinib

TOPKAT_Skin_Irritancy_None_vs_Irritant



$C_{22}H_{23}N_3O_4$

Molecular Weight: 393.43572

ALogP: 4.309

Rotatable Bonds: 10

Acceptors: 7

Donors: 1

Model Prediction

Prediction: Non-Irritant

Probability: 0.119

Enrichment: 0.13

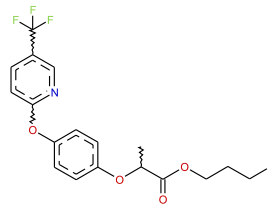
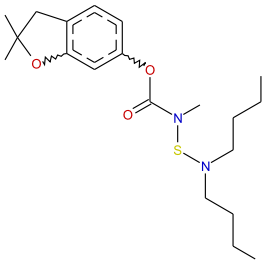
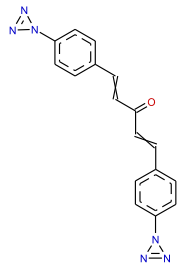
Bayesian Score: -5.76

Mahalanobis Distance: 10.2

Mahalanobis Distance p-value: 0.0333

Prediction: Positive if the Bayesian score is above the estimated best cutoff value from minimizing the false positive and false negative rate.
Probability: The esimated probability that the sample is in the positive category. This assumes that the Bayesian score follows a normal distribution and is different from the prediction using a cutoff.
Enrichment: An estimate of enrichment, that is, the increased likelihood (versus random) of this sample being in the category.
Bayesian Score: The standard Laplacian-modified Bayesian score.
Mahalanobis Distance: The Mahalanobis distance (MD) is the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Propanoic acid, 2-(4-((5-(trifluoromethyl)-2-pyridinyl)oxy)phenoxy) -, butyl ester	Carbamic acid, ((dibutylamino)thio)methyl-, 2,2-dimethyl-2,3-dihydro-7-benzofuranyl ester	1,4-Pentadien-3-one, 1,5-bis(p-azidophenyl)-
Structure			
Actual Endpoint	Irritant	Irritant	Irritant
Predicted Endpoint	Irritant	Irritant	Irritant
Distance	0.776	0.777	0.803
Reference	NNGADV Nippon Noyaku Gakkaishi. Journal of the Pesticide Science Society of Japan. (Nippon Noyaku Gakkai, 1-43-11, Komagome, Toshima-ku, Tokyo 170, Japan) V.1-1976- Volume(issue)/page/year: 15,305,1990	NTIS** National Technical Information Service. (Springfield, VA 22161) Forme rly U.S. Clearinghouse for Scientific & Technical Information. Volume(issue)/pag e/year: OTS0539690	85JCAE "Prehled Prumyslove Toxikologie; Organicke Latky," Marhold, J., Prague , Czechoslovakia, Avicenum, 1986 Volume(issue)/page/year: -,733,1986

Model Applicability

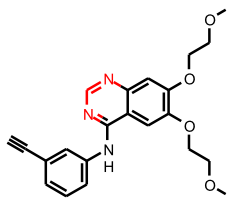
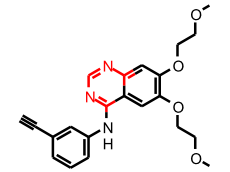
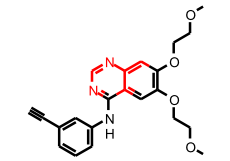
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: 902193919: [*]:[c](:[*])C#C

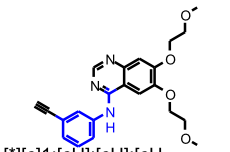
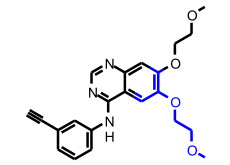
Feature Contribution

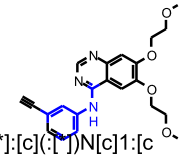
Top features for positive contribution

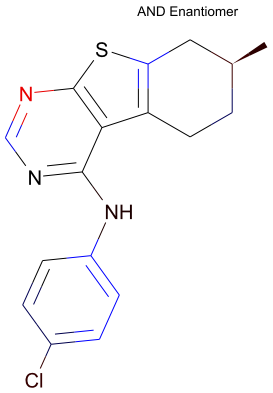
Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set

FCFP_12	-124685461	 [*]:n:[cH]:n:[*]	0.0734	5 out of 5
FCFP_12	-475316933	 [*][c]1:[*]:[c](:[*]) :n:[cH]:n:1	0.0703	4 out of 4
FCFP_12	-1385265413	 [*]:[cH]:[c]1:n:[cH]: n:[*]:[c]:1:[*]	0.0658	3 out of 3

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score	Irritant in training set
FCFP_12	411414971	 [*][c]1:[cH]:[cH]:[cH]:[c](N[c](:[*]):[*]):[cH]:1	-1.31	1 out of 7
FCFP_12	-1059904848	 [*][c](:[*]):[c](OCCO C):[cH]:[*]	-1.04	0 out of 2

FCFP_12	839741273	 [*]:[c](:[*])N[c]1:[cH]:[cH]:[*]:[cH]:[cH]:1	-0.708	4 out of 10



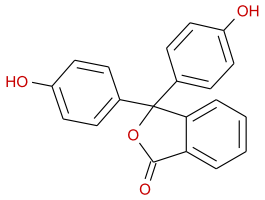
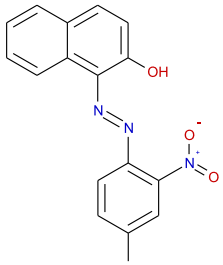
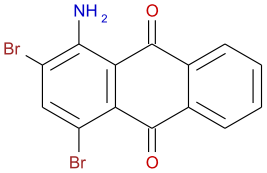
$C_{17}H_{16}ClN_3S$
Molecular Weight: 329.84704
ALogP: 5.5
Rotatable Bonds: 2
Acceptors: 3
Donors: 1

Model Prediction

Prediction: 3.09
Unit: mg/kg_body_weight/day
Mahalanobis Distance: 11.8
Mahalanobis Distance p-value: 4.72e-005

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Phenolphthalein	646	1-Amino-2,4-dibromoanthra-qui-none
Structure			
Actual Endpoint (-log C)	2.43468	0.937339	2.90243
Predicted Endpoint (-log C)	3.66084	3.26294	3.50402
Distance	0.663	0.701	0.750
Reference	CPDB	CPDB	CPDB

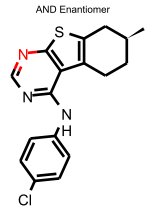
Model Applicability

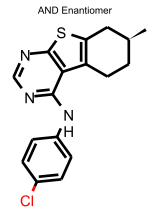
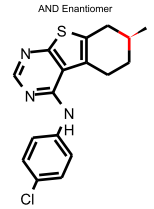
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: 292958156: [*]CC(C)C[*]
3. Unknown ECFP_2 feature: -1672647522: [*]C[c]1:s:[*]:[*]:[c]:1[*]
4. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]

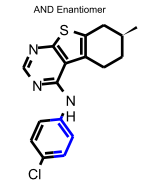
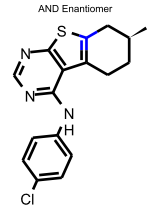
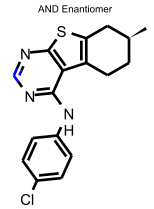
Feature Contribution

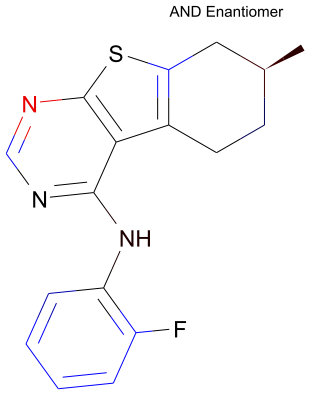
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	655739385	 [*]:n:[*]	0.229

ECFP_6	-817402818	 [*]Cl	0.129
ECFP_6	-167460056	 [*]C([*])[*]	0.0596

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	1996767644	 [*][c](:[*]):[cH]:[cH]:[*]	-0.251
ECFP_6	642810091	 [*][c](:[*]):[*]	-0.247
ECFP_6	-182236392	 [*]:[cH]:[*]	-0.232



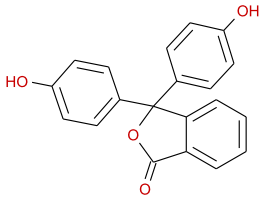
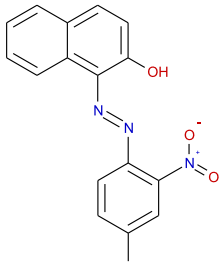
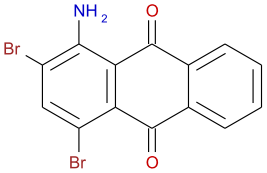
$C_{17}H_{16}FN_3S$
Molecular Weight: 313.39244
ALogP: 5.041
Rotatable Bonds: 2
Acceptors: 3
Donors: 1

Model Prediction

Prediction: 9.29
Unit: mg/kg_body_weight/day
Mahalanobis Distance: 10.9
Mahalanobis Distance p-value: 0.00248

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Phenolphthalein	646	1-Amino-2,4-dibromoanthra-qui-none
Structure			
Actual Endpoint (-log C)	2.43468	0.937339	2.90243
Predicted Endpoint (-log C)	3.66084	3.26294	3.50402
Distance	0.636	0.691	0.731
Reference	CPDB	CPDB	CPDB

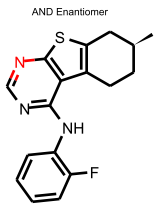
Model Applicability

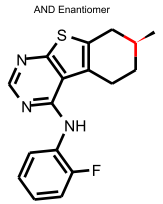
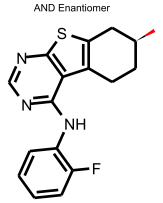
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: 292958156: [*]CC(C)C[*]
3. Unknown ECFP_2 feature: -1672647522: [*]C[c]1:s:[*]:[*]:[c]:1[*]
4. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
5. Unknown ECFP_2 feature: -1311285389: [*][c](:[*]):[c](F):c:[*]

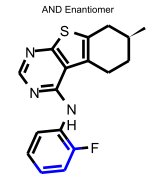
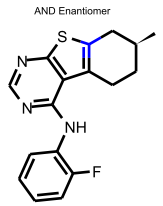
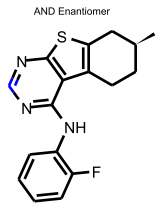
Feature Contribution

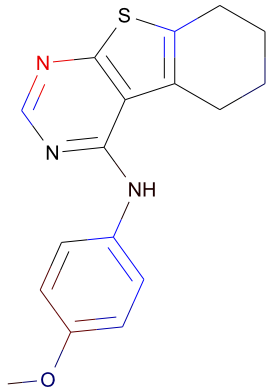
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	655739385	 [*]:n:[*]	0.229

ECFP_6	-167460056	 [*]C([*])[*]	0.0596
ECFP_6	734603939	 [*]C	0.0424

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	1996767644	 [*][c](:[*]):[cH]:[cH]:[*]	-0.251
ECFP_6	642810091	 [*][c](:[*]):[*]	-0.247
ECFP_6	-182236392	 [*]:[cH]:[*]	-0.232



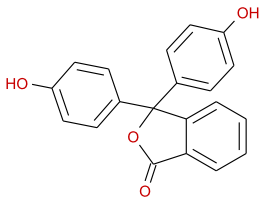
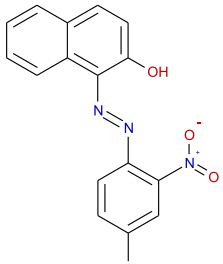
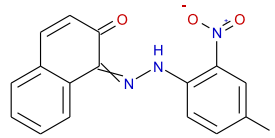
$C_{17}H_{17}N_3OS$
Molecular Weight: 311.40138
ALogP: 4.568
Rotatable Bonds: 3
Acceptors: 4
Donors: 1

Model Prediction

Prediction: 7.19
Unit: mg/kg_body_weight/day
Mahalanobis Distance: 12.3
Mahalanobis Distance p-value: 4.73e-006

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Phenolphthalein	646	C.I. pigment red 3
Structure			
Actual Endpoint (-log C)	2.43468	0.937339	0.937339
Predicted Endpoint (-log C)	3.66084	3.26294	3.17837
Distance	0.626	0.648	0.702
Reference	CPDB	CPDB	CPDB

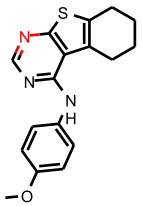
Model Applicability

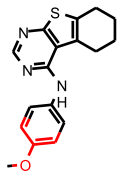
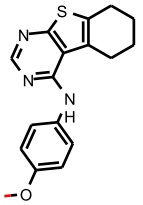
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1672647522: [*]C[c]1:s:[*]:[*]:[c]:1[*]
3. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]

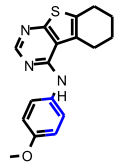
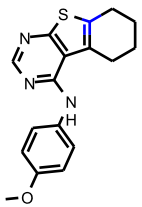
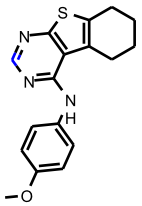
Feature Contribution

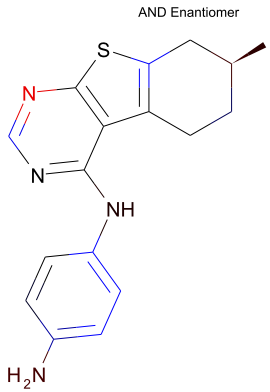
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	655739385	 [*]:n:[*]	0.229

ECFP_6	-176455838	 [*]O[c](:[cH]:[*]):[cH]:[*]	0.0818
ECFP_6	734603939	 [*]C	0.0424

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	1996767644	 [*][c](:[*]):[cH]:[cH]:[*]	-0.251
ECFP_6	642810091	 [*][c](:[*]):[*]	-0.247
ECFP_6	-182236392	 [*]:[cH]:[*]	-0.232



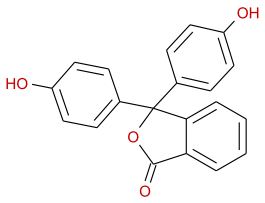
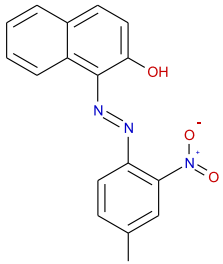
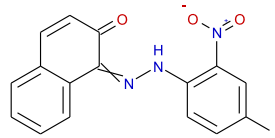
$C_{17}H_{18}N_4S$
Molecular Weight: 310.41662
ALogP: 4.089
Rotatable Bonds: 2
Acceptors: 4
Donors: 2

Model Prediction

Prediction: 3.25
Unit: mg/kg_body_weight/day
Mahalanobis Distance: 11.4
Mahalanobis Distance p-value: 0.000343

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Phenolphthalein	646	C.I. pigment red 3
Structure			
Actual Endpoint (-log C)	2.43468	0.937339	0.937339
Predicted Endpoint (-log C)	3.66084	3.26294	3.17837
Distance	0.596	0.686	0.725
Reference	CPDB	CPDB	CPDB

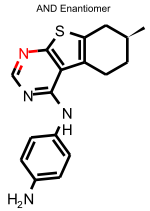
Model Applicability

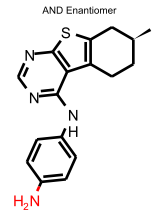
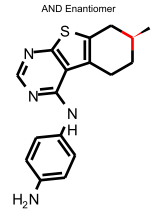
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: 292958156: [*]CC(C)C[*]
3. Unknown ECFP_2 feature: -1672647522: [*]C[c]1:s:[*]:[*]:[c]:1[*]
4. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]

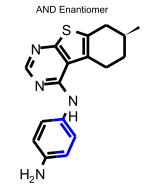
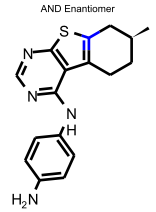
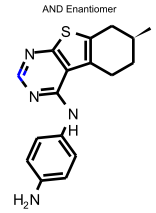
Feature Contribution

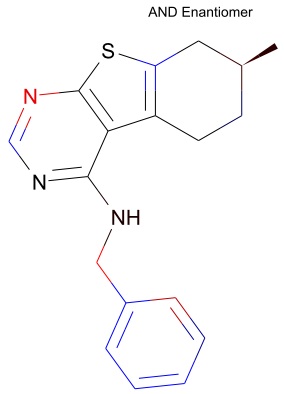
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	655739385	 [*]:n:[*]	0.229

ECFP_6	1572579716	 [*]N	0.225
ECFP_6	-167460056	 [*]C([*])[*]	0.0596

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	1996767644	 [*][c](:[*]):[cH]:[cH]:[*]	-0.251
ECFP_6	642810091	 [*][c](:[*]):[*]	-0.247
ECFP_6	-182236392	 [*]:[cH]:[*]	-0.232



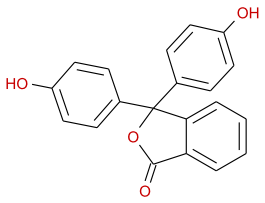
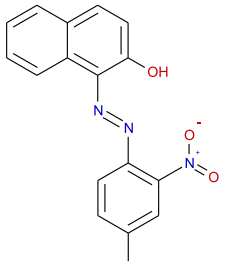
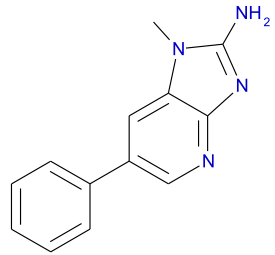
$C_{18}H_{19}N_3S$
Molecular Weight: 309.42856
ALogP: 4.678
Rotatable Bonds: 3
Acceptors: 3
Donors: 1

Model Prediction

Prediction: 4.81
Unit: mg/kg_body_weight/day
Mahalanobis Distance: 10.6
Mahalanobis Distance p-value: 0.00592

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Phenolphthalein	646	1077
Structure			
Actual Endpoint (-log C)	2.43468	0.937339	3.82962
Predicted Endpoint (-log C)	3.66084	3.26294	3.933
Distance	0.634	0.689	0.715
Reference	CPDB	CPDB	CPDB

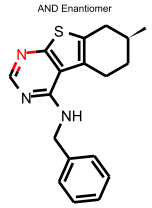
Model Applicability

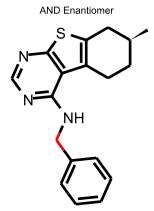
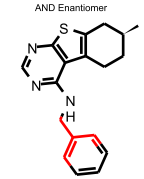
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: 292958156: [*]CC(C)C[*]
3. Unknown ECFP_2 feature: -1672647522: [*]C[c]1:s:[*]:[*]:[c]:1[*]
4. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]

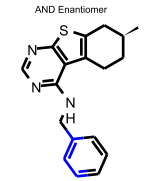
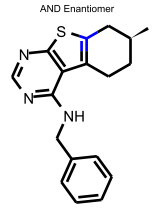
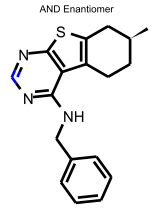
Feature Contribution

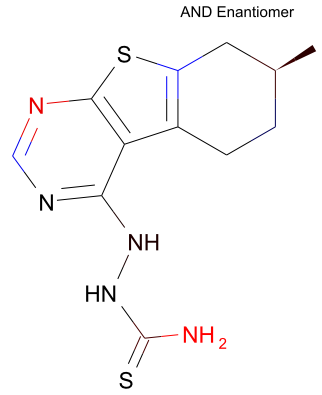
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	655739385	 [*]:n:[*]	0.229

ECFP_6	1559650422	 [*]C[*]	0.203
ECFP_6	-2024255407	 [*]C[c](:[cH]:[*]):[cH]:[*]	0.172

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	1996767644	 [*][c](:[*]):[cH]:[cH]:[*]	-0.251
ECFP_6	642810091	 [*][c](:[*]):[*]	-0.247
ECFP_6	-182236392	 [*]:[cH]:[*]	-0.232



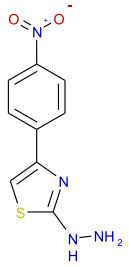
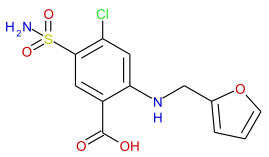
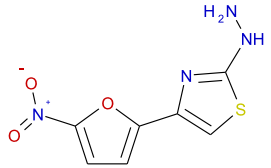
$C_{12}H_{15}N_5S_2$
Molecular Weight: 293.411
ALogP: 3.209
Rotatable Bonds: 3
Acceptors: 4
Donors: 3

Model Prediction

Prediction: 2.92
Unit: mg/kg_body_weight/day
Mahalanobis Distance: 12.9
Mahalanobis Distance p-value: 1.8e-007

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	2-Hydrazino-4-(p-nitrophenyl) thiazole	Furosemide	2-Hydrazino-4-(5-nitro-2-furyl) thi-azole
Structure			
Actual Endpoint (-log C)	4.34807	2.65498	4.13967
Predicted Endpoint (-log C)	4.37858	3.60472	4.34552
Distance	0.685	0.687	0.699
Reference	CPDB	CPDB	CPDB

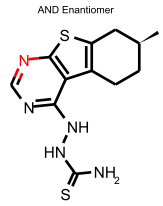
Model Applicability

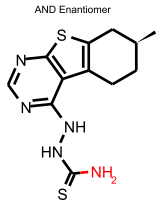
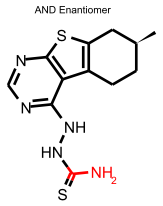
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: 292958156: [*]CC(C)C[*]
3. Unknown ECFP_2 feature: -1672647522: [*]C[c]1:s:[*]:[*]:[c]:1[*]
4. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
5. Unknown ECFP_2 feature: -571028867: [*]NC(=S)N

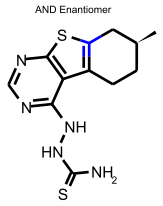
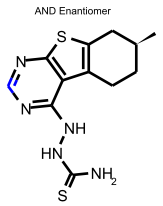
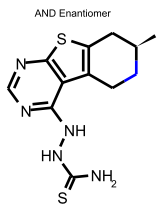
Feature Contribution

Top features for positive contribution

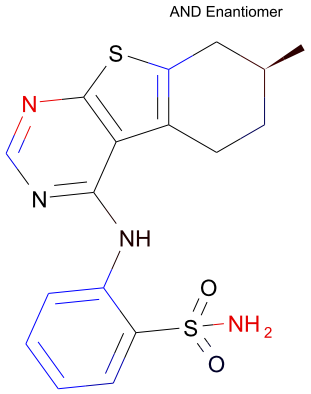
Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	655739385	 [*]:n:[*]	0.229

ECFP_6	1572579716	 [*]N	0.225
ECFP_6	-932108170	 [*]C(=[*])N	0.0784

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	642810091	 [*][c](:[*]):[*]	-0.247
ECFP_6	-182236392	 [*]:[cH]:[*]	-0.232
ECFP_6	-992506539	 [*]C[*]	-0.0852

TOPKAT_Carcinogenic_Potency_TD50_Mouse



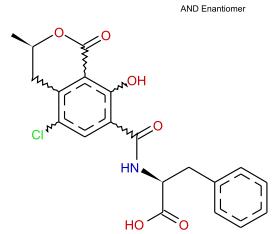
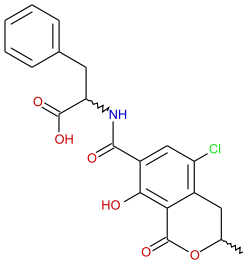
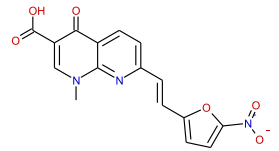
$C_{17}H_{18}N_4O_2S_2$
Molecular Weight: 374.48042
ALogP: 3.541
Rotatable Bonds: 3
Acceptors: 5
Donors: 2

Model Prediction

Prediction: 8.21
Unit: mg/kg_body_weight/day
Mahalanobis Distance: 13.1
Mahalanobis Distance p-value: 8.8e-008

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	542	Ochratoxin A	470
Structure			
Actual Endpoint (-log C)	4.79932	4.79932	4.62839
Predicted Endpoint (-log C)	3.6353	3.6353	3.93264
Distance	0.728	0.728	0.764
Reference	CPDB	CPDB	CPDB

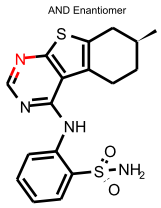
Model Applicability

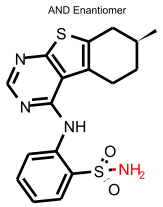
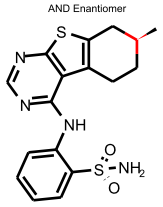
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: 292958156: [*]CC(C)C[*]
3. Unknown ECFP_2 feature: -1672647522: [*]C[c]1:s:[*]:[*]:[c]:1[*]
4. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]

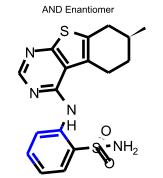
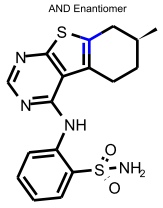
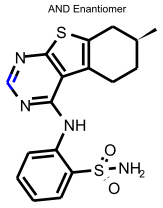
Feature Contribution

Top features for positive contribution

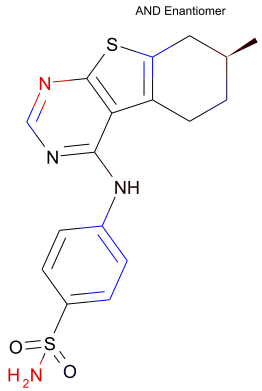
Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	655739385	 [*]:n:[*]	0.229

ECFP_6	1572579716	 [*]N	0.225
ECFP_6	-167460056	 [*]C([*])[*]	0.0596

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	1996767644	 [*][c](:[*]):[cH]:[cH]:[*]	-0.251
ECFP_6	642810091	 [*][c](:[*]):[*]	-0.247
ECFP_6	-182236392	 [*]:[cH]:[*]	-0.232

TOPKAT_Carcinogenic_Potency_TD50_Mouse



$C_{17}H_{18}N_4O_2S_2$

Molecular Weight: 374.48042

ALogP: 3.541

Rotatable Bonds: 3

Acceptors: 5

Donors: 2

Model Prediction

Prediction: 3.51

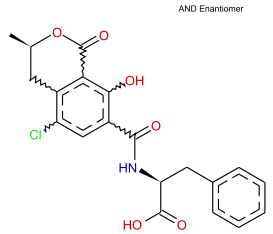
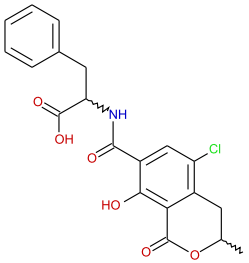
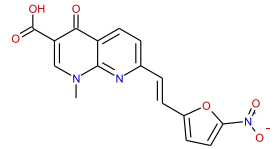
Unit: mg/kg_body_weight/day

Mahalanobis Distance: 12.9

Mahalanobis Distance p-value: 1.99e-007

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	542	Ochratoxin A	470
Structure			
Actual Endpoint (-log C)	4.79932	4.79932	4.62839
Predicted Endpoint (-log C)	3.6353	3.6353	3.93264
Distance	0.735	0.735	0.763
Reference	CPDB	CPDB	CPDB

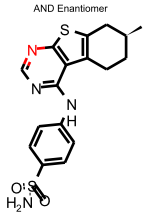
Model Applicability

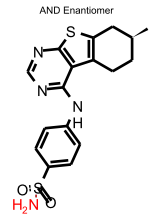
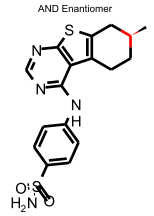
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: 292958156: [*]CC(C)C[*]
3. Unknown ECFP_2 feature: -1672647522: [*]C[c]1:s:[*]:[*]:[c]:1[*]
4. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]

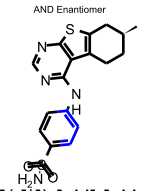
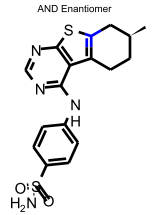
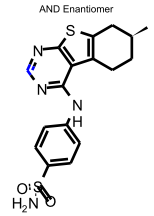
Feature Contribution

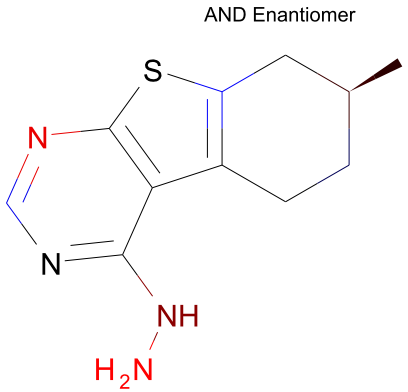
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	655739385	 [*]:n:[*]	0.229

ECFP_6	1572579716	 [*]N	0.225
ECFP_6	-167460056	 [*]C([*])[*]	0.0596

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	1996767644	 [*][c](:[*]):[cH]:[cH]:[*]	-0.251
ECFP_6	642810091	 [*][c](:[*]):[*]	-0.247
ECFP_6	-182236392	 [*]:[cH]:[*]	-0.232



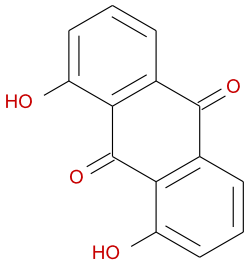
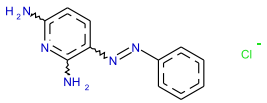
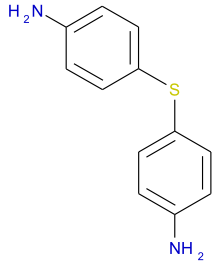
$C_{11}H_{14}N_4S$
Molecular Weight: 234.32065
ALogP: 2.561
Rotatable Bonds: 1
Acceptors: 4
Donors: 2

Model Prediction

Prediction: 2.64
Unit: mg/kg_body_weight/day
Mahalanobis Distance: 10.6
Mahalanobis Distance p-value: 0.00657

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Chrysazin	215	4,4´-Thiodianiline
Structure			
Actual Endpoint (-log C)	3.0774	3.477	3.81392
Predicted Endpoint (-log C)	3.07832	3.97642	3.72747
Distance	0.568	0.618	0.626
Reference	CPDB	CPDB	CPDB

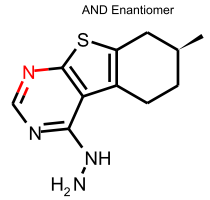
Model Applicability

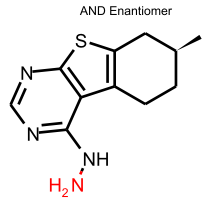
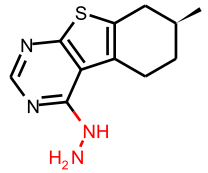
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: 292958156: [*]CC(C)C[*]
3. Unknown ECFP_2 feature: -1672647522: [*]C[c]1:s:[*]:[*]:[c]:1[*]
4. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]

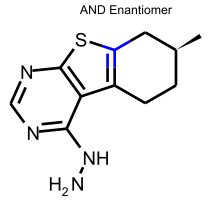
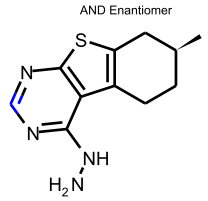
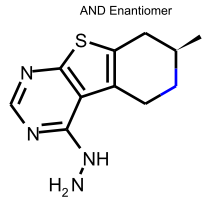
Feature Contribution

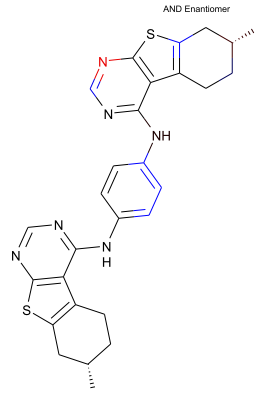
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	655739385	 [*]:n:[*]	0.229

ECFP_6	1572579716	 [*]N	0.225
ECFP_6	-934039951	 [*]NN	0.108

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	642810091	 [*][c](:[*]):[*]	-0.247
ECFP_6	-182236392	 [*]:[cH]:[*]	-0.232
ECFP_6	-992506539	 [*]C[*]	-0.0852



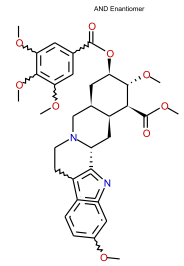
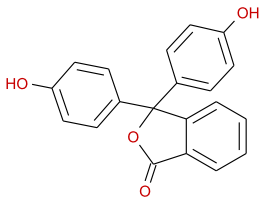
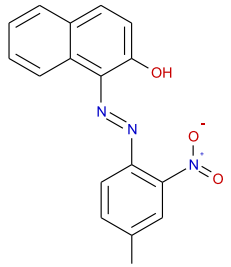
$C_{28}H_{28}N_6S_2$
Molecular Weight: 512.69212
ALogP: 7.842
Rotatable Bonds: 4
Acceptors: 6
Donors: 2

Model Prediction

Prediction: 0.169
Unit: mg/kg_body_weight/day
Mahalanobis Distance: 13.8
Mahalanobis Distance p-value: 1.09e-009

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	223	Phenolphthalein	646
Structure			
Actual Endpoint (-log C)	5.08368	2.43468	0.937339
Predicted Endpoint (-log C)	5.08273	3.66084	3.26294
Distance	1.084	1.139	1.147
Reference	CPDB	CPDB	CPDB

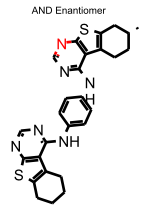
Model Applicability

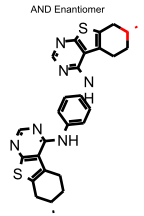
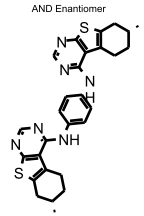
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: 292958156: [*]CC(C)C[*]
3. Unknown ECFP_2 feature: -1672647522: [*]C[c]1:s:[*]:[*]:[c]:1[*]
4. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]

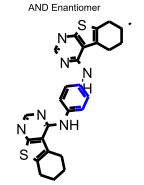
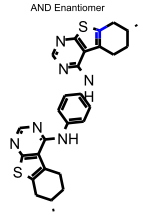
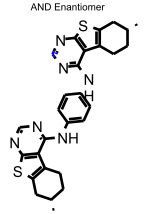
Feature Contribution

Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	655739385	 [*]:n:[*]	0.229

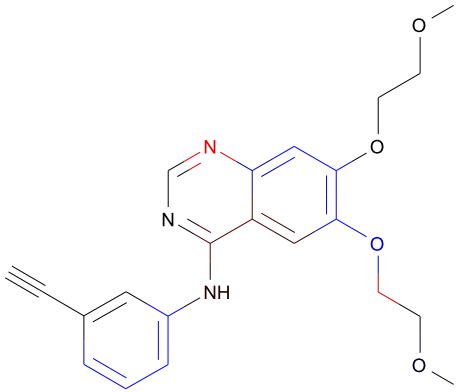
ECFP_6	-167460056	 [*]C([*])[*]	0.0596
ECFP_6	734603939	 [*]C	0.0424

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	1996767644	 [*][c](:[*]):[cH]:[cH]:[*]	-0.251
ECFP_6	642810091	 [*][c](:[*]):[*]	-0.247
ECFP_6	-182236392	 [*]:[cH]:[*]	-0.232

Erlotinib

TOPKAT_Carcinogenic_Potency_TD50_Mouse



$C_{22}H_{23}N_3O_4$

Molecular Weight: 393.43572

ALogP: 4.309

Rotatable Bonds: 10

Acceptors: 7

Donors: 1

Model Prediction

Prediction: 39.8

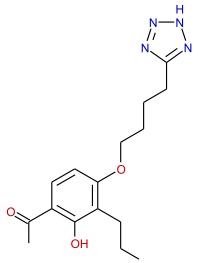
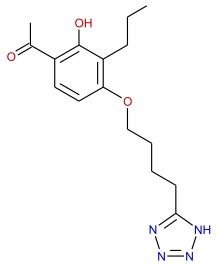
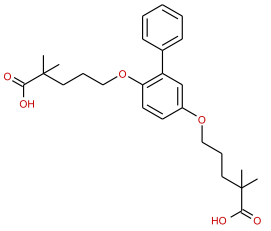
Unit: mg/kg_body_weight/day

Mahalanobis Distance: 16.1

Mahalanobis Distance p-value: 1.15e-016

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Compound LY171883	832	5,5´-(1,1´-Biphenyl)-2,5-dyl-bis (oxy)(2,2-dimethylpentanoic acid)
Structure			
Actual Endpoint (-log C)	3.45372	3.45372	3.90166
Predicted Endpoint (-log C)	2.84749	2.80429	2.75893
Distance	0.772	0.782	0.796
Reference	CPDB	CPDB	CPDB

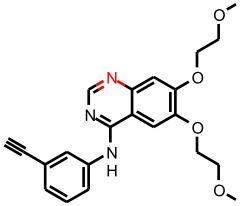
Model Applicability

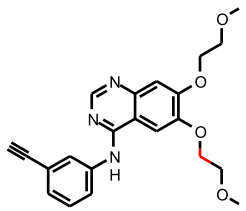
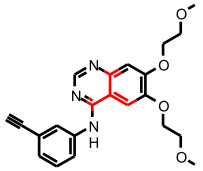
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

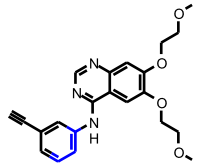
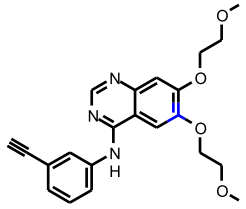
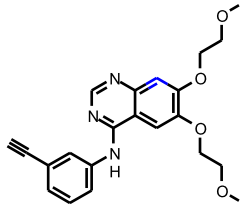
1. OPS PC13 out of range. Value: -3.2209. Training min, max, SD, explained variance: -3.068, 3.6909, 1.329, 0.0220.
2. Unknown ECFP_2 feature: -182178874: [*]#C[c](:c:[*]):c:[*]
3. Unknown ECFP_2 feature: 1139738044: [*]:[c](:[*])C#C
4. Unknown ECFP_2 feature: -1253653003: [*]COC

Feature Contribution

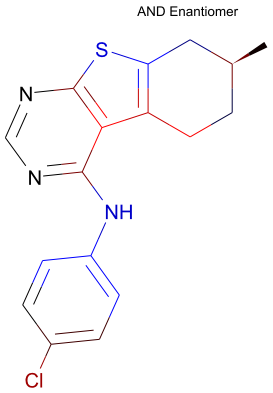
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	655739385	 [*]:n:[*]	0.229

ECFP_6	1559650422	 [*]C[*]	0.203
ECFP_6	1333660716	 [*][c](:[*]):[c](:[cH]:[*]):[c](:[*]):[*]	0.0746

Top Features for negative contribution			
Fingerprint	**Bit/Smiles**	**Feature Structure**	**Score**
ECFP_6	1996767644	 [*][c](:[*]):[cH]:[cH]:[*]	-0.251
ECFP_6	642810091	 [*][c](:[*]):[*]	-0.247
ECFP_6	-182236392	 [*]:[cH]:[*]	-0.232

TOPKAT_Carcinogenic_Potency_TD50_Rat



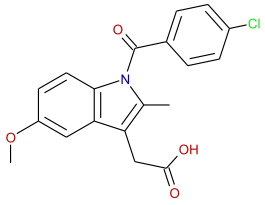
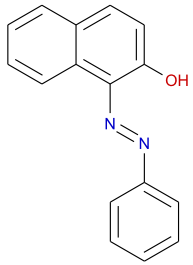
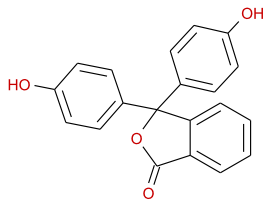
$C_{17}H_{16}ClN_3S$
Molecular Weight: 329.84704
ALogP: 5.5
Rotatable Bonds: 2
Acceptors: 3
Donors: 1

Model Prediction

Prediction: 3.75
Unit: mg/kg_body_weight/day
Mahalanobis Distance: 18.1
Mahalanobis Distance p-value: 1.65e-021

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Indomethacin	45	Phenolphthalein
Structure			
Actual Endpoint (-log C)	5.49293	3.92659	2.54766
Predicted Endpoint (-log C)	4.9569	3.28325	3.7508
Distance	0.621	0.646	0.651
Reference	CPDB	CPDB	CPDB

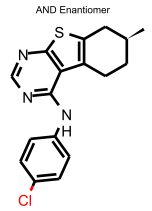
Model Applicability

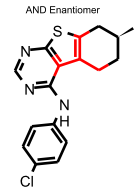
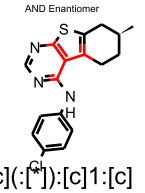
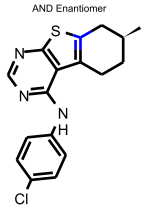
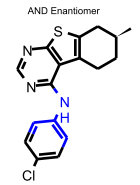
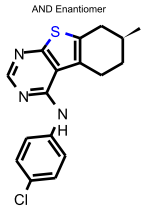
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

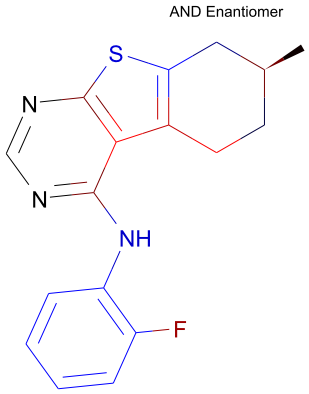
1. All properties and OPS components are within expected ranges.

Feature Contribution

Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_6	32	 [*]Cl	0.154

FCFP_6	203677720	 [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.137
FCFP_6	307419094	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.121
Top Features for negative contribution			
Fingerprint	**Bit/Smiles**	**Feature Structure**	**Score**
FCFP_6	16	 [*][c](:[*]):[*]	-0.354
FCFP_6	590925877	 [*]N[c](:[cH]:[*]):[cH]:[*]	-0.323
FCFP_6	17	 [*]:s:[*]	-0.149



$C_{17}H_{16}FN_3S$

Molecular Weight: 313.39244

ALogP: 5.041

Rotatable Bonds: 2

Acceptors: 3

Donors: 1

Model Prediction

Prediction: 10.5

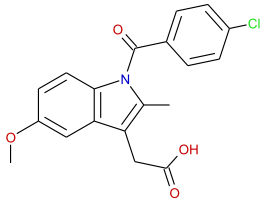
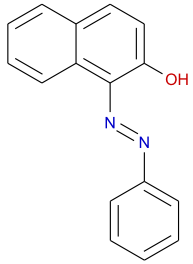
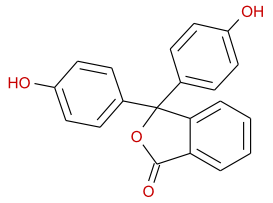
Unit: mg/kg_body_weight/day

Mahalanobis Distance: 18.6

Mahalanobis Distance p-value: 1.03e-023

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Indomethacin	45	Phenolphthalein
Structure			
Actual Endpoint (-log C)	5.49293	3.92659	2.54766
Predicted Endpoint (-log C)	4.9569	3.28325	3.7508
Distance	0.627	0.628	0.630
Reference	CPDB	CPDB	CPDB

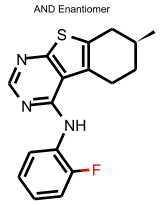
Model Applicability

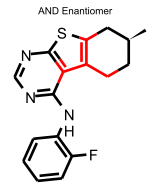
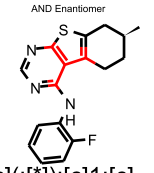
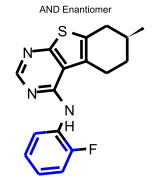
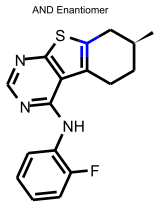
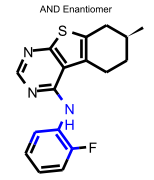
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

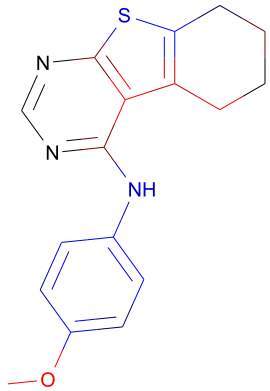
1. All properties and OPS components are within expected ranges.

Feature Contribution

Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_6	32	 [*]Cl	0.154

FCFP_6	203677720	 [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.137
FCFP_6	307419094	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.121
Top Features for negative contribution			
Fingerprint	**Bit/Smiles**	**Feature Structure**	**Score**
FCFP_6	991735244	 [*][c]1:[*]:[cH]:[cH]:[cH]:[cH]:1	-0.422
FCFP_6	16	 [*][c](:[*]):[*]	-0.354
FCFP_6	590925877	 [*]N[c](:[cH]:[*]):[cH]:[*]	-0.323



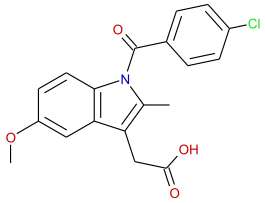
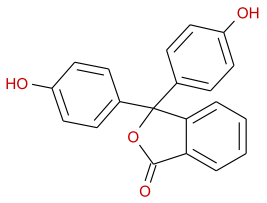
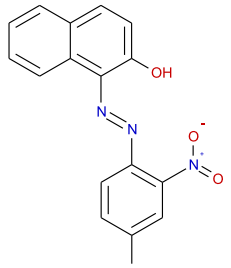
$C_{17}H_{17}N_3OS$
Molecular Weight: 311.40138
ALogP: 4.568
Rotatable Bonds: 3
Acceptors: 4
Donors: 1

Model Prediction

Prediction: 1.42
Unit: mg/kg_body_weight/day
Mahalanobis Distance: 16.7
Mahalanobis Distance p-value: 1.26e-016

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Indomethacin	Phenolphthalein	646
Structure			
Actual Endpoint (-log C)	5.49293	2.54766	2.41938
Predicted Endpoint (-log C)	4.9569	3.7508	3.77987
Distance	0.556	0.608	0.627
Reference	CPDB	CPDB	CPDB

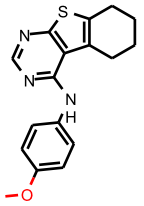
Model Applicability

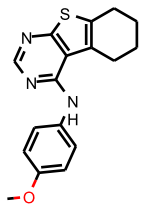
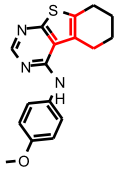
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

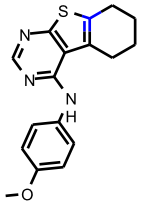
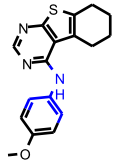
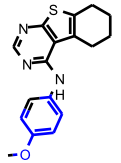
Feature Contribution

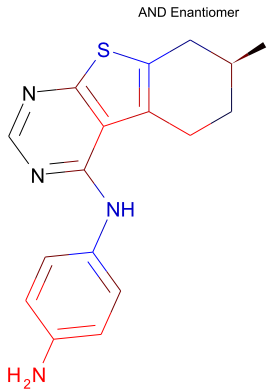
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_6	136627117	 [*]OC	0.69

FCFP_6	1	 [*]O[*]	0.234
FCFP_6	203677720	 [*]C[c]1:[c]([*]):[*] :[*]:[c]:1:[*]	0.137

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_6	16	 [*][c](:[*]):[*]	-0.354
FCFP_6	590925877	 [*]N[c](:[cH]:[*]):[c H]:[*]	-0.323
FCFP_6	1674451008	 [*]O[c]1:[cH]:[*]:[c] ([*]):[cH]:[cH]:1	-0.233



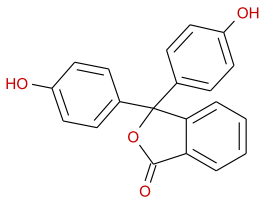
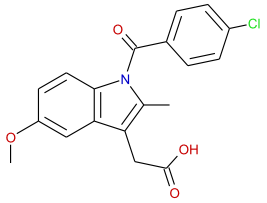
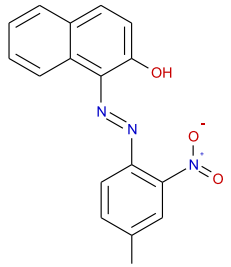
$C_{17}H_{18}N_4S$
Molecular Weight: 310.41662
ALogP: 4.089
Rotatable Bonds: 2
Acceptors: 4
Donors: 2

Model Prediction

Prediction: 2.42
Unit: mg/kg_body_weight/day
Mahalanobis Distance: 16.1
Mahalanobis Distance p-value: 1.25e-014

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Phenolphthalein	Indomethacin	646
Structure			
Actual Endpoint (-log C)	2.54766	5.49293	2.41938
Predicted Endpoint (-log C)	3.7508	4.9569	3.77987
Distance	0.570	0.664	0.682
Reference	CPDB	CPDB	CPDB

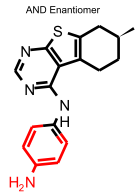
Model Applicability

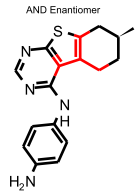
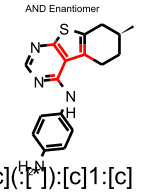
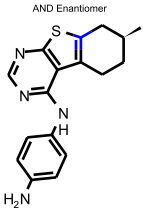
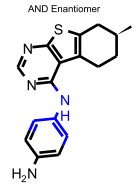
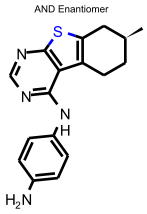
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

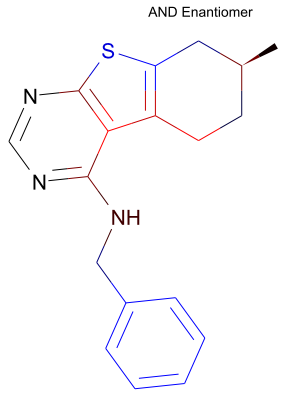
1. All properties and OPS components are within expected ranges.

Feature Contribution

Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_6	-1247245120	 N[c]1:[cH]:[cH]:[*]:[cH]:[cH]:1	0.375

FCFP_6	203677720	 [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.137
FCFP_6	307419094	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.121
Top Features for negative contribution			
Fingerprint	**Bit/Smiles**	**Feature Structure**	**Score**
FCFP_6	16	 [*][c](:[*]):[*]	-0.354
FCFP_6	590925877	 [*]N[c](:[cH]:[*]):[cH]:[*]	-0.323
FCFP_6	17	 [*]:s:[*]	-0.149



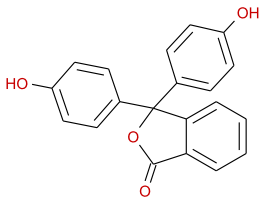
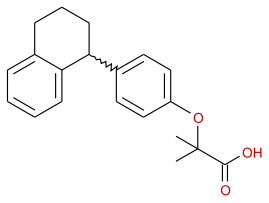
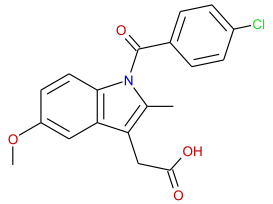
$C_{18}H_{19}N_3S$
Molecular Weight: 309.42856
ALogP: 4.678
Rotatable Bonds: 3
Acceptors: 3
Donors: 1

Model Prediction

Prediction: 29.9
Unit: mg/kg_body_weight/day
Mahalanobis Distance: 17.2
Mahalanobis Distance p-value: 3.34e-018

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Phenolphthalein	Nafenopin s	Indomethacin
Structure			
Actual Endpoint (-log C)	2.54766	4.45051	5.49293
Predicted Endpoint (-log C)	3.7508	3.8403	4.9569
Distance	0.613	0.617	0.622
Reference	CPDB	CPDB	CPDB

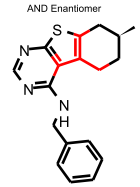
Model Applicability

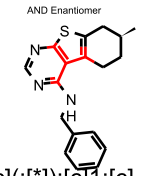
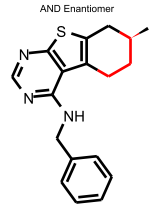
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

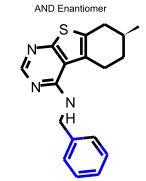
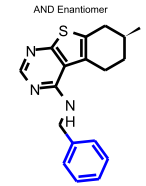
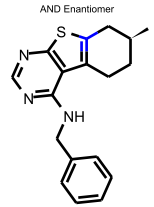
Feature Contribution

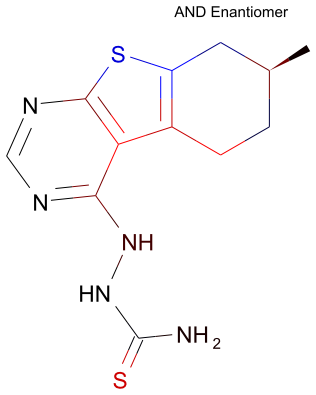
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_6	203677720	 [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.137

FCFP_6	307419094	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.121
FCFP_6	-1272798659	 [*]CCC([*])[*]	0.11

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_6	991735244	 [*][c]1:[*]:[cH]:[cH]:[cH]:[cH]:1	-0.422
FCFP_6	-2093839777	 [*][c]1:[cH]:[cH]:[cH]:[cH]:[cH]:1	-0.378
FCFP_6	16	 [*][c](:[*]):[*]	-0.354



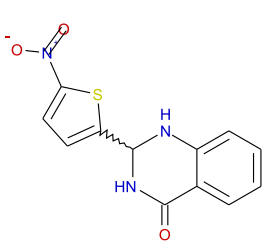
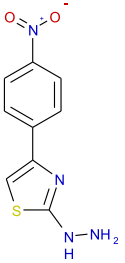
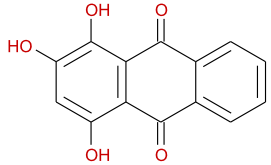
$C_{12}H_{15}N_5S_2$
Molecular Weight: 293.411
ALogP: 3.209
Rotatable Bonds: 3
Acceptors: 4
Donors: 3

Model Prediction

Prediction: 10
Unit: mg/kg_body_weight/day
Mahalanobis Distance: 15.5
Mahalanobis Distance p-value: 1.05e-012

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	1,2-Dihydro-2-(5-nitro-2-thi-enyl) quinazolin-4(3H)-one	2-Hydrazino-4-(p-nitrophenyl) thiazole	Purpurin
Structure			
Actual Endpoint (-log C)	5.25509	4.86687	2.57737
Predicted Endpoint (-log C)	3.89291	5.14723	3.49183
Distance	0.622	0.670	0.681
Reference	CPDB	CPDB	CPDB

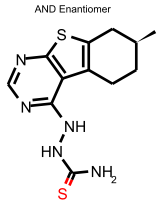
Model Applicability

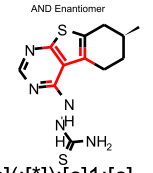
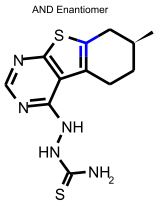
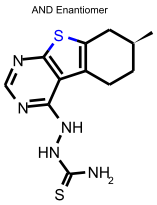
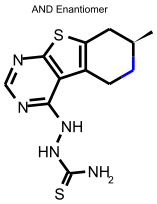
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

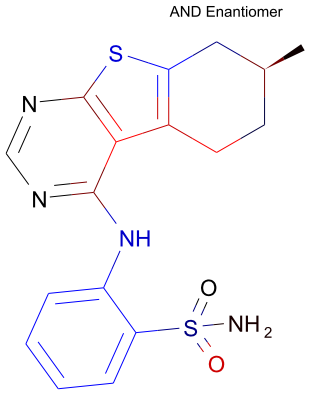
Feature Contribution

Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_6	1	 [*]O[*]	0.234

FCFP_6	203677720	 [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.137
FCFP_6	307419094	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.121
Top Features for negative contribution			
Fingerprint	**Bit/Smiles**	**Feature Structure**	**Score**
FCFP_6	16	 [*][c](:[*]):[*]	-0.354
FCFP_6	17	 [*]:s:[*]	-0.149
FCFP_6	0	 [*]C[*]	-0.115

TOPKAT_Carcinogenic_Potency_TD50_Rat



$C_{17}H_{18}N_4O_2S_2$

Molecular Weight: 374.48042

ALogP: 3.541

Rotatable Bonds: 3

Acceptors: 5

Donors: 2

Model Prediction

Prediction: 29.3

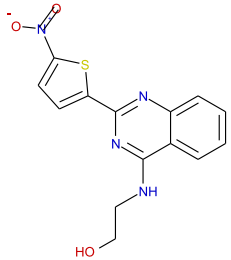
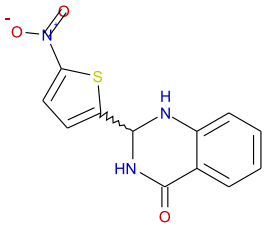
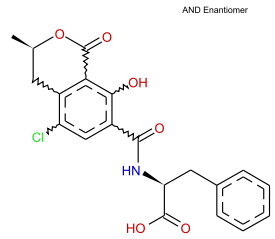
Unit: mg/kg_body_weight/day

Mahalanobis Distance: 17

Mahalanobis Distance p-value: 1.11e-017

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	4-(2-Hydroxyethylamino)-2-(5-nitro-2-thienyl)quinazoline	1,2-Dihydro-2-(5-nitro-2-thi-enyl) quinazolin-4(3H)-one	542
Structure			
Actual Endpoint (-log C)	5.22831	5.25509	6.59334
Predicted Endpoint (-log C)	4.31976	3.89291	5.06501
Distance	0.622	0.662	0.693
Reference	CPDB	CPDB	CPDB

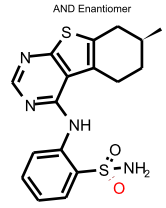
Model Applicability

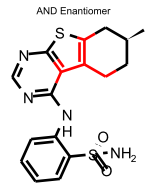
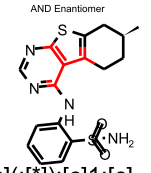
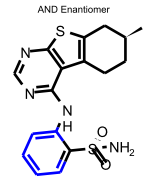
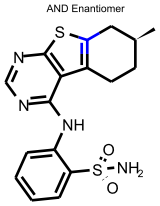
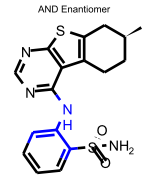
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

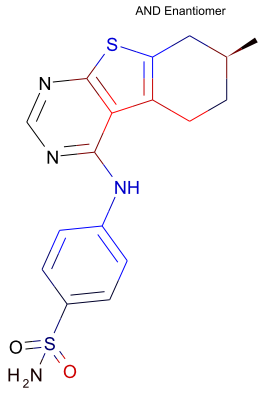
1. All properties and OPS components are within expected ranges.

Feature Contribution

Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_6	1	 [*]O[*]	0.234

FCFP_6	203677720	 [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.137
FCFP_6	307419094	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.121
Top Features for negative contribution			
Fingerprint	**Bit/Smiles**	**Feature Structure**	**Score**
FCFP_6	991735244	 [*][c]1:[*]:[cH]:[cH]:[cH]:[cH]:1	-0.422
FCFP_6	16	 [*][c](:[*]):[*]	-0.354
FCFP_6	590925877	 [*]N[c](:[cH]:[*]):[cH]:[*]	-0.323



$C_{17}H_{18}N_4O_2S_2$

Molecular Weight: 374.48042

ALogP: 3.541

Rotatable Bonds: 3

Acceptors: 5

Donors: 2

Model Prediction

Prediction: 10.7

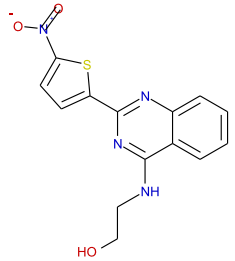
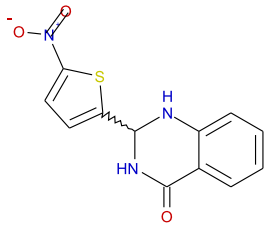
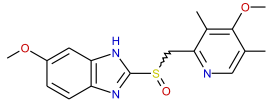
Unit: mg/kg_body_weight/day

Mahalanobis Distance: 16.8

Mahalanobis Distance p-value: 4.07e-017

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	4-(2-Hydroxyethylamino)-2-(5-nitro-2-thienyl)quinazoline	1,2-Dihydro-2-(5-nitro-2-thi-enyl) quinazolin-4(3H)-one	Omeprazole
Structure			
Actual Endpoint (-log C)	5.22831	5.25509	3.4628
Predicted Endpoint (-log C)	4.31976	3.89291	4.7324
Distance	0.626	0.678	0.701
Reference	CPDB	CPDB	CPDB

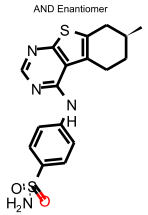
Model Applicability

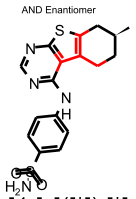
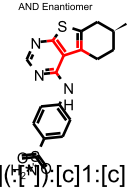
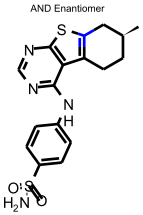
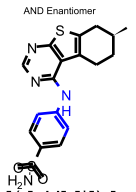
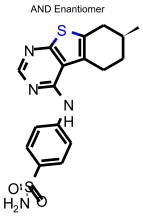
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

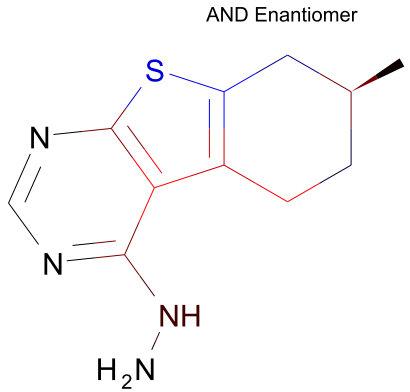
1. All properties and OPS components are within expected ranges.

Feature Contribution

Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_6	1	 [*]O[*]	0.234

FCFP_6	203677720	 [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.137
FCFP_6	307419094	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.121
Top Features for negative contribution			
Fingerprint	**Bit/Smiles**	**Feature Structure**	**Score**
FCFP_6	16	 [*][c](:[*]):[*]	-0.354
FCFP_6	590925877	 [*]N[c](:[cH]:[*]):[cH]:[*]	-0.323
FCFP_6	17	 [*]:s:[*]	-0.149



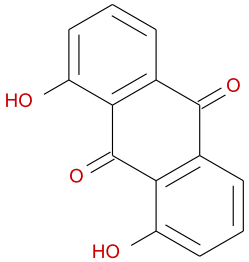
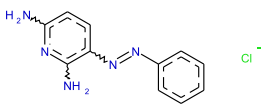
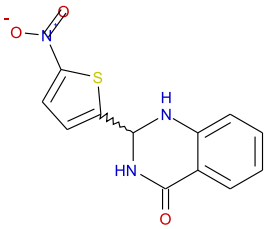
$C_{11}H_{14}N_4S$
Molecular Weight: 234.32065
ALogP: 2.561
Rotatable Bonds: 1
Acceptors: 4
Donors: 2

Model Prediction

Prediction: 9.15
Unit: mg/kg_body_weight/day
Mahalanobis Distance: 16
Mahalanobis Distance p-value: 2.28e-014

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	Chrysazin	215	1,2-Dihydro-2-(5-nitro-2-thi-enyl) quinazolin-4(3H)-one
Structure			
Actual Endpoint (-log C)	2.99143	2.84742	5.25509
Predicted Endpoint (-log C)	3.29868	3.32496	3.89291
Distance	0.552	0.594	0.604
Reference	CPDB	CPDB	CPDB

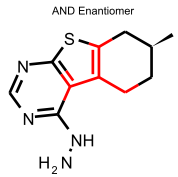
Model Applicability

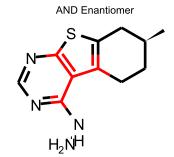
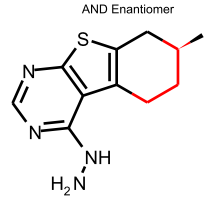
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

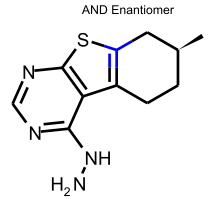
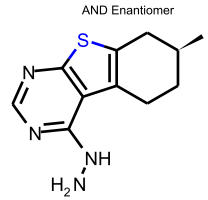
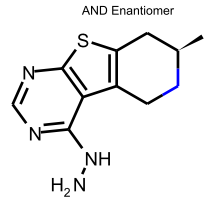
Feature Contribution

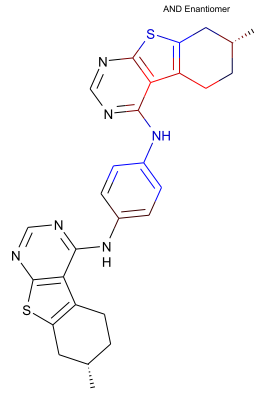
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_6	203677720	 [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.137

FCFP_6	307419094	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.121
FCFP_6	-1272798659	 [*]CCC([*])[*]	0.11

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_6	16	 [*][c](:[*]):[*]	-0.354
FCFP_6	17	 [*]:s:[*]	-0.149
FCFP_6	0	 [*]C[*]	-0.115



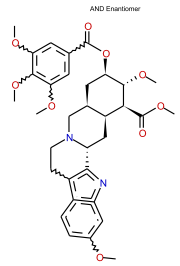
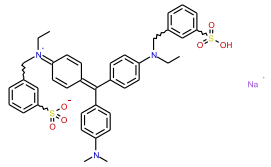
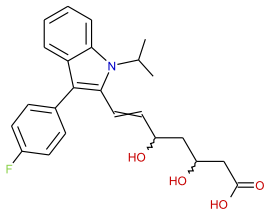
$C_{28}H_{28}N_6S_2$
Molecular Weight: 512.69212
ALogP: 7.842
Rotatable Bonds: 4
Acceptors: 6
Donors: 2

Model Prediction

Prediction: 0.347
Unit: mg/kg_body_weight/day
Mahalanobis Distance: 18.2
Mahalanobis Distance p-value: 4.61e-022

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	223	411	Fluvastatin
Structure			
Actual Endpoint (-log C)	6.29867	3.06566	3.51742
Predicted Endpoint (-log C)	7.5657	4.8672	5.41573
Distance	1.050	1.054	1.066
Reference	CPDB	CPDB	CPDB

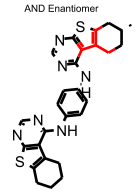
Model Applicability

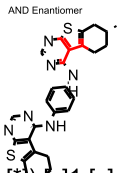
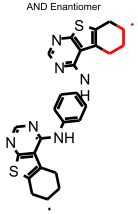
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.

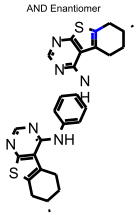
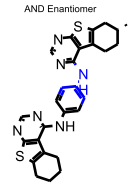
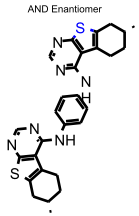
Feature Contribution

Top features for positive contribution

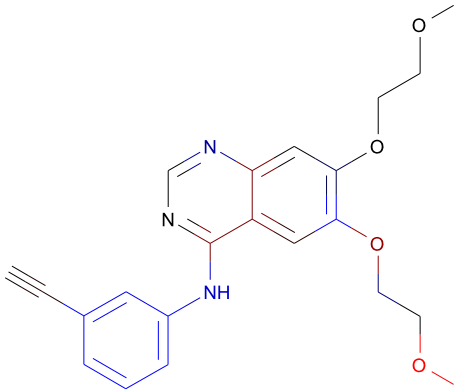
Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_6	203677720	 [*]C[c]1:[c]([*]):[*] :[*]:[c]:1:[*]	0.137

FCFP_6	307419094	 [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	0.121
FCFP_6	-1272798659	 [*]CCC([*])[*]	0.11

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_6	16	 [*][c](:[*]):[*]	-0.354
FCFP_6	590925877	 [*]N[c](:[cH]:[*]):[cH]:[*]	-0.323
FCFP_6	17	 [*]:s:[*]	-0.149

Erlotinib



$C_{22}H_{23}N_3O_4$

Molecular Weight: 393.43572

ALogP: 4.309

Rotatable Bonds: 10

Acceptors: 7

Donors: 1

Model Prediction

Prediction: 8.06

Unit: mg/kg_body_weight/day

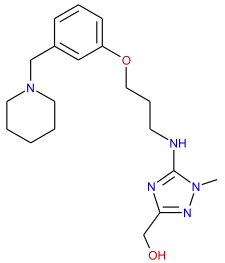
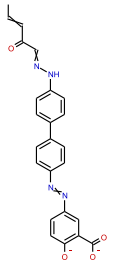
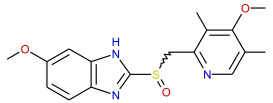
Mahalanobis Distance: 17.7

Mahalanobis Distance p-value: 3.99e-020

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

TOPKAT_Carcinogenic_Potency_TD50_Rat

Structural Similar Compounds

Name	Loxtidine	C.I. direct brown 95	Omeprazole
Structure			
Actual Endpoint (-log C)	2.87532	5.31387	3.4628
Predicted Endpoint (-log C)	3.63996	4.30266	4.7324
Distance	0.685	0.715	0.741
Reference	CPDB	CPDB	CPDB

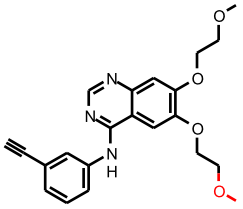
Model Applicability

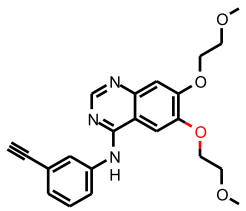
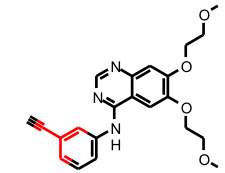
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: 902193919: [*]:[c](:[*])C#C

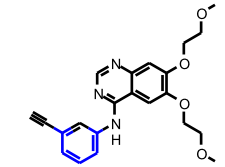
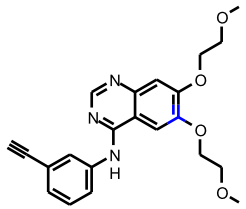
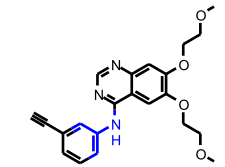
Feature Contribution

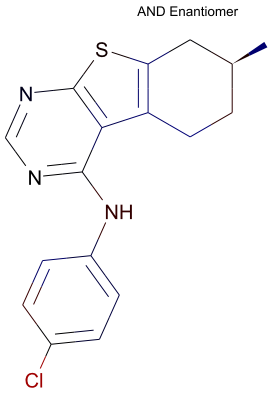
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_6	136627117	 [*]OC	0.69

FCFP_6	1	 [*]O[*]	0.234
FCFP_6	203677720	 [*]C[c]1:[c]([*]):[*] :[*]:[c]:1:[*]	0.137

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_6	991735244	 [*][c]1:[*]:[cH]:[cH] :[cH]:[cH]:1	-0.422
FCFP_6	16	 [*][c](:[*]):[*]	-0.354
FCFP_6	590925877	 [*]N[c](:[cH]:[*]):[c H]:[*]	-0.323



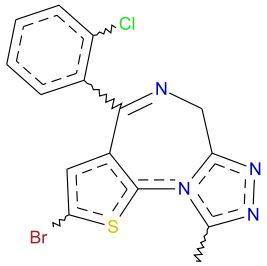
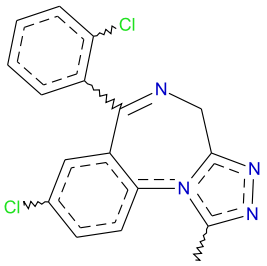
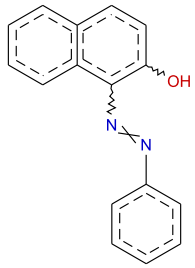
$C_{17}H_{16}ClN_3S$
Molecular Weight: 329.84704
ALogP: 5.5
Rotatable Bonds: 2
Acceptors: 3
Donors: 1

Model Prediction

Prediction: 0.0375
Unit: g/kg_body_weight
Mahalanobis Distance: 33.7
Mahalanobis Distance p-value: 2.01e-031

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	BROTIZOLAM	TRIAZOLAM	C.I. SOLVENT YELLOW 14
Structure			
Actual Endpoint (-log C)	2.99309	3.83659	4.298
Predicted Endpoint (-log C)	3.70649	3.85527	3.36361
Distance	0.589	0.593	0.615
Reference	ARZNEI.FORSCH.36.592. 1986	UPJ-33030	NTP REPORT # 226

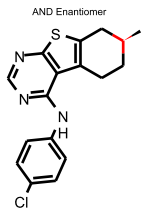
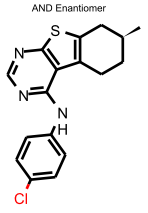
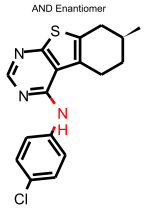
Model Applicability

Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

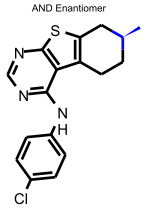
1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_6 feature: 914325265: [*]:s:[*]
3. Unknown ECFP_6 feature: 292958156: [*]CC(C)C[*]
4. Unknown ECFP_6 feature: 53207596: [*]C([*])C[c](:[*]):[*]
5. Unknown ECFP_6 feature: -1672647522: [*]C[c]1:s:[*]:[*]:[c]:1[*]
6. Unknown ECFP_6 feature: -1660340418: [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]
7. Unknown ECFP_6 feature: 51876938: [*]CC[c](:[*]):[*]
8. Unknown ECFP_6 feature: 85262808: [*][c]1:[*]:[*]:[c](:[*]):s:1
9. Unknown ECFP_6 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
10. Unknown ECFP_6 feature: -1661653144: [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]
11. Unknown ECFP_6 feature: 865482986: [*]C([*])C
12. Unknown ECFP_6 feature: -677309799: [*]:[cH]:n:[c](:[*]):[*]
13. Unknown ECFP_6 feature: -710237522: [*]:n:[cH]:n:[*]
14. Unknown ECFP_6 feature: 1049768340: [*]N[c](:n:[*]):[c](:[*]):[*]
15. Unknown ECFP_6 feature: -1242906247: [*]:[c](:[*])N[c](:[*]):[*]
16. Unknown ECFP_6 feature: -177077903: [*]N[c](:[cH]:[*]):[cH]:[*]
17. Unknown ECFP_6 feature: -176494269: [*]:[cH]:[c](Cl):[cH]:[*]
18. Unknown ECFP_6 feature: 99947387: [*]:[c](:[*])Cl

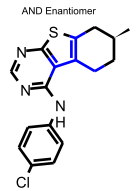
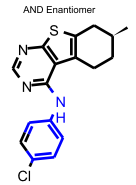
Feature Contribution

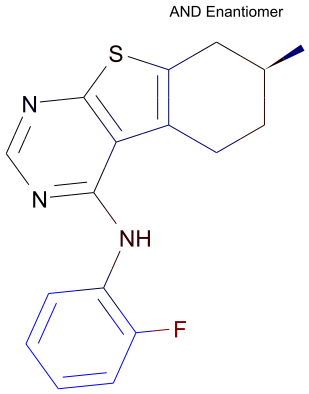
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	-167460056	 [*]C([*])[*]	0.136
FCFP_6	32	 [*]Cl	0.101
FCFP_6	3	 [*]N[*]	0.0924

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_6	136597326	 [*]C([*])C	-0.0815

FCFP_6	203677720	 [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.0713
FCFP_6	-773983804	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	-0.0589



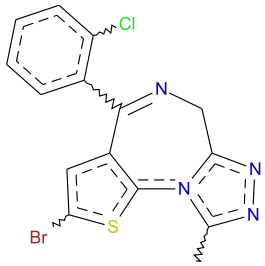
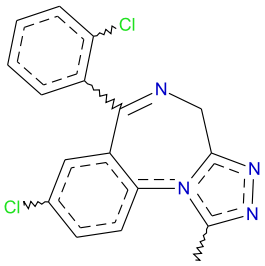
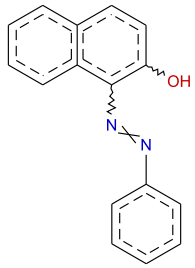
$C_{17}H_{16}FN_3S$
Molecular Weight: 313.39244
ALogP: 5.041
Rotatable Bonds: 2
Acceptors: 3
Donors: 1

Model Prediction

Prediction: 0.0746
Unit: g/kg_body_weight
Mahalanobis Distance: 33.4
Mahalanobis Distance p-value: 9.75e-031

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	BROTIZOLAM	TRIAZOLAM	C.I. SOLVENT YELLOW 14
Structure			
Actual Endpoint (-log C)	2.99309	3.83659	4.298
Predicted Endpoint (-log C)	3.70649	3.85527	3.36361
Distance	0.577	0.582	0.586
Reference	ARZNEI.FORSCH.36.592. 1986	UPJ-33030	NTP REPORT # 226

Model Applicability

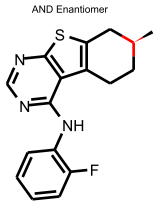
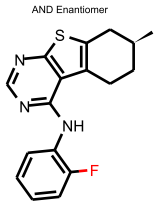
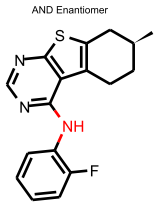
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_6 feature: 914325265: [*]:s:[*]
3. Unknown ECFP_6 feature: -1046436026: [*]F
4. Unknown ECFP_6 feature: 292958156: [*]CC(C)C[*]
5. Unknown ECFP_6 feature: 53207596: [*]C([*])C[c](:[*]):[*]
6. Unknown ECFP_6 feature: -1672647522: [*]C[c]1:s:[*]:[*]:[c]:1[*]
7. Unknown ECFP_6 feature: -1660340418: [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]
8. Unknown ECFP_6 feature: 51876938: [*]CC[c](:[*]):[*]
9. Unknown ECFP_6 feature: 85262808: [*][c]1:[*]:[*]:[c](:[*]):s:1
10. Unknown ECFP_6 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
11. Unknown ECFP_6 feature: -1661653144: [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]
12. Unknown ECFP_6 feature: 865482986: [*]C([*])C
13. Unknown ECFP_6 feature: -677309799: [*]:[cH]:n:[c](:[*]):[*]
14. Unknown ECFP_6 feature: -710237522: [*]:n:[cH]:n:[*]
15. Unknown ECFP_6 feature: 1049768340: [*]N[c](:n:[*]):[c](:[*]):[*]
16. Unknown ECFP_6 feature: -1242906247: [*]:[c](:[*])N[c](:[*]):[*]
17. Unknown ECFP_6 feature: 1335108269: [*]N[c](:[cH]:[*]):[c]([*]):[*]
18. Unknown ECFP_6 feature: -1311285389: [*][c](:[*]):[c](F):[cH]:[*]
19. Unknown ECFP_6 feature: 1997021792: [*]:[cH]:[cH]:[cH]:[*]

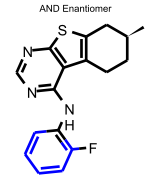
20.	Unknown ECFP_6 feature: 220735655: [*]:[c](:[*])F

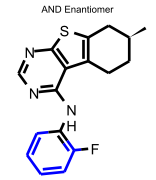
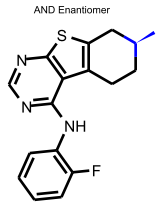
Feature Contribution

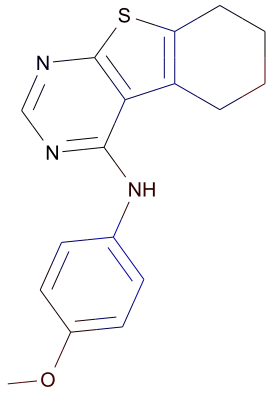
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	-167460056	 [*]C([*])[*]	0.136
FCFP_6	32	 [*]Cl	0.101
FCFP_6	3	 [*]N[*]	0.0924

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_6	991735244	 [*][c]1:[*]:[cH]:[cH] :[cH]:[cH]:1	-0.134

ECFP_6	1564392544	 [*][c]1:[*]:[cH]:[cH] :[cH]:[cH]:1	-0.133
FCFP_6	136597326	 [*]C([*])C	-0.0815



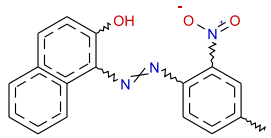
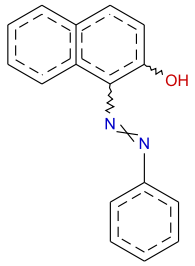
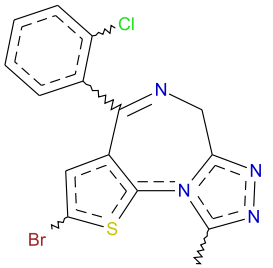
$C_{17}H_{17}N_3OS$
Molecular Weight: 311.40138
ALogP: 4.568
Rotatable Bonds: 3
Acceptors: 4
Donors: 1

Model Prediction

Prediction: 0.0486
Unit: g/kg_body_weight
Mahalanobis Distance: 31.8
Mahalanobis Distance p-value: 7.04e-028

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	C.I. PIGMENT RED 3	C.I. SOLVENT YELLOW 14	BROTIZOLAM
Structure			
Actual Endpoint (-log C)	3.0252	4.298	2.99309
Predicted Endpoint (-log C)	3.34768	3.36361	3.70649
Distance	0.548	0.614	0.619
Reference	NTP REPORT # 407	NTP REPORT # 226	ARZNEI.FORSCH.36.592. 1986

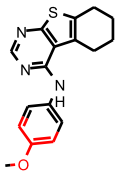
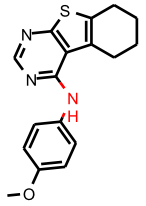
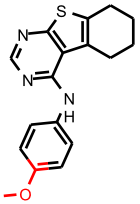
Model Applicability

Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

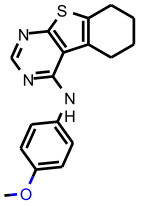
1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_6 feature: 914325265: [*]:s:[*]
3. Unknown ECFP_6 feature: -1332781180: [*]CCC[*]
4. Unknown ECFP_6 feature: 51876938: [*]CC[c](:[*]):[*]
5. Unknown ECFP_6 feature: -1672647522: [*]C[c]1:s:[*]:[*]:[c]:1[*]
6. Unknown ECFP_6 feature: -1660340418: [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]
7. Unknown ECFP_6 feature: 85262808: [*][c]1:[*]:[*]:[c](:[*]):s:1
8. Unknown ECFP_6 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
9. Unknown ECFP_6 feature: -1661653144: [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]
10. Unknown ECFP_6 feature: -677309799: [*]:[cH]:n:[c](:[*]):[*]
11. Unknown ECFP_6 feature: -710237522: [*]:n:[cH]:n:[*]
12. Unknown ECFP_6 feature: 1049768340: [*]N[c](:n:[*]):[c](:[*]):[*]
13. Unknown ECFP_6 feature: -1242906247: [*]:[c](:[*])N[c](:[*]):[*]
14. Unknown ECFP_6 feature: -177077903: [*]N[c](:[cH]:[*]):[cH]:[*]
15. Unknown ECFP_6 feature: 1307307440: [*]:[c](:[*])OC

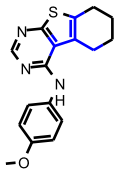
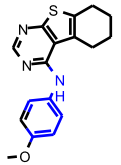
Feature Contribution

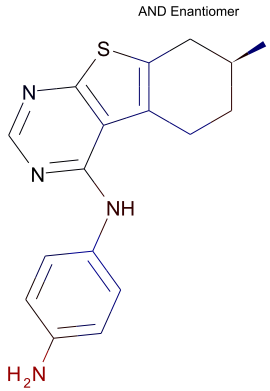
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	-176455838	 [*]O[c](:[cH]:[*]):[cH]:[*]	0.106
FCFP_6	3	 [*]N[*]	0.0924
FCFP_6	1036089772	 [*]:[c](:[*])OC	0.073

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_6	1	 [*]O[*]	-0.102

FCFP_6	203677720	 [*]C[c]1:[c]([*]):[*] :[*]:[c]:1:[*]	-0.0713
FCFP_6	-773983804	 [*]N[c]1:[cH]:[*]:[c] ([*]):[cH]:[cH]:1	-0.0589



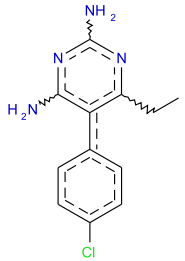
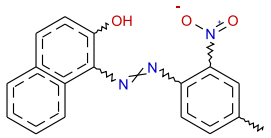
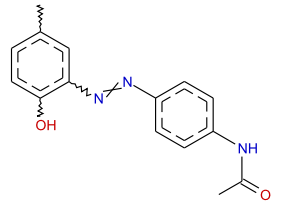
$C_{17}H_{18}N_4S$
Molecular Weight: 310.41662
ALogP: 4.089
Rotatable Bonds: 2
Acceptors: 4
Donors: 2

Model Prediction

Prediction: 0.063
Unit: g/kg_body_weight
Mahalanobis Distance: 33.1
Mahalanobis Distance p-value: 3.04e-030

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

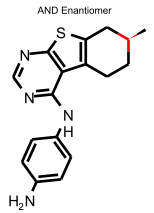
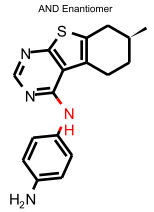
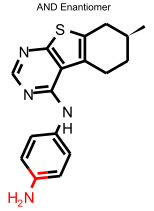
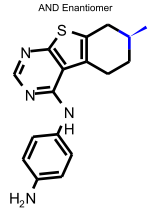
Name	PYRIMETHAMINE	C.I. PIGMENT RED 3	HC BLUE 1
Structure			
Actual Endpoint (-log C)	3.99776	3.0252	3.0323
Predicted Endpoint (-log C)	4.25218	3.34768	2.7171
Distance	0.619	0.621	0.653
Reference	NTP 77 55	NTP REPORT # 407	NTP REPORT # 222

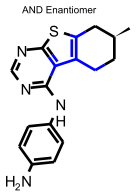
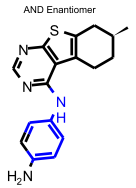
Model Applicability

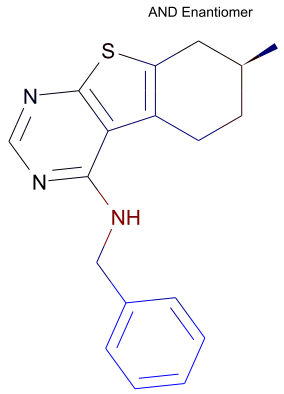
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_6 feature: 914325265: [*]:s:[*]
3. Unknown ECFP_6 feature: 292958156: [*]CC(C)C[*]
4. Unknown ECFP_6 feature: 53207596: [*]C([*])C[c](:[*]):[*]
5. Unknown ECFP_6 feature: -1672647522: [*]C[c]1:s:[*]:[*]:[c]:1[*]
6. Unknown ECFP_6 feature: -1660340418: [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]
7. Unknown ECFP_6 feature: 51876938: [*]CC[c](:[*]):[*]
8. Unknown ECFP_6 feature: 85262808: [*][c]1:[*]:[*]:[c](:[*]):s:1
9. Unknown ECFP_6 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
10. Unknown ECFP_6 feature: -1661653144: [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]
11. Unknown ECFP_6 feature: 865482986: [*]C([*])C
12. Unknown ECFP_6 feature: -677309799: [*]:[cH]:n:[c](:[*]):[*]
13. Unknown ECFP_6 feature: -710237522: [*]:n:[cH]:n:[*]
14. Unknown ECFP_6 feature: 1049768340: [*]N[c](:n:[*]):[c](:[*]):[*]
15. Unknown ECFP_6 feature: -1242906247: [*]:[c](:[*])N[c](:[*]):[*]
16. Unknown ECFP_6 feature: -177077903: [*]N[c](:[cH]:[*]):[cH]:[*]
17. Unknown ECFP_6 feature: 971820502: [*]:[cH]:[c](N):[cH]:[*]
18. Unknown ECFP_6 feature: -938530932: [*]:[c](:[*])N

Feature Contribution

Top features for positive contribution			
Fingerprint	**Bit/Smiles**	**Feature Structure**	**Score**
ECFP_6	-167460056	 [*]C([*])[*]	0.136
FCFP_6	3	 [*]N[*]	0.0924
FCFP_6	1069584379	 [*]:[c](:[*])N	0.0717
Top Features for negative contribution			
Fingerprint	**Bit/Smiles**	**Feature Structure**	**Score**
FCFP_6	136597326	 [*]C([*])C	-0.0815

FCFP_6	203677720	 [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.0713
FCFP_6	-773983804	 [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	-0.0589



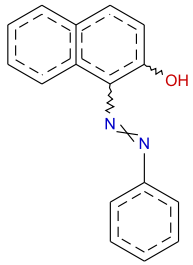
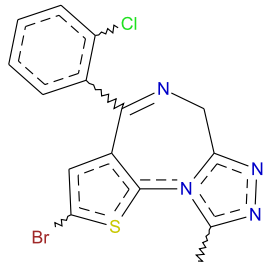
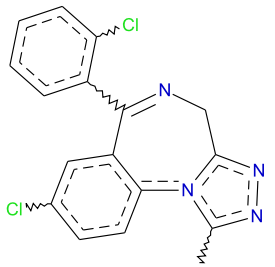
$C_{18}H_{19}N_3S$
Molecular Weight: 309.42856
ALogP: 4.678
Rotatable Bonds: 3
Acceptors: 3
Donors: 1

Model Prediction

Prediction: 0.0709
Unit: g/kg_body_weight
Mahalanobis Distance: 34.6
Mahalanobis Distance p-value: 5.26e-033

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

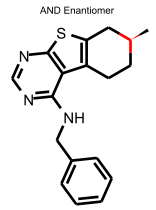
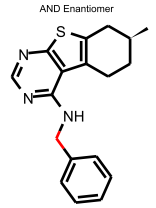
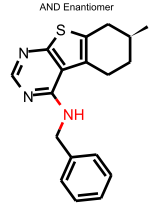
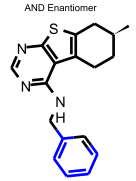
Name	C.I. SOLVENT YELLOW 14	BROTIZOLAM	TRIAZOLAM
Structure			
Actual Endpoint (-log C)	4.298	2.99309	3.83659
Predicted Endpoint (-log C)	3.36361	3.70649	3.85527
Distance	0.589	0.597	0.605
Reference	NTP REPORT # 226	ARZNEI.FORSCH.36.592. 1986	UPJ-33030

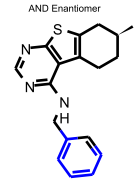
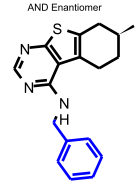
Model Applicability

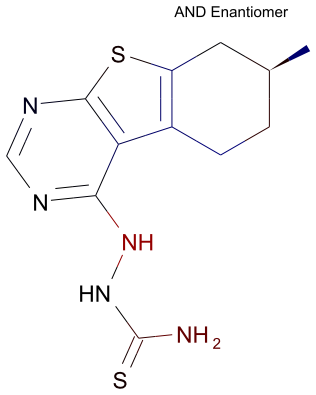
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_6 feature: 914325265: [*]:s:[*]
3. Unknown ECFP_6 feature: 292958156: [*]CC(C)C[*]
4. Unknown ECFP_6 feature: 53207596: [*]C([*])C[c](:[*]):[*]
5. Unknown ECFP_6 feature: -1672647522: [*]C[c]1:s:[*]:[*]:[c]:1[*]
6. Unknown ECFP_6 feature: -1660340418: [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]
7. Unknown ECFP_6 feature: 51876938: [*]CC[c](:[*]):[*]
8. Unknown ECFP_6 feature: 85262808: [*][c]1:[*]:[*]:[c](:[*]):s:1
9. Unknown ECFP_6 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
10. Unknown ECFP_6 feature: -1661653144: [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]
11. Unknown ECFP_6 feature: 865482986: [*]C([*])C
12. Unknown ECFP_6 feature: -677309799: [*]:[cH]:n:[c](:[*]):[*]
13. Unknown ECFP_6 feature: -710237522: [*]:n:[cH]:n:[*]
14. Unknown ECFP_6 feature: 1049768340: [*]N[c](:n:[*]):[c](:[*]):[*]
15. Unknown ECFP_6 feature: 491100606: [*]CN[c](:[*]):[*]
16. Unknown ECFP_6 feature: 769925792: [*]NC[c](:[*]):[*]
17. Unknown ECFP_6 feature: 1997021792: [*]:[cH]:[cH]:[cH]:[*]

Feature Contribution

Top features for positive contribution			
Fingerprint	**Bit/Smiles**	**Feature Structure**	**Score**
ECFP_6	-167460056	 [*]C([*])[*]	0.136
ECFP_6	1559650422	 [*]C[*]	0.129
FCFP_6	3	 [*]N[*]	0.0924
Top Features for negative contribution			
Fingerprint	**Bit/Smiles**	**Feature Structure**	**Score**
FCFP_6	991735244	 [*][c]1:[*]:[cH]:[cH]:[cH]:[cH]:1	-0.134

ECFP_6	1564392544	 [*][c]1:[*]:[cH]:[cH]:[cH]:[cH]:1	-0.133
FCFP_6	-1698724694	 [*]C[c]1:[cH]:[cH]:[cH]:[cH]:[cH]:1	-0.0944



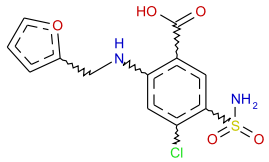
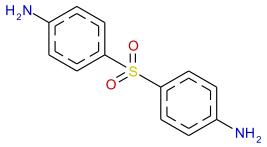
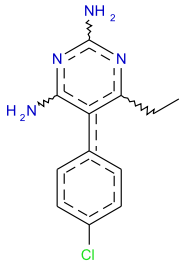
$C_{12}H_{15}N_5S_2$
Molecular Weight: 293.411
ALogP: 3.209
Rotatable Bonds: 3
Acceptors: 4
Donors: 3

Model Prediction

Prediction: 0.122
Unit: g/kg_body_weight
Mahalanobis Distance: 31.9
Mahalanobis Distance p-value: 5.05e-028

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	FUROSEMIDE	DAPSONE	PYRIMETHAMINE
Structure			
Actual Endpoint (-log C)	4.27645	3.6168	3.99776
Predicted Endpoint (-log C)	4.40005	3.43657	4.25218
Distance	0.623	0.702	0.707
Reference	NTP REPORT # 356	NTP 20 47	NTP 77 55

Model Applicability

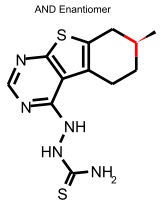
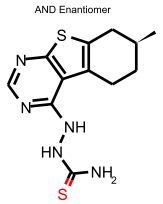
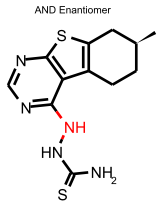
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. OPS PC31 out of range. Value: 5.3583. Training min, max, SD, explained variance: -4.0208, 4.2529, 1.246, 0.0068.
2. Unknown FCFP_2 feature: 1294344583: [*]NN[c](:[*]):[*]
3. Unknown ECFP_6 feature: 914325265: [*]:s:[*]
4. Unknown ECFP_6 feature: 292958156: [*]CC(C)C[*]
5. Unknown ECFP_6 feature: 53207596: [*]C([*])C[c](:[*]):[*]
6. Unknown ECFP_6 feature: -1672647522: [*]C[c]1:s:[*]:[*]:[c]:1[*]
7. Unknown ECFP_6 feature: -1660340418: [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]
8. Unknown ECFP_6 feature: 51876938: [*]CC[c](:[*]):[*]
9. Unknown ECFP_6 feature: 85262808: [*][c]1:[*]:[*]:[c](:[*]):s:1
10. Unknown ECFP_6 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
11. Unknown ECFP_6 feature: -1661653144: [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]
12. Unknown ECFP_6 feature: 865482986: [*]C([*])C
13. Unknown ECFP_6 feature: -677309799: [*]:[cH]:n:[c](:[*]):[*]
14. Unknown ECFP_6 feature: -710237522: [*]:n:[cH]:n:[*]
15. Unknown ECFP_6 feature: 1049768340: [*]N[c](:n:[*]):[c](:[*]):[*]
16. Unknown ECFP_6 feature: -1238415266: [*]NN[c](:[*]):[*]
17. Unknown ECFP_6 feature: 1635339976: [*]NNC(=[*])[*]
18. Unknown ECFP_6 feature: -571028867: [*]NC(=S)N
19. Unknown ECFP_6 feature: -932108170: [*]C(=[*])N

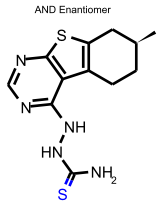
20. Unknown ECFP_6 feature: 1979182050: [*]C(=S)[*]

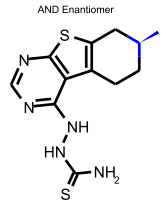
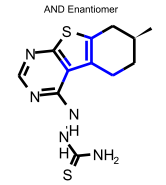
Feature Contribution

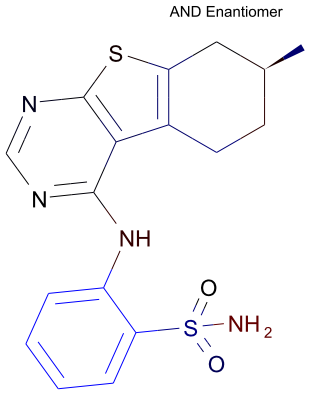
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	-167460056	 [*]C([*])[*]	0.136
ECFP_6	-845108448	 [*]=S	0.105
FCFP_6	3	 [*]N[*]	0.0924

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_6	1	 [*]O[*]	-0.102

FCFP_6	136597326	 [*]C([*])C	-0.0815
FCFP_6	203677720	 [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.0713



$C_{17}H_{18}N_4O_2S_2$

Molecular Weight: 374.48042

ALogP: 3.541

Rotatable Bonds: 3

Acceptors: 5

Donors: 2

Model Prediction

Prediction: 0.323

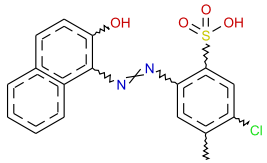
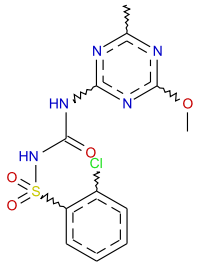
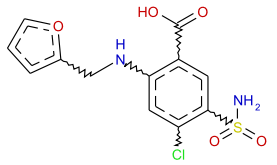
Unit: g/kg_body_weight

Mahalanobis Distance: 35.3

Mahalanobis Distance p-value: 3.24e-034

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	D & C RED 9	CHLORSULFURON	FUROSEMIDE
Structure			
Actual Endpoint (-log C)	3.87715	4.15566	4.27645
Predicted Endpoint (-log C)	3.6546	3.79771	4.40005
Distance	0.600	0.628	0.669
Reference	NTP REPORT # 225	EPA COVER SHEET 0027;880301;(1)	NTP REPORT # 356

Model Applicability

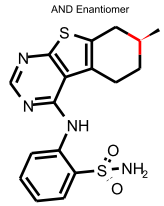
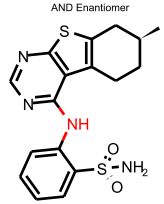
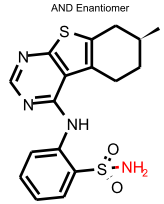
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_6 feature: 914325265: [*]:s:[*]
3. Unknown ECFP_6 feature: -797085356: [*]S(=[*])(=[*])[*]
4. Unknown ECFP_6 feature: 292958156: [*]CC(C)C[*]
5. Unknown ECFP_6 feature: 53207596: [*]C([*])C[c](:[*]):[*]
6. Unknown ECFP_6 feature: -1672647522: [*]C[c]1:s:[*]:[*]:[c]:1[*]
7. Unknown ECFP_6 feature: -1660340418: [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]
8. Unknown ECFP_6 feature: 51876938: [*]CC[c](:[*]):[*]
9. Unknown ECFP_6 feature: 85262808: [*][c]1:[*]:[*]:[c](:[*]):s:1
10. Unknown ECFP_6 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
11. Unknown ECFP_6 feature: -1661653144: [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]
12. Unknown ECFP_6 feature: 865482986: [*]C([*])C
13. Unknown ECFP_6 feature: -677309799: [*]:[cH]:n:[c](:[*]):[*]
14. Unknown ECFP_6 feature: -710237522: [*]:n:[cH]:n:[*]
15. Unknown ECFP_6 feature: 1049768340: [*]N[c](:n:[*]):[c](:[*]):[*]
16. Unknown ECFP_6 feature: -1242906247: [*]:[c](:[*])N[c](:[*]):[*]
17. Unknown ECFP_6 feature: 1335108269: [*]N[c](:[cH]:[*]):[c]([*]):[*]
18. Unknown ECFP_6 feature: 1997021792: [*]:[cH]:[cH]:[cH]:[*]
19. Unknown ECFP_6 feature: 1755253401: [*][c](:[*]):[c](:[cH]:[*])S(=[*])(=[*])[*]

20. Unknown ECFP_6 feature: -2121766239: [*]:[c](:[*])S(=O)(=O)N
21. Unknown ECFP_6 feature: 2102150379: [*]S(=[*])(=O)[*]
22. Unknown ECFP_6 feature: -934226723: [*]S(=[*])(=[*])N

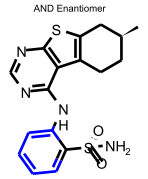
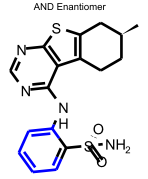
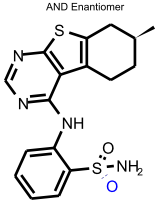
Feature Contribution

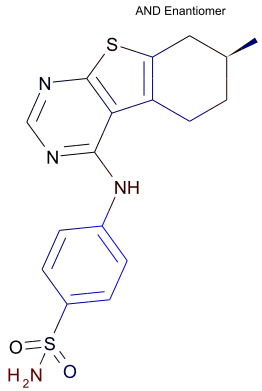
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	-167460056	 [*]C([*])[*]	0.136
FCFP_6	3	 [*]N[*]	0.0924
ECFP_6	1572579716	 [*]N	0.0576

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score

FCFP_6	991735244	 [*][c]1:[*]:[cH]:[cH]:[cH]:[cH]:1	-0.134
ECFP_6	1564392544	 [*][c]1:[*]:[cH]:[cH]:[cH]:[cH]:1	-0.133
FCFP_6	1	 [*]O[*]	-0.102



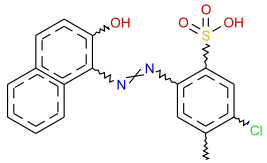
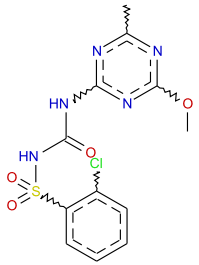
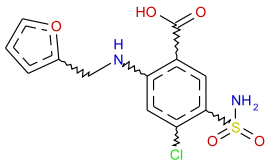
$C_{17}H_{18}N_4O_2S_2$
Molecular Weight: 374.48042
ALogP: 3.541
Rotatable Bonds: 3
Acceptors: 5
Donors: 2

Model Prediction

Prediction: 0.177
Unit: g/kg_body_weight
Mahalanobis Distance: 35.6
Mahalanobis Distance p-value: 1.1e-034

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	D & C RED 9	CHLORSULFURON	FUROSEMIDE
Structure			
Actual Endpoint (-log C)	3.87715	4.15566	4.27645
Predicted Endpoint (-log C)	3.6546	3.79771	4.40005
Distance	0.609	0.641	0.680
Reference	NTP REPORT # 225	EPA COVER SHEET 0027;880301;(1)	NTP REPORT # 356

Model Applicability

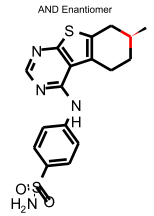
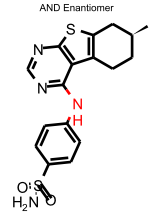
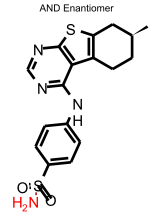
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. OPS PC8 out of range. Value: -5.7967. Training min, max, SD, explained variance: -5.7428, 7.3359, 2.68, 0.0314.
2. Unknown ECFP_6 feature: 914325265: [*]:s:[*]
3. Unknown ECFP_6 feature: -797085356: [*]S(=[*])(=[*])[*]
4. Unknown ECFP_6 feature: 292958156: [*]CC(C)C[*]
5. Unknown ECFP_6 feature: 53207596: [*]C([*])C[c](:[*]):[*]
6. Unknown ECFP_6 feature: -1672647522: [*]C[c]1:s:[*]:[*]:[c]:1[*]
7. Unknown ECFP_6 feature: -1660340418: [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]
8. Unknown ECFP_6 feature: 51876938: [*]CC[c](:[*]):[*]
9. Unknown ECFP_6 feature: 85262808: [*][c]1:[*]:[*]:[c](:[*]):s:1
10. Unknown ECFP_6 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
11. Unknown ECFP_6 feature: -1661653144: [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]
12. Unknown ECFP_6 feature: 865482986: [*]C([*])C
13. Unknown ECFP_6 feature: -677309799: [*]:[cH]:n:[c](:[*]):[*]
14. Unknown ECFP_6 feature: -710237522: [*]:n:[cH]:n:[*]
15. Unknown ECFP_6 feature: 1049768340: [*]N[c](:n:[*]):[c](:[*]):[*]
16. Unknown ECFP_6 feature: -1242906247: [*]:[c](:[*])N[c](:[*]):[*]
17. Unknown ECFP_6 feature: -177077903: [*]N[c](:[cH]:[*]):[cH]:[*]
18. Unknown ECFP_6 feature: -177264675: [*]S(=[*])(=[*])[c](:[cH]:[*]):[cH]:[*]

19. Unknown ECFP_6 feature: -2121766239: [*]:[c](:[*])S(=O)(=O)N
20. Unknown ECFP_6 feature: 2102150379: [*]S(=[*])(=O)[*]
21. Unknown ECFP_6 feature: -934226723: [*]S(=[*])(=[*])N

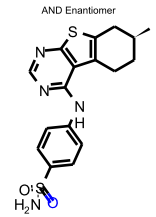
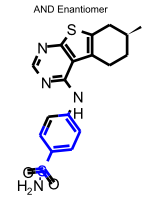
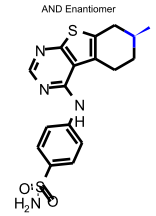
Feature Contribution

Top features for positive contribution

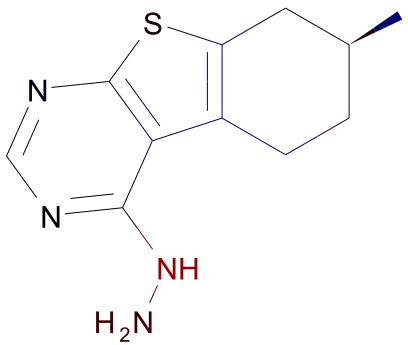
Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	-167460056	 [*]C([*])[*]	0.136
FCFP_6	3	 [*]N[*]	0.0924
ECFP_6	1572579716	 [*]N	0.0576

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score

FCFP_6	1	 [*]O[*]	-0.102
FCFP_6	-453677277	 [*]C[c]1:[cH]:[*]:[cH]:[cH]:[cH]:1	-0.0906
FCFP_6	136597326	 [*]C([*])C	-0.0815

AND Enantiomer



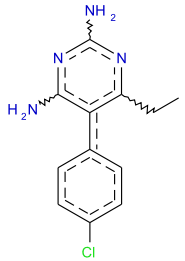
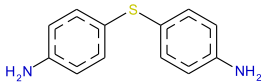
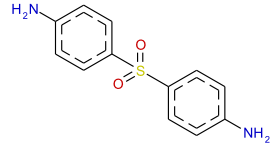
$C_{11}H_{14}N_4S$
Molecular Weight: 234.32065
ALogP: 2.561
Rotatable Bonds: 1
Acceptors: 4
Donors: 2

Model Prediction

Prediction: 0.129
Unit: g/kg_body_weight
Mahalanobis Distance: 36.4
Mahalanobis Distance p-value: 4.74e-036

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	PYRIMETHAMINE	4;4'-THIODIANILINE	DAPSONE
Structure			
Actual Endpoint (-log C)	3.99776	3.46	3.6168
Predicted Endpoint (-log C)	4.25218	3.46805	3.43657
Distance	0.465	0.532	0.559
Reference	NTP 77 55	NTP 47 VIII	NTP 20 47

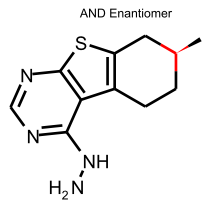
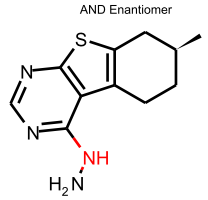
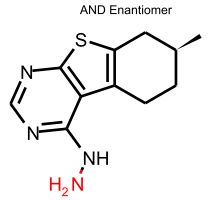
Model Applicability

Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

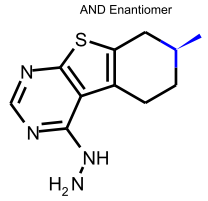
1. OPS PC31 out of range. Value: 4.3094. Training min, max, SD, explained variance: -4.0208, 4.2529, 1.246, 0.0068.
2. Unknown FCFP_2 feature: 1294344583: [*]NN[c](:[*]):[*]
3. Unknown FCFP_2 feature: 1070150408: [*]NN
4. Unknown ECFP_6 feature: 914325265: [*]:s:[*]
5. Unknown ECFP_6 feature: 292958156: [*]CC(C)C[*]
6. Unknown ECFP_6 feature: 53207596: [*]C([*])C[c](:[*]):[*]
7. Unknown ECFP_6 feature: -1672647522: [*]C[c]1:s:[*]:[*]:[c]:1[*]
8. Unknown ECFP_6 feature: -1660340418: [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]
9. Unknown ECFP_6 feature: 51876938: [*]CC[c](:[*]):[*]
10. Unknown ECFP_6 feature: 85262808: [*][c]1:[*]:[*]:[c](:[*]):s:1
11. Unknown ECFP_6 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
12. Unknown ECFP_6 feature: -1661653144: [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]
13. Unknown ECFP_6 feature: 865482986: [*]C([*])C
14. Unknown ECFP_6 feature: -677309799: [*]:[cH]:n:[c](:[*]):[*]
15. Unknown ECFP_6 feature: -710237522: [*]:n:[cH]:n:[*]
16. Unknown ECFP_6 feature: 1049768340: [*]N[c](:n:[*]):[c](:[*]):[*]
17. Unknown ECFP_6 feature: -136863293: [*]:[c](:[*])NN
18. Unknown ECFP_6 feature: -934039951: [*]NN

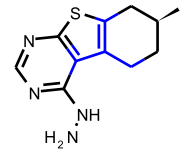
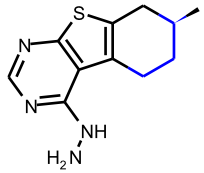
Feature Contribution

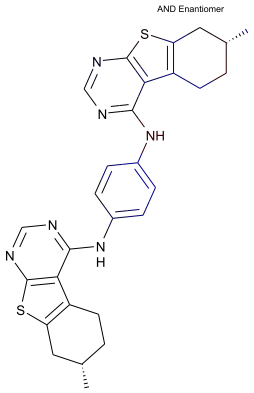
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	-167460056	 [*]C([*])[*]	0.136
FCFP_6	3	 [*]N[*]	0.0924
ECFP_6	1572579716	 [*]N	0.0576

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_6	136597326	 [*]C([*])C	-0.0815

FCFP_6	203677720	AND Enantiomer  [*]C[c]1:[c]([*]):[*] :[*]:[c]:1:[*]	-0.0713
ECFP_6	-1331450522	AND Enantiomer  [*]CCC([*])[*]	-0.0538



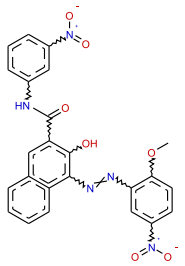
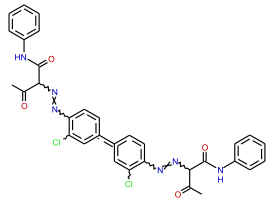
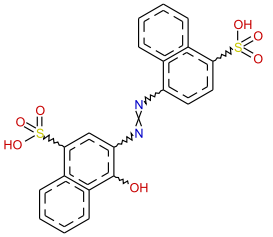
$C_{28}H_{28}N_6S_2$
Molecular Weight: 512.69212
ALogP: 7.842
Rotatable Bonds: 4
Acceptors: 6
Donors: 2

Model Prediction

Prediction: 0.0719
Unit: g/kg_body_weight
Mahalanobis Distance: 33.8
Mahalanobis Distance p-value: 1.77e-031

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	C.I.PIGMENT RED 23	DIARYLANILIDE YELLOW	C.I. ACID RED 14
Structure			
Actual Endpoint (-log C)	2.28997	2.70208	2.8654
Predicted Endpoint (-log C)	3.52921	3.76154	3.29295
Distance	0.862	0.898	0.923
Reference	NTP 411 146	NTP 30 C-4	NTP REPORT # 220

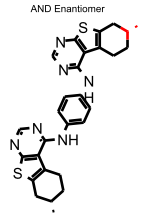
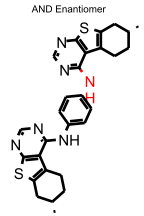
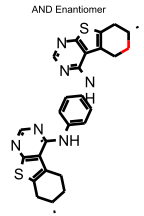
Model Applicability

Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

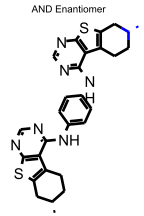
1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_6 feature: 914325265: [*]:s:[*]
3. Unknown ECFP_6 feature: 292958156: [*]CC(C)C[*]
4. Unknown ECFP_6 feature: 53207596: [*]C([*])C[c](:[*]):[*]
5. Unknown ECFP_6 feature: -1672647522: [*]C[c]1:s:[*]:[*]:[c]:1[*]
6. Unknown ECFP_6 feature: -1660340418: [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]
7. Unknown ECFP_6 feature: 51876938: [*]CC[c](:[*]):[*]
8. Unknown ECFP_6 feature: 85262808: [*][c]1:[*]:[*]:[c](:[*]):s:1
9. Unknown ECFP_6 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
10. Unknown ECFP_6 feature: -1661653144: [*][c](:[*]):[c]1:[c]([*]):[*]:[*]:[c]:1:[*]
11. Unknown ECFP_6 feature: 865482986: [*]C([*])C
12. Unknown ECFP_6 feature: -677309799: [*]:[cH]:n:[c](:[*]):[*]
13. Unknown ECFP_6 feature: -710237522: [*]:n:[cH]:n:[*]
14. Unknown ECFP_6 feature: 1049768340: [*]N[c](:n:[*]):[c](:[*]):[*]
15. Unknown ECFP_6 feature: -1242906247: [*]:[c](:[*])N[c](:[*]):[*]
16. Unknown ECFP_6 feature: -177077903: [*]N[c](:[cH]:[*]):[cH]:[*]

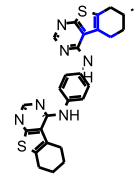
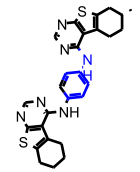
Feature Contribution

Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	-167460056	 [*]C([*])[*]	0.136
FCFP_6	3	 [*]N[*]	0.0924
ECFP_6	-992506539	 [*]C[*]	0.0554

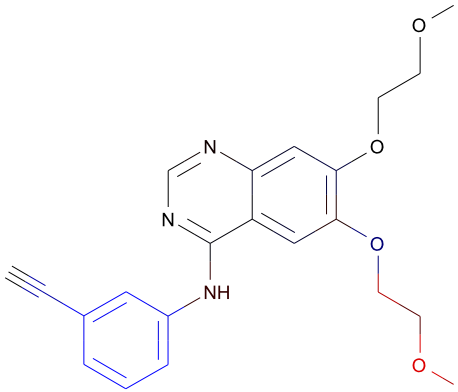
Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_6	136597326	 [*]C([*])C	-0.0815

FCFP_6	203677720	AND Enantiomer  [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.0713
FCFP_6	-773983804	AND Enantiomer  [*]N[c]1:[cH]:[*]:[c]([*]):[cH]:[cH]:1	-0.0589

Erlotinib

TOPKAT_Chronic_LOAEL



$C_{22}H_{23}N_3O_4$

Molecular Weight: 393.43572

ALogP: 4.309

Rotatable Bonds: 10

Acceptors: 7

Donors: 1

Model Prediction

Prediction: 0.0359

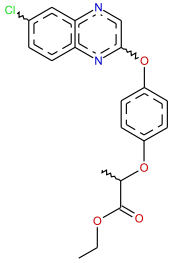
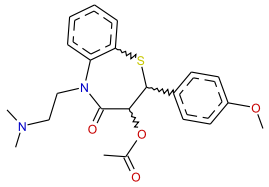
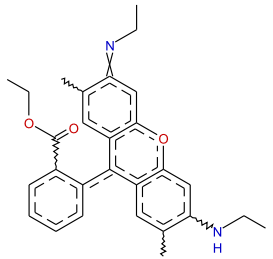
Unit: g/kg_body_weight

Mahalanobis Distance: 34.8

Mahalanobis Distance p-value: 2.91e-033

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	ASSURE	DILTIAZEM	RHODAMINE 6G
Structure			
Actual Endpoint (-log C)	5.00328	4.21961	4.54906
Predicted Endpoint (-log C)	4.27671	4.005	4.6787
Distance	0.611	0.676	0.689
Reference	EPA COVER SHEET 0335;891001;(1)	NDA-18602	NTP 364 39

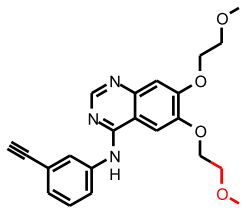
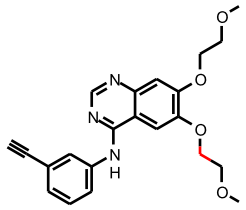
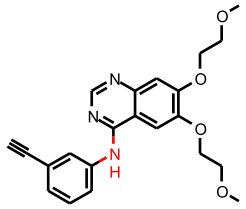
Model Applicability

Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

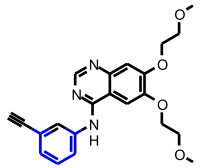
1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: 902193919: [*]:[c](:[*])C#C
3. Unknown FCFP_2 feature: 131784192: [*]C#C
4. Unknown ECFP_6 feature: -1114776580: [*]C#[*]
5. Unknown ECFP_6 feature: -1939823063: [*]#C
6. Unknown ECFP_6 feature: 1410041175: [*]:[cH]:[c](:n:[*]):[c](:[*]):[*]
7. Unknown ECFP_6 feature: 1333660716: [*][c](:[*]):[c](:[cH]:[*]):[c](:[*]):[*]
8. Unknown ECFP_6 feature: -677309799: [*]:[cH]:n:[c](:[*]):[*]
9. Unknown ECFP_6 feature: -710237522: [*]:n:[cH]:n:[*]
10. Unknown ECFP_6 feature: 1049768340: [*]N[c](:n:[*]):[c](:[*]):[*]
11. Unknown ECFP_6 feature: -1255706725: [*]CO[c](:[*]):[*]
12. Unknown ECFP_6 feature: -1790412586: [*]CCO[*]
13. Unknown ECFP_6 feature: -1242906247: [*]:[c](:[*])N[c](:[*]):[*]
14. Unknown ECFP_6 feature: -177077903: [*]N[c](:[cH]:[*]):[cH]:[*]
15. Unknown ECFP_6 feature: 1997021792: [*]:[cH]:[cH]:[cH]:[*]
16. Unknown ECFP_6 feature: -182178874: [*]#C[c](:[cH]:[*]):[cH]:[*]
17. Unknown ECFP_6 feature: 1139738044: [*]:[c](:[*])C#C
18. Unknown ECFP_6 feature: -1545539812: [*]C#C
19. Unknown ECFP_6 feature: -1253653003: [*]COC

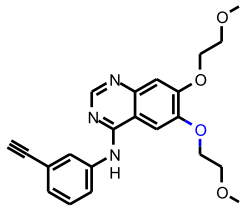
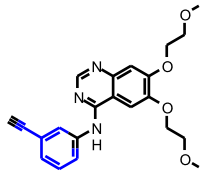
Feature Contribution

Top features for positive contribution

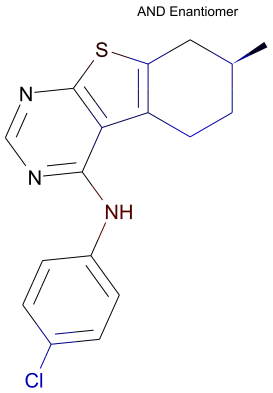
Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_6	-1143715940	 [*]COC	0.13
ECFP_6	1559650422	 [*]C[*]	0.129
FCFP_6	3	 [*]N[*]	0.0924

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_6	991735244	 [*][c]1:[*]:[cH]:[cH] :[cH]:[cH]:1	-0.134

FCFP_6	1	 [*]O[*]	-0.102
FCFP_6	-453677277	 [*]C[c]1:[cH]:[*]:[cH]:[cH]:[cH]:1	-0.0906

TOPKAT_Rat_Maximum_Tolerated_Dose_Feed



$C_{17}H_{16}ClN_3S$

Molecular Weight: 329.84704

ALogP: 5.5

Rotatable Bonds: 2

Acceptors: 3

Donors: 1

Model Prediction

Prediction: 0.13

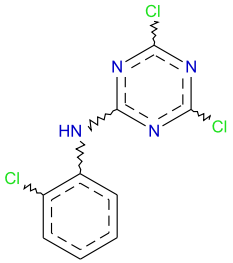
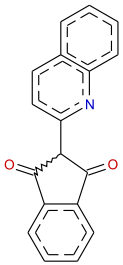
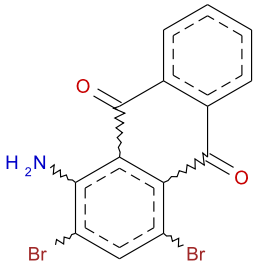
Unit: g/kg_body_weight

Mahalanobis Distance: 11.4

Mahalanobis Distance p-value: 1.36e-007

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	ANILAZINE	D&C YELLOW NO. 11	1-AMINO-2,4-DIBROMOANTHRAQUINONE
Structure			
Actual Endpoint (-log C)	3.78694	4.03869	2.82966
Predicted Endpoint (-log C)	3.42114	3.54593	3.92444
Distance	0.563	0.623	0.632
Reference	NCI/NTP TR-104	NCI/NTP TR-463	NCI/NTP TR-383

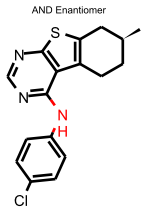
Model Applicability

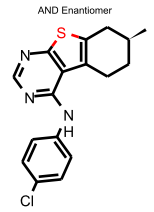
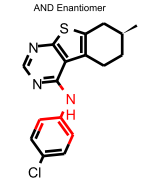
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]

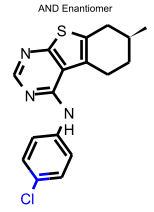
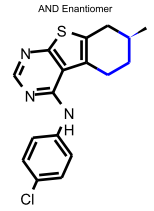
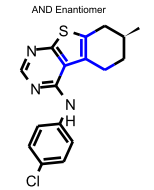
Feature Contribution

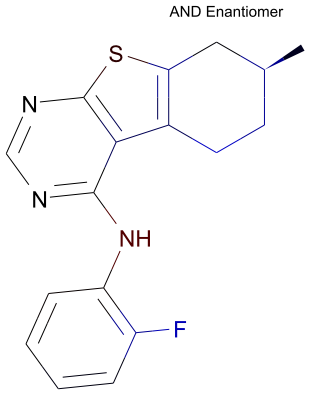
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	3	 [*]N[*]	0.0737

FCFP_2	17	 [*]:s:[*]	0.0441
FCFP_2	590925877	 [*]N[c](:[cH]:[*]):[cH]:[*]	0.00762

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	71476542	 [*]:[c](:[*])Cl	-0.134
FCFP_2	-1272798659	 [*]CCC([*])[*]	-0.111
FCFP_2	203677720	 [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.0829



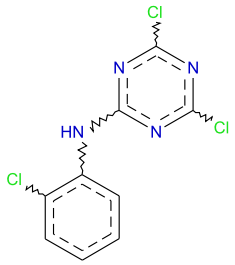
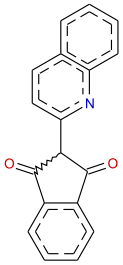
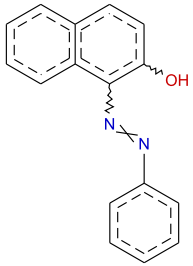
$C_{17}H_{16}FN_3S$
Molecular Weight: 313.39244
ALogP: 5.041
Rotatable Bonds: 2
Acceptors: 3
Donors: 1

Model Prediction

Prediction: 0.138
Unit: g/kg_body_weight
Mahalanobis Distance: 11.6
Mahalanobis Distance p-value: 6.73e-008

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	ANILAZINE	D&C YELLOW NO. 11	C.I. SOLVENT YELLOW 14
Structure			
Actual Endpoint (-log C)	3.78694	4.03869	4.04277
Predicted Endpoint (-log C)	3.42114	3.54593	2.8989
Distance	0.544	0.589	0.612
Reference	NCI/NTP TR-104	NCI/NTP TR-463	NCI/NTP TR-226

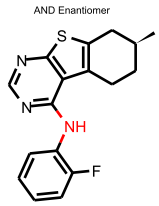
Model Applicability

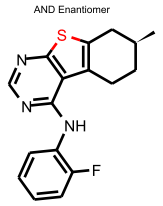
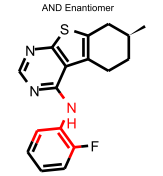
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]

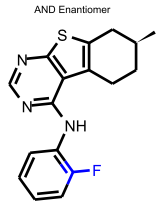
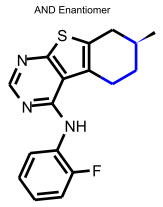
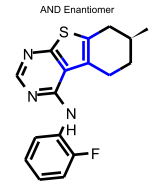
Feature Contribution

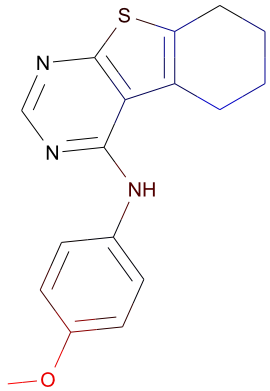
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	3	 [*]N[*]	0.0737

FCFP_2	17	 [*]:s:[*]	0.0441
FCFP_2	590925877	 [*]N[c](:[cH]:[*]):[cH]:[*]	0.00762

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	71476542	 [*]:[c](:[*])Cl	-0.134
FCFP_2	-1272798659	 [*]CCC([*])[*]	-0.111
FCFP_2	203677720	 [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.0829



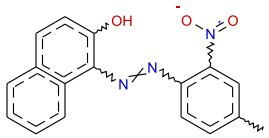
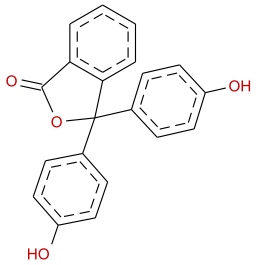
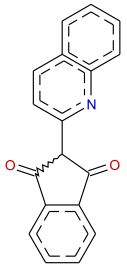
$C_{17}H_{17}N_3OS$
Molecular Weight: 311.40138
ALogP: 4.568
Rotatable Bonds: 3
Acceptors: 4
Donors: 1

Model Prediction

Prediction: 0.0607
Unit: g/kg_body_weight
Mahalanobis Distance: 10.2
Mahalanobis Distance p-value: 2.32e-005

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	C.I.PIGMENT RED 3	PHENOLPHTHALEIN	D&C YELLOW NO. 11
Structure			
Actual Endpoint (-log C)	2.65635	2.20184	4.03869
Predicted Endpoint (-log C)	2.97957	2.8857	3.54593
Distance	0.524	0.579	0.584
Reference	NCI/NTP TR-407	NCI/NTP TR-465	NCI/NTP TR-463

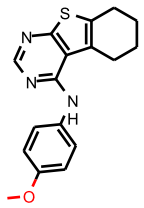
Model Applicability

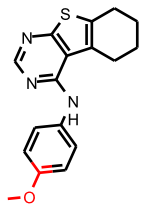
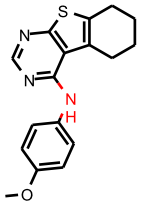
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. OPS PC9 out of range. Value: 3.507. Training min, max, SD, explained variance: -2.8548, 3.3954, 1.263, 0.0360.
2. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]

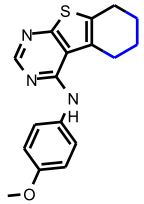
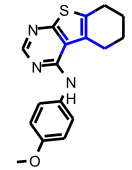
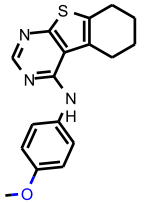
Feature Contribution

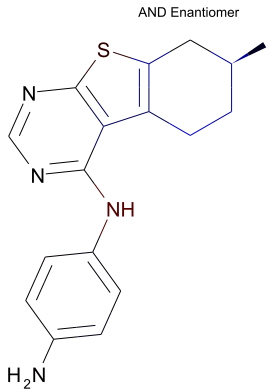
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	136627117	 [*]OC	0.173

FCFP_2	1036089772	 [*]:[c](:[*])OC	0.0749
FCFP_2	3	 [*]N[*]	0.0737

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	-1272798659	 [*]CCC([*])[*]	-0.111
FCFP_2	203677720	 [*]C[c]1:[c]([*]):[*] :[*]:[c]:1:[*]	-0.0829
FCFP_2	1	 [*]O[*]	-0.0796



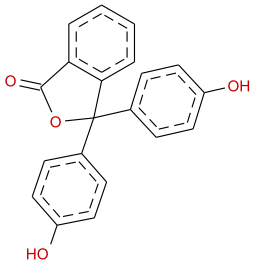
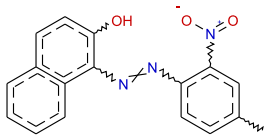
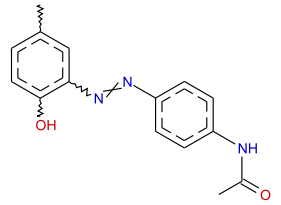
$C_{17}H_{18}N_4S$
Molecular Weight: 310.41662
ALogP: 4.089
Rotatable Bonds: 2
Acceptors: 4
Donors: 2

Model Prediction

Prediction: 0.138
Unit: g/kg_body_weight
Mahalanobis Distance: 9.21
Mahalanobis Distance p-value: 0.000718

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	PHENOLPHTHALEIN	C.I.PIGMENT RED 3	DISPERSE YELLOW 3
Structure			
Actual Endpoint (-log C)	2.20184	2.65635	2.77703
Predicted Endpoint (-log C)	2.8857	2.97957	2.80195
Distance	0.572	0.617	0.650
Reference	NCI/NTP TR-465	NCI/NTP TR-407	NCI/NTP TR-222

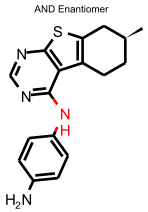
Model Applicability

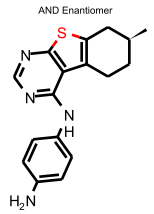
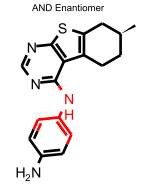
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]

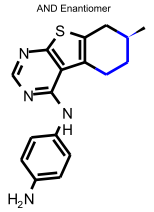
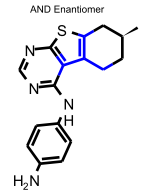
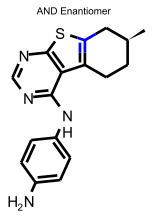
Feature Contribution

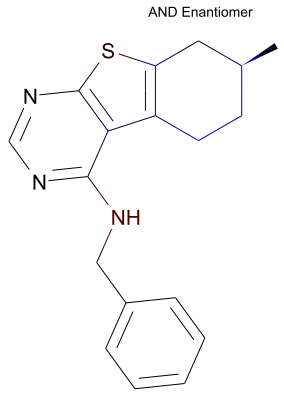
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	3	 [*]N[*]	0.0737

FCFP_2	17	 [*]:s:[*]	0.0441
FCFP_2	590925877	 [*]N[c](:[cH]:[*]):[cH]:[*]	0.00762

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	-1272798659	 [*]CCC([*])[*]	-0.111
FCFP_2	203677720	 [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.0829
FCFP_2	16	 [*][c](:[*]):[*]	-0.0512



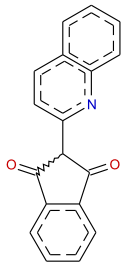
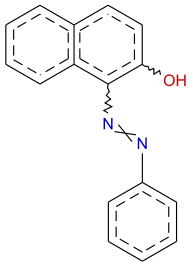
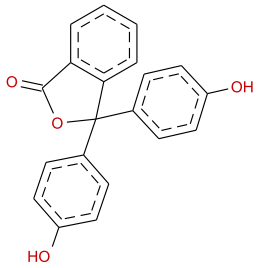
$C_{18}H_{19}N_3S$
Molecular Weight: 309.42856
ALogP: 4.678
Rotatable Bonds: 3
Acceptors: 3
Donors: 1

Model Prediction

Prediction: 0.1
Unit: g/kg_body_weight
Mahalanobis Distance: 10.6
Mahalanobis Distance p-value: 3.79e-006

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	D&C YELLOW NO. 11	C.I. SOLVENT YELLOW 14	PHENOLPHTHALEIN
Structure			
Actual Endpoint (-log C)	4.03869	4.04277	2.20184
Predicted Endpoint (-log C)	3.54593	2.8989	2.8857
Distance	0.569	0.610	0.615
Reference	NCI/NTP TR-463	NCI/NTP TR-226	NCI/NTP TR-465

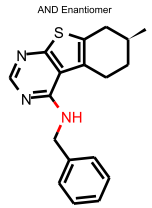
Model Applicability

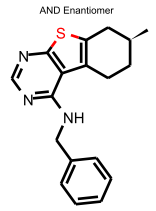
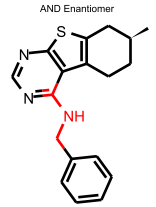
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. OPS PC9 out of range. Value: 3.5628. Training min, max, SD, explained variance: -2.8548, 3.3954, 1.263, 0.0360.
2. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]

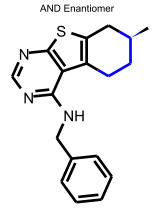
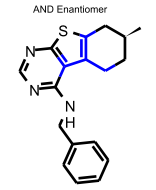
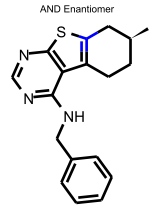
Feature Contribution

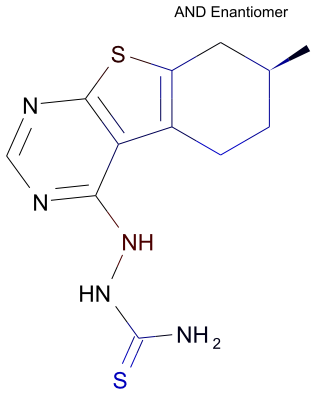
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	3	 [*]N[*]	0.0737

FCFP_2	17	 [*]:s:[*]	0.0441
FCFP_2	1294255210	 [*]CN[c](:[*]):[*]	0.00319

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	-1272798659	 [*]CCC([*])[*]	-0.111
FCFP_2	203677720	 [*]C[c]1:[c]([*]):[*] :[*]:[c]:1:[*]	-0.0829
FCFP_2	16	 [*][c](:[*]):[*]	-0.0512



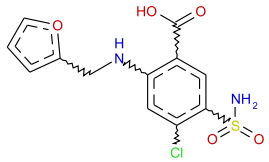
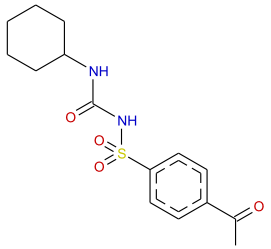
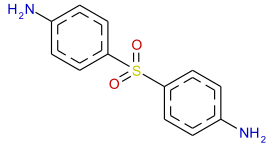
$C_{12}H_{15}N_5S_2$
Molecular Weight: 293.411
ALogP: 3.209
Rotatable Bonds: 3
Acceptors: 4
Donors: 3

Model Prediction

Prediction: 0.222
Unit: g/kg_body_weight
Mahalanobis Distance: 10.6
Mahalanobis Distance p-value: 3.68e-006

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	FUROSEMIDE	ACETOHEXAMIDE	DAPSONE
Structure			
Actual Endpoint (-log C)	4.04236	2.55683	3.66258
Predicted Endpoint (-log C)	2.8614	3.62413	3.26993
Distance	0.571	0.696	0.700
Reference	NCI/NTP TR-356	NCI/NTP TR-050	NCI/NTP TR-20

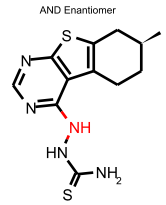
Model Applicability

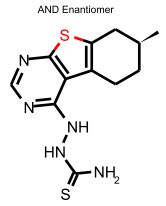
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. OPS PC10 out of range. Value: 3.9942. Training min, max, SD, explained variance: -4.0578, 3.2378, 1.25, 0.0353.
2. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
3. Unknown FCFP_2 feature: -885461129: [*]NNC(=[*])[*]

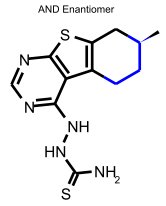
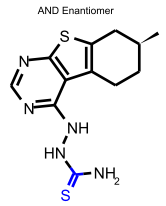
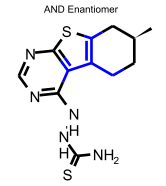
Feature Contribution

Top features for positive contribution

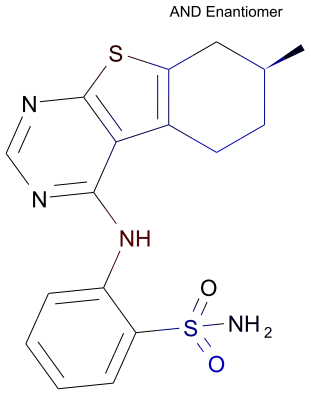
Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	3	 [*]N[*]	0.0737

FCFP_2	17	 [*]:s:[*]	0.0441

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	-1272798659	 [*]CCC([*])[*]	-0.111
FCFP_2	1872154524	 [*]C(=S)[*]	-0.105
FCFP_2	203677720	 [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.0829

TOPKAT_Rat_Maximum_Tolerated_Dose_Feed



$C_{17}H_{18}N_4O_2S_2$

Molecular Weight: 374.48042

ALogP: 3.541

Rotatable Bonds: 3

Acceptors: 5

Donors: 2

Model Prediction

Prediction: 0.109

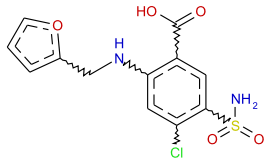
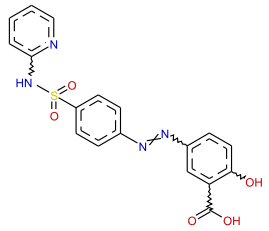
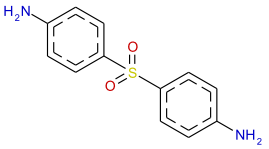
Unit: g/kg_body_weight

Mahalanobis Distance: 11.1

Mahalanobis Distance p-value: 5.29e-007

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	FUROSEMIDE	SALICYLAZOSULFAPYRIDINE	DAPSONE
Structure			
Actual Endpoint (-log C)	4.04236	3.375	3.66258
Predicted Endpoint (-log C)	2.8614	2.80292	3.26993
Distance	0.637	0.660	0.748
Reference	NCI/NTP TR-356	NCI/NTP TR-457	NCI/NTP TR-20

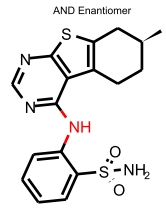
Model Applicability

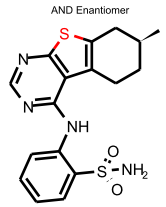
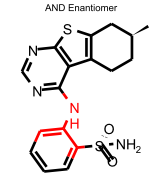
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. OPS PC10 out of range. Value: 3.8932. Training min, max, SD, explained variance: -4.0578, 3.2378, 1.25, 0.0353.
2. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]

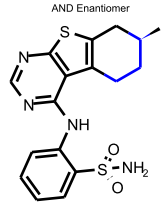
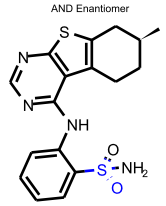
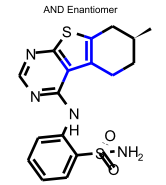
Feature Contribution

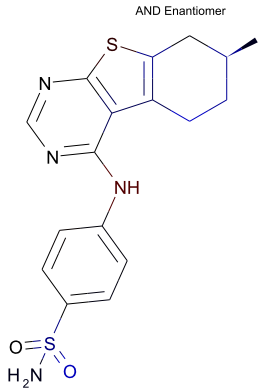
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	3	 [*]N[*]	0.0737

FCFP_2	17	 [*]:s:[*]	0.0441
FCFP_2	590925877	 [*]N[c](:[cH]:[*]):[cH]:[*]	0.00762

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	-1272798659	 [*]CCC([*])[*]	-0.111
FCFP_2	1872154524	 [*]C(=S)[*]	-0.105
FCFP_2	203677720	 [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.0829



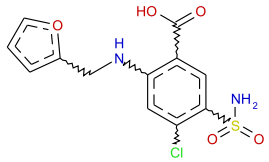
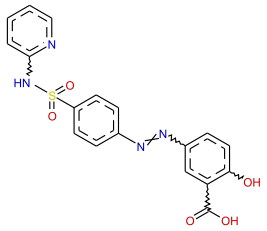
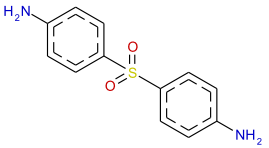
$C_{17}H_{18}N_4O_2S_2$
Molecular Weight: 374.48042
ALogP: 3.541
Rotatable Bonds: 3
Acceptors: 5
Donors: 2

Model Prediction

Prediction: 0.109
Unit: g/kg_body_weight
Mahalanobis Distance: 11.1
Mahalanobis Distance p-value: 5.29e-007

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	FUROSEMIDE	SALICYLAZOSULFAPYRIDINE	DAPSONE
Structure			
Actual Endpoint (-log C)	4.04236	3.375	3.66258
Predicted Endpoint (-log C)	2.8614	2.80292	3.26993
Distance	0.637	0.660	0.748
Reference	NCI/NTP TR-356	NCI/NTP TR-457	NCI/NTP TR-20

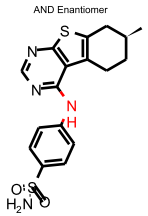
Model Applicability

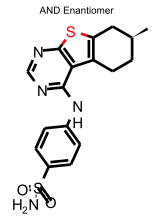
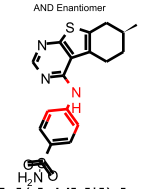
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. OPS PC10 out of range. Value: 3.8932. Training min, max, SD, explained variance: -4.0578, 3.2378, 1.25, 0.0353.
2. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]

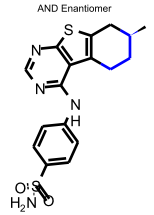
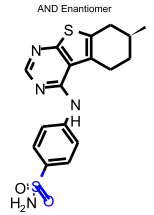
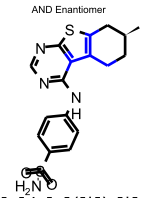
Feature Contribution

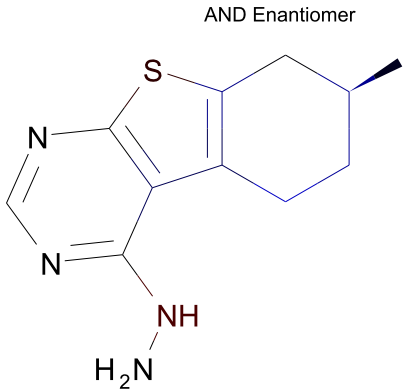
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	3	 [*]N[*]	0.0737

FCFP_2	17	 [*]:s:[*]	0.0441
FCFP_2	590925877	 [*]N[c](:[cH]:[*]):[cH]:[*]	0.00762

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	-1272798659	 [*]CCC([*])[*]	-0.111
FCFP_2	1872154524	 [*]C(=S)[*]	-0.105
FCFP_2	203677720	 [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.0829



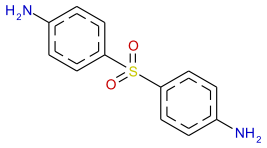
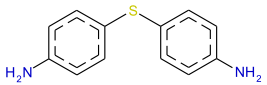
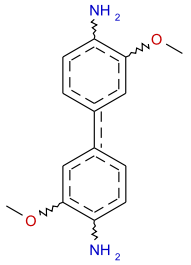
$C_{11}H_{14}N_4S$
Molecular Weight: 234.32065
ALogP: 2.561
Rotatable Bonds: 1
Acceptors: 4
Donors: 2

Model Prediction

Prediction: 0.133
Unit: g/kg_body_weight
Mahalanobis Distance: 10.7
Mahalanobis Distance p-value: 2.76e-006

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	DAPSONE	4,4'-THIODIANILINE	BENZIDINE,3,3'-DIMETHOXY-
Structure			
Actual Endpoint (-log C)	3.66258	3.20473	4.06569
Predicted Endpoint (-log C)	3.26993	3.3362	3.57405
Distance	0.560	0.578	0.611
Reference	NCI/NTP TR-20	NCI/NTP TR-47	NCI/NTP Report 10, Nov. 1987

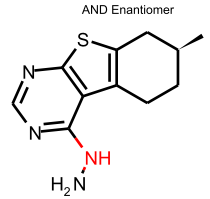
Model Applicability

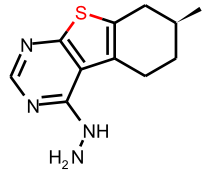
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
3. Unknown FCFP_2 feature: 1070150408: [*]NN

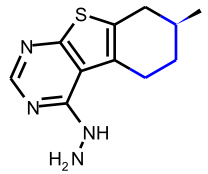
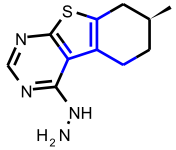
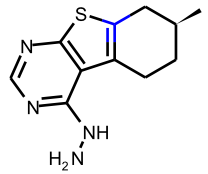
Feature Contribution

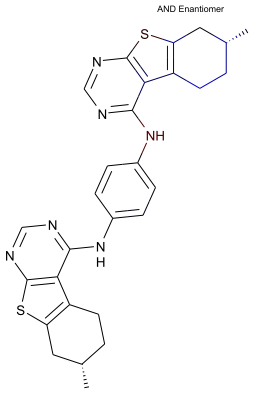
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	3	 [*]N[*]	0.0737

FCFP_2	17	AND Enantiomer  [*]:s:[*]	0.0441

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	-1272798659	AND Enantiomer  [*]CCC([*])[*]	-0.111
FCFP_2	203677720	AND Enantiomer  [*]C[c]1:[c]([*]):[*] :[*]:[c]:1:[*]	-0.0829
FCFP_2	16	AND Enantiomer  [*][c](:[*]):[*]	-0.0512



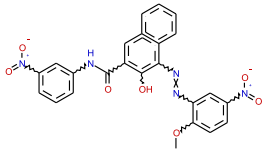
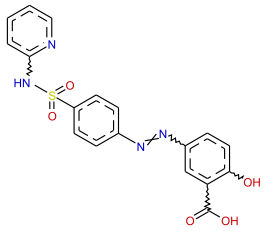
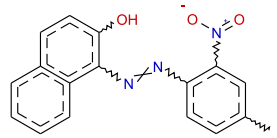
$C_{28}H_{28}N_6S_2$
Molecular Weight: 512.69212
ALogP: 7.842
Rotatable Bonds: 4
Acceptors: 6
Donors: 2

Model Prediction

Prediction: 0.0912
Unit: g/kg_body_weight
Mahalanobis Distance: 13.2
Mahalanobis Distance p-value: 6.77e-011

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	C.I.PIGMENT RED 23	SALICYLAZOSULFAPYRIDINE	C.I.PIGMENT RED 3
Structure			
Actual Endpoint (-log C)	2.30052	3.375	2.65635
Predicted Endpoint (-log C)	3.55333	2.80292	2.97957
Distance	0.888	1.031	1.059
Reference	NCI/NTP TR-411	NCI/NTP TR-457	NCI/NTP TR-407

Model Applicability

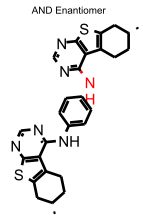
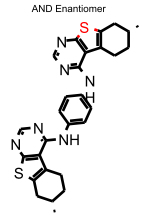
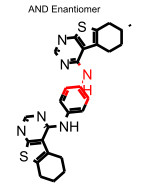
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. ALogP out of range. Value: 7.842. Training min, max, mean, SD: -4.271, 7.574, 2.3494, 1.981.
2. Num_AromaticRings out of range. Value: 5. Training min, max, mean, SD: 0, 4, 1.1685, 0.8469.
3. OPS PC8 out of range. Value: 4.5344. Training min, max, SD, explained variance: -3.8548, 3.9137, 1.331, 0.0400.
4. OPS PC9 out of range. Value: 3.4665. Training min, max, SD, explained variance: -2.8548, 3.3954, 1.263, 0.0360.
5. OPS PC10 out of range. Value: 3.814. Training min, max, SD, explained variance: -4.0578, 3.2378, 1.25, 0.0353.
6. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]

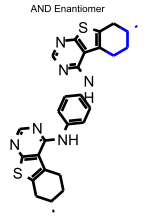
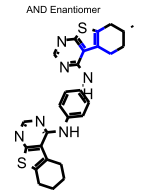
Feature Contribution

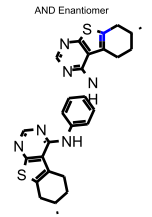
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score

FCFP_2	3	 [*]N[*]	0.0737
FCFP_2	17	 [*]:s:[*]	0.0441
FCFP_2	590925877	 [*]N[c](:[cH]:[*]):[cH]:[*]	0.00762

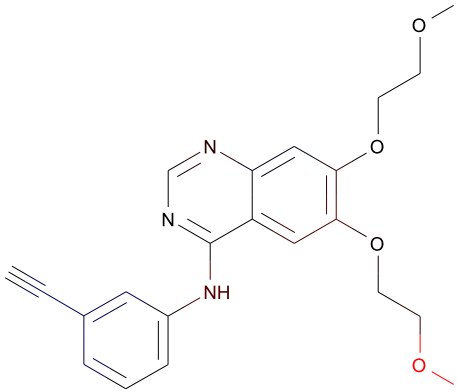
Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	-1272798659	 [*]CCC([*])[*]	-0.111
FCFP_2	203677720	 [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.0829

FCFP_2	16	AND Enantiomer  [*][c](:[*]):[*]	-0.0512

Erlotinib

TOPKAT_Rat_Maximum_Tolerated_Dose_Feed



$C_{22}H_{23}N_3O_4$

Molecular Weight: 393.43572

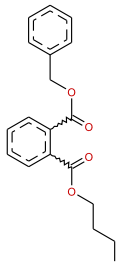
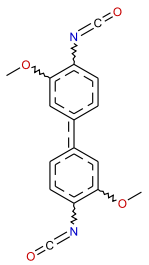
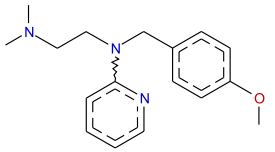
ALogP: 4.309

Rotatable Bonds: 10

Acceptors: 7

Donors: 1

Structural Similar Compounds

Name	BUTYL BENZYL PHTHALATE	3,3'-DIMETHOXYBENZIDINE-4,4'-DIISOCYANATE	PYRILAMINE
Structure			
Actual Endpoint (-log C)	2.79569	2.17504	3.32511
Predicted Endpoint (-log C)	3.18498	3.78717	3.65163
Distance	0.758	0.795	0.820
Reference	NCI/NTP TR-458	NCI/NTP TR-128	NCI/NTP Report 10, Nov. 1987

Model Prediction

Prediction: 0.0828

Unit: g/kg_body_weight

Mahalanobis Distance: 9.37

Mahalanobis Distance p-value: 0.000417

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

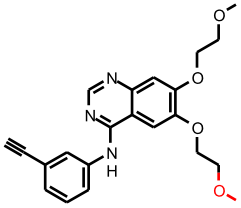
Model Applicability

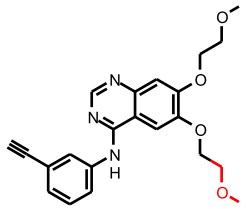
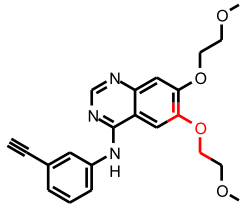
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
3. Unknown FCFP_2 feature: 902193919: [*]:[c](:[*])C#C
4. Unknown FCFP_2 feature: 131784192: [*]C#C

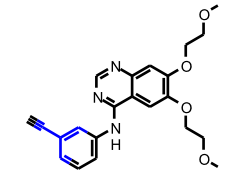
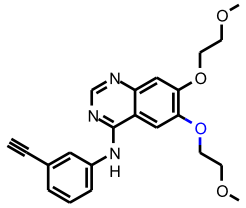
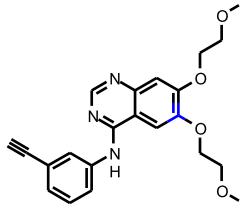
Feature Contribution

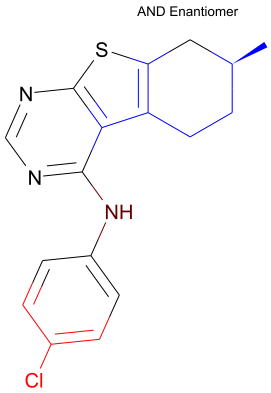
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	136627117	 [*]OC	0.173

FCFP_2	-1143715940	 [*]COC	0.095
FCFP_2	1036089772	 [*]:[c](:[*])OC	0.0749

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	203677720	 [*]C[c]1:[c]([*]):[*] :[*]:[c]:1:[*]	-0.0829
FCFP_2	1	 [*]O[*]	-0.0796
FCFP_2	16	 [*][c](:[*]):[*]	-0.0512



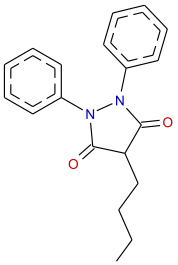
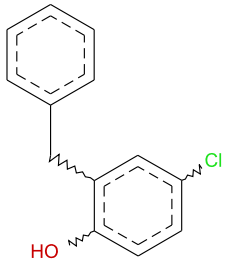
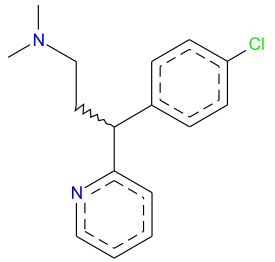
$C_{17}H_{16}ClN_3S$
Molecular Weight: 329.84704
ALogP: 5.5
Rotatable Bonds: 2
Acceptors: 3
Donors: 1

Model Prediction

Prediction: 0.00765
Unit: g/kg_body_weight
Mahalanobis Distance: 9.61
Mahalanobis Distance p-value: 1.91e-005

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	PHENYLBUTAZONE	o-BENZYL-p-CHLOROPHENOL	CHLORPHENIRAMINE MALEATE
Structure			
Actual Endpoint (-log C)	3.48909	3.26063	3.96188
Predicted Endpoint (-log C)	3.17333	3.64448	3.83117
Distance	0.862	0.886	0.887
Reference	NCI/NTP TR-367	NCI/NTP TR-424	NCI/NTP TR-317

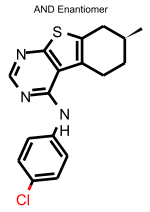
Model Applicability

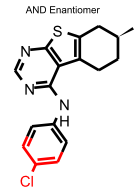
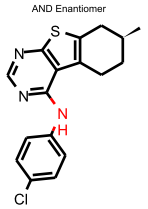
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. Num_AromaticRings out of range. Value: 3. Training min, max, mean, SD: 0, 2, 0.5625, 0.693.
2. OPS PC7 out of range. Value: -2.8755. Training min, max, SD, explained variance: -2.8003, 2.9332, 1.16, 0.0416.
3. Unknown FCFP_2 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
4. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
5. Unknown FCFP_2 feature: 1293778554: [*]:[c](:[*])N[c](:[*]):[*]

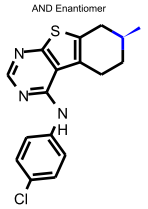
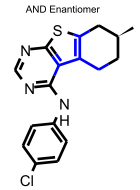
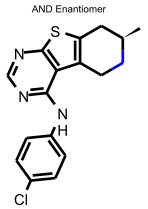
Feature Contribution

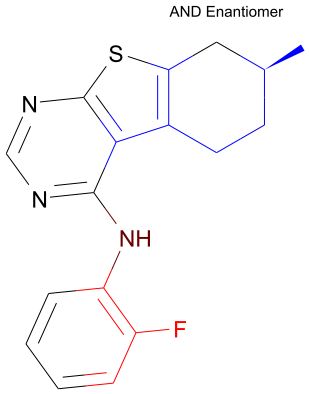
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	32	 [*]Cl	0.526

FCFP_2	367998008	 [*]:[cH]:[c](Cl):[cH]:[*]	0.413
FCFP_2	3	 [*]N[*]	0.104

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	136597326	 [*]C([*])C	-0.489
FCFP_2	203677720	 [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.406
FCFP_2	0	 [*]C[*]	-0.29



$C_{17}H_{16}FN_3S$

Molecular Weight: 313.39244

ALogP: 5.041

Rotatable Bonds: 2

Acceptors: 3

Donors: 1

Model Prediction

Prediction: 0.00972

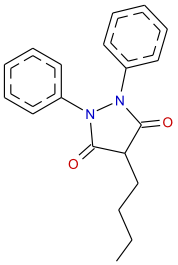
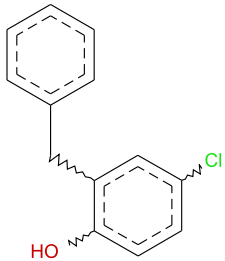
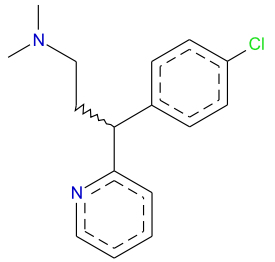
Unit: g/kg_body_weight

Mahalanobis Distance: 9.46

Mahalanobis Distance p-value: 3.06e-005

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	PHENYLBUTAZONE	o-BENZYL-p-CHLOROPHENOL	CHLORPHENIRAMINE MALEATE
Structure			
Actual Endpoint (-log C)	3.48909	3.26063	3.96188
Predicted Endpoint (-log C)	3.17333	3.64448	3.83117
Distance	0.845	0.861	0.867
Reference	NCI/NTP TR-367	NCI/NTP TR-424	NCI/NTP TR-317

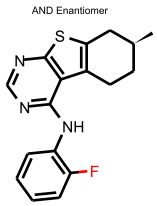
Model Applicability

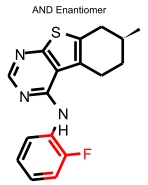
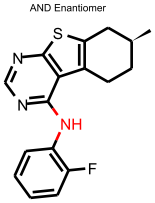
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. Num_AromaticRings out of range. Value: 3. Training min, max, mean, SD: 0, 2, 0.5625, 0.693.
2. OPS PC7 out of range. Value: -2.8344. Training min, max, SD, explained variance: -2.8003, 2.9332, 1.16, 0.0416.
3. Unknown FCFP_2 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
4. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
5. Unknown FCFP_2 feature: 1293778554: [*]:[c](:[*])N[c](:[*]):[*]

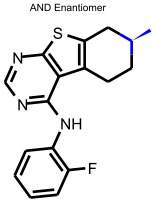
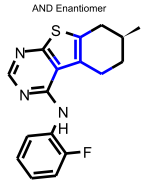
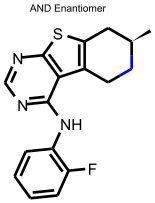
Feature Contribution

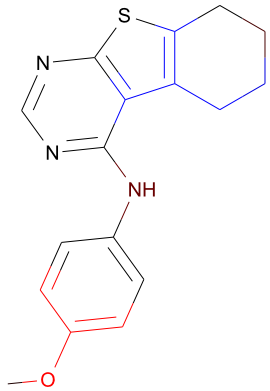
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	32	 [*]Cl	0.526

FCFP_2	367998008	 [*]:[cH]:[c](Cl):[cH]:[*]	0.413
FCFP_2	3	 [*]N[*]	0.104

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	136597326	 [*]C([*])C	-0.489
FCFP_2	203677720	 [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.406
FCFP_2	0	 [*]C[*]	-0.29



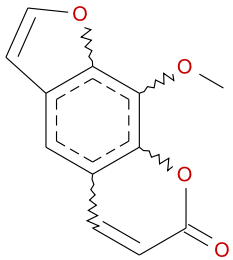
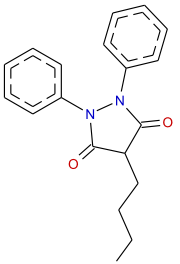
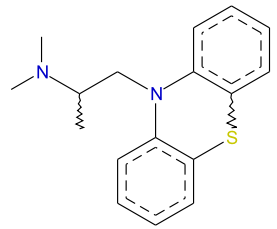
$C_{17}H_{17}N_3OS$
Molecular Weight: 311.40138
ALogP: 4.568
Rotatable Bonds: 3
Acceptors: 4
Donors: 1

Model Prediction

Prediction: 0.00084
Unit: g/kg_body_weight
Mahalanobis Distance: 9.84
Mahalanobis Distance p-value: 9.32e-006

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	8-METHOXYPSORALEN	PHENYLBUTAZONE	PROMETHAZINE.HCL
Structure			
Actual Endpoint (-log C)	3.45978	3.48909	3.93152
Predicted Endpoint (-log C)	4.14745	3.17333	4.72433
Distance	0.819	0.870	0.902
Reference	NCI/NTP TR-359	NCI/NTP TR-367	NCI/NTP TR-425

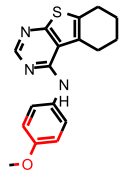
Model Applicability

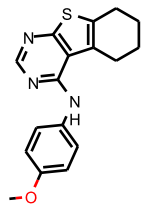
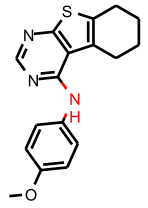
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. Num_AromaticRings out of range. Value: 3. Training min, max, mean, SD: 0, 2, 0.5625, 0.693.
2. OPS PC6 out of range. Value: -3.1044. Training min, max, SD, explained variance: -2.4321, 2.9885, 1.256, 0.0488.
3. Unknown FCFP_2 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
4. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
5. Unknown FCFP_2 feature: 1293778554: [*]:[c](:[*])N[c](:[*]):[*]

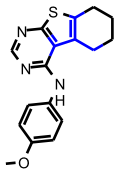
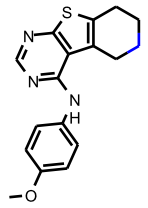
Feature Contribution

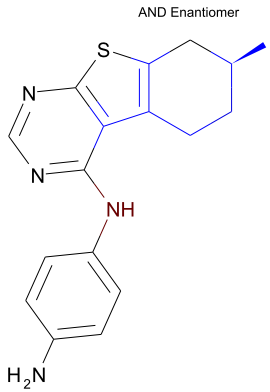
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	332760439	 [*]O[c](:[cH]:[*]):[cH]:[*]	0.672

FCFP_2	1	 [*]O[*]	0.511
FCFP_2	3	 [*]N[*]	0.104

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	203677720	 [*]C[c]1:[c]([*]):[*] :[*]:[c]:1:[*]	-0.406
FCFP_2	0	 [*]C[*]	-0.29



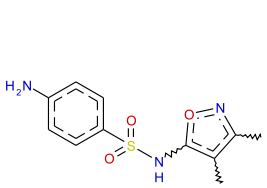
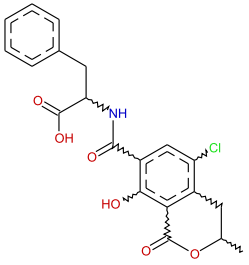
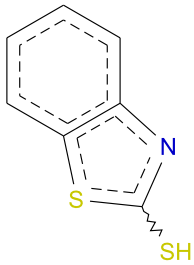
$C_{17}H_{18}N_4S$
Molecular Weight: 310.41662
ALogP: 4.089
Rotatable Bonds: 2
Acceptors: 4
Donors: 2

Model Prediction

Prediction: 0.067
Unit: g/kg_body_weight
Mahalanobis Distance: 10.5
Mahalanobis Distance p-value: 1.12e-006

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	SULFISOOXAZOLE	OCHRATOXIN	2-MERCAPTOBENZOTHIAZOLE
Structure			
Actual Endpoint (-log C)	2.82494	6.28396	2.34829
Predicted Endpoint (-log C)	3.0705	5.12358	3.82125
Distance	0.758	0.915	0.951
Reference	NCI/NTP TR-138	NCI/NTP TR-358	NCI/NTP TR-332

Model Applicability

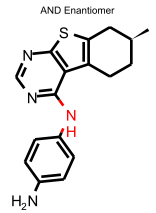
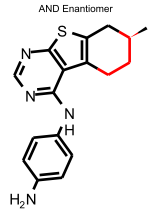
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. Num_AromaticRings out of range. Value: 3. Training min, max, mean, SD: 0, 2, 0.5625, 0.693.
2. OPS PC9 out of range. Value: -2.7349. Training min, max, SD, explained variance: -2.7086, 2.9267, 1.019, 0.0321.
3. Unknown FCFP_2 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
4. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
5. Unknown FCFP_2 feature: 1293778554: [*]:[c](:[*])N[c](:[*]):[*]

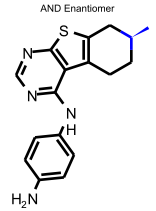
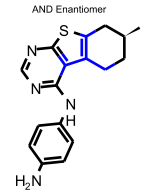
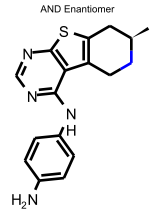
Feature Contribution

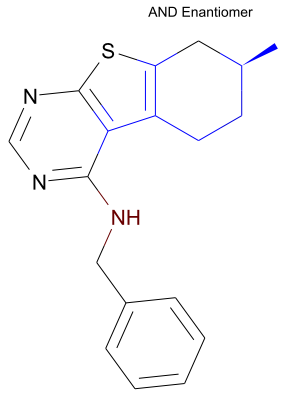
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score

FCFP_2	3	 [*]N[*]	0.104
FCFP_2	-1272798659	 [*]CCC([*])[*]	0.0703

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	136597326	 [*]C([*])C	-0.489
FCFP_2	203677720	 [*]C[c]1:[c]([*]):[*] :[*]:[c]:1:[*]	-0.406
FCFP_2	0	 [*]C[*]	-0.29



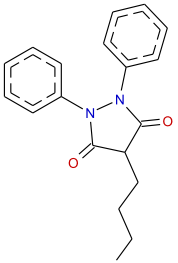
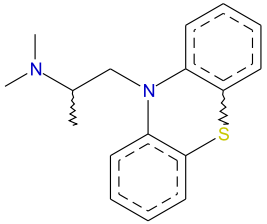
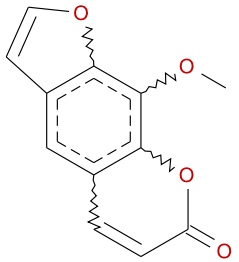
$C_{18}H_{19}N_3S$
Molecular Weight: 309.42856
ALogP: 4.678
Rotatable Bonds: 3
Acceptors: 3
Donors: 1

Model Prediction

Prediction: 0.152
Unit: g/kg_body_weight
Mahalanobis Distance: 10.1
Mahalanobis Distance p-value: 4.04e-006

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	PHENYLBUTAZONE	PROMETHAZINE.HCL	8-METHOXYPSORALEN
Structure			
Actual Endpoint (-log C)	3.48909	3.93152	3.45978
Predicted Endpoint (-log C)	3.17333	4.72433	4.14745
Distance	0.799	0.872	0.883
Reference	NCI/NTP TR-367	NCI/NTP TR-425	NCI/NTP TR-359

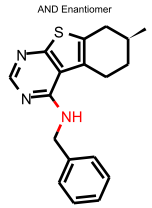
Model Applicability

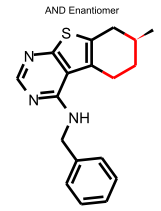
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. Num_AromaticRings out of range. Value: 3. Training min, max, mean, SD: 0, 2, 0.5625, 0.693.
2. Unknown FCFP_2 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]

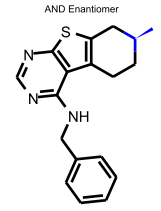
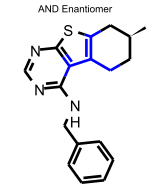
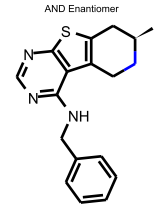
Feature Contribution

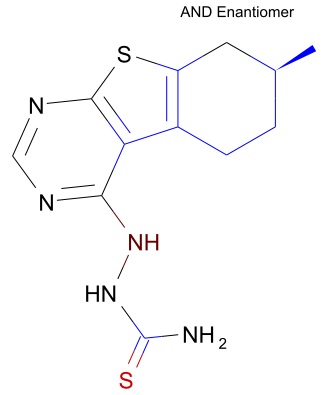
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	3	 [*]N[*]	0.104

FCFP_2	-1272798659	 [*]CCC([*])[*]	0.0703

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	136597326	 [*]C([*])C	-0.489
FCFP_2	203677720	 [*]C[c]1:[c]([*]):[*] :[*]:[c]:1:[*]	-0.406
FCFP_2	0	 [*]C[*]	-0.29



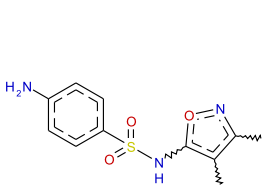
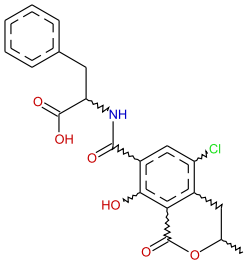
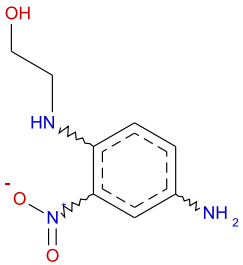
$C_{12}H_{15}N_5S_2$
Molecular Weight: 293.411
ALogP: 3.209
Rotatable Bonds: 3
Acceptors: 4
Donors: 3

Model Prediction

Prediction: 0.32
Unit: g/kg_body_weight
Mahalanobis Distance: 10.7
Mahalanobis Distance p-value: 5.71e-007

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	SULFISOOXAZOLE	OCHRATOXIN	HC RED 3
Structure			
Actual Endpoint (-log C)	2.82494	6.28396	2.59592
Predicted Endpoint (-log C)	3.0705	5.12358	3.285
Distance	0.745	0.779	0.893
Reference	NCI/NTP TR-138	NCI/NTP TR-358	NCI/NTP TR-281

Model Applicability

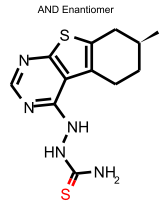
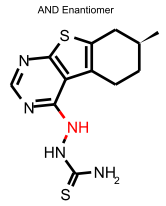
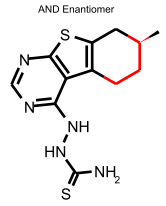
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. Molecular_PolarSASA out of range. Value: 232.59. Training min, max, mean, SD: 0, 223.97, 50.816, 55.15.
2. OPS PC9 out of range. Value: -2.8528. Training min, max, SD, explained variance: -2.7086, 2.9267, 1.019, 0.0321.
3. Unknown FCFP_2 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
4. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
5. Unknown FCFP_2 feature: 1294344583: [*]NN[c](:[*]):[*]
6. Unknown FCFP_2 feature: -885461129: [*]NNC(=[*])[*]
7. Unknown FCFP_2 feature: 1499521844: [*]NC(=S)N

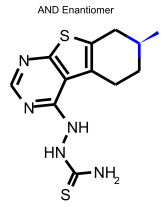
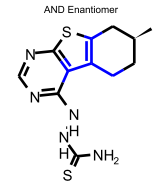
Feature Contribution

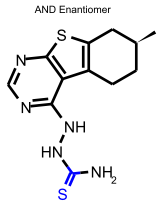
Top features for positive contribution

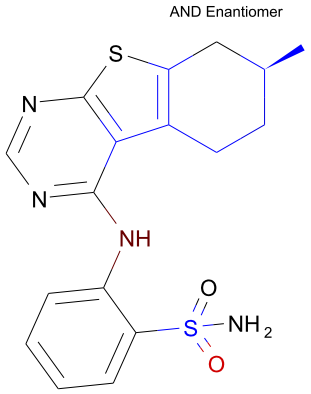
Fingerprint	Bit/Smiles	Feature Structure	Score

FCFP_2	1	 [*]O[*]	0.511
FCFP_2	3	 [*]N[*]	0.104
FCFP_2	-1272798659	 [*]CCC([*])[*]	0.0703

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	136597326	 [*]C([*])C	-0.489
FCFP_2	203677720	 [*]C[c]1:[c]([*]):[*]:[*]:[c]:1:[*]	-0.406

FCFP_2	1872154524	AND Enantiomer  [*]C(=S)[*]	-0.307



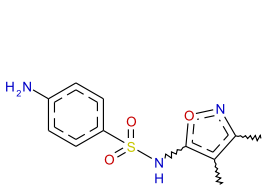
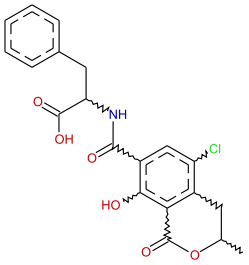
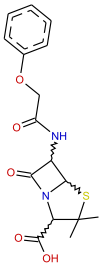
$C_{17}H_{18}N_4O_2S_2$
Molecular Weight: 374.48042
ALogP: 3.541
Rotatable Bonds: 3
Acceptors: 5
Donors: 2

Model Prediction

Prediction: 0.0657
Unit: g/kg_body_weight
Mahalanobis Distance: 9.78
Mahalanobis Distance p-value: 1.14e-005

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	SULFISOOXAZOLE	OCHRATOXIN	PENICILLIN VK
Structure			
Actual Endpoint (-log C)	2.82494	6.28396	2.54455
Predicted Endpoint (-log C)	3.0705	5.12358	3.9702
Distance	0.769	0.786	1.038
Reference	NCI/NTP TR-138	NCI/NTP TR-358	NCI/NTP TR-336

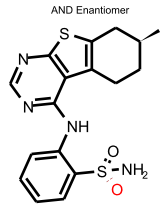
Model Applicability

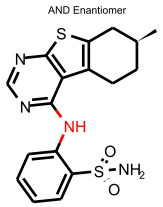
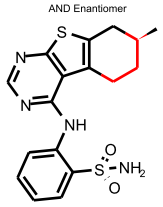
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. Num_AromaticRings out of range. Value: 3. Training min, max, mean, SD: 0, 2, 0.5625, 0.693.
2. OPS PC9 out of range. Value: -2.8441. Training min, max, SD, explained variance: -2.7086, 2.9267, 1.019, 0.0321.
3. Unknown FCFP_2 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
4. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
5. Unknown FCFP_2 feature: 1293778554: [*]:[c](:[*])N[c](:[*]):[*]

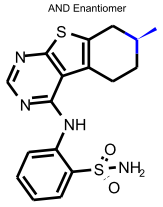
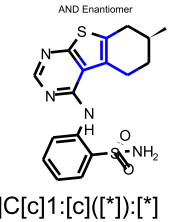
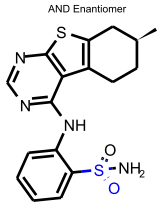
Feature Contribution

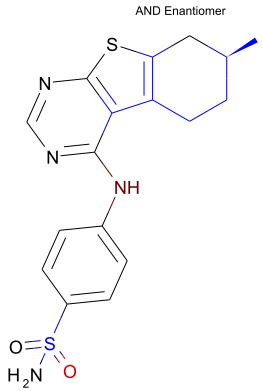
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	1	 [*]O[*]	0.511

FCFP_2	3	 [*]N[*]	0.104
FCFP_2	-1272798659	 [*]CCC([*])[*]	0.0703

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	136597326	 [*]C([*])C	-0.489
FCFP_2	203677720	 [*]C[c]1:[c]([*]):[*] :[*]:[c]:1:[*]	-0.406
FCFP_2	1872154524	 [*]C(=S)[*]	-0.307



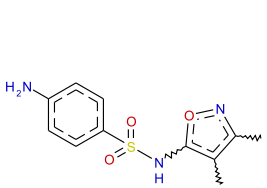
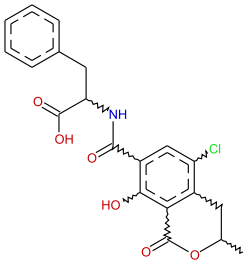
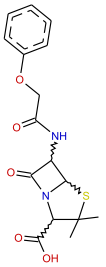
$C_{17}H_{18}N_4O_2S_2$
Molecular Weight: 374.48042
ALogP: 3.541
Rotatable Bonds: 3
Acceptors: 5
Donors: 2

Model Prediction

Prediction: 0.0657
Unit: g/kg_body_weight
Mahalanobis Distance: 9.78
Mahalanobis Distance p-value: 1.14e-005

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	SULFISOOXAZOLE	OCHRATOXIN	PENICILLIN VK
Structure			
Actual Endpoint (-log C)	2.82494	6.28396	2.54455
Predicted Endpoint (-log C)	3.0705	5.12358	3.9702
Distance	0.769	0.786	1.038
Reference	NCI/NTP TR-138	NCI/NTP TR-358	NCI/NTP TR-336

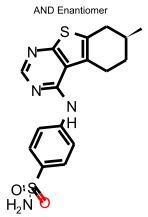
Model Applicability

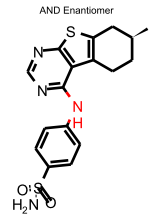
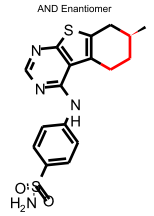
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. Num_AromaticRings out of range. Value: 3. Training min, max, mean, SD: 0, 2, 0.5625, 0.693.
2. OPS PC9 out of range. Value: -2.8441. Training min, max, SD, explained variance: -2.7086, 2.9267, 1.019, 0.0321.
3. Unknown FCFP_2 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
4. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
5. Unknown FCFP_2 feature: 1293778554: [*]:[c](:[*])N[c](:[*]):[*]

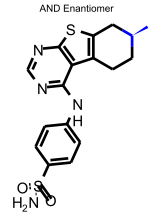
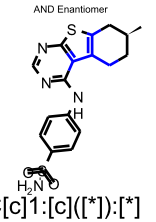
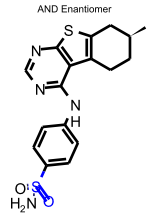
Feature Contribution

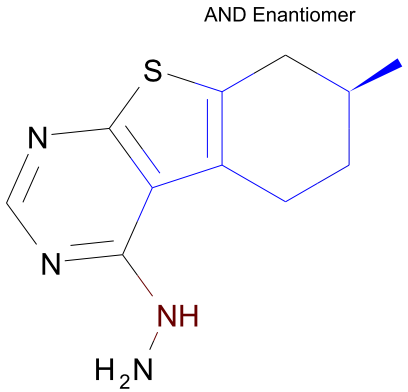
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	1	 [*]O[*]	0.511

FCFP_2	3	 [*]N[*]	0.104
FCFP_2	-1272798659	 [*]CCC([*])[*]	0.0703

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	136597326	 [*]C([*])C	-0.489
FCFP_2	203677720	 [*]C[c]1:[c]([*]):[*] :[*]:[c]:1:[*]	-0.406
FCFP_2	1872154524	 [*]C(=S)[*]	-0.307



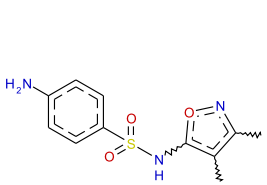
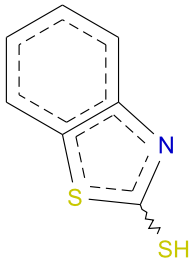
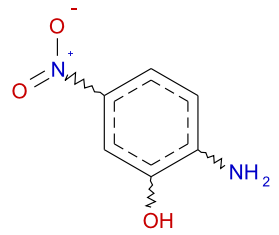
$C_{11}H_{14}N_4S$
Molecular Weight: 234.32065
ALogP: 2.561
Rotatable Bonds: 1
Acceptors: 4
Donors: 2

Model Prediction

Prediction: 0.102
Unit: g/kg_body_weight
Mahalanobis Distance: 8.95
Mahalanobis Distance p-value: 0.00014

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	SULFISOOXAZOLE	2-MERCAPTOBENZOTHIAZOLE	2-AMINO-5-NITROPHENOL
Structure			
Actual Endpoint (-log C)	2.82494	2.34829	2.88684
Predicted Endpoint (-log C)	3.0705	3.82125	3.28491
Distance	0.623	0.783	0.795
Reference	NCI/NTP TR-138	NCI/NTP TR-332	NCI/NTP TR-334

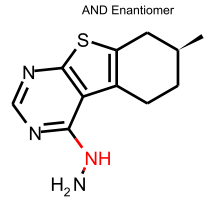
Model Applicability

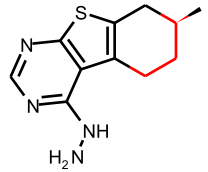
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown FCFP_2 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
4. Unknown FCFP_2 feature: 1294344583: [*]NN[c](:[*]):[*]
5. Unknown FCFP_2 feature: 1070150408: [*]NN

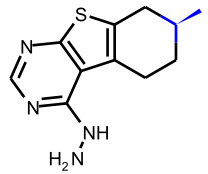
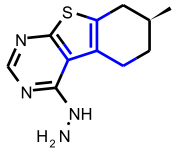
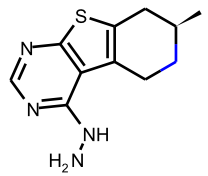
Feature Contribution

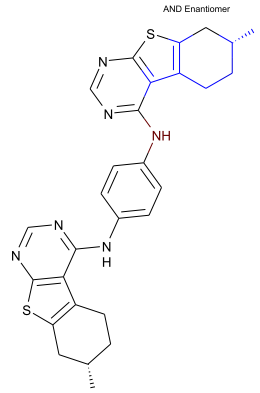
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	3	 [*]N[*]	0.104

FCFP_2	-1272798659	AND Enantiomer  [*]CCC([*])[*]	0.0703

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	136597326	AND Enantiomer  [*]C([*])C	-0.489
FCFP_2	203677720	AND Enantiomer  [*]C[c]1:[c]([*]):[*] :[*]:[c]:1:[*]	-0.406
FCFP_2	0	AND Enantiomer  [*]C[*]	-0.29



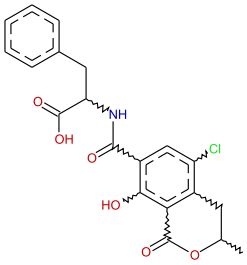
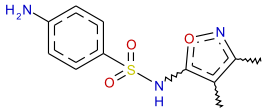
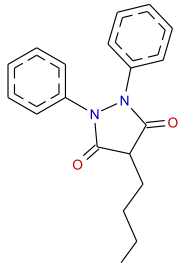
$C_{28}H_{28}N_6S_2$
Molecular Weight: 512.69212
ALogP: 7.842
Rotatable Bonds: 4
Acceptors: 6
Donors: 2

Model Prediction

Prediction: 0.00163
Unit: g/kg_body_weight
Mahalanobis Distance: 17.8
Mahalanobis Distance p-value: 9.44e-017

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	OCHRATOXIN	SULFISOOXAZOLE	PHENYLBUTAZONE
Structure			
Actual Endpoint (-log C)	6.28396	2.82494	3.48909
Predicted Endpoint (-log C)	5.12358	3.0705	3.17333
Distance	1.371	1.541	1.694
Reference	NCI/NTP TR-358	NCI/NTP TR-138	NCI/NTP TR-367

Model Applicability

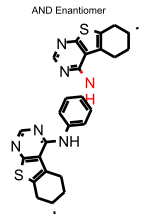
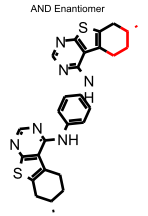
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. Molecular_Weight out of range. Value: 512.69. Training min, max, mean, SD: 68.074, 434.63, 171.13, 85.06.
2. Num_AromaticRings out of range. Value: 5. Training min, max, mean, SD: 0, 2, 0.5625, 0.693.
3. OPS PC6 out of range. Value: -3.2739. Training min, max, SD, explained variance: -2.4321, 2.9885, 1.256, 0.0488.
4. OPS PC9 out of range. Value: -2.9987. Training min, max, SD, explained variance: -2.7086, 2.9267, 1.019, 0.0321.
5. Unknown FCFP_2 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
6. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
7. Unknown FCFP_2 feature: 1293778554: [*]:[c](:[*])N[c](:[*]):[*]

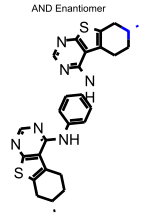
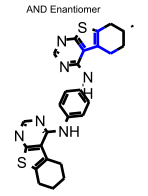
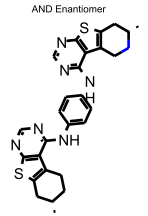
Feature Contribution

Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score

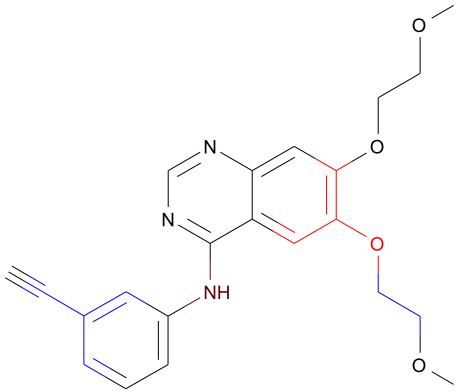
FCFP_2	3	 [*]N[*]	0.104
FCFP_2	-1272798659	 [*]CCC([*])[*]	0.0703

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	136597326	 [*]C([*])C	-0.489
FCFP_2	203677720	 [*]C[c]1:[c]([*]):[*] :[*]:[c]:1:[*]	-0.406
FCFP_2	0	 [*]C[*]	-0.29

Erlotinib

TOPKAT_Rat_Maximum_Tolerated_Dose_Gavage



$C_{22}H_{23}N_3O_4$

Molecular Weight: 393.43572

ALogP: 4.309

Rotatable Bonds: 10

Acceptors: 7

Donors: 1

Model Prediction

Prediction: 0.000344

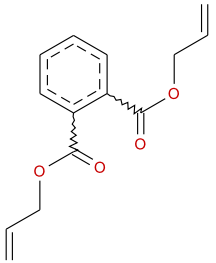
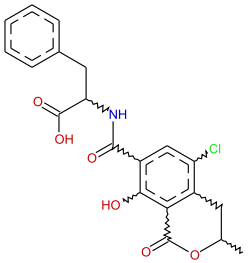
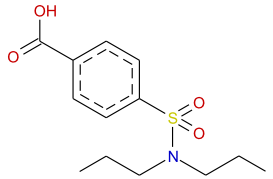
Unit: g/kg_body_weight

Mahalanobis Distance: 11.7

Mahalanobis Distance p-value: 2.74e-008

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	DIALLYL PHTHALATE	OCHRATOXIN	PROBENECID
Structure			
Actual Endpoint (-log C)	3.3914	6.28396	2.85333
Predicted Endpoint (-log C)	3.50093	5.12358	2.4258
Distance	1.113	1.136	1.152
Reference	NCI/NTP TR-284	NCI/NTP TR-358	NCI/NTP TR-395

Model Applicability

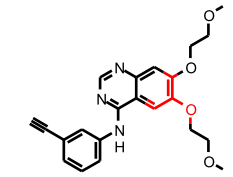
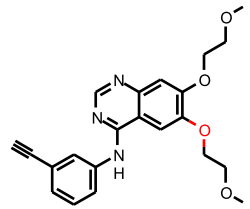
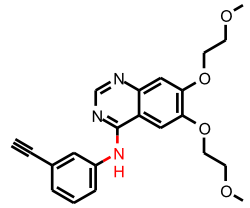
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. Num_H_Acceptors out of range. Value: 7. Training min, max, mean, SD: 0, 6, 1.6146, 1.644.
2. Num_AromaticRings out of range. Value: 3. Training min, max, mean, SD: 0, 2, 0.5625, 0.693.
3. OPS PC6 out of range. Value: -3.0997. Training min, max, SD, explained variance: -2.4321, 2.9885, 1.256, 0.0488.
4. Unknown FCFP_2 feature: -124685461: [*]:n:c:n:[*]
5. Unknown FCFP_2 feature: 1293778554: [*]:[c](:[*])N[c](:[*]):[*]
6. Unknown FCFP_2 feature: 902193919: [*]:[c](:[*])C#C
7. Unknown FCFP_2 feature: 131784192: [*]C#C

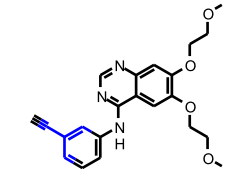
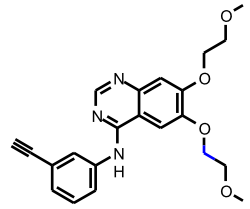
Feature Contribution

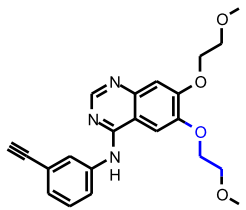
Top features for positive contribution

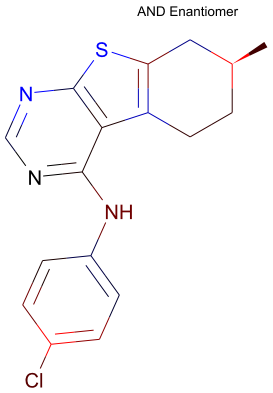
Fingerprint	Bit/Smiles	Feature Structure	Score

FCFP_2	332760439	 [*]O[c](:[cH]:[*]):[c H]:[*]	0.672
FCFP_2	1	 [*]O[*]	0.511
FCFP_2	3	 [*]N[*]	0.104

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
FCFP_2	203677720	 [*]C[c]1:[c]([*]):[*] :[*]:[c]:1:[*]	-0.406
FCFP_2	0	 [*]C[*]	-0.29

FCFP_2	-1272768868	 [*]CCO[*]	-0.271



$C_{17}H_{16}ClN_3S$

Molecular Weight: 329.84704

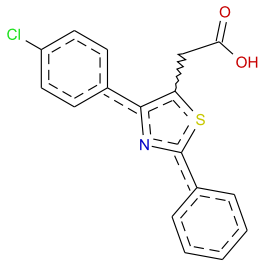
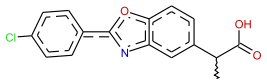
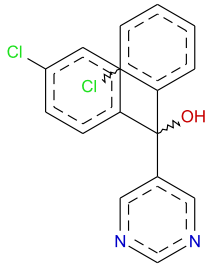
ALogP: 5.5

Rotatable Bonds: 2

Acceptors: 3

Donors: 1

Structural Similar Compounds

Name	FENTIAZAC	BENOXAPROFEN	.alpha.-(2-CHLOROPHENYL)-.alpha.-(4-CHLOROPHENYL)-5-PYRIMIDINE METHANOL
Structure			
Actual Endpoint (-log C)	2.907	3.408	2.122
Predicted Endpoint (-log C)	2.69613	2.85166	2.72534
Distance	0.554	0.558	0.592
Reference	NIIRDN 6;APP-17;82	YACHDS 9;4445;81	FMCHA2 -;C254;89

Model Prediction

Prediction: 0.483

Unit: g/kg_body_weight

Mahalanobis Distance: 19.6

Mahalanobis Distance p-value: 1.23e-007

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Model Applicability

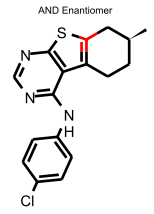
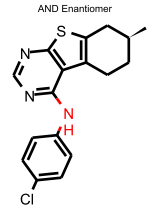
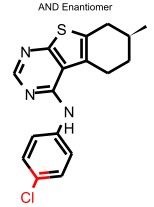
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_6 feature: 16: [*][c](:[*]):[*]
4. Unknown FCFP_6 feature: 1747237384: [*][c]1:[*]:[*]:[c](:[*]):s:1
5. Unknown FCFP_6 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
6. Unknown FCFP_6 feature: -124685461: [*]:n:[cH]:n:[*]
7. Unknown FCFP_6 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]
8. Unknown FCFP_6 feature: 1293778554: [*]:[c](:[*])N[c](:[*]):[*]
9. Unknown FCFP_6 feature: 1618154665: [*][c](:[*]):[cH]:[cH]:[*]
10. Unknown FCFP_6 feature: 71476542: [*]:[c](:[*])Cl

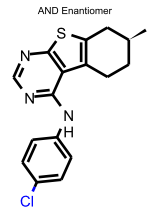
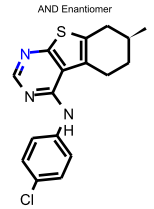
Feature Contribution

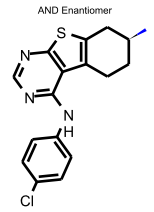
Top features for positive contribution

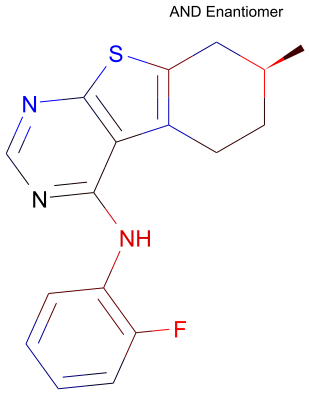
Fingerprint	Bit/Smiles	Feature Structure	Score

ECFP_6	642810091	 [*][c](:[*]):[*]	0.281
ECFP_6	-1897341097	 [*]N[*]	0.216
ECFP_6	99947387	 [*]:[c](:[*])Cl	0.181

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	-817402818	 [*]Cl	-0.263
ECFP_6	655739385	 [*]:n:[*]	-0.239

ECFP_6	734603939	AND Enantiomer  [*]C	-0.201



$C_{17}H_{16}FN_3S$

Molecular Weight: 313.39244

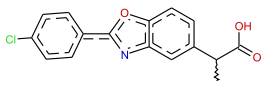
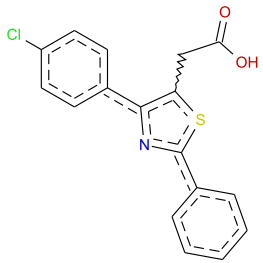
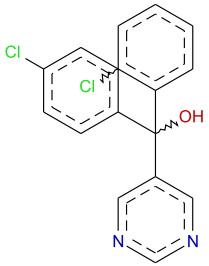
ALogP: 5.041

Rotatable Bonds: 2

Acceptors: 3

Donors: 1

Structural Similar Compounds

Name	BENOXAPROFEN	FENTIAZAC	.alpha.-(2-CHLOROPHENYL)-.alpha.-(4-CHLOROPHENYL)-5-PYRIMIDINE METHANOL
Structure			
Actual Endpoint (-log C)	3.408	2.907	2.122
Predicted Endpoint (-log C)	2.85166	2.69613	2.72534
Distance	0.530	0.554	0.570
Reference	YACHDS 9;4445;81	NIIRDN 6;APP-17;82	FMCHA2 -;C254;89

Model Prediction

Prediction: 0.212

Unit: g/kg_body_weight

Mahalanobis Distance: 20.3

Mahalanobis Distance p-value: 6.1e-010

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Model Applicability

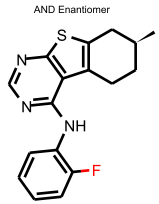
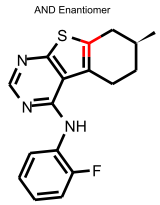
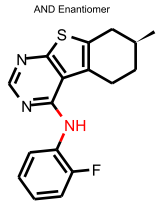
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_6 feature: 16: [*][c](:[*]):[*]
4. Unknown FCFP_6 feature: 1747237384: [*][c]1:[*]:[*]:[c](:[*]):s:1
5. Unknown FCFP_6 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
6. Unknown FCFP_6 feature: -124685461: [*]:n:[cH]:n:[*]
7. Unknown FCFP_6 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]
8. Unknown FCFP_6 feature: 1293778554: [*]:[c](:[*])N[c](:[*]):[*]
9. Unknown FCFP_6 feature: 1618154665: [*][c](:[*]):[cH]:[cH]:[*]
10. Unknown FCFP_6 feature: 71476542: [*]:[c](:[*])Cl

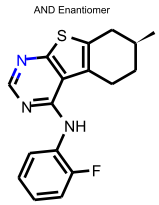
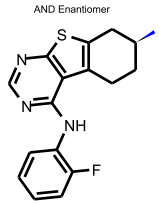
Feature Contribution

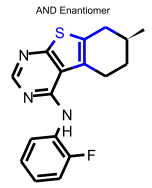
Top features for positive contribution

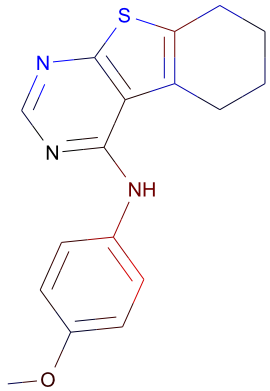
Fingerprint	Bit/Smiles	Feature Structure	Score

ECFP_6	-1046436026	 [*]F	0.349
ECFP_6	642810091	 [*][c](:[*]):[*]	0.281
ECFP_6	-1897341097	 [*]N[*]	0.216

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	655739385	 [*]:n:[*]	-0.239
ECFP_6	734603939	 [*]C	-0.201

FCFP_6	-1539132615	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	-0.2



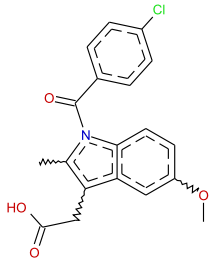
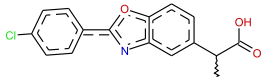
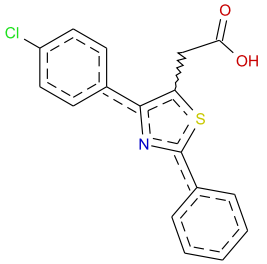
$C_{17}H_{17}N_3OS$
Molecular Weight: 311.40138
ALogP: 4.568
Rotatable Bonds: 3
Acceptors: 4
Donors: 1

Model Prediction

Prediction: 0.45
Unit: g/kg_body_weight
Mahalanobis Distance: 18.2
Mahalanobis Distance p-value: 0.000275

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	INDOMETHAZINE	BENOXAPROFEN	FENTIAZAC
Structure			
Actual Endpoint (-log C)	5.17	3.408	2.907
Predicted Endpoint (-log C)	3.33605	2.85166	2.69613
Distance	0.516	0.541	0.552
Reference	ARZNAD 25;1526;75	YACHDS 9;4445;81	NIIRDN 6;APP-17;82

Model Applicability

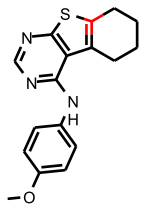
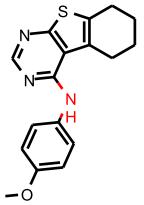
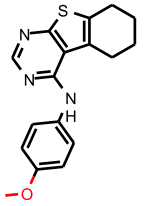
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_6 feature: 16: [*][c](:[*]):[*]
4. Unknown FCFP_6 feature: 1747237384: [*][c]1:[*]:[*]:[c](:[*]):s:1
5. Unknown FCFP_6 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
6. Unknown FCFP_6 feature: -124685461: [*]:n:[cH]:n:[*]
7. Unknown FCFP_6 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]
8. Unknown FCFP_6 feature: 1293778554: [*]:[c](:[*])N[c](:[*]):[*]
9. Unknown FCFP_6 feature: 1618154665: [*][c](:[*]):[cH]:[cH]:[*]

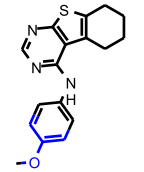
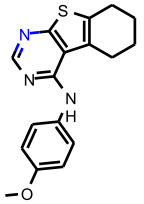
Feature Contribution

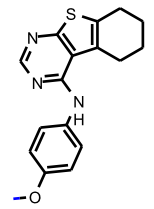
Top features for positive contribution

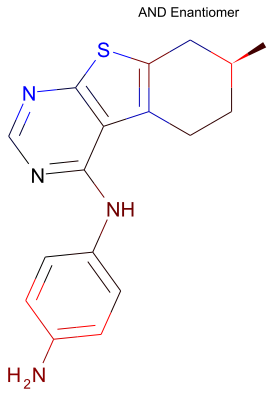
Fingerprint	Bit/Smiles	Feature Structure	Score

ECFP_6	642810091	 [*][c](:[*]):[*]	0.281
ECFP_6	-1897341097	 [*]N[*]	0.216
FCFP_6	136627117	 [*]OC	0.17

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	-176455838	 [*]O[c](:[cH]:[*]):[c H]:[*]	-0.257
ECFP_6	655739385	 [*]:n:[*]	-0.239

ECFP_6	734603939	 [*]C	-0.201



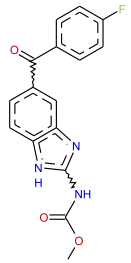
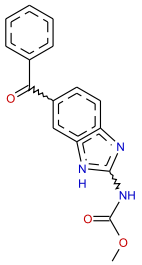
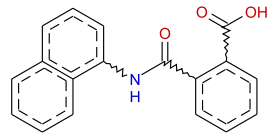
$C_{17}H_{18}N_4S$
Molecular Weight: 310.41662
ALogP: 4.089
Rotatable Bonds: 2
Acceptors: 4
Donors: 2

Model Prediction

Prediction: 0.611
Unit: g/kg_body_weight
Mahalanobis Distance: 20.4
Mahalanobis Distance p-value: 2.67e-010

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	FLUBENDAZOLE	CARBAMIC ACID; N-(5-BENZOYLBENZIMIDAZOL-2-YL)-; METHYL ESTER	NAPTALAM
Structure			
Actual Endpoint (-log C)	2.088	2.617	1.551
Predicted Endpoint (-log C)	2.69288	2.2368	1.89036
Distance	0.574	0.582	0.644
Reference	YRTMA6 9;11;78	IYKEDH 19;735;88	FMCHA2 -;C206;89

Model Applicability

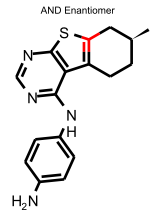
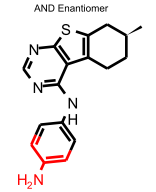
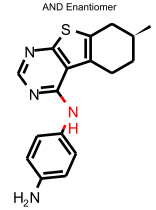
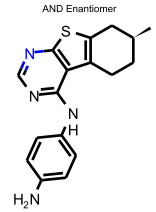
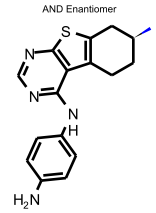
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

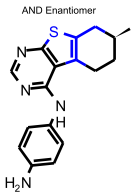
1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_6 feature: 16: [*][c](:[*]):[*]
4. Unknown FCFP_6 feature: 1747237384: [*][c]1:[*]:[*]:[c](:[*]):s:1
5. Unknown FCFP_6 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
6. Unknown FCFP_6 feature: -124685461: [*]:n:[cH]:n:[*]
7. Unknown FCFP_6 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]
8. Unknown FCFP_6 feature: 1293778554: [*]:[c](:[*])N[c](:[*]):[*]
9. Unknown FCFP_6 feature: 1618154665: [*][c](:[*]):[cH]:[cH]:[*]
10. Unknown FCFP_6 feature: 1069584379: [*]:[c](:[*])N

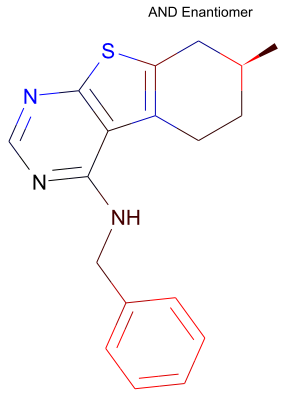
Feature Contribution

Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score

ECFP_6	642810091	 [*][c](:[*]):[*]	0.281
ECFP_6	971820502	 [*]:[cH]:[c](N):[cH]: [*]	0.276
ECFP_6	-1897341097	 [*]N[*]	0.216
Top Features for negative contribution			
Fingerprint	**Bit/Smiles**	**Feature Structure**	**Score**
ECFP_6	655739385	 [*]:n:[*]	-0.239
ECFP_6	734603939	 [*]C	-0.201

FCFP_6	-1539132615	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	-0.2



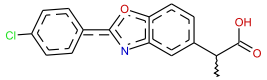
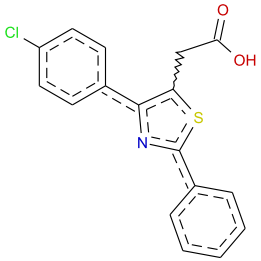
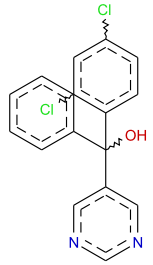
$C_{18}H_{19}N_3S$
Molecular Weight: 309.42856
ALogP: 4.678
Rotatable Bonds: 3
Acceptors: 3
Donors: 1

Model Prediction

Prediction: 0.36
Unit: g/kg_body_weight
Mahalanobis Distance: 19.8
Mahalanobis Distance p-value: 2.15e-008

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	BENOXAPROFEN	FENTIAZAC	TRIARIMOL
Structure			
Actual Endpoint (-log C)	3.408	2.907	2.742
Predicted Endpoint (-log C)	2.85166	2.69613	2.87257
Distance	0.497	0.539	0.557
Reference	YACHDS 9;4445;81	NIIRDN 6;APP-17;82	FMCHA2 -;C293;89

Model Applicability

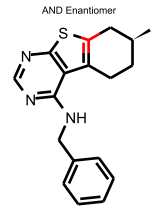
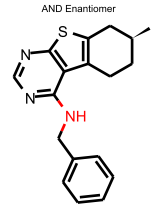
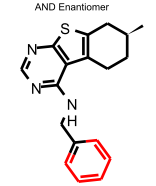
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_6 feature: 16: [*][c](:[*]):[*]
4. Unknown FCFP_6 feature: 1747237384: [*][c]1:[*]:[*]:[c](:[*]):s:1
5. Unknown FCFP_6 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
6. Unknown FCFP_6 feature: -124685461: [*]:n:[cH]:n:[*]
7. Unknown FCFP_6 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]
8. Unknown FCFP_6 feature: 907096426: [*]NC[c](:[*]):[*]
9. Unknown FCFP_6 feature: 1618154665: [*][c](:[*]):[cH]:[cH]:[*]

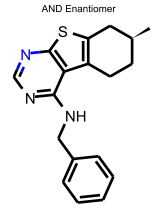
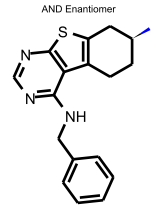
Feature Contribution

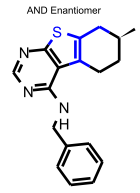
Top features for positive contribution

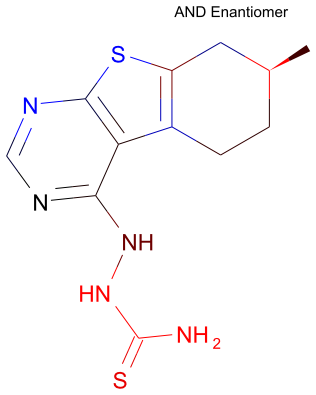
Fingerprint	Bit/Smiles	Feature Structure	Score

ECFP_6	642810091	 [*][c](:[*]):[*]	0.281
ECFP_6	-1897341097	 [*]N[*]	0.216
ECFP_6	1571214559	 [*]1:[cH]:[cH]:[cH]:[cH]:[cH]:1	0.19

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	655739385	 [*]:n:[*]	-0.239
ECFP_6	734603939	 [*]C	-0.201

FCFP_6	-1539132615	AND Enantiomer  [*]C[c]1:s:[*]:[*]:[c]:1[*]	-0.2



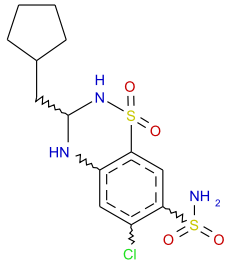
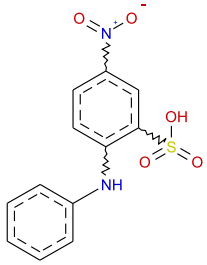
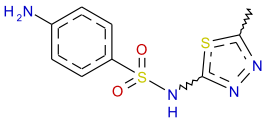
$C_{12}H_{15}N_5S_2$
Molecular Weight: 293.411
ALogP: 3.209
Rotatable Bonds: 3
Acceptors: 4
Donors: 3

Model Prediction

Prediction: 0.169
Unit: g/kg_body_weight
Mahalanobis Distance: 23.1
Mahalanobis Distance p-value: 4.71e-021

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	3-CYCLOPENTYLMETHYLHYDROCHLOROTHIAZIDE	2-ANILINO-5-NITROBENZENESULFONIC ACID; SODIUM SALT (Na STRIPPED)	SULFAMETHIZOLE
Structure			
Actual Endpoint (-log C)	2.58	2.126	1.687
Predicted Endpoint (-log C)	1.91133	2.19141	1.85826
Distance	0.709	0.714	0.735
Reference	YAKUD5 21;775;79	85JCAE -;1061;86	NIIRDN 6;388;82

Model Applicability

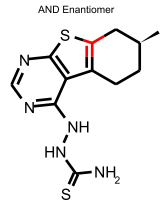
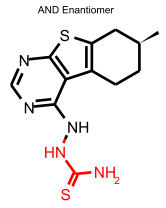
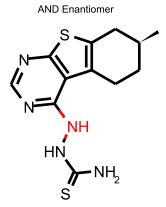
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_6 feature: 16: [*][c](:[*]):[*]
4. Unknown FCFP_6 feature: 1747237384: [*][c]1:[*]:[*]:[c](:[*]):s:1
5. Unknown FCFP_6 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
6. Unknown FCFP_6 feature: -124685461: [*]:n:[cH]:n:[*]
7. Unknown FCFP_6 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]
8. Unknown FCFP_6 feature: 1294344583: [*]NN[c](:[*]):[*]
9. Unknown FCFP_6 feature: -885461129: [*]NNC(=[*])[*]

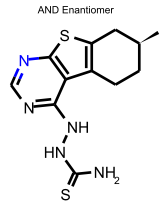
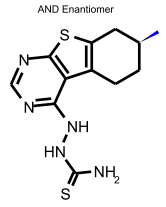
Feature Contribution

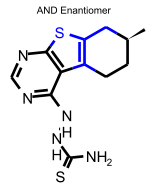
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score

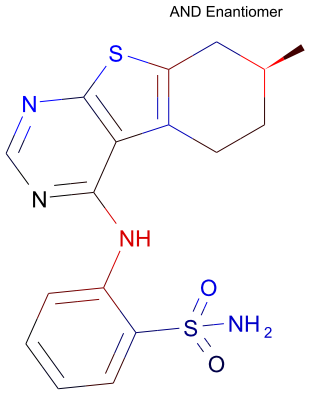
ECFP_6	642810091	 [*][c](:[*]):[*]	0.281
FCFP_6	1499521844	 [*]NC(=S)N	0.258
ECFP_6	-1897341097	 [*]N[*]	0.216

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	655739385	 [*]:n:[*]	-0.239
ECFP_6	734603939	 [*]C	-0.201

FCFP_6	-1539132615	 [*]C[c]1:s:[*]:[*]:[c]:1[*]	-0.2

TOPKAT_Rat_Oral_LD50



$C_{17}H_{18}N_4O_2S_2$

Molecular Weight: 374.48042

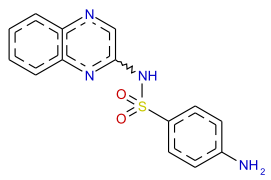
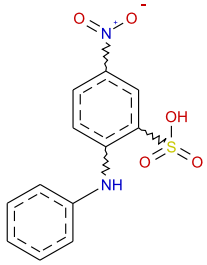
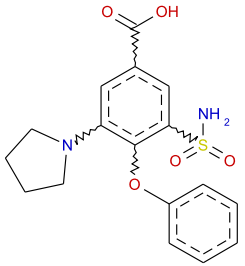
ALogP: 3.541

Rotatable Bonds: 3

Acceptors: 5

Donors: 2

Structural Similar Compounds

Name	SULFAQUINOXALINE	2-ANILINO-5-NITROBENZENESULFONIC ACID; SODIUM SALT (Na STRIPPED)	PIRETANIDE
Structure			
Actual Endpoint (-log C)	2.341	2.126	1.811
Predicted Endpoint (-log C)	2.42674	2.19141	1.83976
Distance	0.631	0.658	0.662
Reference	MahWM# 16NOV82	85JCAE -;1061;86	DRFUD4 2;393;77

Model Prediction

Prediction: 2.95

Unit: g/kg_body_weight

Mahalanobis Distance: 20.8

Mahalanobis Distance p-value: 1.37e-011

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Model Applicability

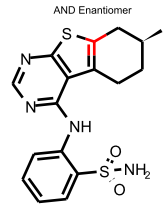
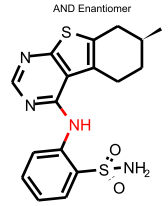
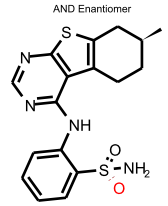
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_6 feature: 16: [*][c](:[*]):[*]
4. Unknown FCFP_6 feature: 1747237384: [*][c]1:[*]:[*]:[c](:[*]):s:1
5. Unknown FCFP_6 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
6. Unknown FCFP_6 feature: -124685461: [*]:n:[cH]:n:[*]
7. Unknown FCFP_6 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]
8. Unknown FCFP_6 feature: 1293778554: [*]:[c](:[*])N[c](:[*]):[*]
9. Unknown FCFP_6 feature: 1618154665: [*][c](:[*]):[cH]:[cH]:[*]

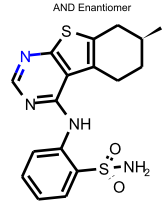
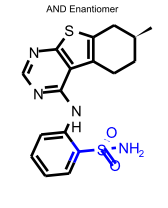
Feature Contribution

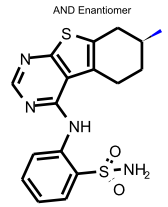
Top features for positive contribution

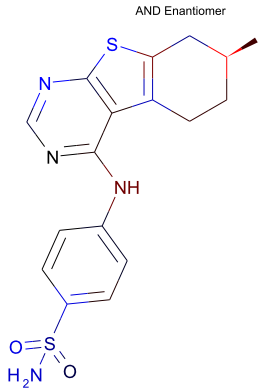
Fingerprint	Bit/Smiles	Feature Structure	Score

ECFP_6	642810091	 [*][c](:[*]):[*]	0.281
ECFP_6	-1897341097	 [*]N[*]	0.216
ECFP_6	-1074141656	 [*]=O	0.142

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	655739385	 [*]:n:[*]	-0.239
FCFP_6	-1096219292	 [*]:[c](:[*])S(=O)(=O)N	-0.225

ECFP_6	734603939	AND Enantiomer  [*]C	-0.201



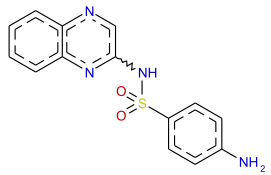
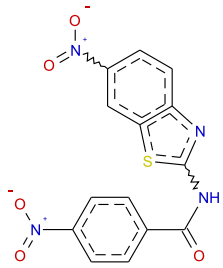
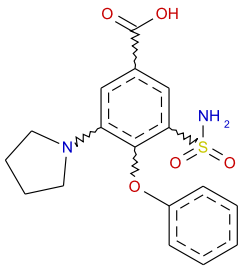
$C_{17}H_{18}N_4O_2S_2$
Molecular Weight: 374.48042
ALogP: 3.541
Rotatable Bonds: 3
Acceptors: 5
Donors: 2

Model Prediction

Prediction: 2.61
Unit: g/kg_body_weight
Mahalanobis Distance: 20.8
Mahalanobis Distance p-value: 9.44e-012

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	SULFAQUINOXALINE	BENZOTHIAZOLE; 6-NITRO-2-(p-NITROBENZOYLAMINO)-	PIRETANIDE
Structure			
Actual Endpoint (-log C)	2.341	2.361	1.811
Predicted Endpoint (-log C)	2.42674	2.96257	1.83976
Distance	0.626	0.667	0.672
Reference	MahWM# 16NOV82	JPETAB 90;260;47	DRFUD4 2;393;77

Model Applicability

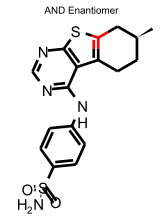
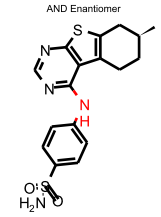
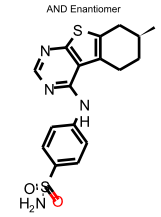
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_6 feature: 16: [*][c](:[*]):[*]
4. Unknown FCFP_6 feature: 1747237384: [*][c]1:[*]:[*]:[c](:[*]):s:1
5. Unknown FCFP_6 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
6. Unknown FCFP_6 feature: -124685461: [*]:n:[cH]:n:[*]
7. Unknown FCFP_6 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]
8. Unknown FCFP_6 feature: 1293778554: [*]:[c](:[*])N[c](:[*]):[*]
9. Unknown FCFP_6 feature: 1618154665: [*][c](:[*]):[cH]:[cH]:[*]

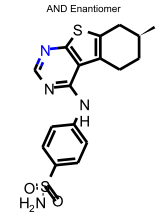
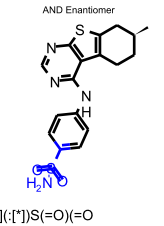
Feature Contribution

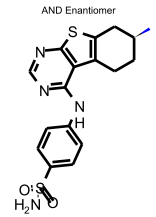
Top features for positive contribution

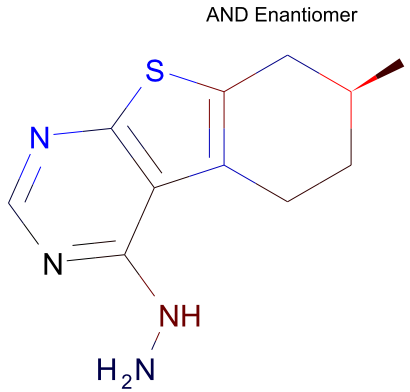
Fingerprint	Bit/Smiles	Feature Structure	Score

ECFP_6	642810091	 [*][c](:[*]):[*]	0.281
ECFP_6	-1897341097	 [*]N[*]	0.216
ECFP_6	-1074141656	 [*]=O	0.142

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	655739385	 [*]:n:[*]	-0.239
FCFP_6	-1096219292	 [*]:[c](:[*])S(=O)(=O)N	-0.225

ECFP_6	734603939		-0.201



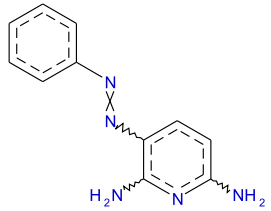
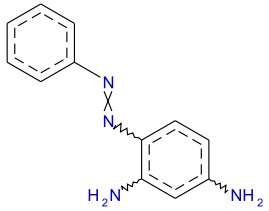
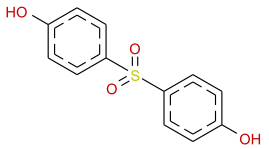
$C_{11}H_{14}N_4S$
Molecular Weight: 234.32065
ALogP: 2.561
Rotatable Bonds: 1
Acceptors: 4
Donors: 2

Model Prediction

Prediction: 0.467
Unit: g/kg_body_weight
Mahalanobis Distance: 20.5
Mahalanobis Distance p-value: 1.49e-010

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	PHENAZOPYRIDINE .HCl (HCl STRIPPED)	m-PHENYLENEDIAMINE; 4-(PHENYLAZO)-	4;4'-SULFONYLDIPHENOL
Structure			
Actual Endpoint (-log C)	2.724	2.109	1.74
Predicted Endpoint (-log C)	2.95034	2.69628	2.31209
Distance	0.497	0.527	0.530
Reference	TXAPA9 1;42;59	85JCAE -;1308;86	BIOFX* 601-05501;74

Model Applicability

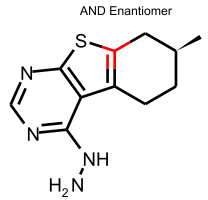
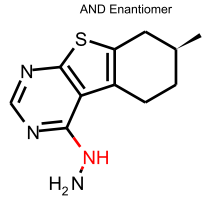
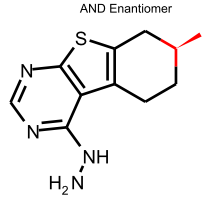
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_6 feature: 16: [*][c](:[*]):[*]
4. Unknown FCFP_6 feature: 1747237384: [*][c]1:[*]:[*]:[c](:[*]):s:1
5. Unknown FCFP_6 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
6. Unknown FCFP_6 feature: -124685461: [*]:n:[cH]:n:[*]
7. Unknown FCFP_6 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]
8. Unknown FCFP_6 feature: 1294344583: [*]NN[c](:[*]):[*]
9. Unknown FCFP_6 feature: 1070150408: [*]NN

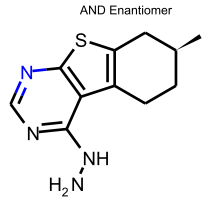
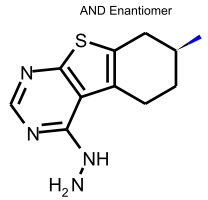
Feature Contribution

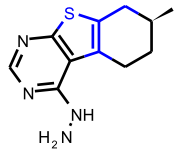
Top features for positive contribution

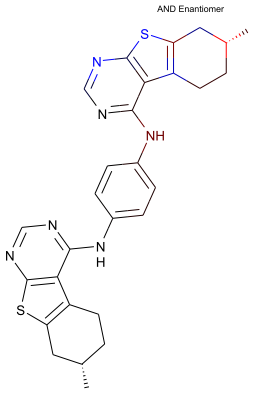
Fingerprint	Bit/Smiles	Feature Structure	Score

ECFP_6	642810091	 [*][c](:[*]):[*]	0.281
ECFP_6	-1897341097	 [*]N[*]	0.216
ECFP_6	865482986	 [*]C([*])C	0.132

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	655739385	 [*]:n:[*]	-0.239
ECFP_6	734603939	 [*]C	-0.201

FCFP_6	-1539132615	AND Enantiomer  [*]C[c]1:s:[*]:[*]:[c]:1[*]	-0.2



$C_{28}H_{28}N_6S_2$

Molecular Weight: 512.69212

ALogP: 7.842

Rotatable Bonds: 4

Acceptors: 6

Donors: 2

Model Prediction

Prediction: 0.705

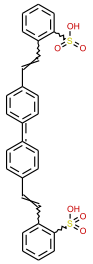
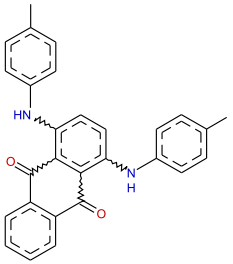
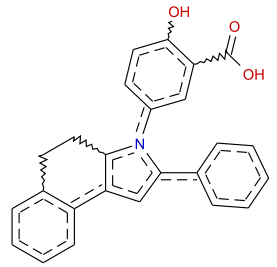
Unit: g/kg_body_weight

Mahalanobis Distance: 25.3

Mahalanobis Distance p-value: 7.16e-033

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	BENZENESULFONIC ACID; 2;2'-(4;4'-BIPHENYLYLENEDIVINYLENE)DI-; DISODIUM SALT (Na STRIPPED)	ANTHRAQUINONE; 1;4-bis-(p-TOLYLAMINO)-	FENDOSAL
Structure			
Actual Endpoint (-log C)	1.968	2.058	2.928
Predicted Endpoint (-log C)	1.72109	1.57464	2.59
Distance	0.793	0.960	1.025
Reference	MVCRB3 2;193;73	85JCAE -;1330;86	AGACBH 8;209;78

Model Applicability

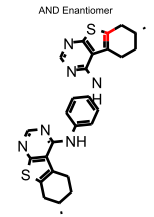
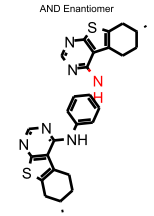
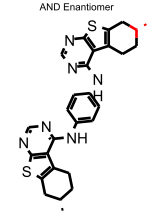
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: -1597579789: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
3. Unknown FCFP_6 feature: 16: [*][c](:[*]):[*]
4. Unknown FCFP_6 feature: 1747237384: [*][c]1:[*]:[*]:[c](:[*]):s:1
5. Unknown FCFP_6 feature: -1564473960: [*]:n:[c]1:s:[*]:[*]:[c]:1:[*]
6. Unknown FCFP_6 feature: -124685461: [*]:n:[cH]:n:[*]
7. Unknown FCFP_6 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]
8. Unknown FCFP_6 feature: 1293778554: [*]:[c](:[*])N[c](:[*]):[*]
9. Unknown FCFP_6 feature: 1618154665: [*][c](:[*]):[cH]:[cH]:[*]

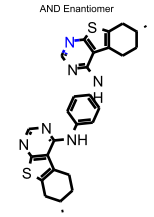
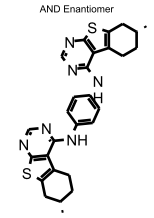
Feature Contribution

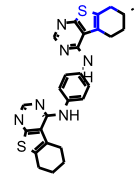
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score

ECFP_6	642810091	 [*][c](:[*]):[*]	0.281
ECFP_6	-1897341097	 [*]N[*]	0.216
ECFP_6	865482986	 [*]C([*])C	0.132

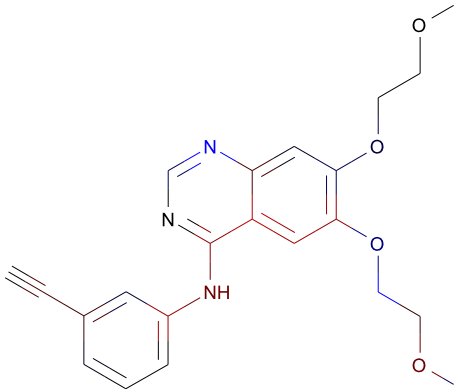
Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	655739385	 [*]:n:[*]	-0.239
ECFP_6	734603939	 [*]C	-0.201

FCFP_6	-1539132615	AND Enantiomer  [*]C[c]1:s:[*]:[*]:[c]:1[*]	-0.2

Erlotinib

TOPKAT_Rat_Oral_LD50



$C_{22}H_{23}N_3O_4$

Molecular Weight: 393.43572

ALogP: 4.309

Rotatable Bonds: 10

Acceptors: 7

Donors: 1

Model Prediction

Prediction: 0.662

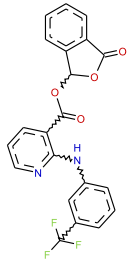
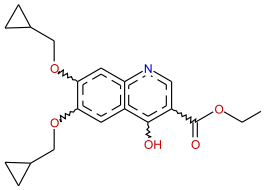
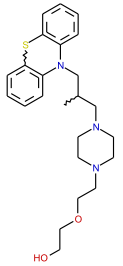
Unit: g/kg_body_weight

Mahalanobis Distance: 20.8

Mahalanobis Distance p-value: 9.57e-012

Mahalanobis Distance: The Mahalanobis distance (MD) is a generalization of the Euclidean distance that accounts for correlations among the X properties. It is calculated as the distance to the center of the training data. The larger the MD, the less trustworthy the prediction.
Mahalanobis Distance p-value: The p-value gives the fraction of training data with an MD greater than or equal to the one for the given sample, assuming normally distributed data. The smaller the p-value, the less trustworthy the prediciton. For highly non-normal X properties (e.g., fingerprints), the MD p-value is wildly inaccurate.

Structural Similar Compounds

Name	TALNIFLUMATE	3-QUINOLINECARBOXYLIC ACID; 6;7-bis-(CYCLOPROPYLMETHOXY)-4-HYDROXY-; ETHYL ESTER	DIXYRAZINE .HCl (HCl STRIPPED)
Structure			
Actual Endpoint (-log C)	1.538	2.076	3.029
Predicted Endpoint (-log C)	2.82541	2.50101	2.47585
Distance	0.615	0.615	0.654
Reference	FRPSAX 36;372;81	TXAPA9 18;185;71	ANPBAZ 61;669;61

Model Applicability

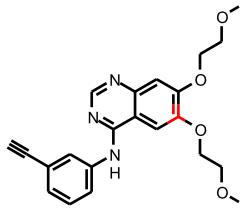
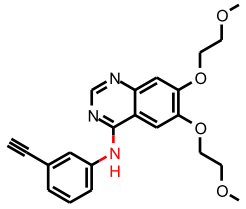
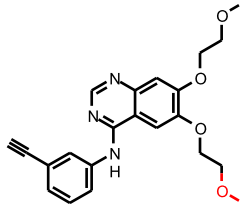
Unknown features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.

1. All properties and OPS components are within expected ranges.
2. Unknown ECFP_2 feature: 1139738044: [*]:[c](:[*])C#C
3. Unknown FCFP_6 feature: 16: [*][c](:[*]):[*]
4. Unknown FCFP_6 feature: 1618154665: [*][c](:[*]):[cH]:[cH]:[*]
5. Unknown FCFP_6 feature: 1747237384: [*][c]1:[*]:[*]:[c](:[*]):s:1
6. Unknown FCFP_6 feature: -124685461: [*]:n:[cH]:n:[*]
7. Unknown FCFP_6 feature: -1151884458: [*]N[c](:n:[*]):[c](:[*]):[*]
8. Unknown FCFP_6 feature: 1293778554: [*]:[c](:[*])N[c](:[*]):[*]
9. Unknown FCFP_6 feature: 902193919: [*]:[c](:[*])C#C
10. Unknown FCFP_6 feature: 131784192: [*]C#C

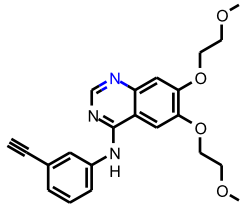
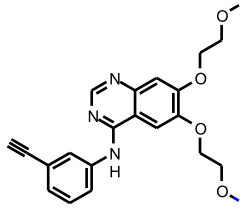
Feature Contribution

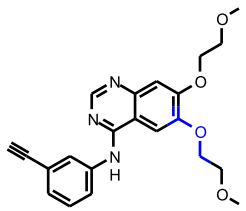
Top features for positive contribution

Fingerprint	Bit/Smiles	Feature Structure	Score

ECFP_6	642810091	 [*][c](:[*]):[*]	0.281
ECFP_6	-1897341097	 [*]N[*]	0.216
FCFP_6	136627117	 [*]OC	0.17

Top Features for negative contribution

Fingerprint	Bit/Smiles	Feature Structure	Score
ECFP_6	655739385	 [*]:n:[*]	-0.239
ECFP_6	734603939	 [*]C	-0.201

FCFP_6	1036089772	 [*]:[c](:[*])OC	-0.136