

Supporting Information for: Assessment of chemistry knowledge in large language models that generate code

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I. DESCRIPTION OF NLCC TOOLS

As part of this study and our previous perspective article, we have developed the Natural Language in Computational Chemistry (nlcc) command line open-source software tool. This python-based tool is available at the web address <https://github.com/whitead/nlcc> and can be installed simply using the command ‘pip install nlcc’. This tool provides a simple interface for querying natural language models accessible via internet application programming interfaces (APIs), with those from organizations OpenAI and Huggingface being the ones currently implemented. In this sense, the nlcc tool is not really chemistry specific, but can be used for most code-generating scenarios.


In addition to its general features, the nlcc library has two features specific to this work. The first is the ‘nlcc-eval’ tool, which allows us to systematically evaluate the examples in our chemistry benchmark database, described next. This tool retrieves multiple alternative outputs from an API for a given prompt, attempts to evaluate the code in python, and compares the result returned by the code to some correctness criterion provided in the database. The result of nlcc-eval can be viewed in a format that is friendly for command line use and testing, but also used to generate a public available website showing the results (<https://ur-whitelab.github.io/nlcc-data/>). The second is the inclusion of ‘contexts.’ Contexts are short snippets of text that we prepend to the user’s prompt in order to give the model more information. For example, the ‘matplotlib’ context imports the matplotlib library as well as the numpy library, runs a command to use the ‘Agg’ backend (which allows plot generation without an interactive display), and runs a simple numpy command. Using this context for any plotting related tasks makes the output of the model more homogeneous and more likely to be correct. See the attached supplemental file for the full details of all contexts.

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II. EXAMPLE USE OF CHATGPT


A


 Replace [insert] with the correct text:

```
import math
import sys
def claussius(HVap, T1, P1, T2):
    """
    This function returns the phase
    transition pressure at temperature T2
    given a heat of vaporization HVap,
    and and reference temperature and
    pressure T1 and P1
    """
    [insert]
    return P2
```

 `import math`
`import sys`
`def claussius(HVap, T1, P1, T2):`
 `"""`
 `This function returns the phase`
 `transition pressure at temperature T2`
 `given a heat of vaporization HVap,`
 `and and reference temperature and`
 `pressure T1 and P1`
 `"""`
 `P2 = P1 * math.exp((HVap/ 8.314) * ((1/T1) - (1/T2)))`
 `return P2`


C


 You are a chat bot that can solve chemistry questions. What is the phase transition pressure at temperature T2, given a heat of vaporization HVap, and and reference temperature and pressure T1 and P1.

 The phase transition pressure at temperature T2 can be calculated using the Clausius-Clapeyron equation:

$$\ln(P2/P1) = (HVap/R) * ((1/T1) - (1/T2))$$

where P2 is the phase transition pressure at temperature T2, P1 is the reference pressure, HVap is the heat of vaporization, R is the ideal gas constant, and T1 and T2 are the reference temperature and the temperature at which the phase transition pressure is being calculated, respectively.


 Now solve for P2


 To solve for P2, you would plug in the known values for HVap, R, T1, T2 and P1 into the Clausius-Clapeyron equation and then solve for P2.

$$P2 = P1 * e^{((HVap/R) * ((1/T1) - (1/T2)))}$$

where e is the mathematical constant approximately equal to 2.71828.


It is important to note that this equation is only approximate and assumes ideal gas behavior and constant heat of vaporization. In reality, the heat of vaporization can change with temperature, and the equation should only be used for estimation purposes.


 And what is R?

 R is the ideal gas constant, it is a physical constant that relates the energy of a sample of gas to its temperature and number of moles. It is denoted by the symbol R and its value is approximately 8.314 J/mol-K in the International System of Units (SI) and 1.987 cal/mol-K in the calorie-based system of units (cgs). It's also commonly used in other fields of science and engineering.

ChatGPT Jan 9 Version. Free Research Preview. Our goal is to make AI systems more natural and safe to interact with. Your feedback

B

 Explain this to me like I'm taking general chemistry

 Sure! The code you've provided is a Python function called "claussius" that calculates the pressure at which a substance will transition from a liquid to a gas (or vice versa) at a given temperature. The function takes four inputs: the heat of vaporization (HVap) of the substance, a reference temperature (T1) and pressure (P1) at which the heat of vaporization was measured, and the temperature (T2) at which you want to calculate the phase transition pressure.

The heat of vaporization is a measure of the amount of energy required to turn a substance from a liquid to a gas (or vice versa) at a constant temperature and pressure. The Clausius-Clapeyron equation, which is used in this function, relates the heat of vaporization to the change in pressure and temperature as a substance goes through a phase transition.

The function uses the Clausius-Clapeyron equation to calculate the pressure (P2) at the given temperature (T2) using the heat of vaporization, reference temperature and pressure as inputs. The equation is:
 $P2 = P1 * e^{((HVap/R) * ((1/T1) - (1/T2)))}$, where R is the gas constant.

Once the pressure is calculated, the function returns it as the output. This function will be useful for determining the phase transition pressure of a substance at any temperature, as long as you know its heat of vaporization and reference temperature and pressure.

FIG. S1. (a) ChatGPT can solve the problems in our database by asking it to replace “[insert]” with correct text. With an API, we would expect the same performance from ChatGPT as the underlying model in this mode. (b) Continuation of the same conversation shows the AI can explain the problem that was posed only as code generation. (c) A typical use of ChatGPT for the same problem would be to describe the problems in words, and have a conversation about the results. The solution produced is the same, but with more annotation.

III. FOREIGN LANGUAGE PROMPTS

Examples of prompts where tasks are specified in Mandarin.

Prompt

```
def cal_correl_fun(x,y):
    """
    此函数计算两个给定数据集x，y的相关函数C_xy并返回C_xy。
    """
    [insert]
    return C_xy
```

Output

```
def cal_correl_fun(x,y):
    """
    此函数计算两个给定数据集x，y的相关函数C_xy并返回C_xy。
    """
    C_xy = np.zeros((len(x),len(y)))
    for i in range(len(x)):
        for j in range(len(y)):
            C_xy[i,j] = np.corrcoef(x[i],y[j])[0,1]
    return C_xy
```

Prompt

```
def cal_correl_fun(x,y):
    """
    此函数计算两个给定数据集x，y的相关函数C_xy并返回C_xy。
    """
    [insert]
    return corr
```

Output

```
def cal_correl_fun(x,y):
    """
    此函数计算两个给定数据集x，y的相关函数C_xy并返回C_xy。
    """
    corr = np.corrcoef(x,y)
    return corr
```

FIG. S2. Two results for the prompt “This function computes the correlation function C_{xy} for two given datasets x , y and returns C_{xy} ” written in Mandarin. Both use the numpy context (not shown) and the insertion capability of codex, with default parameters described in the paper. The only difference between the two is the name of the returned variable; in the second case, the variable `corr` evidently suggests to the model to use the numpy `corrcoef` function which is a more direct solution when using numpy.

Prompt

```
def remove_water(traj_file,top_file):
    """
    这个函数从加载的traj_file和top_file中除掉溶剂分子，返回动力学轨迹文件
    """
    [insert]
    return trj
```

Output (mdtraj context)

```
def remove_water(traj_file,top_file):
    """
    这个函数从加载的traj_file和top_file中除掉溶剂分子，返回动力学轨迹文件
    """
    trj = md.load(traj_file,top=top_file)
    trj.remove_solvent()
    return trj
```

Output (MDAnalysis context)

```
def remove_water(traj_file,top_file):
    """
    这个函数从加载的traj_file和top_file中除掉溶剂分子，返回动力学轨迹文件
    """
    u = MDAnalysis.Universe(top_file,traj_file)
    u.select_atoms("not resname SOL")
    trj = u.trajectory
    u.trajectory.close()
    return trj
```

FIG. S3. Two results for the prompt “This function removes solvent molecules from the loaded traj_file and top_file and returns the trajectory file” written in Mandarin. The first uses the mdtraj context and the second the MDAnalysis context (not shown).

IV. ALL MODELS COMPARED

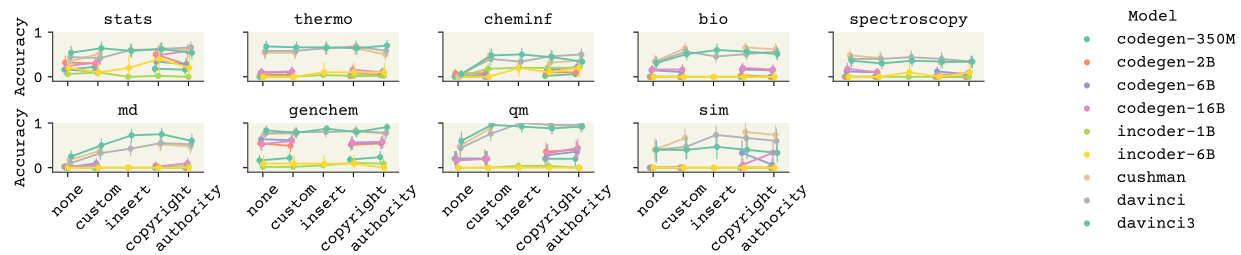


FIG. S4. A comparison of accuracy of the LLMs compared in this study across different contexts. Adding context – short comments/imports – generally improves accuracy across topic and model. Error bars are 95% confidence intervals from bootstrapping across individual prompts, temperature, and from multiple completions.

V. ACCURACY ON ALL PROMPTS

Accuracy on all automatic evaluable prompts is shown in Figure S6

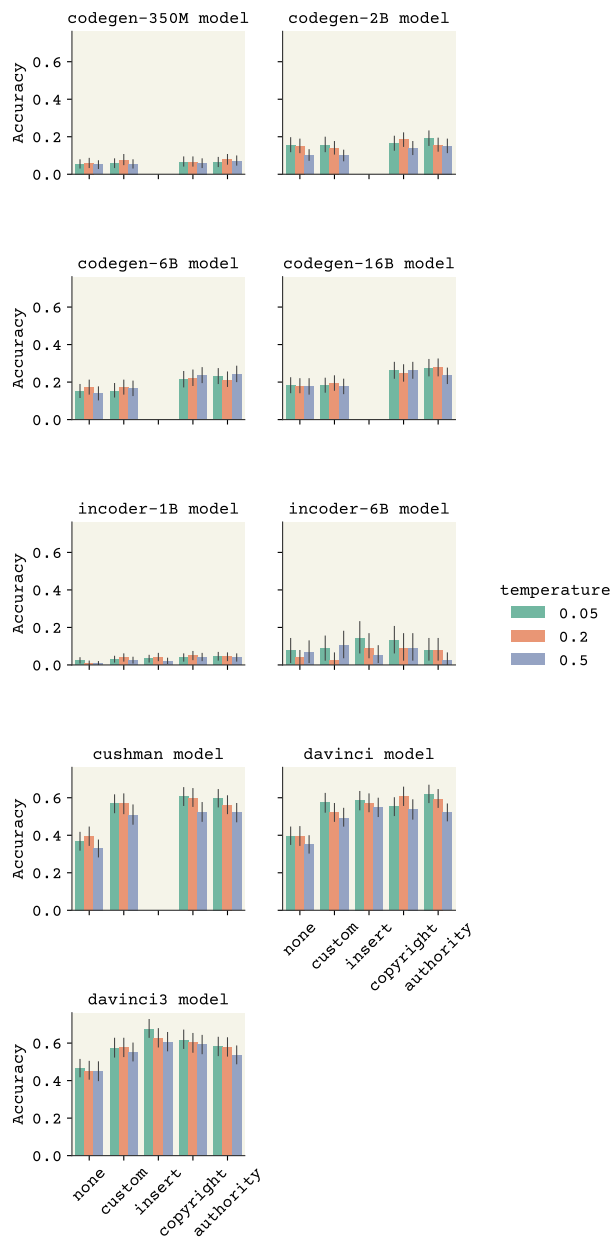


FIG. S5. Comparison of context effect across models and temperatures. Having a custom context is most important. Note that insert, copyright, and authority include the “custom” context. Error bars are 95% confidence intervals from bootstrapping across individual prompts, temperature, and from multiple completions. Cushman and Codegen cannot do insertions.

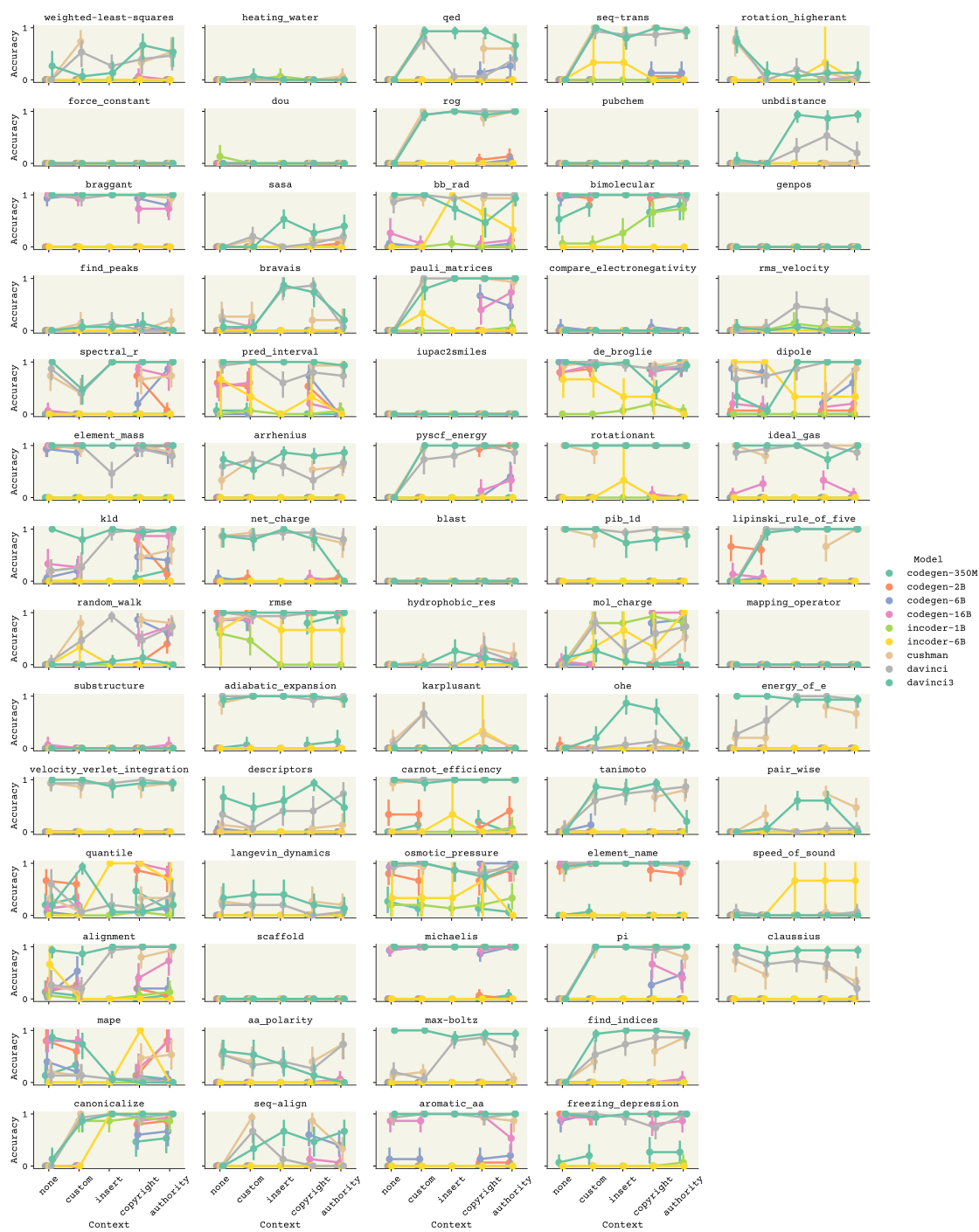


FIG. S6. Accuracy on multiple top-k/temperatures for different models broken out by specific prompt.

VI. GENERATED MOLECULES

This task was to generate SMILES given a sentence about a molecule. The generated SMILES were created from the following prompts, where the SMILES strings are the completions from InstructGPT.

1. This is a drug-like molecule with a tertiary amine and phenol:
SMILES: CCN(CC)CCOc1ccc(cc1)c2cc(ccc12)C#N
2. This is a drug-like molecule with a bicyclic ring:
SMILES: CC1=C(C=CC=C1)C2=CC=CC=C2
3. This is a weakly lipophilic drug-like molecule with two rings:
SMILES: C1CC2C(C1)CC(C2)C3=CC=CC=C3
4. This is a very lipophilic drug-like molecule with two rings:
SMILES: CCCCC...

where the red character was deleted to make the SMILES valid and the final molecule SMILES was 505 Cs.

VII. NOMENCLATURE

This task was to predict IUPAC name from SMILES. The following is a table of IUPAC names and predicted IUPAC names from InstructGPT by completing the following prompt:

```
This program provides SMILES for the given molecule.
It looks them up in a database, so it cannot be wrong.
Molecule 1: 3-(3,4-dichlorophenyl)-1,1-dimethylurea
SMILES: CN(C)C(=O)Nc1ccc(Cl)c(Cl)c1

Molecule 2: 7-methoxy-N-[4-(4-quinoxalin-5-ylpiperazin-1-yl)butyl]-1-benzofuran-2-carboxamide
SMILES: COc1cccc2cc(C(=O)NCCCC3CCN(c4cccc5nccnc54)CC3)oc21

Molecule 3: (4-phenylphenyl) acetate
SMILES: CC(=O)OC1=CC=C(C=C1)C2=CC=CC=C2

Molecule 4: [insert]
SMILES: [SMILES]
```

where [SMILES] are taken from the reference molecule. 0 of the 100 attempts were correct. We tried multiple prompts and Davinci and adjusting temperature without success.

True Name	Predicted Name
methyl 2-(2-chloroanilino)-2-(3-chlorophenyl)acetate	2,2-dichloro-N-(2-chlorophenyl)-N-(4-chlorophenyl)acetamide
3-oxo-4H-1,4-benzoxazine-7-carbohydrazide	2-oxiranecarboxylic acid
2-(4-bromo-2-chlorophenoxy)-1-(4-methylphenyl)propan-1-one	4-bromo-2-chloro-5-fluorophenyl acetate
N-(8-azabicyclo[3.2.1]octan-3-yl)-N-methylquinolin-4-amine	2-cyano-N-(4-methoxyphenyl)-3-phenylpropanamide
N-[[2-(ethoxymethyl)phenyl]methyl]-4-nitrobenzamide	2-chloro-N-(3-methoxypropyl)-5-nitrobenzamide
3-(4-methyl-2-pyridin-4-ylpyrimidin-5-yl)propanoic acid	2-chloro-N-(2-chlorophenyl)-N-(methoxycarbonyl)acetamide
2-(2-chlorophenyl)sulfinyl-1-(4-propylphenyl)ethanamine	4-chloro-2-methylphenol
1-cyclopropyl-3-(2-phenylmethoxypropanoylamino)urea	2-chloro-N-(2-chloroethyl)-N-(2-chlorophenyl)-urea
4-hydroxy-1-[4-hydroxy-2-(hydroxymethyl)butyl]pyridin-2-one	2-ethyl-1-hexanol
(2R)-2-amino-N-(3-hydroxypropyl)-3-methylbutanamide	2-chloro-N-(2-chlorophenyl)-N-(methoxycarbonyl)acetamide
2-chloro-4-(2-propan-2-ylphenyl)pyrimidine	2-chloro-N-(2-chlorophenyl)-N-(methylamino)cyclohexan-1-amine
1-(4,4-dimethylcyclohexyl)-2-(furan-2-yl)ethanamine	2-chloro-N-(2-chlorophenyl)-N-(methoxycarbonyl)acetamide
2-hydroxy-N-piperidin-4-yl-N-propylbenzamide	2-cyano-N-(4-methoxy-3-nitrophenyl)-N-(2-thienylmethyl)-acetamide
N'-[4-(4-methylpiperidin-1-yl)phenyl]hexane-1,6-diamine	3-methyl-2-oxiranecarboxylic acid
5-chloro-2-(5-methyl-2-propan-2-ylcyclohexyl)oxyaniline	2-chloro-N-(2-chlorophenyl)-N-(methoxycarbonyl)acetamide
2-(2-nitrophenyl)oxolane-3-carboxylic acid	2-phenylpropanoic acid
dimethyl 2-ethyl-5-methyloxane-3,3-dicarboxylate	2,2,2-trifluoroethyl acetate
5-ethyl-6-naphthalen-1-yl-4,5-dihydropyridazin-3-amine	2-amino-5-chloro-N-(2-chloroethyl)-benzamide
1-[4-(4,5-dihydroimidazol-1-yl)phenyl]ethanone	2-methyl-2-propanol
5-(1H-indol-3-yl)-2-methyl-6-oxo-3H-pyran-2-carbonitrile	2-chloro-5-fluoroaniline
3-ethoxy-2-(thiophen-3-ylmethyl)prop-2-enoic acid	2-thiophenecarboxaldehyde
chloro-(2-fluorophenyl)diazene	2-chloro-N,N-diphenylformamide
2-[(5-pyridin-3-yl-1H-pyrazol-4-yl)methylamino]acetic acid	2-cyano-N-(2-methoxyethyl)-5-methylbenzamide
1,4-dibromo-2-[(R)-chloro-(4-ethylphenyl)methyl]benzene	2-bromo-4-(bromomethyl)phenyl chloride
2-ethyl-5-propan-2-ylbenzene-1,4-diol	2-butanol
1-[1-(methoxymethylsulfanyl)-2-methylpropyl]benzotriazole	2-amino-5-chloro-N-(2-methoxyethyl)-benzamide
4-methyl-3-(oxiran-2-ylmethyl)benzenesulfonic acid	2-thiophenecarboxylic acid
2-[[2-(1-oxophthalazin-2-yl)acetyl]amino]propanoic acid	2-chloro-N-(2-chlorophenyl)-N-methoxyacetamide
3-(2-chlorophenyl)-2-cyano-N-(4-nitrophenyl)prop-2-enamide	2-chloro-5-(trifluoromethyl)benzaldehyde
5-(2-hydroxypropoxy)hexane-1,1,4-triol	2-butanol
3-bromo-N-(4-iodophenyl)-4-prop-2-enoxybenzamide	2-bromo-3-iodo-5-nitrobenzene
2-piperidin-1-yl-5-(2-pyridin-3-ylethynyl)pyridine	2-methyl-5-phenyl-1H-pyrazolo[3,4-b]pyridine
[ethoxy(phenoxy)phosphoryl]methylbenzene	2,2,2-trifluoroethyl acetate
1-(4-methylphenyl)sulfonyl-3-pyridin-2-ylurea	2-thiophenecarboxaldehyde
1-cyclopropyl-2-[2-(4-methoxyphenyl)ethyl]guanidine	2-methyl-2-propanol
(3-chloro-2-methylpropyl) 4-methylbenzenesulfonate	4-chloro-2-fluoro-benzenesulfonic acid
2-amino-N-ethyl-N-(oxolan-3-ylmethyl)pent-4-ynamide	2-amino-5-chloro-N-(2-methoxyethyl)-benzamide
1-(2-ethoxyethyl)-4-pyridin-2-ylpiperazine	2-amino-5-chloro-N-(2-methoxyethyl)-benzamide
1-(3-cyanophenyl)-3-(2,6-dimethylphenyl)-1-methylthiourea	2-amino-5-chloro-N-(2-methoxyethyl)-benzamide
5,7-dimethyl-2-piperidin-4-ylpyrazolo[1,5-a]pyrimidine	2-amino-5-chloro-N-(2-methoxyethyl)-benzamide
[2,6-dibromo-4-(4-pentylcyclohexyl)phenyl] 4-heptylbenzoate	4-bromo-2-(4-bromophenyl)-5-methylphenyl acetate
4-chloroiminocyclohexan-1-one	2-chloro-N-(4-methoxy-phenyl)-acetamide
(5,10-dioxobenzo[g]quinolin-3-yl)methyl N-phenylcarbamate	2-methyl-2-propanol
(10-methylphenothiazin-2-yl) acetate	2-amino-5-methylthiophene
(3-nitrophenyl) 4-bromo-3-nitrobenzoate	2-bromo-3-methyl-1-butanol
3-(ethylamino)-4-(2-methylpropoxy)butan-1-ol	2-chloro-N-(2,6-dichlorophenyl)-acetamide
1-butylsulfonylpyrrolidine-2-carbonyl chloride	2-chloro-N-(2-chloroethyl)-N-methylethanamine
2-(cycloheptylamino)-2-oxoacetate	2-methyl-2-propanol
[2-(2-chlorophenyl)morpholin-4-yl]-pyridin-4-ylmethanone	2-chloro-N-(2-chlorophenyl)-3-methylbutanamide
methyl 2-[3-(methoxycarbonylamino)phenoxy]acetate	2-chloro-N-(2-methoxyethyl)-N-(2-methoxyethyl)acetamide
4-(3-fluoro-4-methoxyphenyl)-2-phenylpyridine	2-fluoro-N-(4-fluorophenyl)-3-methylbenzamide
3-[(2R)-6-ethoxy-2-methyl-4-oxo-3H-chromen-2-yl]propanoate	2-butanol
N-(2-aminobutyl)-2-methylpropanamide	3-methyl-2-oxetanone
3-phenyl-4-(3-phenylpropoxy)aniline	2-amino-5-chloro-N-(2-methoxyethyl)-benzamide
1,6-dimorpholin-4-ylhexane-1,6-dithione	2-(2-chlorophenyl)-N-(4-methoxyphenyl)-5-oxazolamine
5-(2-ethylmorpholin-4-yl)-4-fluoro-2-nitrobenzoic acid	2-fluoro-N-(4-methoxyphenyl)acetamide
3-chloro-2-fluoro-5-(4-methylphenyl)sulfanylpyridine	2-(2-fluorophenyl)-N-(4-methoxyphenyl)acetamide
N-but-2-enylcyclohexanamine	2-chloro-N-(2-chlorophenyl)-N-(methoxycarbonyl)acetamide

True Name	Predicted Name
3-(1-methylindol-7-yl)-5-(pyridin-3-ylamino)phenol	2-cyano-N-(2,6-dimethylphenyl)-3-methylbutanamide
2-but-3-enoxybenzamide	2-chloro-N-(2-chlorophenyl)-N-(methoxycarbonyl)acetamide
2-oxo-N-quinolin-2-ylnonanamide	dodecane
2-[(4-carbamoylphenyl)sulfonylamino]-5-chlorobenzoic acid	2-chloro-5-fluorophenyl acetic acid
4-(2-aminobutyl)-N-ethyl-N-(2-methoxyethyl)-2-methylaniline	2-chloro-N-(2-chloroethyl)-N-methylethanamine
1-[(3-aminophenyl)methyl]-1-cyclopropyl-3-propylurea	2-chloro-N-(2-chloroethyl)-N-methylethanamine
ethyl 2-[2-(3-amino-2-hydroxypropyl)imidazol-1-yl]benzoate	2-amino-5-chloro-N-(2-methoxyethyl)-benzamide
2-(benzenesulfonamido)-3-phenylpentanedioic acid	2-hydroxy-5-oxo-5H-pyrrolo[3,4-b]pyridine-3-carboxylic acid
ethyl N-(pyrazol-3-ylidenemethylamino)carbamate	2-methyl-2-propanol
1-[2-(3,5-dimethylpyrazol-1-yl)phenyl]-N-methylethanamine	2-amino-5-chloro-N-(2-fluorophenyl)-benzamide
1-propyl-3-[(Z)-pyridin-2-ylmethylideneamino]thiourea	2-amino-5-chloro-N-(2-fluorophenyl)-benzamide
N-(3-methylcyclopentyl)-3-(2H-tetrazol-5-yl)aniline	2-methyl-2-propanol
oxolan-3-yl 4-(methylamino)butanoate	2-cyano-N-(4-methoxyphenyl)-N-(2-phenylethyl)acetamide
2-carboxyoxycarbonyl-6-tetradecylbenzoic acid	2-chloro-N-(2-chlorophenyl)-N-(methoxyimino)acetamide
2-(5-phenyl-1,3-oxazol-4-yl)acetonitrile	2-cyano-N-(2-methoxyethyl)-5-nitrobenzamide
4-chloro-N-[[4-(trifluoromethoxy)phenyl]methyl]benzamide	2-chloro-5-(trifluoromethyl)benzaldehyde
N-(2,3-dimethylbutyl)-2-(2-hydroxyphenyl)acetamide	2-methyl-2-propanol
2-fluoro-N-heptan-2-yl-5-morpholin-4-ylsulfonylbenzamide	hexamethylcyclotrisiloxane
(3-formylphenyl)methanesulfonate	2-chloroacetophenone
4-(4,4-dimethylpentan-2-yl)cyclohex-2-en-1-one	2-methyl-2-propanol
2-[[2-(methanesulfonamido)phenyl]sulfamoyl]propanoic acid	2-amino-5-chloro-N-(2-methoxyethyl)-benzene-1-sulfonamide
4-[(4-chloro-2-methylanilino)methyl]piperidin-4-ol	2-chloro-N-(4-methoxyphenyl)-acetamide
(5,5-dimethyl-1,4-dioxan-2-yl)methylmethanesulfonate	2-methyl-2-propanol
2-[2-methoxy-5-(thiophen-3-ylmethylamino)phenoxy]ethanol	2-amino-5-methylthiophene
2-(3,4-difluorophenyl)sulfinyl-1-(4-methylphenyl)ethanamine	2-fluoro-5-methylphenol
3-methoxy-N-propan-2-ylthiophene-2-carboxamide	2-cyano-N-(4-methoxy-3-nitrophenyl)-3-pyridinecarboxamide
2-(4-phenylmethoxybutyl)tridecane-1,2-diol	12-crown-4
1-(1-but-3-ynoxy-2-nitroethyl)-2-chlorobenzene	2-chloro-N-(2-chlorophenyl)-N-(4-methoxyphenyl)acetamide
1-[methyl-[(1-methylpyrazol-4-yl)methyl]amino]propan-2-one	2-cyano-N-(4-methoxy-3-nitrophenyl)-3-pyridinecarboxamide
2-methyl-N-[2-(2-phenoxyethoxy)propyl]butan-2-amine	2-chloro-N-(2-chloroethyl)-N-methylethanamine
2-[(2S)-1-aminopropan-2-yl]-4-chlorophenol	2-chloro-N-(2-chlorophenyl)-N-(methoxycarbonyl)acetamide
7-fluoro-2-(2-hydroxyethyl)-3,4-dihydroisoquinolin-1-one	2-fluoro-5-methylbenzotrile
2-[2-amino-2-(3-chlorothiophen-2-yl)ethoxy]acetamide	2-chloro-N-(2-chlorophenyl)-3-methylbutanamide
1-benzyl-3-[(4-methoxyphenyl)carbamothioylamino]thiourea	2-chloro-N-(2-chloro-5-fluorophenyl)-N-methylacetamide
2-(4-chlorophenyl)sulfonyl-5-nitro-1,3-thiazole	2-chloro-5-(trifluoromethyl)benzene
1-butyl-N-[(5-chlorofuran-2-yl)methyl]piperidin-4-amine	2-chloro-N-(2-chlorophenyl)-N-(4-methoxyphenyl)acetamide
1-ethyl-2-(2,4,6-trimethylphenyl)azepan-3-amine	3-methyl-2-oxiranecarboxylic acid
1-methyl-4-(2-methylimidazol-1-yl)piperidine	2-cyano-N-(4-methoxy-3-nitrophenyl)-3-phenylpropanamide
2-bromo-1-fluoro-3-[(3-fluorophenyl)sulfonylmethyl]benzene	2-bromo-4-fluoro-5-methylbenzene
N-[(1R)-1-(2,5-dimethoxyphenyl)ethyl]-2-methylaniline	2-methyl-2-propanol
N,N-bis[(4-nitrophenyl)methyl]-1,3-thiazol-2-amine	2-chloro-N-(2-chlorophenyl)-N-methoxyacetamide
2-ethylbicyclo[2.2.1]heptane-2-carbaldehyde	2-chloro-N-(2-chlorophenyl)-N-(methoxycarbonyl)acetamide