Supporting Information for

SMARTCyp – a 2D-method for Prediction of Cytochrome P450 Mediated Drug Metabolism

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Table S1. SMARTS rules and corresponding energies.

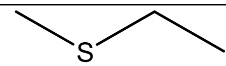
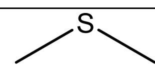
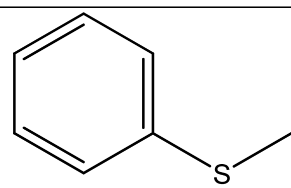
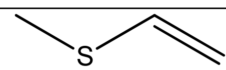
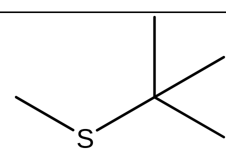
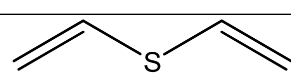
Table S2. Structures and information on all QM calculations for all SMARTS rules.

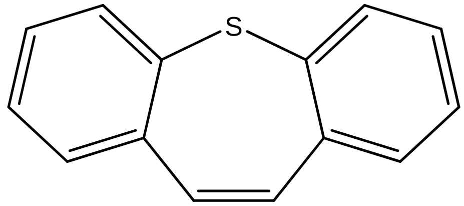
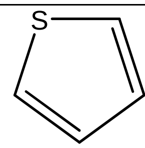
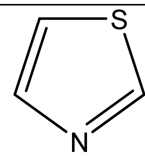
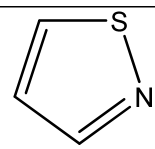
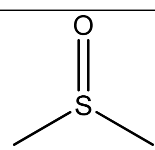
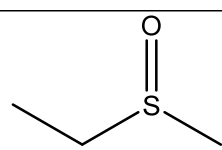
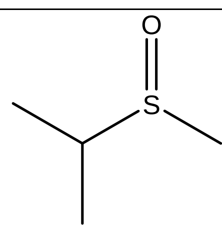
Table S1. SMARTS rules and corresponding energies (kJ/mol).

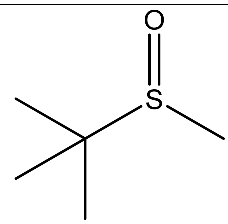
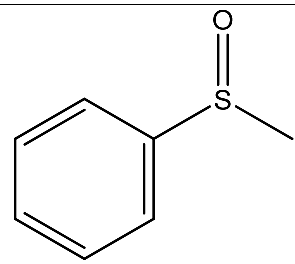
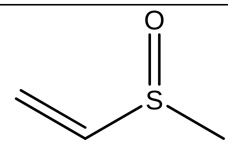
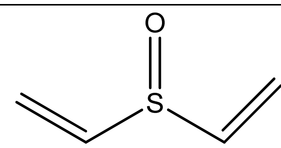
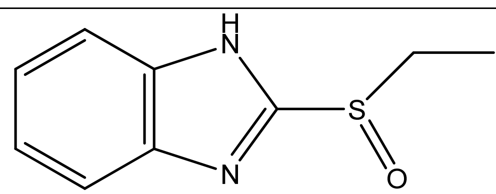
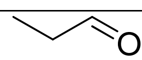
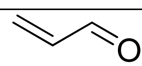
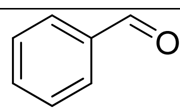
Sulphur atoms	
[SX2H1]	41.5
[$([SX2H0]);!$([S][*^2]);!$([S][CX4H0])]	26.3
[$([SX2H0][*^2]);!$([S](~[^2])[^2]);!$([S][CX4H0])]	34.4
[$([S][*D4H0]);$([SX2H0])]	44.4
[$([SX2H0]([*^2])[*^2]);!$([S][CX4H0])]	46.9
[sX2r5]	70.0
[$([#16X3](=[OX1]));$([#16]);!$([#16X3](=[OX1])[#6^2](~[#7^2]))]	30.4
[$([#16X3](=[OX1]));$([#16]);$([#16X3](=[OX1])[#6^2](~[#7^2]))]	46.9
Aldehyde carbon atoms	
[$([CX3H1](=O)[#6])]	40.2
Phosphor with double bonded sulphur	
[$([PX4]);$([P]=[S])]	13.3
sp3 hybridized carbon atoms	
[$([CX4]([#6^2])([#6^2])[#6^2]);!$([CH0])]	33.1
[$([CX4][N]);!$([CH0]);!$([C][N]([*^2])[*^2]);!$([C][N]=[#6X3]);!$([CX4][NX3][C]=[O])]	39.8
[!$([CH0]);$([CX4]([#6^2])[#6^2]),$([CX4][#7]=[#6X3]),$([CX4]([#8])[#8]);!$([CX4]([#8])[#8][C]=[O])]	48.6
[$([CX4][S]);!$([CH0]);!$([C][S]=[O])]	57.7
[$([CX4][#6^2]~[#8]),$([CX4][#6^2](~[#7])~[#7]),$([CX4][#6^1]),$([CX4][C^2]=[C^2]-[#6^2]); !$([CH0]);!$([CX4][C](=[O])[NX3]);!$([CX4][#6^2](=[#8])-[#8]);!$([CX4][C^2]([C^2])=[C^2]-[#6^2])]	60.0
[$([CX4][O]);!$([CH0]);!$([C][O][C]=[O]);!$([CX4]1[O][C]1)]	62.2
[$([CX4][#6^2]);!$([CH0]);!$([CX4][C](=[O])[NX3])]	66.7
[$([CX4][#7](~[*^2])~[*^2]);!$([CH0])]	69.1
[$([CX4][S](=[O])=[O]);!$([CH0])]	69.5
[CX4;CH1,CH2;!$([CX4][NX3H1][C]=[O])]	77.7
[CX4H3;!$([CX4][NX3H1][C]=[O])]	89.6
[$([CX4][NX3H1][C]=[O]);!$([CH0])]	94.6
sp2 hybridized carbon atoms	
[$([CX3H2]);$([C]=[*^2]-[*^2])]	40.1
[$([CX3H1]);$([C]=[*^2]-[*^2]);!$([C](-[*^2])=[*^2]-[*^2])]	52.4
[$([cH1]);$([c](:[#7]):[#7])]	55.8
[$([ch1]);!$([ch1]1:[c](-[N^3]-[*^2]):[c]:[c]:[c]:[c]1);!$([c]1:[c]:[c]:[c](-[N^3]-[*^2]):[c]:[c]1); $([ch1]1:[c](-[N^3]):[c]:[c]:[c]:[c]1),$([c]1:[c]:[c]:[c](-[N^3]):[c]:[c]1)]	59.5
[$([CX3]);$([CX3]=[CX3]);!$([CH0]);!$([CX3](-[*^2])=[CX3]);!$([CX3]=[CX3]-[*^2])]	65.6
[$([cH1]);$([c]:[#16])]	67.1
[$([ch1]);$([c]1:[c]:[c]:[c](~[#7X2H0]~[c^2,C^2]):[c]:[c]1),$([c]1:[c]:[c]:[c](~[#7X3H1]~[c^2,C^2]):[c]:[c]1); !$([c]1:[c]:[c]:[c](-[NH]-[C]=[O]):[c]:[c]1)]	69.2
[$([ch1]);!$([c]1:[c]:[c]:[c](-[O]-[C]=[O]):[c]:[c]1);$([c]1:[c]:[c]:[c](-[NH]-[C]=[O]):[c]:[c]1),	75.3

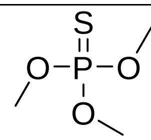
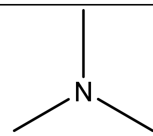
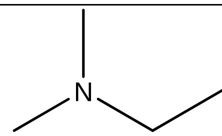
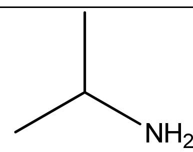
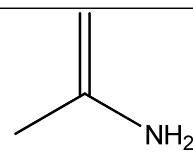
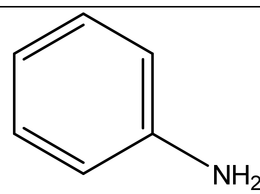
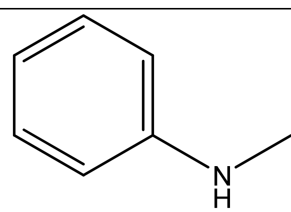
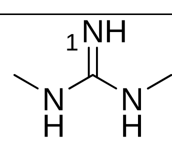
$([c]1:[c]:[c]:[c](-[O,SX2]):[c]:[c]1)]	
[$([cH1]);$([c]1:[c]:[#16]:[c]:[c]1)]	76.7
[$([ch1]);$([ch1]1:[c](~[#7X2H0]~[c^2,C^2]):[c]:[c]:[c]:[c]1),$([ch1]1:[c](~[#7X3H1]~[c^2,C^2]):[c]:[c]:[c]:[c]1),$([ch1]:[c]-[O,SX2]);!$([ch1]:[c]-[O]-[C]=[O])]	77.3
[$([CX3H1,cX3H1]);!$([ch1]1:[c]:[c]:[#7]:[c]:[c]1);!$([ch1]1:[c]:[#7]:[c]:[c]:[c]1);!$([ch1]1:[c]:[#7]:[c]:[c]1);!$([ch1]:[#7])]	82.3
[$([ch1]1:[c]:[c]:[#7]:[c]:[c]1),$([ch1]1:[c]:[#7]:[c]:[c]:[c]1),$([ch1]1:[c]:[#7]:[c]:[c]1),$([ch1]:[#7])]	89.6
Nitrogen atoms	
[$([N^3H0]);!$([N^3][*^2])]	41.0
[$([N^3]);$([H1,H2])]	54.1
[$([N]([#6^2]1)[#6^2]=[#6^2][#6^3][#6^2]=1)]	61.9
[$([N^3H0]);$([N^3][*^2]);!$([N^3]([*^2])[*^2])]	63.9
[$([nr6]),$([N^2]=[C])]	75.6
[$([N]);$([NX3H0]([*^2])[*^2]),$([N^2H1][C]=[O])]	89.6
[nr5H0]	92.1

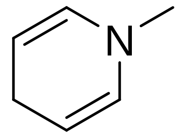
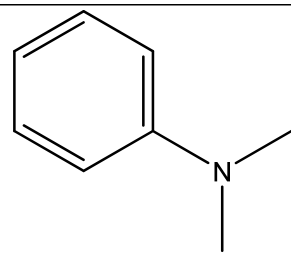
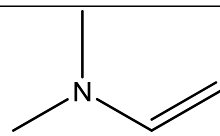
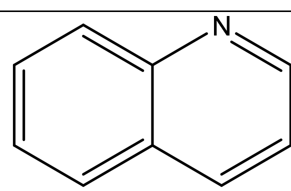
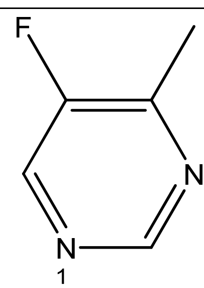
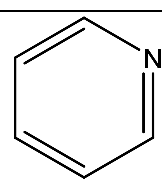
Table S2. Structures and information on all QM calculations for all SMARTS rules. Spin state in parenthesis after compound name (d is doublet, q is quartet). If there are multiple possible sites the computed site is marked with the number 1 unless otherwise written.

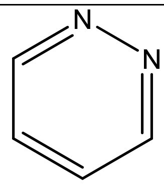
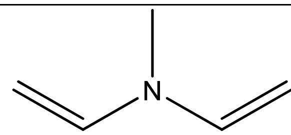
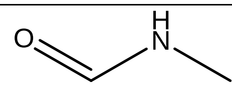
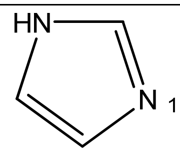
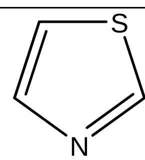
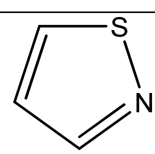
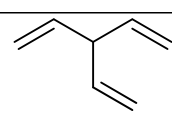
Sulphur Oxidations		
[SX2H1]		**Energy** (kJ/mol)
Methylsulfane (d)		41.5
[$([SX2H0]);!$([S][*^2]);!$([S][CX4H0])]		**Energy** (kJ/mol)
Methylethylsulfane (d)		28.7[a]
Dimethylsulfane (d)		23.8[b]
	Average:	26.3
	Standard deviation:	3.5
[$([SX2H0][*^2]);!$([S](~[^2])[^2]);!$([S][CX4H0])]		**Energy** (kJ/mol)
Phenylmethylsulfane (d)		33.8[a]
Vinylmethylsulfane (d)		35.0[a]
	Average:	34.4
	Standard deviation:	0.9
[$([S][*D4H0]);$([SX2H0])]		**Energy** (kJ/mol)
Tertbutylmethylsulfane (d)		44.4[a]
[$([SX2H0]([*^2])[*^2]);!$([S][CX4H0])]		**Energy** (kJ/mol)
Divinylsulfane (d)		45.1[a]

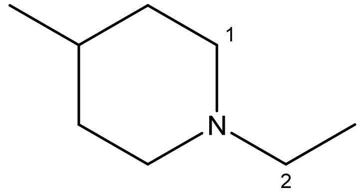
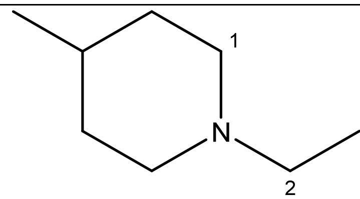
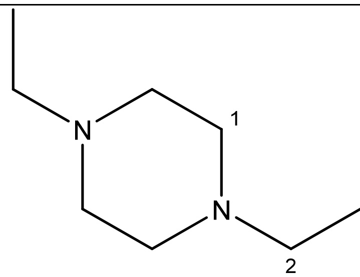
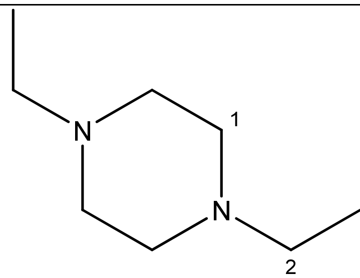
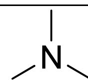
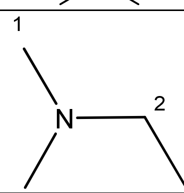
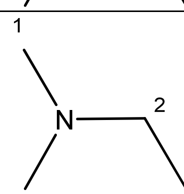
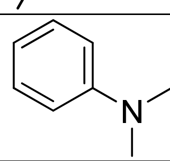
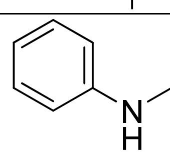
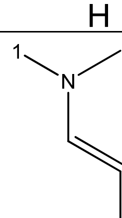
Dibenzo[b,f]thiepine (d)		48.8[a]
	Average:	46.9
	Standard deviation:	2.6
[sX2r5]		**Energy** (kJ/mol)
Thiophene (d)		69.1
Thiazole (d)		74.0
Isothiazole (d)		66.9
	Average:	70.0
	Standard deviation:	3.6
[$([#16X3](=[OX1]));$([#16]);!$([#16X3](=[OX1])[#6^2](~[#7^2]))]		**Energy** (kJ/mol)
Dimethylsulfoxide (d)		27.3[b]
Methylsulfinylethane (d)		25.3[a]
Methylsulfinylisopropane (d)		33.6[a]

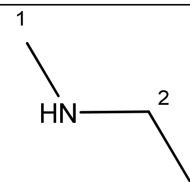
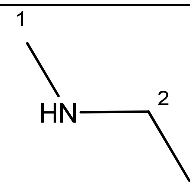
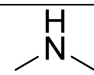
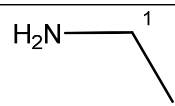
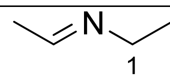
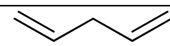
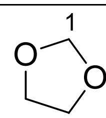
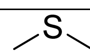
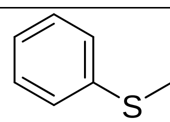
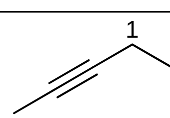
Methylsulfinyltertbutane (d)		34.8[a]
Methylsulfinylbenzene (d)		31.3[a]
Methylsulfinylethene (d)		27.4[a]
Divinylsulfoxide (d)		32.8[a]
	Average:	30.4
	Standard deviation:	3.7
[$([#16X3](=[OX1]));$([#16]);$([#16X3](=[OX1])[#6^2](~[#7^2]))]		**Energy** (kJ/mol)
2-(ethylsulfinyl)-1H-benzo[d]imidazole (d)		46.9[a]
	Aldehyde oxidation (of C=O carbon)	
[$([CX3H1](=O)[#6])]		**Energy** (kJ/mol)
Propionaldehyde (q)		37.0
Acrylaldehyde (q)		42.5
Benzaldehyde (q)		41.1
	Average:	40.2
	Standard deviation:	2.8

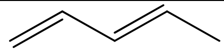
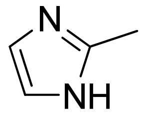
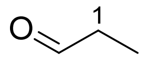
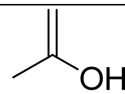
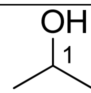
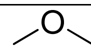
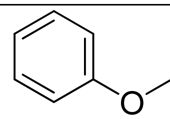
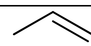
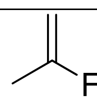
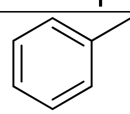
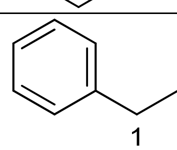
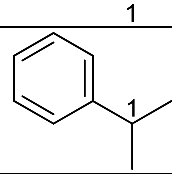
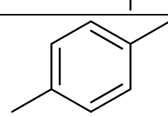
Phosphor with double bonded sulphur (desulphurization)		
[$([PX4]);$([P]=[S])]		**Energy** (kJ/mol)
O,O,O-trimethyl phosphorothioate (d)		13.3[c]
Nitrogen oxidations		
[$([N^3H0]);!$([N^3][*^2])]		**Energy** (kJ/mol)
Trimethylamine (d)		39.8[b]
N-ethyl-dimethylamine (d)		42.3
	Average:	41.0
	Standard deviation:	1.7
[$([N^3]);$([H1,H2])]		**Energy** (kJ/mol)
Propane-2-amine (d)		51.6[a]
Propene-2-amine (d)		55.9[a]
Aniline (d)		56.3
N-methylaniline (d)		50.0
1,3-dimethylguanidine (d)		56.9[a]

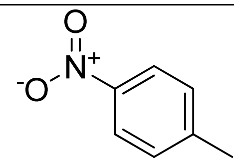
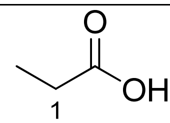
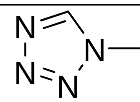
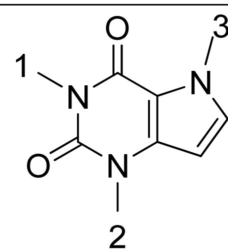
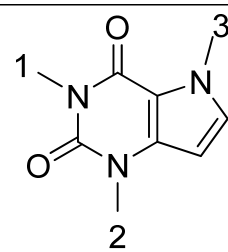
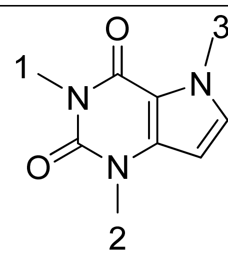
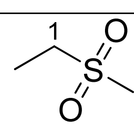
	Average:	54.1
	Standard deviation:	3.1
[$([N]([#6^2]1)[#6^2]=[#6^2][#6^3][#6^2]=1)]		**Energy** (kJ/mol)
1-methyl-4-hydropyridine (d)		61.9
[$([N^3H0]);$([N^3][*^2]);!$([N^3]([*^2])[*^2])]		**Energy** (kJ/mol)
N,*N*-dimethylaniline (d)		62.5
N,*N*-dimethylethenamine (d)		65.3
	Average:	63.9
	Standard deviation:	2.0
[$([nr6]),$([N^2]=[C])]		**Energy** (kJ/mol)
Quinoline (d)		72.7
5-fluoro-4-methylpyrimidine (d)		83.5
Pyridine (d)		71.0

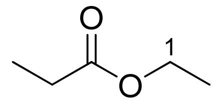
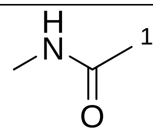
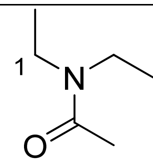
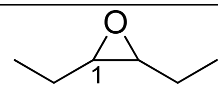
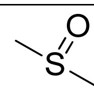
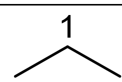
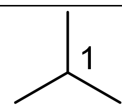
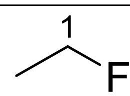
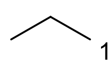
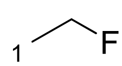
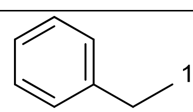
Pyridazine (d)		75.0
	Average:	75.6
	Standard deviation:	5.5
[$([N]);$([NX3H0]([*^2])[*^2]),$([N^2H1][C]=[O])]		**Energy** (kJ/mol)
N,*N*-divinylmethaneamine (d)		93.1
N-methylformamide (d)		86.2
	Average:	89.6
	Standard deviation:	4.9
[nr5H0]		**Energy** (kJ/mol)
Imidazole (d)		85.8
Thiazole (d)		88.4
Isothiazole (d)		102.1
	Average:	92.1
	Standard deviation:	9.4
sp^3 carbons		
[$([CX4]([#6^2])([#6^2])[#6^2]);!$([CH0])]		**Energy** (kJ/mol)
3-vinylpenta-1,4-diene (q)		33.1
[$([CX4][N]);!$([CH0]);!$([C][N]([*^2])[*^2]); !$([C][N]=[#6X3]);!$([CX4][NX3][C]=[O])]		**Energy** (kJ/mol)

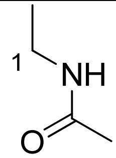
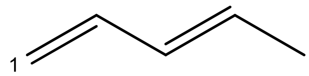
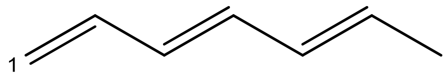
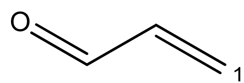
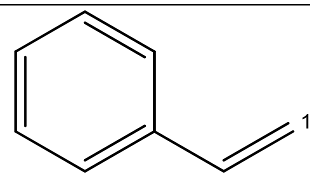
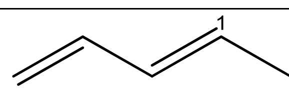
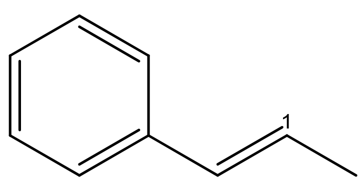
1-ethyl-4-methylpiperidine (q) (1)		35.9
1-ethyl-4-methylpiperidine (q) (2)		37.5
1,4-diethylpiperazine (q) (1)		44.5
1,4-diethylpiperazine (q) (2)		39.6
Trimethylamine (q)		38.4[b]
N-ethyl –dimethylamine (q) (1)		38.8
N-ethyl –dimethylamine (q) (2)		37.1
N,*N*-dimethyl aniline (q)		40.7[d]
N-methyl aniline (q)		44.0[d]
Dimethylpropenamine (q)		32.9

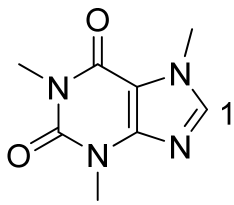
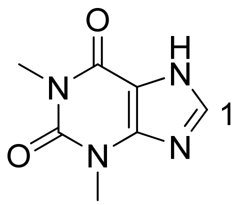
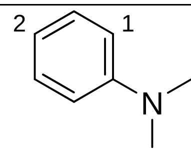
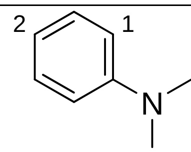
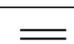
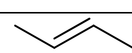
N-ethyl-methylamine (q) (1)		41.9
N-ethyl-methylamine (q) (2)		39.5
Dimethylamine (q)		42.6[d]
Ethanamine (q) (1)		43.5
	Average:	39.8
	Standard deviation:	3.3
[!$([CH0]);$([CX4]([#6^2])[#6^2]),$([CX4][#7]=[#6X3]), $([CX4]([#8])[#8]);!$([CX4]([#8])[#8][C]=[O])]		**Energy** (kJ/mol)
N-ethylideneethaneamine (q)		48.6
Penta-1,4-diene (q)		48.4
1,3-dioxolane (q)		48.7
	Average:	48.6
	Standard deviation:	0.1
[$([CX4][S]);!$([CH0]);!$([C][S]=[O])]		**Energy** (kJ/mol)
Dimethylsulfane (q)		58.1[b]
Methyl(phenyl)sulfane (q)		57.3[d]
	Average:	57.7
	Standard deviation:	0.5
[$([CX4][#6^2]~[#8]),$([CX4][#6^2](~[#7])~[#7]),$([CX4][#6^1]), $([CX4][C^2]=[C^2]-[#6^2]);!$([CH0]);!$([CX4][C](=[O])[NX3]); !$([CX4][#6^2](=[#8])-[#8]);!$([CX4][C^2]([C^2])=[C^2]-[#6^2])]		**Energy** (kJ/mol)
Pent-2-yne (q)		62.3

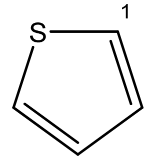
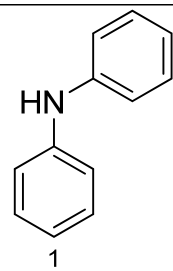
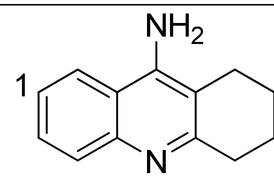
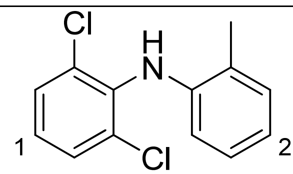
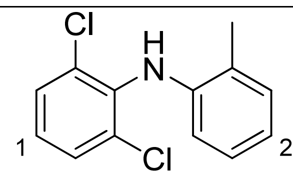
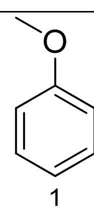
Penta-1,3-diene (q)		57.7
2-methyl-1*H*-imidazole (q)		59.1
Propionaldehyde (q)		61.3
Prop-1-en-2-ol (q)		59.4[d]
	Average:	60.0
	Standard deviation:	1.8
[$([CX4][O]);!$([CH0]);!$([C][O][C]=[O]);!$([CX4]1[O][C]1)]		**Energy** (kJ/mol)
Isopropanol (q)		55.7
Dimethylether (q)		63.1[d]
Anisole (q)		68.0[d]
	Average:	62.2
	Standard deviation:	6.2
[$([CX4][#6^2]);!$([CH0]);!$([CX4][C](=[O])[NX3])]		**Energy** (kJ/mol)
Propene (q)		67.0[d]
2-fluoro-prop-1-ene (q)		69.1[d]
Toluene (q)		67.3[d]
Ethylbenzene (q)		64.6[d]
1-methylethylbenzene (q)		69.7[d]
Para-xylene (q)		65.9[d]

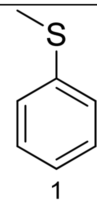
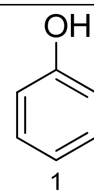
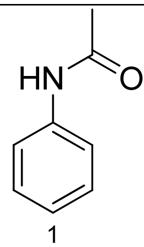
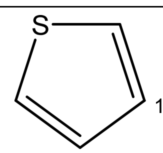
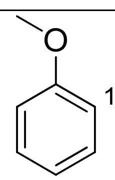
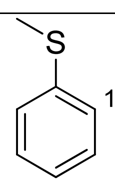
1-methyl-4-nitro-benzene (q)		62.6[d]
Propionic acid (q)		67.2
	Average:	66.7
	Standard deviation:	2.3
[$([CX4][#7](~[*^2])~[*^2]);!$([CH0])]		**Energy** (kJ/mol)
1-methyl-1*H*-tetrazole (q)		65.7
Caffeine (q) (1)		75.8[e]
Caffeine (q) (2)		70.1[e]
Caffeine (q) (3)		64.7[e]
	Average:	69.1
	Standard deviation:	5.0
[$([CX4][S](=[O])=[O]);!$([CH0])]		**Energy** (kJ/mol)
Methylethylsulfone (q)		69.5
[CX4;CH1,CH2;!$([CX4][NX3H1][C]=[O])]		**Energy** (kJ/mol)

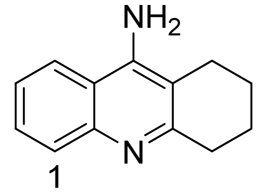
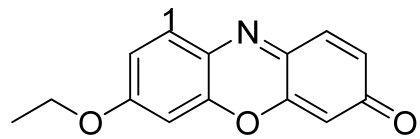
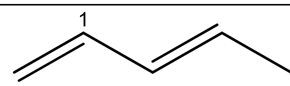
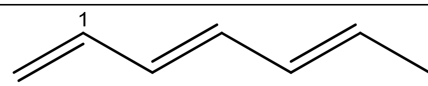
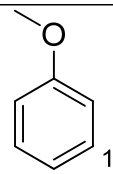
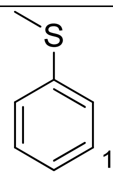
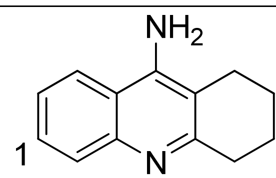
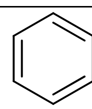
Ethyl propionate (q)		81.9
N-methylacetamide (q)		81.7
N,*N*-diethylacetamide (q)		79.6
2,3-diethyloxirane (q)		73.0
Dimethylsulphoxide (q)		77.0 [b]
Propane (q)		77.0[d]
Isobutane (q)		74.7[d]
Fluoroethane (q)		76.5[d]
	Average:	77.7
	Standard deviation:	2.3
[CX4H3;!$([CX4][NX3H1][C]=[O])]		**Energy** (kJ/mol)
Propane (q)		88.4[d]
Fluoroethane (q)		93.0[d]
Ethylbenzene (q)		87.4[d]
	Average:	89.6
	Standard deviation:	3.0
[$([CX4][NX3H1][C]=[O]);!$([CH0])]		**Energy** (kJ/mol)

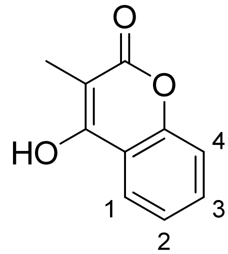
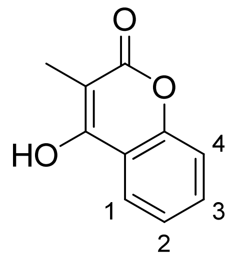
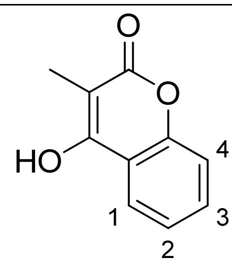
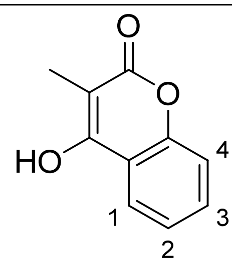
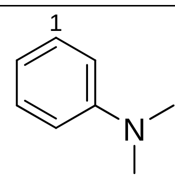
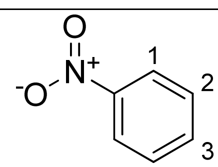
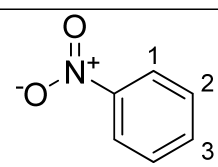
N-ethylacetamide (q)		94.6
sp^2 carbons		
[$([CX3H2]);$([C]=[*^2]-[*^2])]		**Energy** (kJ/mol)
Penta-1,3-diene (q)		44.0
Hepta-1,3,5-triene (q)		29.3
Acrylaldehyde (q)		42.2
Styrene (q)		44.9
	Average:	40.1
	Standard deviation:	7.3
[$([CX3H1]);$([C]=[*^2]-[*^2]);!$([C](-[*^2])=[*^2]-[*^2])]		**Energy** (kJ/mol)
Penta-1,3-diene (q)		52.5
Methylstyrene (q)		52.3
	Average:	52.4
	Standard deviation:	0.1
[$([cH1]);$([c](:[#7]):[#7])]		**Energy** (kJ/mol)

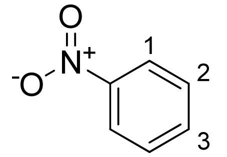
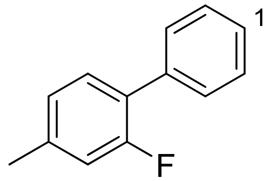
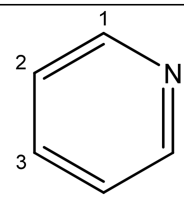
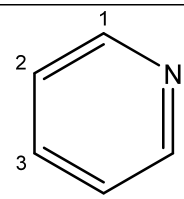
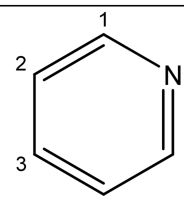
Caffeine (d)		54.4[e]
Theophylline (d)		57.1[e]
	Average:	55.8
	Standard deviation:	1.9
[$([ch1]);!$([ch1]1:[c](-[N^3]-[*^2]):[c]:[c]:[c]:[c]1); !$([c]1:[c]:[c]:[c](-[N^3]-[*^2]):[c]:[c]1); $([ch1]1:[c](-[N^3]):[c]:[c]:[c]:[c]1),$([c]1:[c]:[c]:[c](-[N^3]):[c]:[c]1)]		**Energy** (kJ/mol)
N,*N*-dimethylaniline (d) (1)		58.8[f]
N,*N*-dimethylaniline (d) (2)		60.2[f]
	Average:	59.5
	Standard deviation:	0.9
[$([CX3]);$([CX3]=[CX3]);!$([CH0]);!$([CX3](-[*^2])=[CX3]); !$([CX3]=[CX3]-[*^2])]		**Energy** (kJ/mol)
Ethene (q)		67.5[f]
2-butene (d)		63.6[f]
	Average:	65.6
	Standard deviation:	2.7
[$([cH1]);$([c]:[#16])]		**Energy** (kJ/mol)

Thiophene (d)		67.1
[$([ch1]);$([c]1:[c]:[c]:[c](~[#7X2H0]~[c^2,C^2]):[c]:[c]1), $([c]1:[c]:[c]:[c](~[#7X3H1]~[c^2,C^2]):[c]:[c]1); !$([c]1:[c]:[c]:[c](-[NH]-[C]=[O]):[c]:[c]1)]		**Energy** (kJ/mol)
Diphenylamine (d)		64.9
Tacrine (d)		68.6[e]
2,6-dichloro-N-o-tolylaniline (d) (1)		69.3[f]
2,6-dichloro-N-o-tolylaniline (d) (2)		73.9[f]
	Average:	69.2
	Standard deviation:	3.7
[$([ch1]);!$([c]1:[c]:[c]:[c](-[O]-[C]=[O]):[c]:[c]1); $([c]1:[c]:[c]:[c](-[NH]-[C]=[O]):[c]:[c]1), $([c]1:[c]:[c]:[c](-[O,SX2]):[c]:[c]1)]		**Energy** (kJ/mol)
Anisole (d)		74.4

Methyl(phenyl)sulfane (d)		74.3
Phenol (d)		75.9
N-phenylacetamide (d)		76.7
	Average:	75.3
	Standard deviation:	1.2
[$([cH1]);$([c]1:[c]:[#16]:[c]:[c]1)]		**Energy** (kJ/mol)
Thiophene (d)		76.7
[$([ch1]);$([ch1]1:[c](~[#7X2H0]~[c^2,C^2]):[c]:[c]:[c]:[c]1), $([ch1]1:[c](~[#7X3H1]~[c^2,C^2]):[c]:[c]:[c]:[c]1), $([ch1]:[c]-[O,SX2]);!$([ch1]:[c]-[O]-[C]=[O])]		**Energy** (kJ/mol)
Anisole (d)		78.2
Methyl(phenyl)sulfane (d)		77.2

Tacrine (d)		76.5[e]
7-ethoxyresorufin (d)		77.3[e]
	Average:	77.3
	Standard deviation:	0.7
[$([CX3H1,cX3H1]);!$([ch1]1:[c]:[c]:[#7]:[c]:[c]1);!$([ch1]1:[c]:[#7]:[c]:[c]:[c]1);!$([ch1]1:[c]:[#7]:[c]:[c]1);!$([ch1]:[#7])]		**Energy** (kJ/mol)
Penta-1,3-diene (d)		81.8
Hepta-1,3,5-triene (q)		77.0
Anisole (d)		85.8
Methyl(phenyl)sulfane (d)		87.1
Tacrine (d)		82.0[e]
Benzene (d)		87.3[f]

Warfarin (d) (1)		83.4[f]
Warfarin (d) (2)		80.8[f]
Warfarin (d) (3)		81.0[f]
Warfarin (d) (4)		78.7[f]
N,*N*-dimethylaniline (d)		86.7[f]
Nitrobenzene (q) (1)		78.5[f]
Nitrobenzene (d) (2)		84.5[f]

Nitrobenzene (q) (3)		79.2[f]
2-fluoro-4-methylbiphenyl (d)		80.7[f]
	Average:	82.3
	Standard deviation:	3.4
[$([ch1]1:[c]:[c]:[#7]:[c]:[c]1),$([ch1]1:[c]:[#7]:[c]:[c]:[c]1), $([ch1]1:[c]:[#7]:[c]:[c]1),$([ch1]:[#7])]		**Energy** (kJ/mol)
Pyridine (q) (1)		90.6
Pyridine (d) (2)		85.5
Pyridine (q) (3)		92.6
	Average:	89.6
	Standard deviation:	3.6

[a] Transition state geometry from scan crossing point.

[b] Taken from the publication: P. Rydberg, U. Ryde, L. Olsen, *J. Chem. Theory Comput.* 2008, 4, 1369-1377

[c] Energy taken from the calculation with the small basis set relative to reactant complex.

[d] Taken from the publication: L. Olsen, P. Rydberg, TH. Rod, U. Ryde, *J. Med. Chem.* 2006, 49, 6489-6499.

[e] Taken from the publication: P. Rydberg, P. Vasanthanathan, C. Oostenbrink, L. Olsen, *ChemMedChem* 2009, 4, 2070-2079.

[f] Taken from the publication: P. Rydberg, U. Ryde, L. Olsen, *J. Phys. Chem. A* 2008, 112, 13058-13065.