

Supplementary Material

Chapter 7

June 18, 2016

In chapter 7, the whole dataset, i.e., 668 molecules, were classified into seven queries based on their element type and chemical properties. We list molecular name, PubChem ID, and experimental solvation free energies in Tables 1-7.

Table S1: Molecules in the 1st query which only contain Hydrogen and Carbon elements.

Solute Name	Pubchem ID	Exptl ΔG
cyclohexene	8079	0.14
1,2,2-trifluoroethoxybenzene	21269179	-1.29
m-bis(trifluoromethyl)benzene	223106	1.07
fluoromethane	11638	-0.22
1,1-difluoroethane	6368	-0.11
Trifluoromethane	6373	0.81
trifluoromethylbenzene	7368	-0.25
1,1,2,3,3,3-Hexafluoro-1-propene	8302	2.31
1,2-bis(trifluoromethyl)benzene	9818	1.07
octafluorocyclobutane	8263	3.43
1,1-diphenylethene	10740	-2.78
anthracene	8418	-3.95
1-ethyl-2-methylbenzene	11903	-0.85
9,10-dihydroanthracene	11940	-3.78
ethane	6324	1.83
biphenyl	7095	-2.7
Ethyne	6326	-0.01
prop-1-yne	6335	-0.48
but-1-yne	7846	-0.16
pent-1-yne	12309	0.01
hept-1-yne	12350	0.6
oct-1-yne	12370	0.71
hex-1-yne	12732	0.29
1-Nonyne	18937	1.05
ethylene	6325	1.28
but-1-ene	7844	1.38
pent-1-ene	8004	1.68
1-OCTENE	8125	2.08
prop-1-ene	8252	1.32
2-methylprop-1-ene	8255	1.16
2-methylbut-2-ene	10553	1.31
3-methylbut-1-ene	11239	1.83
1-methylcyclohexene	11574	0.67
hex-1-ene	11597	1.58
hept-1-ene	11610	1.66
hept-2-ene	11611	1.68
4-Methyl-1-pentene	12724	1.91
2-methylpent-1-ene	12986	1.47
non-1-ene	31285	2.06
trans-2-Heptene	639662	1.66
cis-2-PENTENE	5326160	1.31

Table 1 – continued from previous page		
Solute Name	Pubchem ID	Exptl ΔG
trans-2-Pentene	5326161	1.34
cyclopentene	8882	0.56
isoprene	6557	0.68
butadiene	7845	0.56
2,3-dimethylbuta-1,3-diene	10566	0.4
penta-1,4-diene	11587	0.93
hexa-1,5-diene	11598	1.01
cyclohepta-1,3,5-triene	11000	-0.99
isopropenylbenzene	7407	-1.24
styrene	7501	-1.24
2-methylstyrene	11904	-1.24
octane	356	2.88
propane	6334	2
cyclopropane	6351	0.75
isobutane	6360	2.3
2,2-dimethylbutane	6403	2.51
isopentane	6556	2.38
2,3-dimethylbutane	6589	2.34
3-methylpentane	7282	2.51
methylcyclopentane	7296	1.59
n-butane	7843	2.1
isohexane	7892	2.51
2,4-dimethylpentane	7907	2.83
methylcyclohexane	7962	1.7
n-pentane	8003	2.3
hexane	8058	2.48
cyclohexane	8078	1.23
nonane	8141	3.13
heptane	8900	2.67
cyclopentane	9253	1.2
Cycloheptane	9265	0.8
Cyclooctane	9266	0.86
neopentane	10041	2.51
2,2,4-trimethylpentane	10907	2.89
3,3-dimethylpentane	11229	2.56
2,3-dimethylpentane	11260	2.52
2,3,4-trimethylpentane	11269	2.56
1,2-dimethylcyclohexane	11416	1.58
3-methylhexane	11507	2.71
3-methylheptane	11519	2.97
1,4-dimethylcyclohexane	11523	2.11
2,2-dimethylpentane	11542	2.88
2-methylhexane	11582	2.93
decane	15600	3.16
propylcyclopentane	16270	2.13
cis-1,2-Dimethylcyclohexane	16628	1.58
2,2,5-trimethylhexane	19041	2.93
pentylcyclopentane	19540	2.55
naphthalene	931	-2.4
fluorobenzene	10008	-0.8
phenanthrene	995	-3.88
toluene	1140	-0.9
acenaphthene	6734	-3.15
9H-fluorene	6853	-3.35
1-methylnaphthalene	7002	-2.44
o-xylene	7237	-0.9
1,2,4-trimethylbenzene	7247	-0.86
tert-butylbenzene	7366	-0.44

Table 1 – continued from previous page		
Solute Name	Pubchem ID	Exptl ΔG
cumene	7406	-0.3
1-isopropyl-4-methyl-benzene	7463	-0.68
ethylbenzene	7500	-0.79
1,1'-Methylenebisbenzene	7580	-2.82
propylbenzene	7668	-0.53
butylbenzene	7705	-0.4
p-xylene	7809	-0.8
m-xylene	7929	-0.83
mesitylene	7947	-0.9
sec-butylbenzene	8680	-0.45
indane	10326	-1.46
1,2,3-trimethylbenzene	10686	-1.21
pentylbenzene	10864	-0.23
isobutylbenzene	10870	0.16
1,4-dimethylnaphthalene	11304	-2.82
1,3-dimethylnaphthalene	11327	-2.47
2,3-dimethylnaphthalene	11386	-2.78
2,6-dimethylnaphthalene	11387	-2.63
1-ethyl-4-methyl-benzene	12160	-0.95
hexylbenzene	14109	-0.04
1-ethylnaphthalene	14315	-2.4
1,1-Dimethylpropyl benzene	16295	-0.18
pyrene	31423	-4.52
1-Buten-3-yne	12720	0.04
methane	297	2.00

Table S2: Molecules in the 2nd query which only contain Hydrogen, Carbon, and Oxygen elements.

Solute Name	Pubchem ID	Exptl ΔG
dibenzo-p-dioxin	9216	-3.15
1,4-dioxane	31275	-5.06
2-methylbenzaldehyde	10722	-3.93
hexyl acetate	8908	-2.26
(2S,5R)-2-isopropyl-5-methylcyclohexanone	26447	-2.53
(1R,2S,5R)-2-isopropyl-5-methylcyclohexanol	16666	-3.2
(2R,3R,4R,5R)-Hexan-1,2,3,4,5,6-hexol	6251	-23.62
2-ethylphenol	6997	-5.66
tetrahydropyran	8894	-3.12
diphenyl ether	7583	-2.87
1,2-dimethoxybenzene	7043	-5.33
4-(1-Methylethenyl)-1-cyclohexene-1-carboxaldehyde	16441	-4.09
2-hydroxybenzaldehyde	6998	-4.68
(3R)-3,7-Dimethylocta-1,6-dien-3-yl acetate	442474	-2.49
2-ethoxyethyl acetate	8095	-5.31
(2R,5R)-2-methyl-5-(1-methylethenyl)-cyclohexanone	22227	-3.75
6-isopropyl-3-methyl-1-cyclohex-2-enone	61362	-4.51
(1S,5R)-2-methyl-5-(1-methylethenyl)-2-cyclohexen-1-ol	94221	-4.44
(2E)-3,7-dimethylocta-2,6-dien-1-ol	637566	-4.45
(2Z)-3,7-dimethylocta-2,6-dien-1-ol	643820	-4.78
1-butoxy-2-propanol	21210	-5.73
2-methoxyphenol	460	-5.94
4-methyl-2-methoxyphenol	7144	-5.8
4-propylguaiacol	17739	-5.26
2,6-dimethoxyphenol	7041	-6.96
Flurbiprofen	3394	-8.42
(+)-ibuprofen	3672	-7

Table 2 – continued from previous page		
Solute Name	Pubchem ID	Exptl ΔG
glycerol	753	-13.43
Ketoprofen	3825	-10.78
diflunisal	3059	-9.4
naproxen	156391	-10.21
acetylsalicylic acid	2244	-9.94
D-xylose	135191	-20.52
D-glucose	5793	-25.47
propyl paraben	7175	-9.37
butyl paraben	7184	-8.72
methyl paraben	7456	-9.51
ethyl paraben	8434	-9.2
3,5,5-trimethylcyclohex-2-en-1-one	6544	-5.18
1,1-diethoxyethane	7765	-3.28
dimethoxymethane	8020	-2.93
1-acetoxyethyl acetate	222536	-4.97
diethyl propanedioate	7761	-6
2-acetoxyethyl acetate	8121	-6.34
2,3-diacetoxypropyl acetate	5541	-8.84
1,2-diethoxyethane	12375	-3.54
phenyl formate	74626	-3.82
trimethoxymethylbenzene	69720	-4.04
diethoxymethoxybenzene	84440	-5.23
trimethoxymethane	9005	-4.42
1,1,1-trifluoro-2,2,2-trimethoxyethane	18927701	-0.8
1,1,1-trimethoxyethane	15050	-4.42
1,1,1,2-tetramethoxyethane	141897	-5.73
acetaldehyde	177	-3.5
butanal	261	-3.18
octanal	454	-2.29
propanal	527	-3.43
formaldehyde	712	-2.75
hexanal	6184	-2.81
2-methylpropanal	6561	-2.86
pentanal	8063	-3.03
heptanal	8130	-2.67
nonanal	31289	-2.07
benzaldehyde	240	-4.02
acetic acid	176	-6.69
butyric acid	264	-6.35
propionic acid	1032	-6.46
pentanoic acid	7991	-6.16
hexanoic acid	8892	-6.21
3-methylbutanoic acid	10430	-6.09
methyl acetate	6584	-3.13
isobutyl 2-methylpropanoate	7351	-1.69
ethyl propanoate	7749	-2.68
ethyl butanoate	7762	-2.49
propyl butanoate	7770	-2.28
Heptanoic acid ethyl ester	7797	-2.3
propyl propanoate	7803	-2.44
methyl hexanoate	7824	-2.49
isopropyl acetate	7915	-2.64
propyl acetate	7997	-2.79
isobutyl acetate	8038	-2.36
methyl octanoate	8091	-2.04
ethyl acetate	8857	-2.94
ethyl pentanoate	10882	-2.49
methyl propanoate	11124	-2.93

Table 2 – continued from previous page		
Solute Name	Pubchem ID	Exptl ΔG
methyl butanoate	12180	-2.83
methyl pentanoate	12206	-2.56
pentyl propanoate	12217	-2.11
pentyl acetate	12348	-2.51
Propanoic acid 1-methylethyl ester	12508	-2.22
methyl cyclohexanecarboxylate	20748	-3.3
ethyl hexanoate	31265	-2.23
butyl acetate	31272	-2.64
isopentyl acetate	31276	-2.21
methyl 2,2-dimethylpropanoate	69027	-2.4
methyl cyclopropanecarboxylate	76122	-4.1
diethyl butanedioate	31249	-5.71
methyl benzoate	7150	-3.92
ethyl benzoate	7165	-3.64
1,2-ethanediol	66750	-7.75
acetone	180	-3.8
3,3-dimethylbutan-2-one	6416	-3.11
butanone	6569	-3.71
3-PENTANONE	7288	-3.41
pentan-2-one	7895	-3.52
4-methylpentan-2-one	7909	-3.05
cyclohexanone	7967	-4.91
heptan-2-one	8051	-3.04
octan-2-one	8093	-2.88
2-Undecanone	8163	-2.16
cyclopentanone	8452	-4.7
5-Nonanone	10405	-2.65
3-methylbutan-2-one	11251	-3.24
2,4-dimethylpentan-3-one	11271	-2.74
hexan-2-one	11583	-3.28
decan-2-one	12741	-2.34
1-cyclopropylethanone	13004	-4.61
nonan-2-one	13187	-2.49
1-cyclohexylethanone	13207	-3.9
heptan-4-one	31246	-2.92
2-Adamantanone	64151	-4.46
1-phenylethanone	7410	-4.58
1-(p-tolyl)ethanone	8500	-4.7
butan-1-ol	263	-4.72
ethanol	702	-5
methanol	887	-5.1
octan-1-ol	957	-4.09
propan-1-ol	1031	-4.85
propan-2-ol	3776	-4.74
pentan-1-ol	6276	-4.57
2-methylpropan-2-ol	6386	-4.47
2-methylbutan-2-ol	6405	-4.43
2-methylpropan-1-ol	6560	-4.5
butan-2-ol	6568	-4.62
cyclopentanol	7298	-5.49
4-methylpentan-2-ol	7910	-3.73
cyclohexanol	7966	-5.46
hexan-1-ol	8103	-4.4
heptan-1-ol	8129	-4.21
Decyl Alcohol	8174	-3.64
2-methylbutan-1-ol	8723	-4.42
1-Nonanol	8914	-3.89
cycloheptanol	10399	-5.48

Table 2 – continued from previous page		
Solute Name	Pubchem ID	Exptl ΔG
2-methylpentan-3-ol	11264	-3.88
pentan-3-ol	11428	-4.35
4-Heptanol	11513	-4.01
2-methylpentan-2-ol	11543	-3.92
2,3-Dimethyl-2-butanol	11670	-3.91
hexan-3-ol	12178	-4.06
pentan-2-ol	22386	-4.39
3-methylbutan-1-ol	31260	-4.42
H ₂ O	962	-6.3
ethylene glycol	174	-9.3
phenylmethanol	244	-6.62
2-phenylethanol	6054	-6.79
3-phenylpropan-1-ol	31234	-6.92
o-cresol	335	-5.9
m-cresol	342	-5.49
2-fluorophenol	9707	-5.29
Phenol	996	-6.61
p-cresol	2879	-6.13
naphthalen-1-ol	7005	-7.67
3,4-dimethylphenol	7249	-6.5
2,5-dimethylphenol	7267	-5.91
4-tert-butylphenol	7393	-5.91
2,4-dimethylphenol	7771	-6.01
3,5-dimethylphenol	7948	-6.27
naphthalen-2-ol	8663	-8.11
2,3-dimethylphenol	10687	-6.16
2,6-dimethylphenol	11335	-5.26
3-ethylphenol	12101	-6.25
4-propylphenol	12580	-5.21
4-ethylphenol	31242	-6.13
ethoxyethane	3283	-1.59
2-methyltetrahydrofuran	7301	-3.3
2-isopropoxypropane	7914	-0.53
tetrahydrofuran	8028	-3.47
1-propoxypropane	8114	-1.16
methoxymethane	8254	-1.91
1-butoxybutane	8909	-0.83
methoxyethane	10903	-2.1
1-methoxypropane	11182	-1.66
2-methoxypropane	11721	-2.01
1-Ethoxypropane	12340	-1.81
1,3-Dioxolane	12586	-4.1
2,5-dimethyltetrahydrofuran	13855	-2.92
2-methoxy-2-methyl-propane	15413	-2.21
1,2-dimethoxyethane	8071	-4.84
anisole	7519	-2.45
ethoxybenzene	7674	-2.22
oct-2-enal	16900	-3.43
but-2-enal	447466	-4.22
(2E)-hex-2-enal	5281168	-3.68
E-oct-2-enal	5283324	-3.44
trans,trans-2,4-Hexadienal	637564	-4.63
3-hydroxybenzaldehyde	101	-9.52
4-hydroxybenzaldehyde	126	-8.83
methyl formate	7865	-2.78
ethyl formate	8025	-2.56
isopentyl formate	8052	-2.13
isopropyl formate	12257	-2.02

Table S3: Molecules in the 3rd query which only contain Hydrogen, Carbon, and Nitrogen (or Hydrogen, Carbon, Nitrogen, and Oxygen) elements.

Solute Name	Pubchem ID	Exptl ΔG
piperidine	8082	-5.11
Amitriptyline	2160	-7.43
2-chloroaniline	7240	-4.91
4-chloroaniline	7812	-5.9
3-chloroaniline	7932	-5.82
2-chloropyridine	7977	-4.39
3-chloropyridine	12287	-4.01
pebulate	14215	-3.64
N,N-dipropyl(propylsulfanyl)formamide	16003	-4.13
1-benzylimidazole	77918	-7.63
4-dimethylamino-azobenzene	6053	-6.66
imidazole	795	-9.63
acetonitrile	6342	-3.88
propanenitrile	7854	-3.84
butanenitrile	8008	-3.64
dichlobenil	3031	-4.71
pentanenitrile	8061	-3.52
benzonitrile	7505	-4.1
methanamine	6329	-4.55
ethanamine	6341	-4.5
propan-1-amine	7852	-4.39
cyclohexanamine	7965	-4.59
butan-1-amine	8007	-4.24
pentan-1-amine	8060	-4.09
hexan-1-amine	8102	-3.95
heptan-1-amine	8127	-3.79
octan-1-amine	8143	-3.65
1,2-Ethanediamine	3301	-7.6
N-methylmethanamine	674	-4.29
N-isopropylpropan-2-amine	7912	-3.22
N-ethylethanamine	8021	-4.07
N-butylbutan-1-amine	8148	-3.24
N-propylpropan-1-amine	8902	-3.65
Aziridine	9033	-5.42
azetidine	10422	-5.56
Octahydroazocine	14276	-4.4
pyrrolidine	31268	-5.48
piperazine	4837	-7.4
N-methylaniline	7515	-4.69
N,N-dimethylmethanamine	1146	-3.2
1-Methylpyrrolidine	8454	-3.98
N,N-diethylethanamine	8471	-3.22
1-methylpiperidine	12291	-3.88
1,4-dimethylpiperazine	7818	-7.58
N-methyl-N-(2,2,2-trifluoroethyl)aniline	13238893	-1.92
Methenamine	4101	-4.56
N,N-dimethylaniline	949	-3.45
aniline	6115	-5.49
2,6-dimethylaniline	6896	-5.21
naphthalen-2-amine	7057	-7.47
2-methylaniline	7242	-5.53
4-methylaniline	7813	-5.57
naphthalen-1-amine	8640	-7.28
1-methylpiperazine	53167	-7.77
pyridine	1049	-4.69

Table 3 – continued from previous page

Solute Name	Pubchem ID	Exptl ΔG
3-methyl-1H-indole	6736	-5.88
quinoline	7047	-5.72
1-methylpyrrole	7304	-2.89
2-ethylpyridine	7523	-4.33
2,4-dimethylpyridine	7936	-4.86
2,6-dimethylpyridine	7937	-4.59
4-methylpyridine	7963	-4.93
3-methylpyridine	7970	-4.77
2-methylpyridine	7975	-4.63
pyrrole	8027	-4.78
4-ethylpyridine	10822	-4.73
3-ethylpyridine	10823	-4.59
3,4-dimethylpyridine	11417	-5.22
2,3-dimethylpyridine	11420	-4.82
2,5-dimethylpyridine	11526	-4.72
3,5-dimethylpyridine	11565	-4.84
4-1,1-Dimethylethyl-pyridine	19878	-4.46
2,6-Bis-1,1-Dimethylethyl-pyridine	68510	-0.41
pyridine-3-carbonitrile	79	-6.75
pyridine-4-carbonitrile	7506	-6.02
n-propyl-guanidine	447907	-10.91
9-methyl-adenine	69689	-13.6
2-methylpyrazine	7976	-5.51
2-ethylpyrazine	26331	-5.45
2-isobutylpyrazine	34591	-5.04
1-methylimidazole	1390	-8.41
1-N,1-N-diethyl-2,6-dinitro-4-(trifluoromethyl)benzene-1,3-diamine	34468	-5.66
trifluralin	5569	-3.25
N-butyl-N-ethyl-2,6-dinitro-4-(trifluoromethyl)aniline	2319	-3.51
profluralin	33500	-2.45
chlorimuronethyl	56160	-14.01
5-chlorouracil	15758	-17.74
6-chlorouracil	73272	-15.83
5-Amino-4-chloro-2-phenylpyridazin-3(2H)-one	15546	-16.43
bensulfuron	107828	-17.17
thifensulfuron	91729	-16.23
sulfometuron-methyl	52997	-20.25
metsulfuronmethyl	52999	-15.54
5-fluorouracil	3385	-16.92
5-trifluoromethyluracil	5899	-15.46
5-bromouracil	5802	-18.17
bromacil	9411	-9.73
Uracil	1174	-16.59
cyanuric acid	7956	-18.06
1-methyl-uracil	12009	-14
2-(2,3-dimethylphenyl)aminobenzoic acid	4044	-6.78
HEXYL NITRATE	30209	-1.66
3-nitrooxypropyl nitrate	96257	-4.8
1,3-bis-(nitrooxy)butane	138747	-4.29
1,4-diamino-9,10-anthracenedione	31420	-11.85
1-amino-9,10-anthracenedione	6710	-9.44
2-amino-9,10-anthraquinone	8341	-11.53
1-(2-hydroxyethylamino)-9,10-anthraquinone	20528	-14.21
1-amino-4-hydroxy-9,10-anthracenedione	8323	-9.53
[2-benzhydryloxyethyl]-dimethyl-amine	3100	-9.34
phthalimide	6809	-9.61
caffeine	2519	-12.64
isobutyl nitrate	10974	-1.88

Table 3 – continued from previous page

Solute Name	Pubchem ID	Exptl ΔG
butyl nitrate	13567	-2.09
[(2S)-butan-2-yl] nitrate	79123	-1.82
1,2-dinitroxyethane	40818	-5.73
1,2-dinitroxypropane	21075956	-4.95
fenuron	7560	-9.13
1,4,5,8-tetramino-anthraquinone	17190	-8.94
1-amino-4-anilino-anthraquinone	20419	-7.44
4-amino-4'-nitroazobenzene	12896	-11.24
carbofuran	2566	-9.61
dinoseb	6950	-6.23
nitroxyacetone	81226	-5.99
2-(nitrooxy)ethan-1-ol	85254	-8.18
pirimor	31645	-9.41
naphthalen-1-yl N-methylcarbamate	6129	-9.45
N,N-4-trimethylbenzamide	84179	-9.76
alachlor	2078	-8.21
4-methoxy-N,N-dimethyl-benzamide	81713	-11.01
2-nitropropane	398	-3.13
nitromethane	6375	-4.02
1-nitroethane	6587	-3.71
1-nitropropane	7903	-3.34
1-nitrobutane	12302	-3.09
1-nitropentane	220639	-2.82
1-methyl-2-nitro-benzene	6944	-3.58
nitrobenzene	7416	-4.12
1-methyl-3-nitro-benzene	7422	-3.45
acetamide	178	-9.71
propionamide	6578	-9.4
hexanamide	12332	-9.31
benzamide	2331	-11
N-methylacetamide	6582	-10
1-pyrrolidin-1-ylethanone	77650	-9.8
3,3,3-trimethoxypropanenitrile	144381	-6.4
1-methyl-cytosine	79143	-18.4
N,N-dimethylformamide	6228	-7.81
nitralin	20848	-7.98
pyridine-3-carbaldehyde	10371	-7.1
pyridine-4-carbaldehyde	13389	-7
9-methyl-guanine	79639	-22.4
N,N-dimethyl-4-nitro-benzamide	138975	-11.95
1-(3-pyridyl)ethanone	9589	-8.26
1-(4-pyridyl)ethanone	14282	-7.62
2-nitroaniline	6946	-7.37
3-nitroaniline	7423	-8.84
4-nitroaniline	7475	-9.82
3-Methoxy-1-propanamine	1672	-6.93
2-methoxyethanamine	8018	-6.55
2-methoxyaniline	7000	-6.12
4-methoxyaniline	7732	-7.48
3-methoxyaniline	10824	-7.29
morpholine	8083	-7.17
methyl 4-nitrobenzoate	12083	-6.88
4-methylmorpholine	7972	-6.32
4-hydroxybenzonitrile	13019	-10.17
3-hydroxybenzonitrile	13394	-9.65
4-nitrophenol	980	-10.64
2-nitrophenol	6947	-4.58
3-nitrophenol	11137	-9.62

Table 3 – continued from previous page		
Solute Name	Pubchem ID	Exptl ΔG
2-2-Methylpropyl-3-methoxy-pyrazine	32594	-3.68
2-N-ethyl-6-(methylsulfanyl)-4-N-(propan-2-yl)-1,3,5-triazine-2,4-diamine	13263	-7.65
terbutryn	13450	-6.68
captan	8606	-9.01
prometryn	4929	-8.43
N-(3,4-dichlorophenyl)propanimidic acid	4933	-7.78
terbacil	22188	-11.14
aldicarb	9570071	-9.84
oxamyl	9595287	-10.18
methomyl	4109	-10.65
simazine	5216	-10.22
2-Ethyl-3-methoxypyrazine	33135	-4.4
2-[(1R)-1-methylpropyl]-4,6-dinitro-phenolate	688400	-6.23

Table S4: Molecules in the 4th query which only contain Hydrogen, Carbon, Oxygen, and Chlorine elements.

Solute Name	Pubchem ID	Exptl ΔG
2-chlorosyringaldehyde	53479	-7.78
2,6-dichlorosyringaldehyde	53476	-8.68
3,4-dichlorophenol	7258	-7.29
3,5-dichloro-2,6-dimethoxyphenol	93462	-6.44
1-chlorodibenzo-p-dioxin	37207	-3.52
2-chlorodibenzo-p-dioxin	38252	-3.10
2,3-dichlorodibenzo-p-dioxin	34586	-3.56
2,7-dichlorodibenzo-p-dioxin	36613	-3.67
1,2,4-trichlorodibenzo-p-dioxin	38253	-4.05
2,3,7,8-tetrachlorodibenzo-p-dioxin	15625	-3.37
1,2,3,4-tetrachlorodibenzo-p-dioxin	35454	-3.81
1,2,3,7-tetrachlorodibenzo-p-dioxin	48889	-3.84
1,2,3,4,7,8-hexachlorodibenzo-p-dioxin	38251	-3.71
1,2,3,4,7-pentachlorodibenzo-p-dioxin	38254	-4.15
endosulfan alpha	12309460	-4.23
dicamba	3030	-9.86
endrin	3048	-4.82
endrin	46174049	-4.82
2-chloro-1,1,1-trimethoxy-ethane	144702	-4.59
methyl 2-chloroacetate	7295	-4.00
4-chloro-3-methyl-phenol	1732	-6.79
4-chlorophenol	4684	-7.03
2-chlorophenol	7245	-4.55
3-chlorophenol	7933	-6.62

Table S5: Molecules in the 5th query which only contain Hydrogen, Carbon, and Chlorine elements.

Solute Name	Pubchem ID	Exptl ΔG
1,1,1,2-tetrachloroethane	12418	-1.43
1,1,1,2,2-pentachloroethane	6419	-1.23
chloroethane	6337	-0.63
1,1-Thiobis(2-Chloroethane)	10461	-3.92
1,2-dichloroethane	11	-1.79
1,1-dichloroethane	6365	-0.84
1,1,2-trichloroethane	6574	-1.99
1,1,2,2-tetrachloroethane	6591	-2.37

Table 5 – continued from previous page

Solute Name	Pubchem ID	Exptl ΔG
1-chloro-2-phenyl-benzene	249266	-2.69
1,4-dichloro-2-phenyl-benzene	36980	-2.46
1,3,5-trichloro-2-phenyl-benzene	37247	-2.16
1,3-dichloro-2-(2,6-dichlorophenyl)benzene	27588	-2.28
1,2,3,4-tetrachloro-5-phenyl-benzene	36401	-3.48
1,2,3-trichloro-5-(2,5-dichlorophenyl)benzene	63088	-3.61
1,3,5-trichloro-2-(2,6-dichlorophenyl)benzene	91662	-1.96
1,2,3,4-tetrachloro-5-(3,4-dichlorophenyl)benzene	38019	-3.04
1,2,4,5-tetrachloro-3-(3,4-dichlorophenyl)benzene	63079	-4.38
1,2,3,4-tetrachloro-5-(2,3,4-trichlorophenyl)benzene	37037	-4.4
1,2,3,4-tetrachloro-5-(3,4,5-trichlorophenyl)benzene	38306	-3.17
1,2,3,4-tetrachloro-5-(2,3,4,6-tetrachlorophenyl)benzene	39253	-4.61
1,1,1-trichloroethane	6278	-0.19
heptachlor	3589	-2.55
chlordane	5993	-3.44
benzyl chloride	7503	-1.93
chloromethane	6327	-0.55
2-chloropropane	6361	-0.25
2-chlorobutane	6563	0
1-chlorobutane	8005	-0.16
2-chloro-2-methyl-propane	10486	1.09
1-chloropropane	10899	-0.33
1-CHLOROPENTANE	10977	-0.07
1-chlorohexane	10992	0
3-Chloropentane	12016	0.04
2-Chloropentane	12245	0.07
chloro-difluoro-methane	6372	-0.5
chloro-fluoro-methane	11643	-0.77
1-chloroheptane	12371	0.29
dichloromethane	6344	-1.31
1-chloro-2-(2-chloroethoxy)ethane	8115	-4.23
1,2-dichloropropane	6564	-1.27
1,4-dichlorobutane	8059	-2.32
1,3-dichloropropane	8881	-1.89
1,1-Dichlorobutane	10926	-0.7
1,4-dichloropentane	221525	-2.32
Acetic acid methyl ester	6845	-3.32
1-chloro-2-methyl-benzene	7238	-1.14
chlorobenzene	7964	-1.12
1,4-dichlorobenzene	4685	-1.01
1,2-dichlorobenzene	7239	-1.36
1,3-dichlorobenzene	10943	-0.98
1,2,4-trichlorobenzene	13	-1.12
1,2,3-trichlorobenzene	6895	-1.24
1,3,5-trichlorobenzene	7950	-0.78
1,2,4,5-tetrachlorobenzene	7270	-1.34
1,2,3,4-tetrachlorobenzene	12463	-1.34
1,2,3,5-tetrachlorobenzene	12468	-1.62
3-chloroprop-1-ene	7850	-0.57
1,1,2-trichloroethylene	6575	-0.44
chloroform	6212	-1.08
1,1-dichloroethylene	6366	0.25
(E)-1,2-dichloroethylene	638186	-0.78
(Z)-1,2-dichloroethylene	643833	-1.17
chloroethylene	6338	-0.59
hexachloroethane	6214	-0.64
carbon tetrachloride	5943	0.08
lindane	727	-5.44

Table 5 – continued from previous page		
Solute Name	Pubchem ID	Exptl ΔG
1,2,3,4,5-pentachloro-6-(2,3,4,5,6-pentachlorophenyl)benzene	16318	-2.98
hexachlorobenzene	8370	-2.33
trichloro(nitro)methane	6423	-1.45
1,1,2-trichloro-1,2,2-trifluoro-ethane	6428	1.77
1,1,2,2-Tetrachloro-1,2-difluoroethane	6427	0.82
Chloropentafluoroethane	6430	2.86
Dichlorodifluoromethane	6391	1.69
1,2-Dichloro-1,1,2,2-tetrafluoroethane	6429	2.32
1,1-Dichlorotetrafluoroethane	9775	2.51
pentachloronitrobenzene	6720	-5.22
2-chloro-1,1,1-trifluoro-ethane	6408	0.06
Chlorotrifluoromethane	6392	2.52
2-chloro-2-(difluoromethoxy)-1,1,1-trifluoro-ethane	11095291	0.1
1,2,3,4,6,7,8,9-octachlorodibenzo-p-dioxin	18636	-4.53
2,2-dichloro-1,1-difluoro-1-methoxy-ethane	4116	-1.12
1,1,2,2-tetrachloroethylene	31373	0.1

Table S6: Molecules in the 6th query which only contain Hydrogen and Sulfur elements.

Solute Name	Pubchem ID	Exptl ΔG
ethylsulfanylethane	9609	-1.46
hydrogen sulfide	402	-0.7
methanethiol	878	-1.2
ethanethiol	6343	-1.14
propanethiol	7848	-1.1
butane-1-thiol	8012	-0.99
methylsulfanylmethane	1068	-1.61
1-propylsulfanylpropane	8118	-1.28
2-isopropylsulfanylpropane	12264	-1.21
methylsulfanylbenzene	7520	-2.73
benzyl bromide	7498	-2.38
thiophene	8030	-1.4
2-methylthiophene	11126	-1.38
1,1-Thiobisethene	12321	-1.43
ethyldisulfanylethane	8077	-1.64
methyldisulfanylmethane	12232	-1.83

Table S7: Molecules in the 7th query (mixed).

Solute Name	Pubchem ID	Exptl ΔG
ethion	3286	-6.10
malathion	4004	-8.15
phorate	4790	-4.37
hydrazine	9321	-9.30
ammonia	222	-4.29
dialifor	25146	-5.74
carbophenothion	13081	-6.50
chlorpyrifos	2730	-5.04
methanesulfonyl chloride	31297	-4.87
sulfolane	31347	-8.61
methylsulfonylmethane	6213	-10.08
methyl methanesulfonate	4156	-4.87
dimethyl sulfate	6497	-5.10

Table 7 – continued from previous page		
Solute Name	Pubchem ID	Exptl ΔG
methylsulfinylmethane	679	-9.28
trichlorfon	5853	-12.74
chlorfenvinphos	5377791	-7.07
azinphosmethyl	2268	-10.03
parathion	991	-6.74
methyparathion	4130	-7.19
diazinon	3017	-6.48
Trimethyl phosphate	10541	-8.70