Supporting Information for

Predicting protein-ligand binding affinity and correcting crystal structures with quantum mechanical calculations: Lactate Dehydrogenase A .

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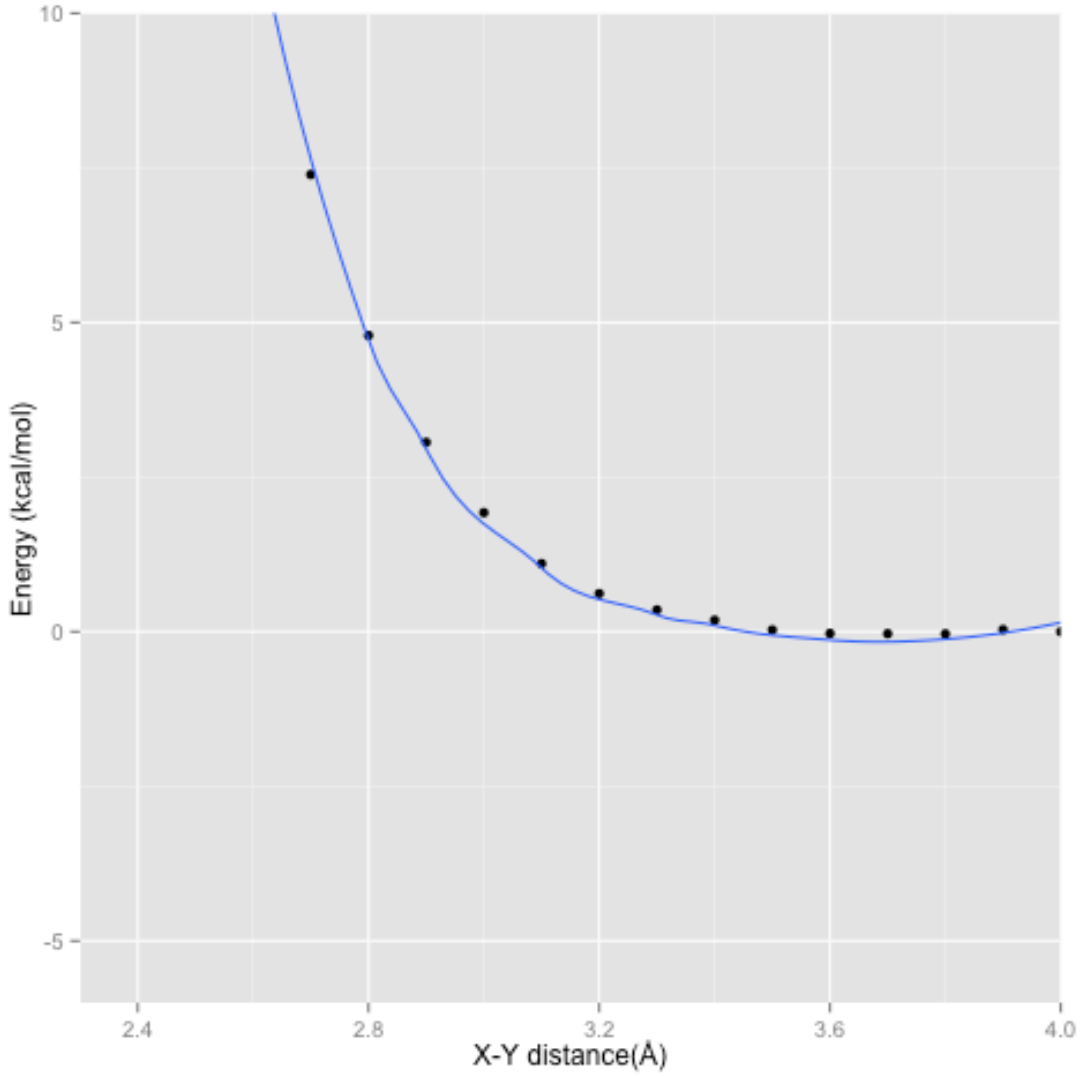
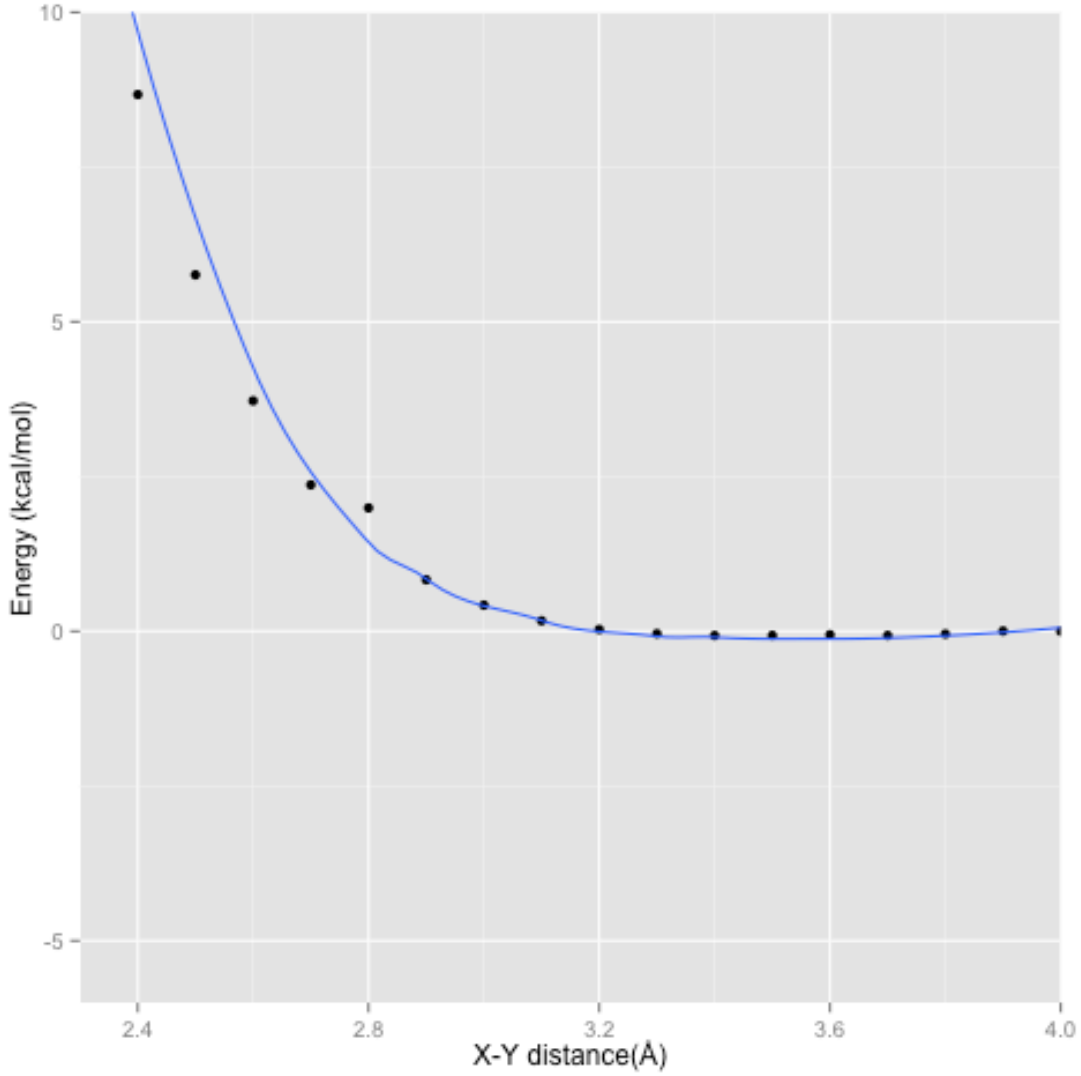
S1. Interaction potential curves for a range of functional groups computed at the M06/6-31+G** level.

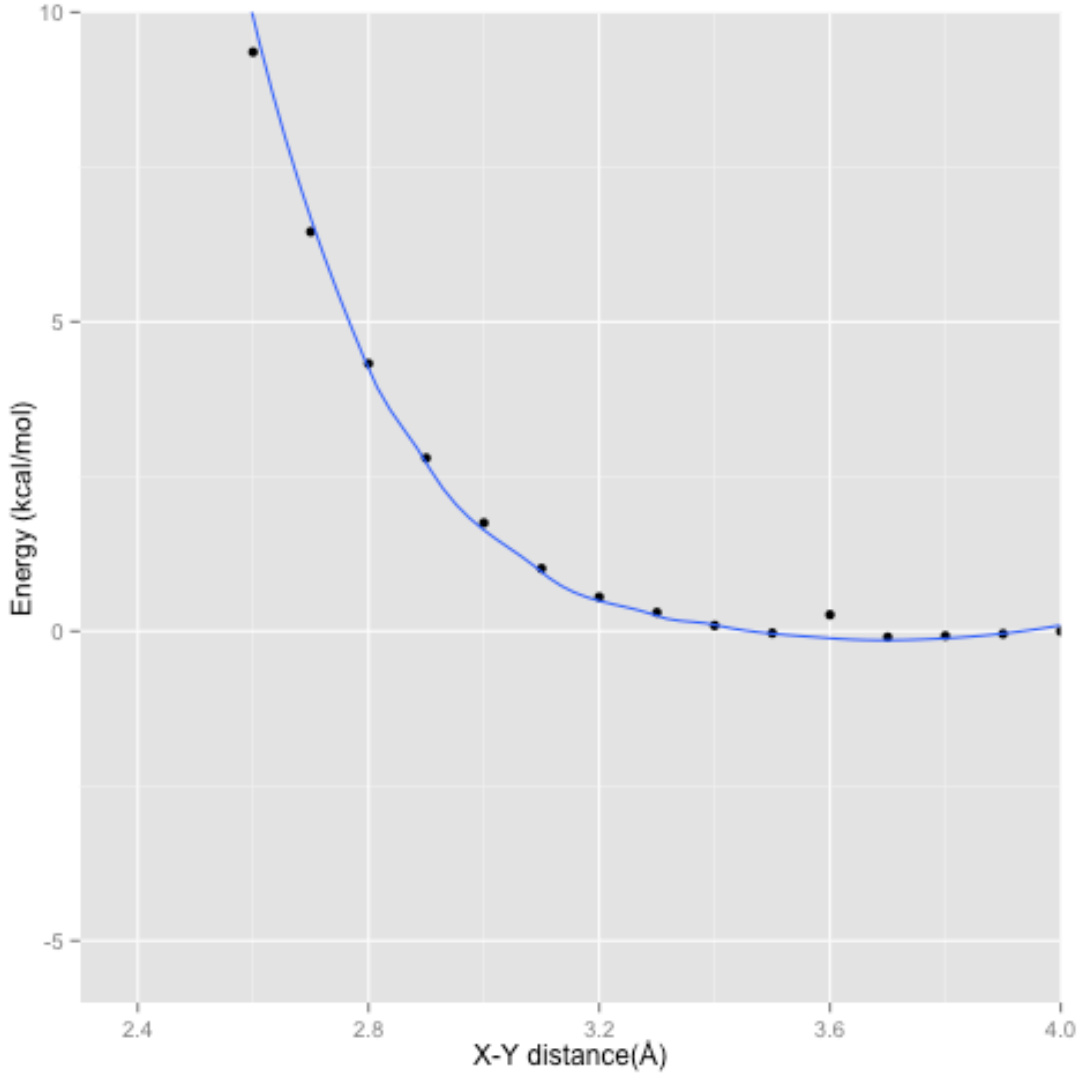
Methane with Methane [non-polar – non-polar]



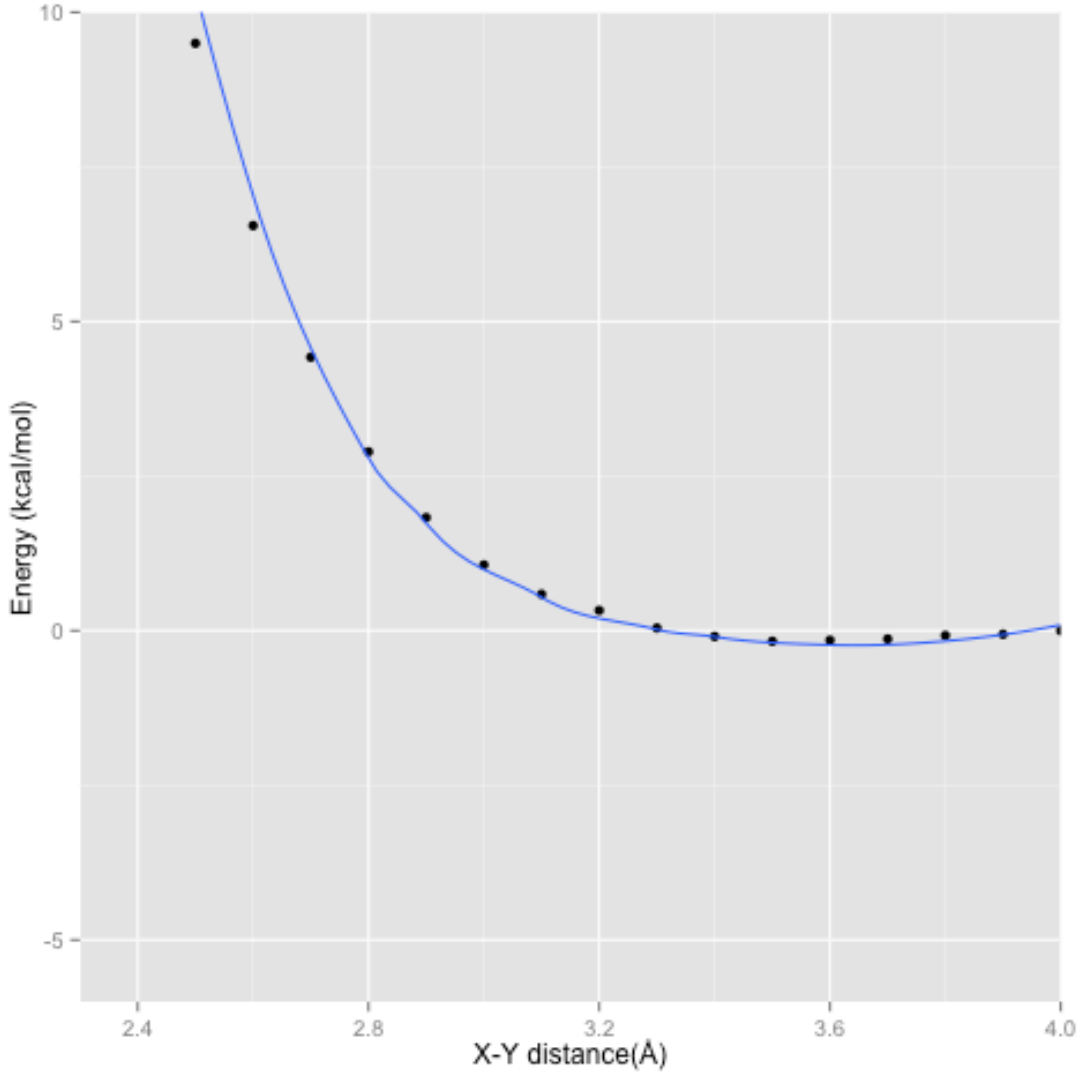
Methane with Water [non-polar – polar]



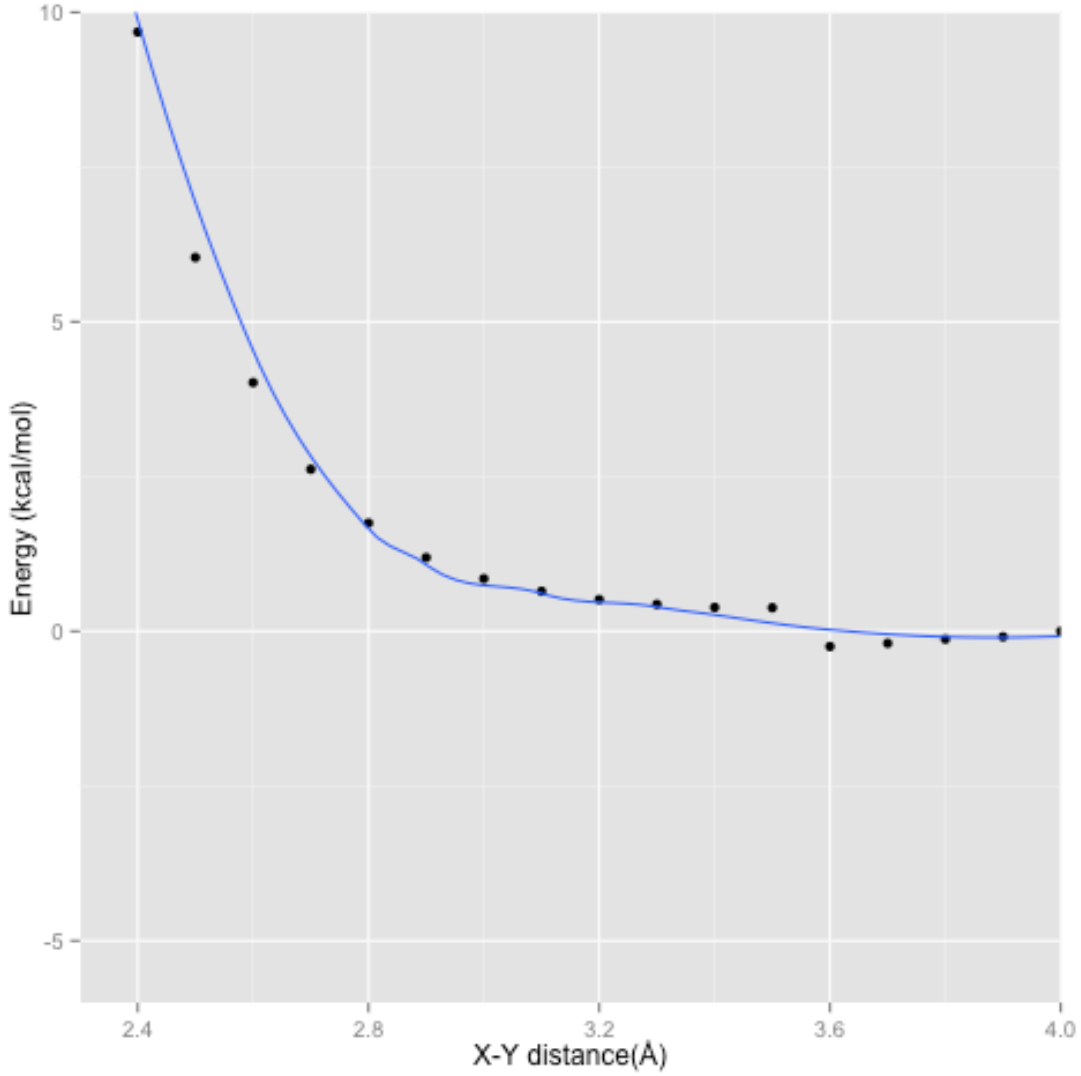
Methane with Benzene [non-polar – non-polar]



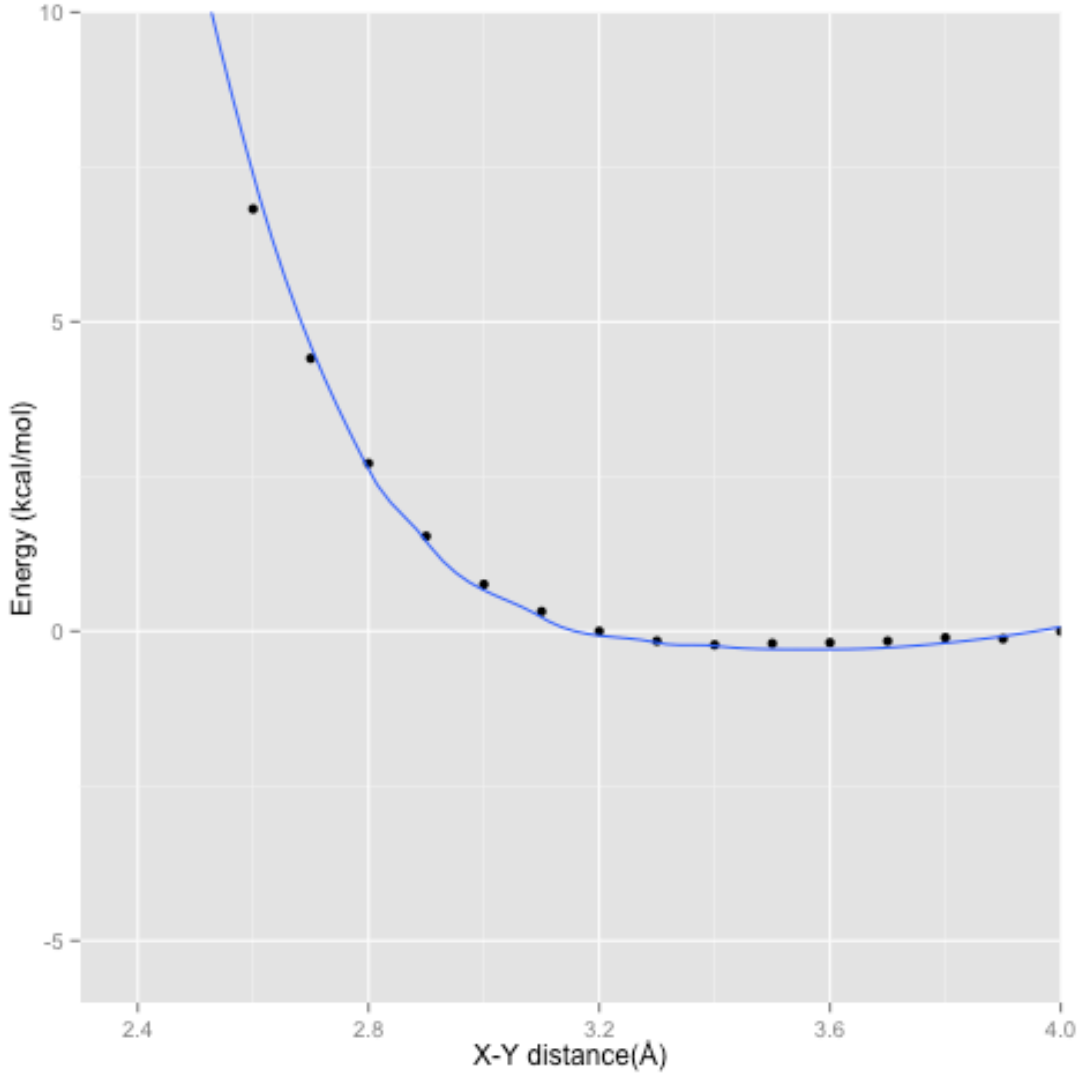
Methane with Pyridine [non-polar – polar]



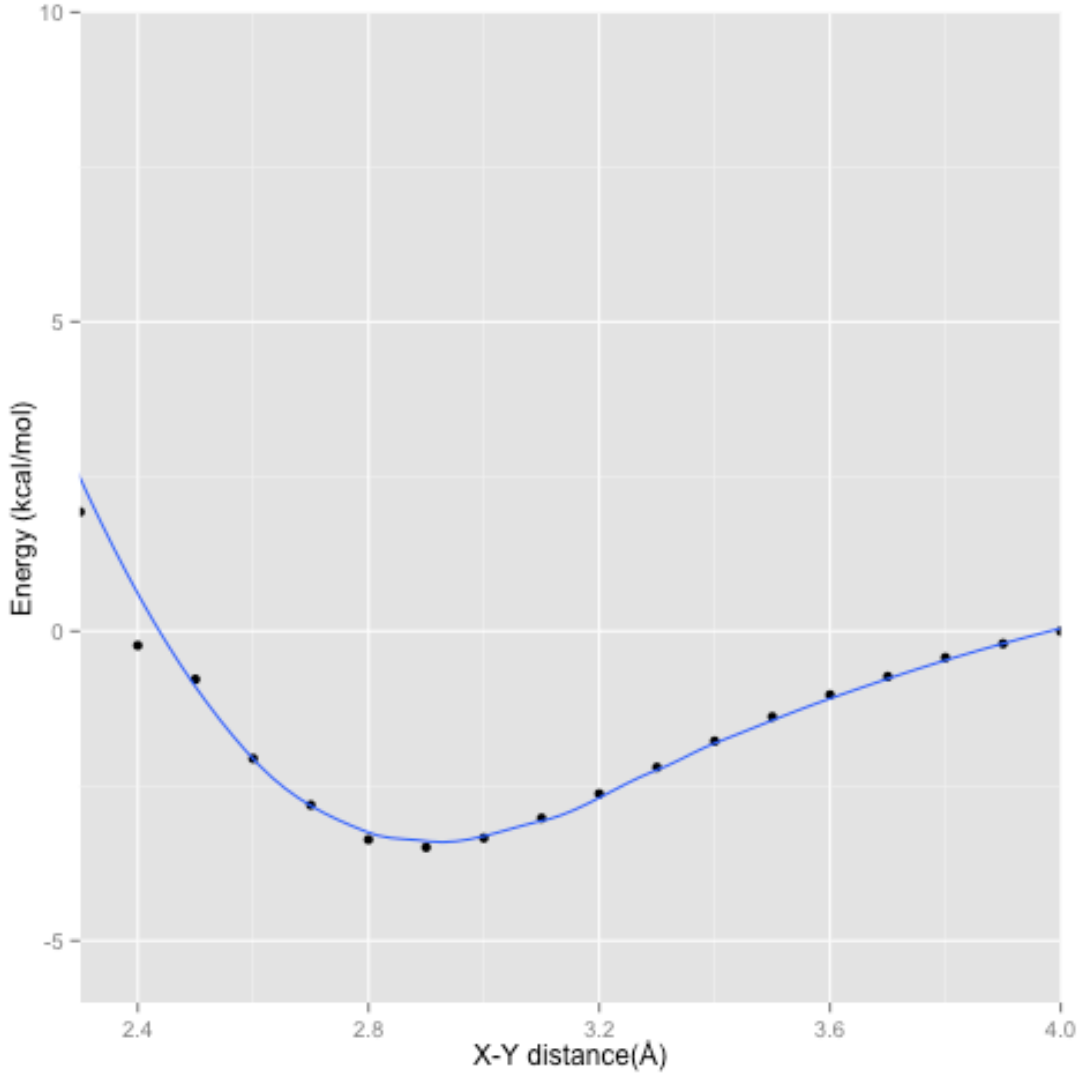
Methane with Amide carbonyl [non-polar – polar]



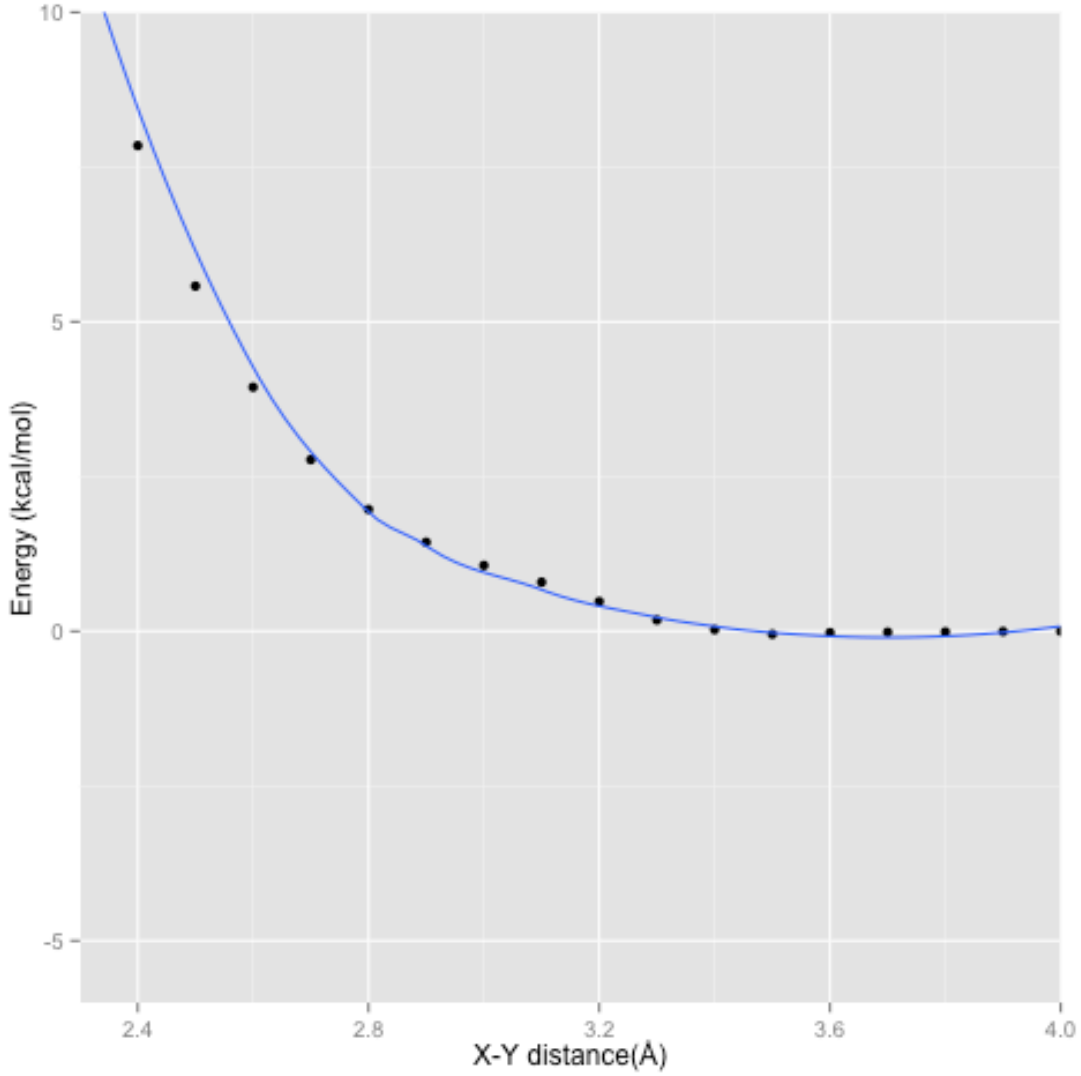
Methane with Amide NH [non-polar – polar]



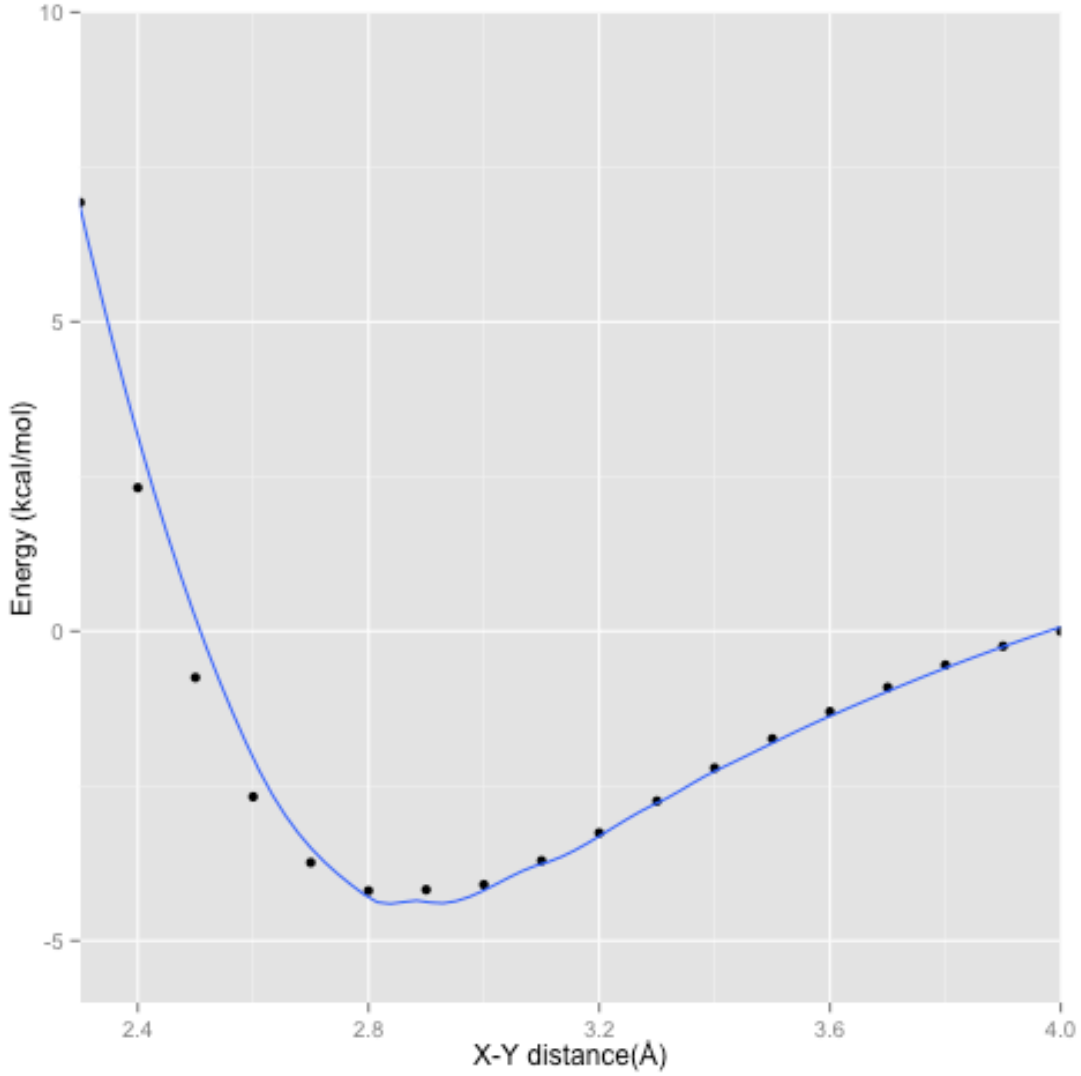
Water with Water [polar – polar]



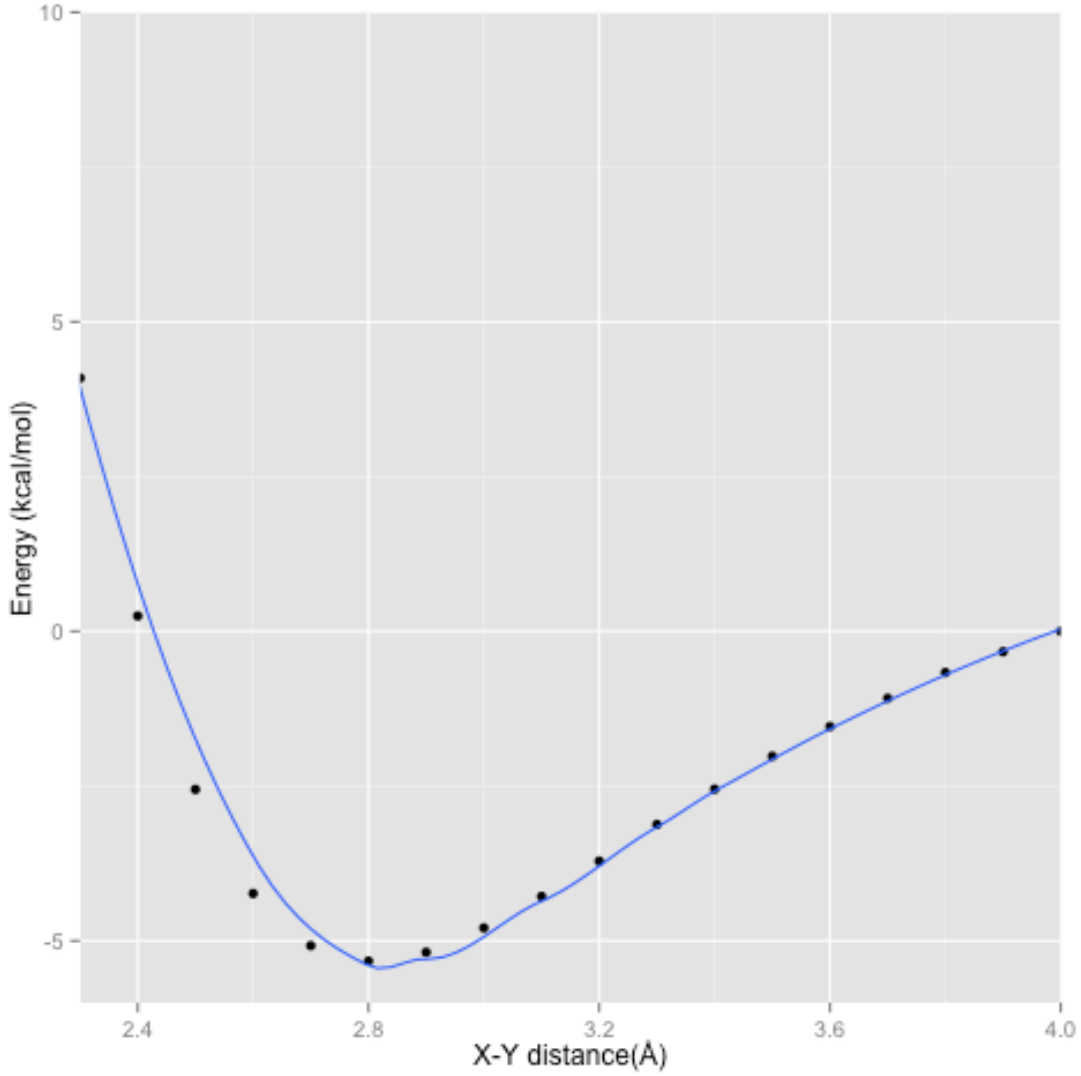
Water with Benzene [polar – non-polar]



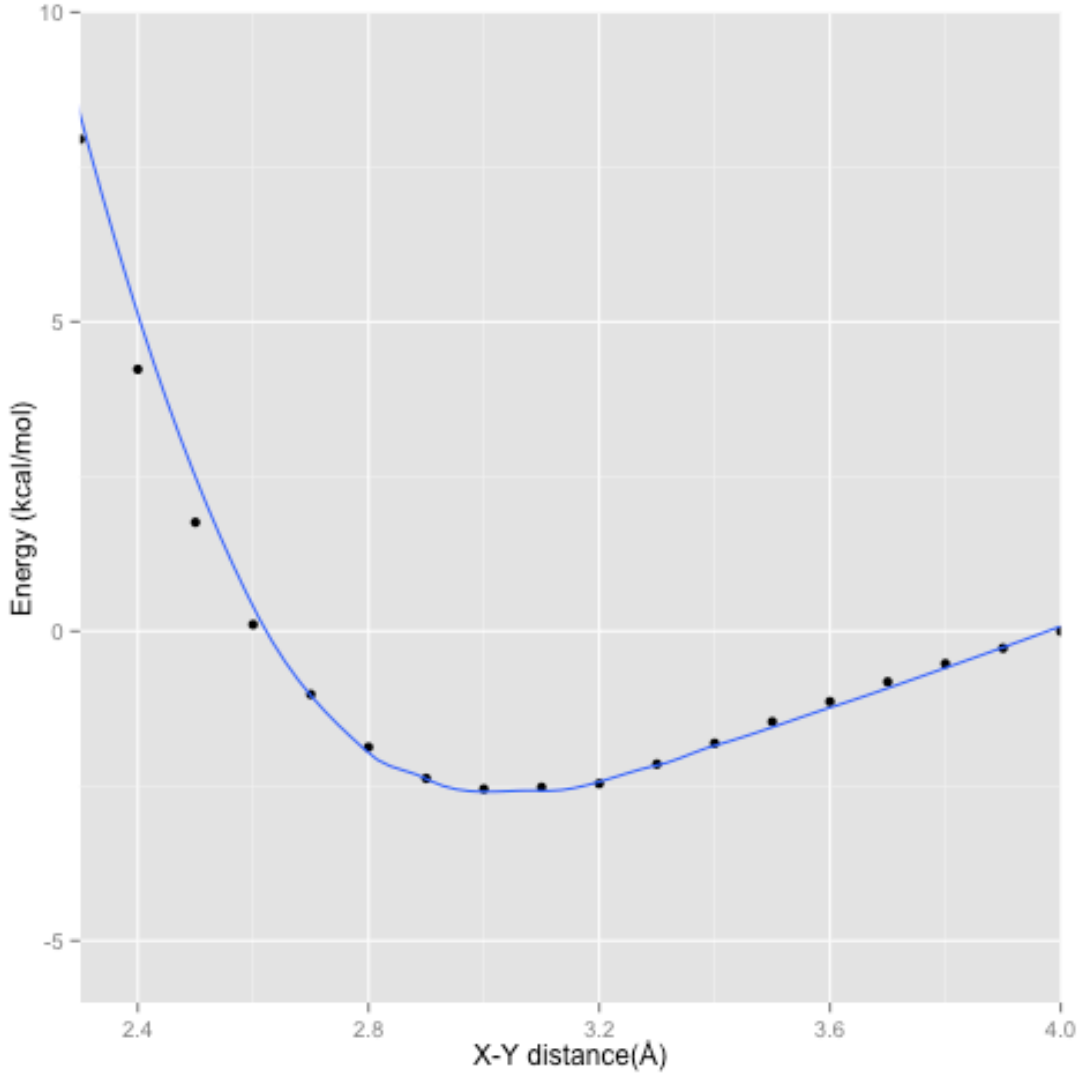
Water with Pyridine [polar – polar]



Water with Amide Carbonyl [polar – polar]

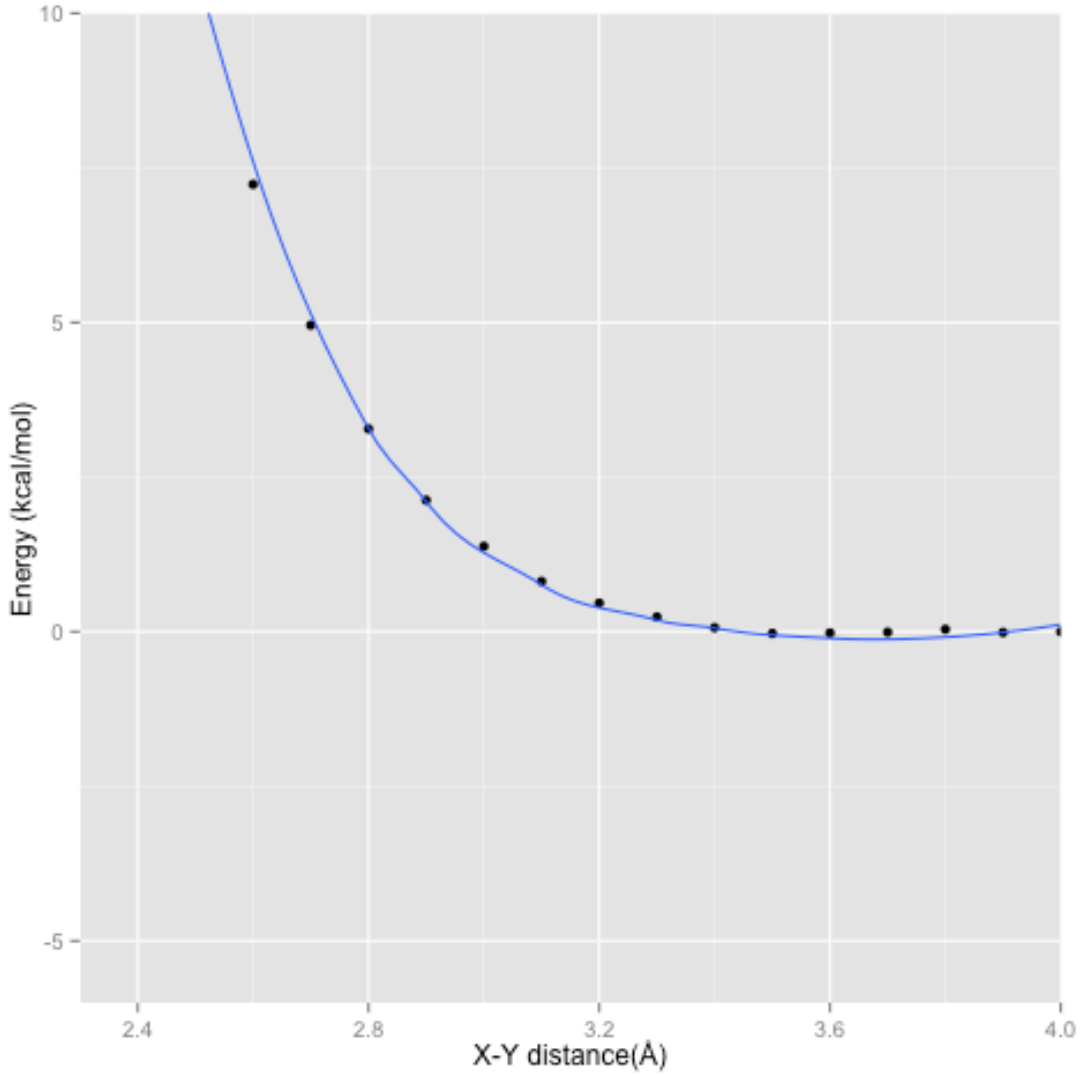


Water with Amide NH [polar – polar]

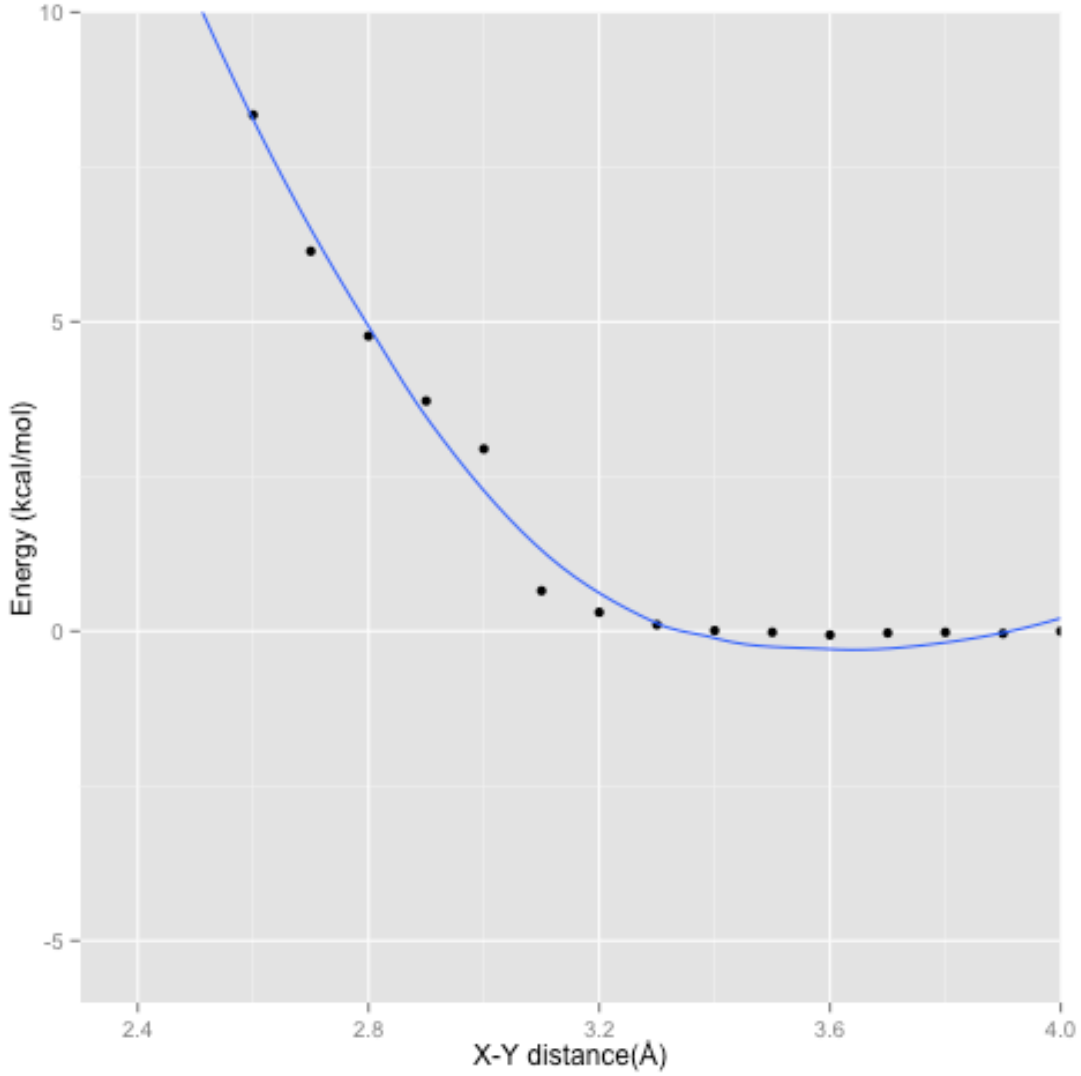


Benzene with Benzene [non-polar – non-polar]

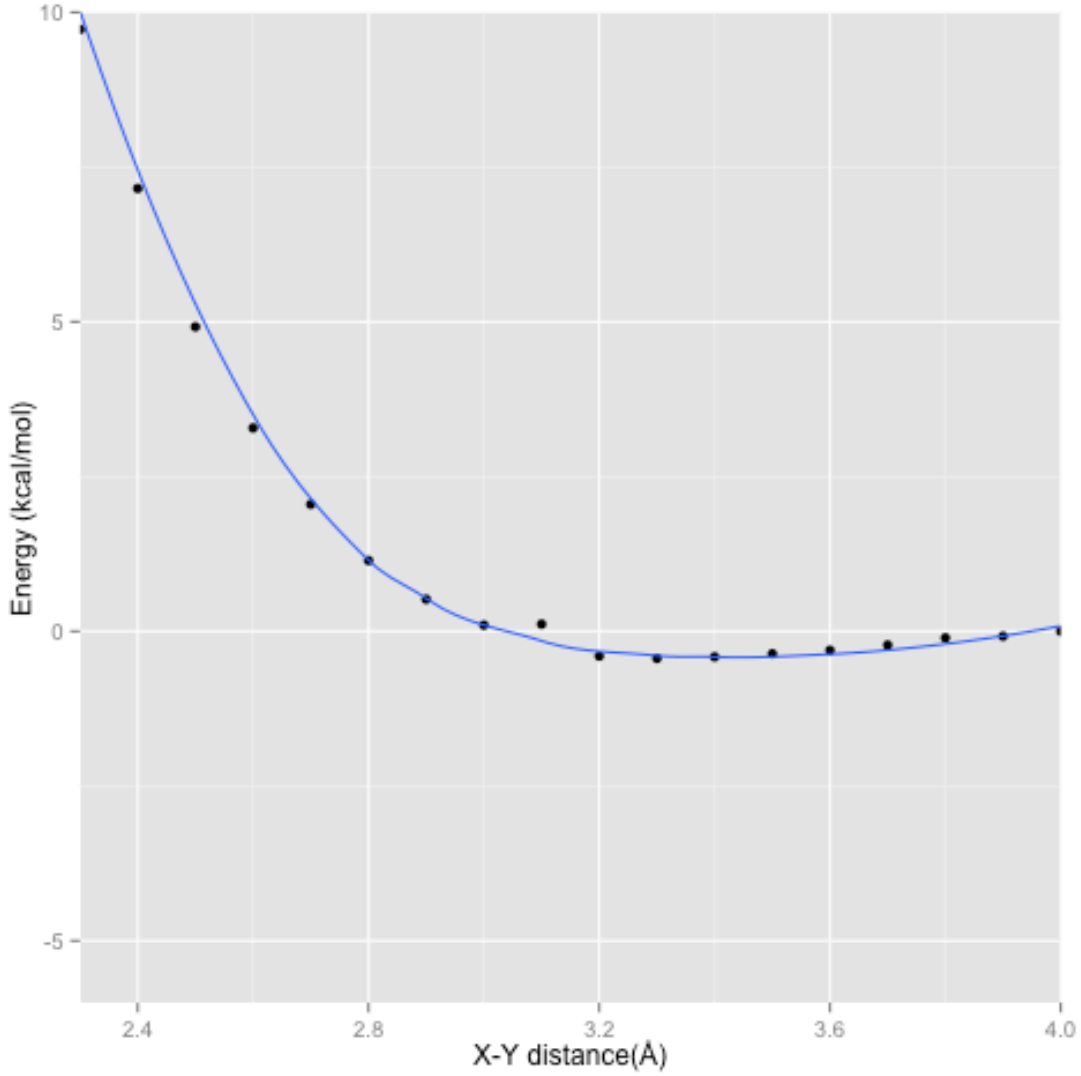
Examples involving aromatic compounds such as this are likely to be in error thanks to known problems with reproducing the interaction curves for higher levels of theory which suggest that minima might be at -1.7 to -2.8 kcal/mol.[1]



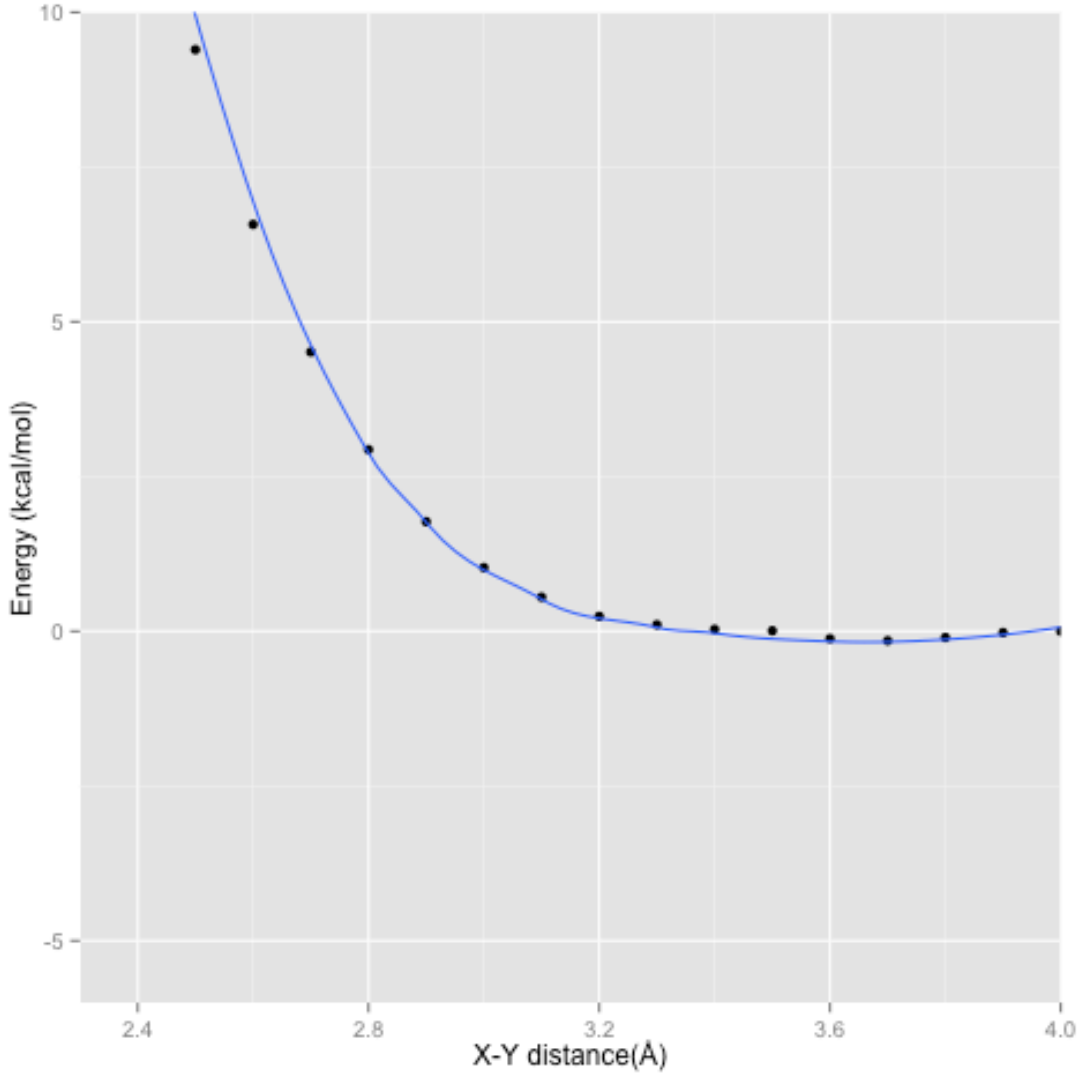
Benzene with Pyridine [non-polar – polar]



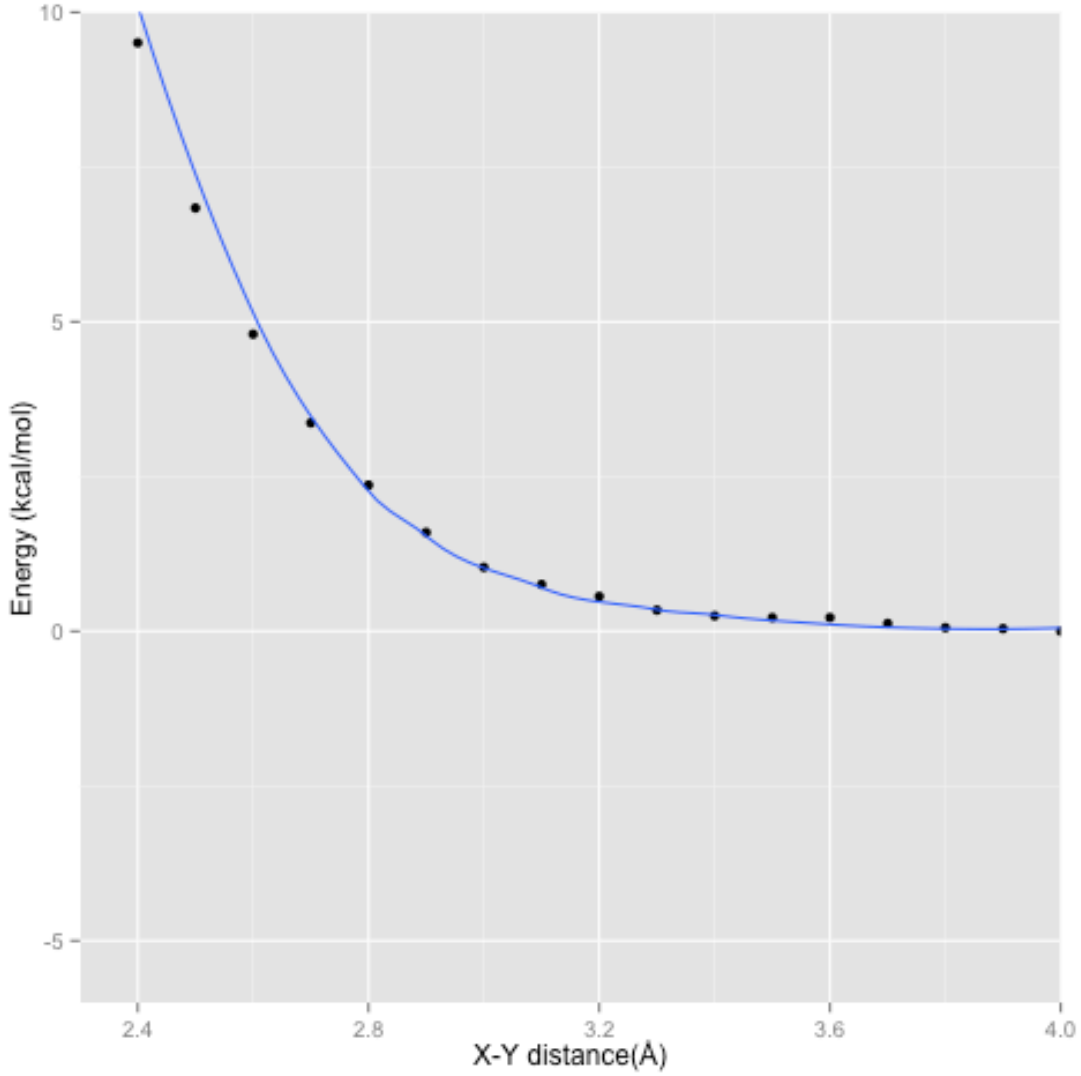
Benzene with Amide Carbonyl [non-polar – polar]



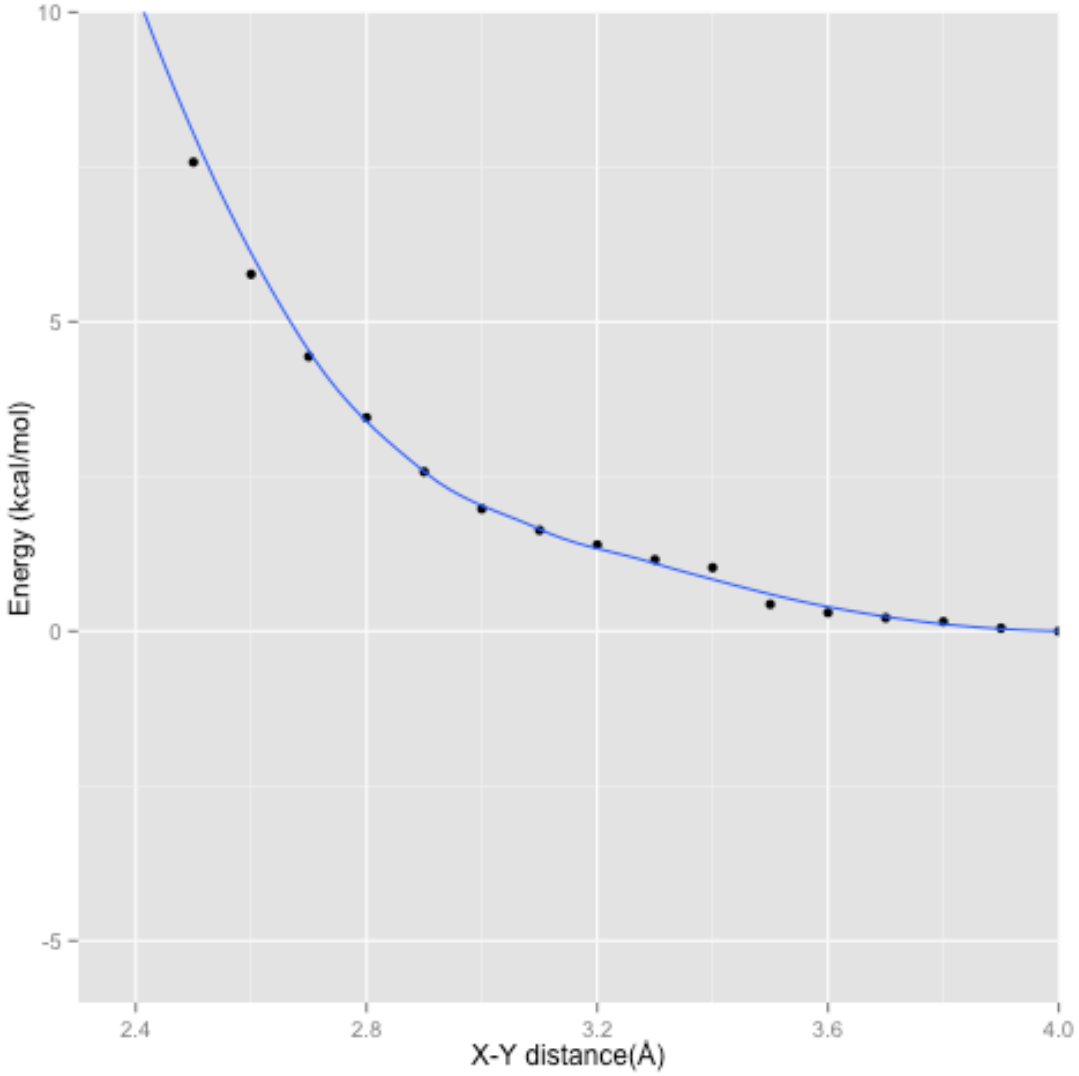
Benzene with Amide NH [non-polar – polar]



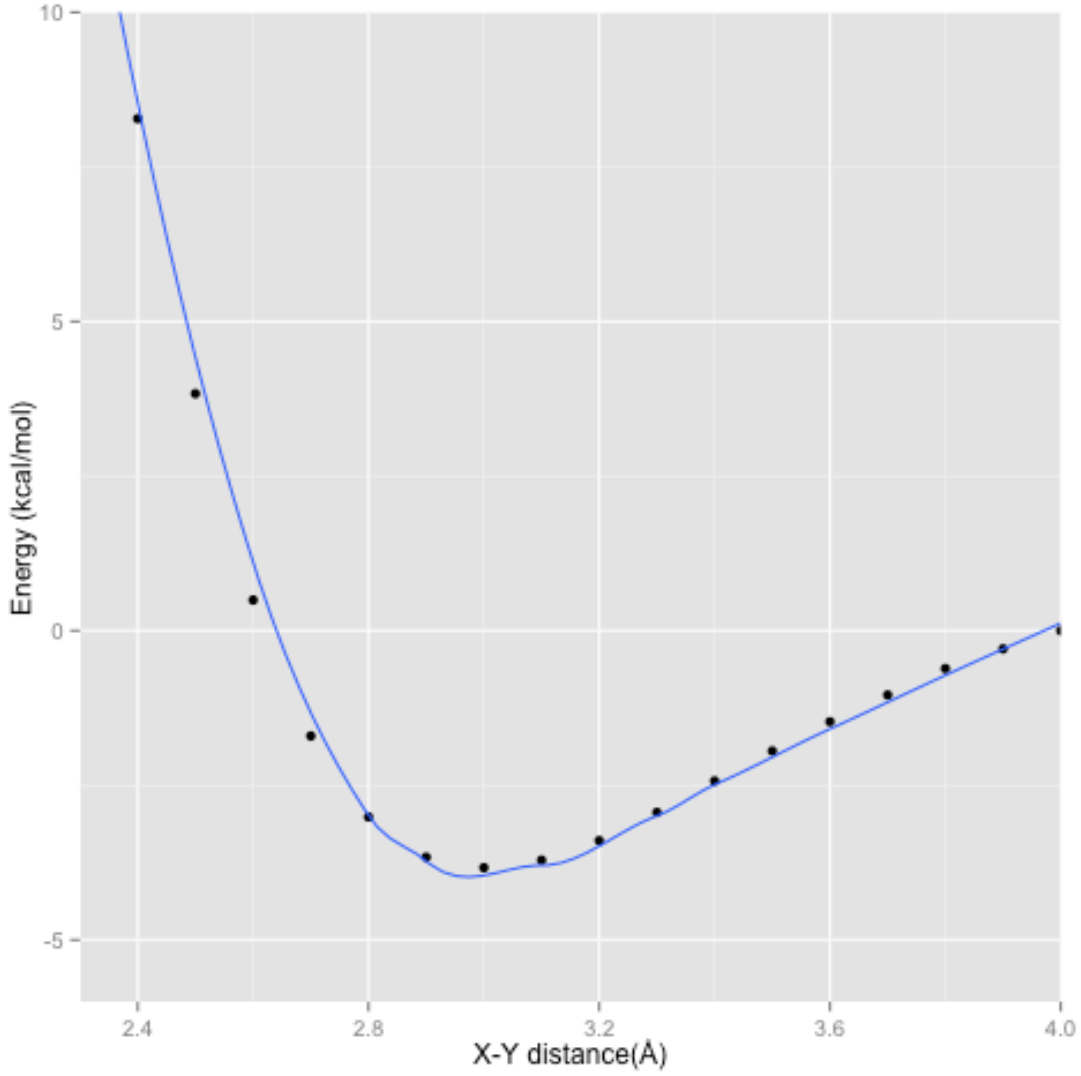
Pyridine with Pyridine [polar – polar MISMATCHED]



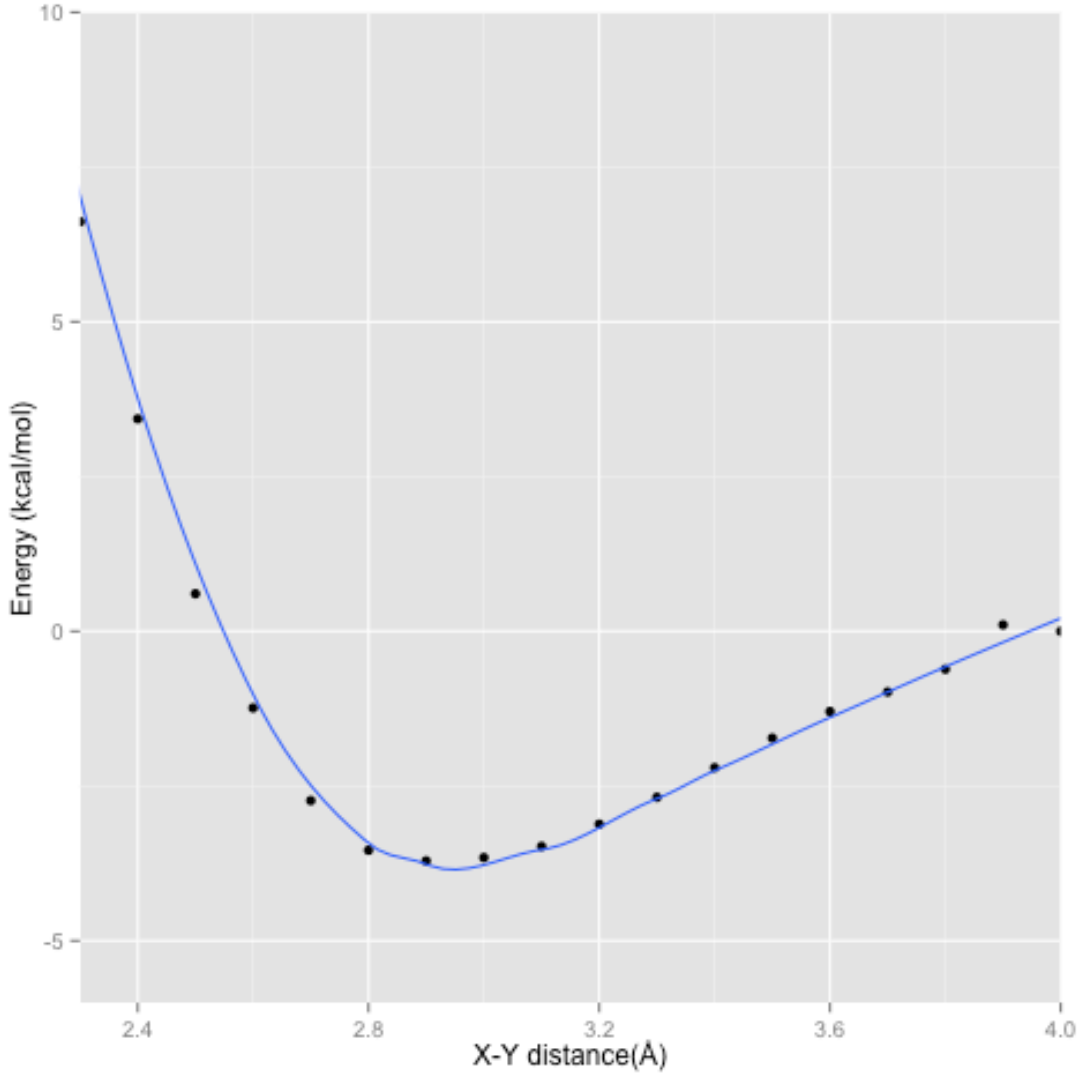
Pyridine with Amide Carbonyl [polar – polar MISMATCHED]



Pyridine with Amide NH [polar – polar]



Amide Carbonyl with Amide NH [polar – polar]

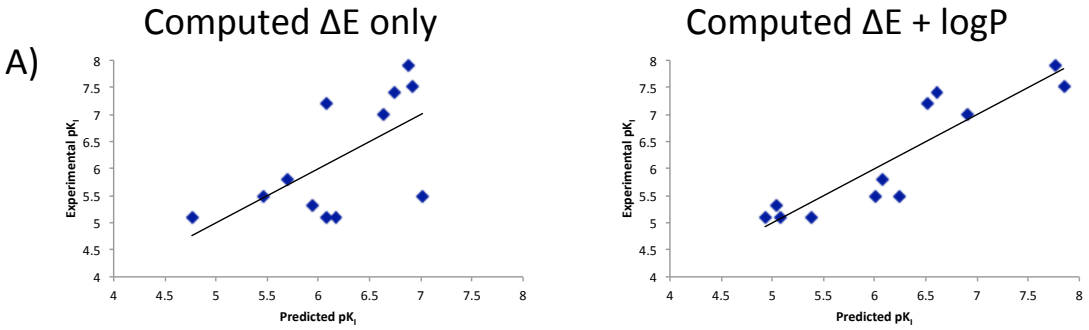


S2. Quantum mechanical binding energies, logPs and observed affinities used to create Table 1 in the main text

A – Mineralocorticoid Receptor.[2]

ΔE (kcal/mol) M06-2X	logD (measured)	pKi
0	1.2	7.4
-0.6	1.8	7.9
0.5	1.5	7
-0.8	1.8	7.5
3.6	1	5.3
8.9	2.2	5.1
3	1.8	7.2
3	0.8	5.1
2.6	1	5.1
5.8	2.1	5.5
4.7	1.9	5.8
-1.2	0.7	5.5

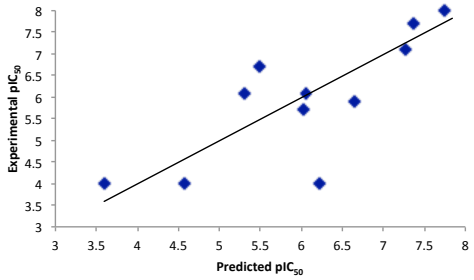
A)

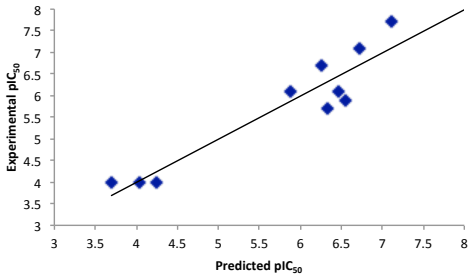


B – Inducible NO synthase.[3]

ΔE (kcal/mol) M06-HF	clogP (from paper)	pIC_{50}
-35.1	3.93	8
-27.58	2.26	4
-29.65	3.83	5.9
-26.52	4.39	5.7
	5.85	4
-19.4	4.37	4
-14.53	5.07	4
-23	4.86	6.1
-32.72	3.24	7.1
-35.55	4.06	8.7
-26.68	4.46	6.1
-23.92	4.95	6.7
-33.25	3.43	7.7

B)



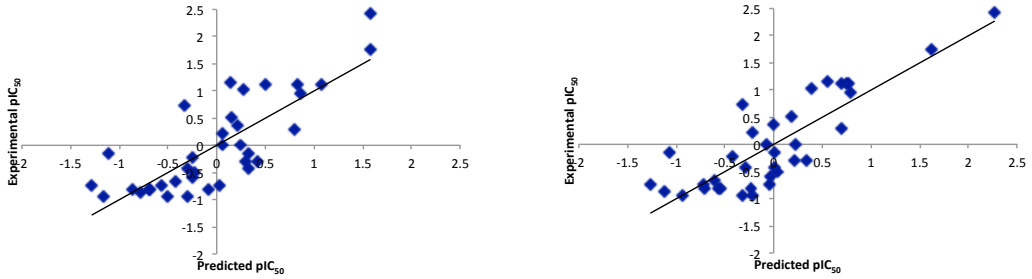


C – Beta-secretase inhibitors.[4]

ΔE (kcal/mol) B3LYP/6-31G** + solvation using SM8 and B3LYP/6-31+G**	clogP (from paper)	Free-Wilson contributions to pIC_{50}
-1.1	0	-0.293365943
-2.9	-0.4	0.293365943
0.9	0	-0.220024457
1.2	0.8	0.733414856
-3.9	-1.5	1.100122284
2.8	-0.4	-0.880097828
-3	-0.5	1.100122284
-0.2	0	0
-3.1	-0.3	0.953439313
-5.7	-0.3	1.760195655
-0.2	-0.6	0.220024457
2.5	1.5	-0.806756342
-1.5	0	-0.293365943
0.3	0	-0.806756342
1.5	0	-0.660073371
-1.2	-1	-0.440048914
-1.2	-1	-0.146682971
-0.6	0.5	0.513390399
-0.8	-0.5	0.366707428
-0.1	0.2	-0.733414856
0.9	1.6	-0.586731885
-0.5	2.2	1.17346377
-1	0.8	1.026780799
-1.8	1.4	1.100122284
-5.7	2.4	2.420269026
1.8	1.6	-0.953439313
4.2	2.2	-0.953439313
1.1	0.8	-0.440048914
2.5	0.9	-0.806756342
0.8	1.8	-0.513390399
3.1	2.4	-0.806756342
1.1	1.1	-0.953439313

2	0.2	-0.733414856
4.6	1.4	-0.733414856
4	1.4	-0.146682971
-0.9	0.3	0

C)

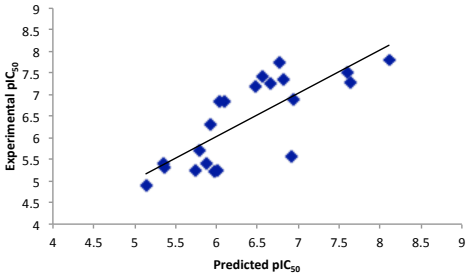


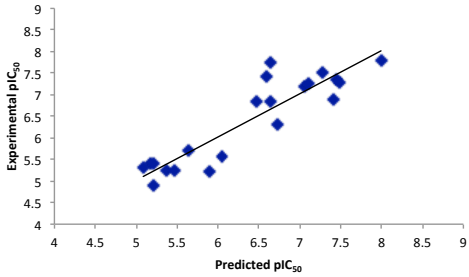
D – CDK2 inhibitors.[5]

An experimental value of ΔG for binding was converted to a pK_D using $-\log_{10}(e^{-\Delta G/RT})$.

ΔE (kcal/mol) TPSS/TZVPP	SlogP (calculated in MOE from Chemical Computing Group)	pK_D (from experimental ΔG for binding)
-103.7	4.93	4.90
-112.1	5.70	6.31
-106	4.64	5.41
-113.9	5.40	6.84
-106.1	4.52	5.30
-113.3	5.28	6.85
-112.7	4.69	5.21
-122.8	5.26	6.89
-121.5	5.46	7.34
-111.6	4.03	5.40
-121	4.60	7.74
-118.8	4.80	7.43
-110.6	4.64	5.70
-118	5.40	7.19
-113.1	4.04	5.25
-122.6	3.74	5.57
-129.9	4.30	7.50
-130.2	4.50	7.28
-135.3	4.50	7.82
-110.1	4.49	5.26
-119.9	5.25	7.27

D)



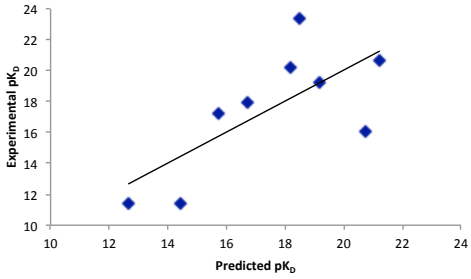


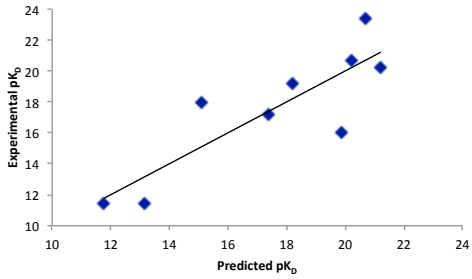
E – Octa-acid cavitand.[6]

An experimental value of ΔG for binding was converted to a pK_D using $-\log_{10}(e^{-\Delta G/RT})$.

ΔE (kcal/mol) BP86/TZVP+COSMO	AlogP computed in Chemdoodle	pK_D
-92.3	1.38	11.44
-112.9	1.69	17.97
-134.5	1.95	19.22
-152.6	2.04	20.61
-148.5	2.04	16.06
-103.8	2.29	17.24
-128.5	2.53	23.32
-76.9	1.9	11.44
-125.7	2.68	20.24

E)



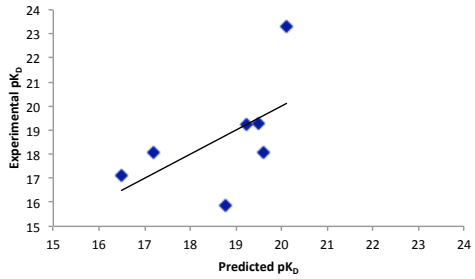


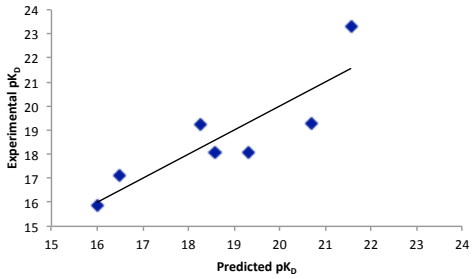
F – Cyclodextrin.[7]

An experimental value of ΔG for binding was converted to a pK_D using $-\log_{10}(e^{-\Delta G/RT})$.

ΔE (kcal/mol)	AlogP computed in Chemdoodle	pK_D
-6.23	0.92	17.16
-2.60	1.31	15.84
-5.10	1.7	18.04
-1.85	2.09	19.22
-1.27	2.48	18.04
-1.44	2.87	19.29
-0.46	3.26	23.32

F)


Experimental pK$_D$
Predicted pK$_D$
24
23
22
21
20
19
18
17
16
15
15 16 17 18 19 20 21 22 23 24


Experimental pK$_D$
Predicted pK$_D$
24
23
22
21
20
19
18
17
16
15
15 16 17 18 19 20 21 22 23 24

S3. Statistics and coefficients for approach employing Number of hydrophobic atoms in place of logP

Number of hydrophobic atoms was computed in MOE but fluorines were subsequently removed from the count.

Label	System	ΔE + random		ΔE + $N_{hydrophobic}$		α	β	γ
		R^2	RMSE	R^2	RMSE			
A	MR agonists	0.51	0.85	0.68	0.68	-0.26	0.64	2.21
B	iNOS inhibitors	0.67	1.00	0.88	0.62	-0.22	0.52	-4.17
C	BACE inhibitors	0.67	0.52	0.65	0.53	-0.28	0.03	-0.22
D	CDK2 inhibitors	0.61	0.65	0.69	0.59	-0.08	0.30	-9.73
E	Octa-acid cavitand + carboxylic acids	0.55	3.11	0.57	3.06	-0.06	1.98	-2.62
F	Cyclodextrin + nitriles	0.33	2.37	0.75	1.45	-0.50	1.32	10.75

S4. XYZ coordinates for theoceptor complexes

Compound **1**

C	75.66007	-11.66308	15.23803
C	77.07691	-11.69092	14.67699
C	77.18143	-12.18806	13.25156
N	78.10923	-11.54706	12.50137
O	76.50315	-13.11870	12.83091
C	78.76855	-18.41407	3.83893
C	78.54363	-19.37282	5.02015
C	78.58739	-18.64992	6.34095
O	77.40926	-18.41301	6.85592
O	79.65053	-18.30442	6.84360
C	81.20205	-16.81002	-0.49800
C	81.77493	-16.49998	0.89199
C	81.33972	-15.12486	1.37126
C	82.04881	-14.67521	2.63431
N	81.54359	-13.36256	3.01607
C	81.97983	-12.63296	4.05452
N	81.42600	-11.45051	4.32190
N	83.02172	-13.03194	4.78848
C	77.10000	-19.40200	10.72203
C	76.18100	-18.17096	10.59491
C	76.92779	-16.95234	10.15949
C	77.15575	-15.76173	10.80263
N	77.56908	-16.92529	8.93882
C	78.17100	-15.75427	8.85445
N	77.94485	-15.01504	9.95500
C	83.79101	-20.52901	11.86214
C	84.68695	-20.21104	13.08288
C	85.53620	-18.96108	12.82361
O	84.86676	-17.87584	12.70968
O	86.76803	-19.08043	12.72684
C	86.30574	-18.19906	7.05052
C	86.55272	-19.36878	8.04815
C	86.46116	-18.85905	9.47838
C	85.55094	-20.48718	7.79711
C	88.40513	-11.84600	8.83004
C	89.16677	-12.84604	9.72498
C	88.32525	-13.62524	10.69744
C	88.44968	-13.42274	12.07333
C	87.44050	-14.62998	10.28181
C	87.71855	-14.16276	12.99618
C	86.70716	-15.39019	11.18506
C	86.83227	-15.16892	12.57230
O	86.15620	-15.84077	13.48398
H	75.19092	-12.64672	15.13490
H	77.69630	-12.37364	15.27726

H	77.54232	-10.69987	14.76962
H	78.41919	-11.93413	11.60441
H	78.69731	-10.84720	12.92708
H	79.74207	-17.91485	3.91891
H	79.33607	-20.13044	5.03194
H	77.57754	-19.87760	4.91185
H	81.56543	-16.08700	-1.23864
H	82.87320	-16.54882	0.85635
H	81.45512	-17.26228	1.61651
H	80.25260	-15.13700	1.55819
H	81.51903	-14.38129	0.57858
H	83.13109	-14.60012	2.45701
H	81.88334	-15.40498	3.44348
H	80.61433	-13.13790	2.68372
H	81.57893	-11.11152	5.29099
H	80.57225	-11.19596	3.84954
H	83.17025	-12.49422	5.64941
H	83.23731	-14.01985	4.83297
H	77.59446	-19.61257	9.76667
H	75.68742	-17.96491	11.55353
H	75.38436	-18.38729	9.86769
H	76.82305	-15.36576	11.75344
H	78.77281	-15.40901	8.02189
H	78.32741	-14.07778	10.10174
H	84.40212	-20.71949	10.96948
H	85.35132	-21.05526	13.30347
H	84.05002	-20.02479	13.95845
H	85.30995	-17.77050	7.23375
H	87.57049	-19.75444	7.87100
H	86.65915	-19.63689	10.22630
H	87.17767	-18.05127	9.67865
H	85.45253	-18.46581	9.69028
H	85.70054	-21.31748	8.49923
H	84.52132	-20.12347	7.93429
H	85.63241	-20.88587	6.77618
H	87.91460	-11.07653	9.44244
H	89.94100	-12.29960	10.28412
H	89.71020	-13.54513	9.06950
H	89.16609	-12.67634	12.42807
H	87.33481	-14.84057	9.21420
H	87.83611	-14.01743	14.06957
H	86.04747	-16.18849	10.84669
H	85.65867	-16.67170	13.10682
H	75.03563	-10.94167	14.69877
H	75.66642	-11.38651	16.29737
H	77.99657	-17.63598	3.81071
H	78.74206	-18.96117	2.89000
H	80.10607	-16.75791	-0.48949
H	81.48601	-17.81115	-0.83767

H	76.53142	-20.29111	11.01742
H	77.88260	-19.22685	11.46880
H	83.14324	-19.67082	11.65069
H	83.16066	-21.41019	12.03428
H	87.61807	-12.35422	8.25802
H	89.08014	-11.34942	8.12255
O	81.92231	-19.29723	8.36526
H	81.11625	-18.91198	7.98425
H	82.00713	-18.92211	9.24694
H	77.49753	-17.84314	7.74670
H	86.34567	-18.53757	6.00622
H	87.04504	-17.39902	7.18791
Cl	81.89496	-7.84150	11.15322
Cl	84.96018	-12.41703	11.56200
Cl	79.33835	-15.02131	5.01350
C	83.21505	-8.81008	11.81899
C	84.04984	-8.16008	12.71510
C	85.14029	-8.81342	13.26061
C	85.42708	-10.14713	12.92580
N	86.47979	-10.82574	13.48356
C	84.55356	-10.77182	12.00224
C	83.43300	-10.14230	11.43604
C	82.58488	-10.88096	10.42604
C	81.09977	-11.00024	10.75322
C	80.36893	-11.84540	9.72701
C	80.86749	-11.85854	8.38695
S	79.98313	-12.82272	7.19294
C	81.00672	-14.27886	7.06174
C	80.74143	-15.22762	6.06911
C	81.52573	-16.36168	5.89636
C	82.60552	-16.58696	6.74058
C	82.87645	-15.67319	7.75774
C	82.08992	-14.53752	7.91225
C	82.00966	-11.12847	7.97924
O	82.45073	-11.08622	6.79830
C	82.78321	-10.34676	9.01265
O	79.35452	-12.47012	10.09219
H	83.84456	-7.12609	12.97949
H	85.77539	-8.27449	13.95702
H	86.68782	-11.75212	13.11351
H	82.95523	-11.91177	10.41067
H	80.60838	-10.01721	10.78803
H	80.95781	-11.47591	11.73219
H	81.25352	-17.09649	5.14333
H	83.17868	-17.50567	6.64755
H	83.69452	-15.85568	8.45275
H	82.30759	-13.83042	8.71001
H	83.84228	-10.38761	8.72521
H	82.47783	-9.29249	8.93478

C	87.55030	-10.16546	14.20006
C	88.35498	-11.16323	15.02023
C	88.50037	-9.39440	13.28072
H	87.10136	-9.45524	14.91755
C	89.49178	-10.44975	15.73074
H	88.77773	-11.93118	14.35818
H	87.70599	-11.67429	15.74356
C	89.63395	-8.78818	14.08913
H	88.90691	-10.09419	12.53387
H	87.96159	-8.60921	12.73252
H	90.12655	-11.15798	16.27255
H	89.08659	-9.72750	16.46719
H	90.37003	-8.29641	13.44439
H	89.23290	-8.02398	14.78566
O	90.33635	-9.76796	14.82398

Compound **2**

C	74.49081	-10.79680	15.80484
C	75.96223	-10.58525	15.41917
C	76.36233	-11.29658	14.13250
N	77.40650	-10.73996	13.46672
O	75.79433	-12.31005	13.74424
C	79.10954	-17.75690	4.91998
C	78.92061	-18.70709	6.12401
C	78.52721	-18.07812	7.45240
O	79.21532	-18.33839	8.46415
O	77.46975	-17.37096	7.44333
C	77.03904	-18.57789	11.63002
C	76.09391	-17.37416	11.58002
C	76.77223	-16.17871	11.01069
C	77.14118	-14.98602	11.57098
N	77.24291	-16.16324	9.71494
C	77.88014	-15.02506	9.50307
N	77.83611	-14.28270	10.60830
C	83.68548	-18.81118	13.37984
C	84.19639	-18.44771	14.78321
C	84.53875	-16.96982	15.01541
O	84.66060	-16.22434	13.98229
O	84.69288	-16.61989	16.19544
C	86.42505	-17.05311	8.35891
C	86.74098	-18.15083	9.41516
C	87.19851	-17.51382	10.71936
C	85.51727	-19.02773	9.64367
C	88.10505	-10.68891	10.14339
C	89.03408	-11.60911	10.93162
C	88.25245	-12.33013	11.99750
C	88.10333	-11.77815	13.27243
C	87.52176	-13.48875	11.70871
C	87.24583	-12.33605	14.21139

C	86.65227	-14.06042	12.63186
C	86.48098	-13.47242	13.89871
O	85.62063	-13.91938	14.80328
O	81.92272	-19.29711	8.36498
H	73.82219	-10.35612	15.05742
H	74.26595	-11.86610	15.85652
H	76.61468	-10.98296	16.21013
H	76.19441	-9.51403	15.34213
H	77.81595	-11.19364	12.65056
H	77.90029	-9.94549	13.84233
H	79.35870	-18.32483	4.01475
H	78.19343	-17.18164	4.73793
H	79.92364	-17.04151	5.10746
H	79.83950	-19.28794	6.27603
H	78.12402	-19.42255	5.87371
H	76.52272	-19.46611	12.01035
H	77.44177	-18.80901	10.63567
H	75.73104	-17.12167	12.58387
H	75.20838	-17.61698	10.97570
H	76.95207	-14.57272	12.55235
H	77.22764	-16.86875	8.89826
H	78.37059	-14.75905	8.57785
H	83.42444	-19.87608	13.31106
H	82.79768	-18.22127	13.12041
H	84.45069	-18.59679	12.62306
H	85.10640	-19.01995	15.01643
H	83.46531	-18.73180	15.55119
H	86.06509	-17.49413	7.42059
H	85.64072	-16.38450	8.74337
H	87.31193	-16.44346	8.14262
H	87.55563	-18.77893	9.01754
H	87.43806	-18.26836	11.47935
H	88.08380	-16.88011	10.57976
H	86.40186	-16.88239	11.13996
H	85.72819	-19.83497	10.35732
H	84.69527	-18.43002	10.06551
H	85.14888	-19.47503	8.71155
H	88.63075	-10.14867	9.34407
H	87.29011	-11.26630	9.68837
H	87.64075	-9.95064	10.81012
H	89.84569	-11.02289	11.38677
H	89.50813	-12.33048	10.24945
H	88.66474	-10.87713	13.52932
H	87.61883	-13.94996	10.72208
H	87.13530	-11.90536	15.20555
H	86.08470	-14.96125	12.40112
H	85.21438	-14.81553	14.54147
H	80.99395	-18.97250	8.38582
H	82.02464	-19.78808	9.18528

H	78.29127	-13.35811	10.70673
H	74.27692	-10.33950	16.77626
H	77.89405	-18.36995	12.28271
Cl	81.19859	-15.91976	7.28623
O	81.92540	-10.83267	7.31280
C	81.41208	-10.60787	8.44456
C	81.41144	-9.18654	10.53109
C	81.22747	-7.78567	11.11219
C	81.59241	-7.91987	12.59640
C	82.60872	-9.02964	12.57799
C	82.54744	-9.73029	11.37017
C	79.91125	-11.10454	10.36369
O	79.02665	-11.75324	10.93191
C	80.63870	-11.51567	9.19036
S	80.36486	-13.11537	8.50297
C	81.47931	-14.19176	9.40880
C	81.97916	-13.87246	10.67557
C	82.82427	-14.74536	11.35336
C	83.17314	-15.96756	10.78307
C	82.66806	-16.32303	9.53473
C	81.83361	-15.43193	8.86950
C	81.41799	-16.76105	-0.10107
C	81.99402	-16.37200	1.26601
C	81.11430	-15.39919	2.04650
C	81.68389	-15.03433	3.41482
N	80.88197	-13.96422	4.01034
C	81.28754	-13.09912	4.95722
N	80.58815	-11.99573	5.20010
N	82.42451	-13.29809	5.63505
H	80.43973	-17.24508	0.00825
H	81.28436	-15.87799	-0.73859
H	82.71390	-14.66465	3.31811
H	81.70541	-15.91909	4.07196
H	80.11225	-15.83864	2.18392
H	80.98121	-14.47543	1.46133
H	82.99013	-15.92474	1.13170
H	82.14807	-17.27901	1.86941
H	79.90689	-13.91836	3.74355
H	80.87632	-11.42768	6.01758
H	79.85122	-11.69874	4.58166
H	82.57221	-12.62181	6.39345
H	82.63809	-14.26128	5.88199
H	81.70253	-12.92399	11.13016
H	83.20492	-14.49479	12.34300
H	83.82470	-16.64023	11.34161
H	82.88299	-17.28821	9.07418
H	82.08049	-17.45718	-0.62485
C	81.59024	-9.22665	9.03168
O	80.17679	-9.88619	10.88848

H	80.85815	-8.55823	8.55042
C	83.43854	-10.76559	11.10180
C	84.36929	-11.12293	12.07668
C	83.53111	-9.39198	13.55168
C	84.40207	-10.45094	13.29853
H	83.41613	-11.29932	10.15194
H	85.07583	-11.93328	11.89654
H	85.12606	-10.76600	14.04745
H	83.57783	-8.85544	14.49863
H	81.94224	-7.11529	10.61390
H	80.21382	-7.41317	10.92276
H	81.98160	-6.98950	13.02782
H	80.71030	-8.20819	13.18641
H	82.58833	-8.86369	8.75698

Compound **3**

C	74.49101	-10.79701	15.80499
C	75.96200	-10.58499	15.41900
C	76.37949	-11.34153	14.17117
N	77.31118	-10.71148	13.41495
O	75.92898	-12.44671	13.89329
C	79.10964	-17.75690	4.91998
C	78.92051	-18.70712	6.12401
C	78.66244	-17.96085	7.42365
O	79.63167	-17.68775	8.17010
O	77.45180	-17.64984	7.65313
C	77.03897	-18.57799	11.63003
C	76.09403	-17.37400	11.57996
C	76.78521	-16.17155	11.03616
C	77.09473	-14.95942	11.59181
N	77.34545	-16.18096	9.77595
C	77.97883	-15.03722	9.57781
N	77.84319	-14.26863	10.65912
C	83.68500	-18.81097	13.37997
C	84.19703	-18.44805	14.78301
C	84.33537	-16.92896	14.94222
O	84.97458	-16.34100	13.99745
O	83.85353	-16.37999	15.94426
C	86.42498	-17.05306	8.35897
C	86.74100	-18.15092	9.41508
C	86.92725	-17.52717	10.79097
C	85.63198	-19.19461	9.43592
C	88.10402	-10.68799	10.14102
C	89.03499	-11.61003	10.93398
C	88.35134	-12.38654	12.02135
C	88.46958	-12.01368	13.36267
C	87.57012	-13.51034	11.72801
C	87.82868	-12.72017	14.37359
C	86.92264	-14.23219	12.72173

C	87.03839	-13.83706	14.06673
O	86.41123	-14.46399	15.05886
C	83.90588	-12.46308	13.99576
C	84.56901	-11.62469	13.10091
C	83.86064	-10.68069	12.36480
C	82.47367	-10.54393	12.49285
C	81.82300	-11.37890	13.40961
C	82.53015	-12.32753	14.14886
C	81.72942	-9.50763	11.66030
C	82.23333	-9.42506	10.21935
C	81.89219	-10.64330	9.38868
O	82.59888	-10.86784	8.37171
C	80.77763	-11.43149	9.77883
C	79.91300	-11.05934	10.84477
O	78.90213	-11.71041	11.19585
C	80.22955	-9.77035	11.58022
S	80.39086	-12.86246	8.81643
C	81.40270	-14.13710	9.56441
C	81.93360	-13.98144	10.85060
C	82.73689	-14.95723	11.43024
C	83.04287	-16.13104	10.73725
C	82.55502	-16.31116	9.45729
C	81.74322	-15.32620	8.88255
N	81.34065	-15.52314	7.51154
O	82.07107	-16.19633	6.77353
O	80.34480	-14.93590	7.09115
C	81.77303	-16.24999	0.53702
C	82.22296	-15.85902	1.94498
C	81.50813	-14.65765	2.54334
C	81.99446	-14.40568	3.96199
N	81.46215	-13.14517	4.47394
C	81.89677	-12.52716	5.58211
N	81.41991	-11.32888	5.91231
N	82.86918	-13.05172	6.33214
O	81.92282	-19.29696	8.36501
H	73.82091	-10.38139	15.04423
H	74.27632	-11.86676	15.88627
H	76.61066	-10.94838	16.22917
H	76.17989	-9.51397	15.30789
H	77.76217	-11.17412	12.61891
H	77.67396	-9.81738	13.70666
H	79.25942	-18.32295	3.99285
H	78.22934	-17.11384	4.79948
H	79.98623	-17.11338	5.08235
H	79.81961	-19.32631	6.24137
H	78.06834	-19.37016	5.92961
H	76.52324	-19.46760	12.00723
H	77.43308	-18.80983	10.63292
H	75.71457	-17.13433	12.58065

H	75.21989	-17.61174	10.95725
H	76.83721	-14.52027	12.54785
H	77.34235	-16.92202	8.97818
H	78.53500	-14.79269	8.68154
H	83.55592	-19.89335	13.25240
H	82.71762	-18.33170	13.18030
H	84.39792	-18.45698	12.62478
H	85.18896	-18.89578	14.94050
H	83.52701	-18.82667	15.56392
H	86.28037	-17.48864	7.36161
H	85.50102	-16.52414	8.63666
H	87.23268	-16.31179	8.30326
H	87.68270	-18.64248	9.11829
H	87.16945	-18.27989	11.55225
H	87.72929	-16.77771	10.79508
H	86.00626	-17.02737	11.12971
H	85.83125	-19.98045	10.17594
H	84.66659	-18.74015	9.70233
H	85.50291	-19.67533	8.45709
H	88.63988	-10.15421	9.34587
H	87.28855	-11.26045	9.68045
H	87.64285	-9.94433	10.80479
H	89.84649	-11.01072	11.37270
H	89.51952	-12.30683	10.23213
H	89.08036	-11.14608	13.61965
H	87.46390	-13.83230	10.68879
H	87.91440	-12.42298	15.41676
H	86.31647	-15.10566	12.48716
H	85.80346	-15.19398	14.69199
H	84.44918	-13.21997	14.56132
H	85.64482	-11.71454	12.96206
H	84.41207	-10.04978	11.66953
H	80.74362	-11.32654	13.54484
H	82.00103	-12.98349	14.83723
H	81.88103	-8.52042	12.12665
H	83.31419	-9.27299	10.14044
H	81.76967	-8.55589	9.72388
H	79.74532	-8.94303	11.03735
H	79.76090	-9.81385	12.56866
H	81.71958	-13.07347	11.40974
H	83.13343	-14.81383	12.43691
H	83.65758	-16.89355	11.21198
H	82.74895	-17.22548	8.89982
H	80.70701	-16.50914	0.52082
H	81.92606	-15.42727	-0.17327
H	83.30425	-15.65466	1.93596
H	82.08881	-16.71855	2.61893
H	80.42025	-14.83326	2.55129
H	81.68882	-13.76439	1.92459

H	83.09144	-14.32951	3.96469
H	81.71383	-15.23911	4.62393
H	80.56910	-12.84243	4.10858
H	81.68008	-10.96072	6.84087
H	80.73564	-10.86804	5.33629
H	83.05315	-12.56365	7.21450
H	83.02212	-14.05467	6.31385
H	81.08192	-18.78773	8.36626
H	82.28391	-19.13480	7.48813
H	78.27295	-13.33244	10.77615
H	74.26816	-10.31589	16.76271
H	77.89571	-18.37337	12.28137
H	82.33322	-17.11682	0.17267

Compound **4**

Compound **5**

C	74.49100	-10.79700	15.80499
C	75.96200	-10.58501	15.41901
C	76.40905	-11.35243	14.18823
N	77.46207	-10.79703	13.53810
O	75.88165	-12.40028	13.83513
C	79.10960	-17.75690	4.92000
C	78.92050	-18.70710	6.12400
C	78.57582	-18.06854	7.46470
O	79.26887	-18.36459	8.46494
O	77.55343	-17.31393	7.48293
C	77.03899	-18.57800	11.62999
C	76.09401	-17.37400	11.58001
C	76.79857	-16.16863	11.05738
C	77.14291	-14.98882	11.65965
N	77.33449	-16.12832	9.78499
C	77.98166	-14.98483	9.62902
N	77.88440	-14.26718	10.74656
C	83.68500	-18.81101	13.38001
C	84.19700	-18.44808	14.78298
C	84.42846	-16.95080	15.03575
O	84.66989	-16.21994	14.01317
O	84.40462	-16.57354	16.21714
C	86.42498	-17.05312	8.35901
C	86.74102	-18.15088	9.41509
C	86.93554	-17.52351	10.78812
C	85.61828	-19.18105	9.43794
C	88.10401	-10.68799	10.14101
C	89.03498	-11.61002	10.93399
C	88.27402	-12.33954	12.00775
C	88.25246	-11.86978	13.32347
C	87.46568	-13.44151	11.70519
C	87.45009	-12.45694	14.29315

C	86.65191	-14.04300	12.65883
C	86.61713	-13.54128	13.97303
O	85.82693	-14.02715	14.92341
C	81.77300	-16.25000	0.53700
C	82.22300	-15.85900	1.94500
C	81.46468	-14.68580	2.54774
C	81.94338	-14.39209	3.96121
N	81.30783	-13.18265	4.47625
C	81.74379	-12.46998	5.52728
N	81.23760	-11.26680	5.78162
N	82.73726	-12.92573	6.29698
O	81.92280	-19.29700	8.36500
H	73.82128	-10.40815	15.03017
H	74.28038	-11.86501	15.91533
H	76.61005	-10.92074	16.24224
H	76.17291	-9.51473	15.28619
H	77.94513	-11.28851	12.78124
H	77.90139	-9.96686	13.90526
H	79.27016	-18.32729	3.99738
H	78.22743	-17.11823	4.79404
H	79.98378	-17.10628	5.07199
H	79.82111	-19.32065	6.25299
H	78.09314	-19.39403	5.89335
H	76.51195	-19.47749	11.96679
H	77.47514	-18.78079	10.64350
H	75.70224	-17.14028	12.57734
H	75.22771	-17.60162	10.94300
H	76.90727	-14.59173	12.63847
H	77.33317	-16.81369	8.95024
H	78.51315	-14.69557	8.73262
H	83.54982	-19.89518	13.26611
H	82.72397	-18.32235	13.17417
H	84.39563	-18.46707	12.61752
H	85.16110	-18.94563	14.96754
H	83.51355	-18.81302	15.55989
H	86.27495	-17.48995	7.36324
H	85.50414	-16.52293	8.64144
H	87.23510	-16.31480	8.29951
H	87.67614	-18.65309	9.11617
H	87.16745	-18.27515	11.55337
H	87.74344	-16.78089	10.79036
H	86.01938	-17.00953	11.11585
H	85.79053	-19.95017	10.20232
H	84.65706	-18.69643	9.66685
H	85.49976	-19.67951	8.46723
H	88.63541	-10.13921	9.35177
H	87.29780	-11.26611	9.67277
H	87.62995	-9.95844	10.81085
H	89.84610	-11.02053	11.38564

H	89.51148	-12.32544	10.24654
H	88.87599	-11.01368	13.59063
H	87.46205	-13.83801	10.68642
H	87.43205	-12.08699	15.31666
H	86.03283	-14.90613	12.41619
H	85.32919	-14.85958	14.62657
H	80.71524	-16.54107	0.52796
H	81.89509	-15.41592	-0.16583
H	83.29626	-15.61696	1.93105
H	82.12055	-16.72730	2.61316
H	80.38546	-14.90931	2.56496
H	81.59931	-13.78970	1.92153
H	83.03027	-14.22955	3.96657
H	81.73363	-15.25057	4.61799
H	80.42126	-12.91250	4.07199
H	81.48964	-10.83901	6.68912
H	80.59895	-10.82307	5.14271
H	82.91115	-12.35661	7.13340
H	82.78124	-13.92963	6.44434
H	80.98082	-19.00663	8.38907
H	82.05452	-19.78241	9.18423
H	78.35264	-13.35514	10.89756
H	74.26324	-10.28982	16.74797
H	77.87002	-18.38785	12.31810
H	82.35547	-17.09584	0.15882
Cl	80.89152	-15.61996	7.36507
Cl	81.03386	-6.76525	11.86913
Cl	84.48194	-10.82980	13.28411
O	79.14215	-11.83258	11.37007
C	80.12906	-11.16790	10.98528
O	82.43120	-10.67225	8.17681
C	80.60040	-10.03303	11.87299
C	80.84352	-11.41374	9.77665
S	80.44576	-12.84816	8.82334
C	81.51266	-14.09052	9.56615
C	82.15346	-13.91743	10.79871
C	82.94285	-14.92130	11.35128
C	83.10685	-16.12706	10.67514
C	82.48190	-16.33227	9.44823
C	81.69642	-15.31648	8.91925
C	81.87808	-10.56476	9.30302
C	82.36163	-9.44969	10.20343
C	82.08933	-9.76789	11.66944
C	82.73127	-8.80409	12.63532
C	82.34294	-7.46919	12.81872
C	82.95573	-6.60804	13.72145
C	84.02033	-7.07020	14.48302
C	84.46324	-8.37528	14.32799
C	83.82859	-9.21727	13.41894

H	80.38966	-10.32614	12.91003
H	79.98928	-9.14648	11.65156
H	82.02640	-12.98159	11.33706
H	83.42142	-14.78803	12.32248
H	83.71095	-16.91212	11.12751
H	82.57194	-17.27863	8.91289
H	81.87402	-8.51144	9.89775
H	83.43573	-9.32776	10.01329
H	82.57907	-10.73067	11.85378
H	82.59634	-5.58696	13.81226
H	84.50901	-6.40890	15.19381
H	85.30051	-8.76016	14.90311

Compound **6**

C	74.49099	-10.79700	15.80500
C	75.96201	-10.58499	15.41900
C	76.41379	-11.54118	14.31968
N	77.75273	-11.65070	14.15639
O	75.61648	-12.15201	13.61235
C	79.10962	-17.75689	4.91997
C	78.92046	-18.70712	6.12404
C	78.95010	-17.95858	7.44514
O	79.94754	-17.21295	7.67492
O	77.98030	-18.12733	8.22935
C	77.03898	-18.57797	11.63003
C	76.09403	-17.37404	11.57995
C	76.77082	-16.14780	11.06094
C	76.73932	-14.84127	11.47112
N	77.63332	-16.19841	9.98101
C	78.10310	-14.98000	9.74622
N	77.57294	-14.13612	10.62834
C	83.68500	-18.81100	13.38001
C	84.19700	-18.44811	14.78299
C	84.30370	-16.93577	15.01794
O	84.86317	-16.27191	14.08498
O	83.86670	-16.47569	16.08889
C	86.42500	-17.05312	8.35901
C	86.74100	-18.15088	9.41509
C	86.94184	-17.51755	10.78495
C	85.62059	-19.18025	9.45440
C	88.10400	-10.68800	10.14100
C	89.03500	-11.61000	10.93400
C	88.24645	-12.30244	12.01662
C	87.91670	-11.62615	13.19640
C	87.67538	-13.56306	11.82157
C	87.04564	-12.16920	14.13079
C	86.80360	-14.13074	12.74719
C	86.46276	-13.42909	13.91650
O	85.60262	-13.89169	14.82288

C	81.77299	-16.25002	0.53698
C	82.22302	-15.85897	1.94501
C	81.11539	-15.22673	2.78426
C	81.53597	-15.00927	4.23058
N	80.53049	-14.21564	4.94289
C	80.58711	-13.93010	6.26743
N	80.09217	-12.77790	6.71708
N	81.12361	-14.79396	7.12364
O	81.92280	-19.29700	8.36500
H	73.85012	-10.69920	14.92416
H	74.33690	-11.80242	16.21033
H	76.62633	-10.69680	16.28974
H	76.12411	-9.56341	15.04656
H	78.10016	-12.19004	13.37367
H	78.44674	-11.20155	14.74995
H	79.03959	-18.30180	3.97109
H	78.35176	-16.96300	4.91677
H	80.09655	-17.28335	4.97019
H	79.73769	-19.44160	6.14133
H	77.97486	-19.25355	6.04605
H	76.53334	-19.44533	12.06662
H	77.37923	-18.85908	10.62668
H	75.69442	-17.14624	12.57569
H	75.22956	-17.61255	10.94365
H	76.20378	-14.34882	12.27465
H	77.85581	-17.03759	9.35104
H	78.82699	-14.70738	8.98879
H	83.65327	-19.89779	13.22683
H	82.67376	-18.41513	13.21989
H	84.33746	-18.36563	12.62026
H	85.20472	-18.86854	14.91951
H	83.55559	-18.87649	15.56265
H	86.29073	-17.48725	7.35999
H	85.49595	-16.53343	8.63148
H	87.22743	-16.30589	8.31158
H	87.67470	-18.65378	9.11256
H	87.16262	-18.26740	11.55535
H	87.76129	-16.78688	10.78233
H	86.03064	-16.99124	11.10649
H	85.82501	-19.97030	10.18878
H	84.67749	-18.69733	9.74614
H	85.45527	-19.65106	8.47698
H	88.62676	-10.16439	9.32855
H	87.28037	-11.26612	9.70440
H	87.65664	-9.93473	10.80084
H	89.85829	-11.02370	11.36864
H	89.49076	-12.35073	10.26134
H	88.34219	-10.63624	13.37722
H	87.90561	-14.11675	10.90740

H	86.78457	-11.63157	15.04038
H	86.36860	-15.11685	12.58871
H	85.26715	-14.82441	14.58772
H	80.96074	-16.98599	0.57586
H	81.40469	-15.37766	-0.01827
H	83.07428	-15.16499	1.88815
H	82.59696	-16.75259	2.46739
H	80.21257	-15.85657	2.76106
H	80.83076	-14.26043	2.33356
H	82.51213	-14.49947	4.27355
H	81.65948	-15.97442	4.73614
H	80.03857	-13.53406	4.37906
H	80.11474	-12.63337	7.75218
H	79.96477	-11.99553	6.09452
H	81.16975	-14.46138	8.09107
H	80.91895	-15.80161	7.02877
H	81.33904	-18.53410	8.20566
H	82.14126	-19.25857	9.30036
H	77.85660	-13.13606	10.63868
H	74.17761	-10.06544	16.55709
H	77.92290	-18.35734	12.23889
H	82.59582	-16.68871	-0.03651
Cl	83.43522	-11.23045	15.20457
C	78.28724	-11.98878	19.03550
C	79.09746	-11.66000	17.79130
C	80.40324	-12.42680	17.73963
C	81.41599	-12.18198	18.66728
C	82.60392	-12.91099	18.62527
C	82.79605	-13.88764	17.65109
C	81.79048	-14.13403	16.71993
C	80.60336	-13.40987	16.76839
N	79.32019	-10.20801	17.76407
C	79.88264	-9.62503	16.64720
C	80.19169	-8.23309	16.63200
N	80.74584	-7.67474	15.57781
C	81.08636	-8.47399	14.54639
C	80.84277	-9.83260	14.57228
N	80.18104	-10.38353	15.61212
C	81.32323	-10.79002	13.54482
C	80.59410	-11.05124	12.38787
C	81.00506	-12.02666	11.47496
C	82.17089	-12.75055	11.73411
C	82.91401	-12.51814	12.88646
C	82.48911	-11.53600	13.77602
C	80.15979	-12.31441	10.26716
O	80.67018	-13.01279	9.33715
O	78.98238	-11.86916	10.25165
N	79.84865	-7.44457	17.72555
H	78.50895	-11.95974	16.90526

H	77.31339	-11.47805	19.02754
H	78.10698	-13.06691	19.08676
H	78.83105	-11.69602	19.94258
H	81.28111	-11.40315	19.41931
H	83.38883	-12.70372	19.35081
H	83.71792	-14.45975	17.57072
H	81.97255	-14.89041	15.95869
H	79.83001	-13.58054	16.01745
H	78.63040	-9.64383	18.24852
H	81.59541	-8.00946	13.70375
H	79.67757	-10.49668	12.18890
H	82.48804	-13.51359	11.02835
H	83.80756	-13.09763	13.11583
H	80.24115	-6.51343	17.64417
H	80.06271	-7.87136	18.62086

Compound **7**

C	74.49100	-10.79701	15.80501
C	75.96201	-10.58499	15.41899
C	76.69235	-11.79035	14.85874
N	77.92434	-11.49764	14.35065
O	76.24496	-12.93161	14.86669
C	79.10960	-17.75690	4.92000
C	78.92050	-18.70710	6.12399
C	78.95744	-17.88710	7.41161
O	80.01618	-17.20762	7.64332
O	77.96023	-17.89870	8.16706
C	77.03903	-18.57797	11.63001
C	76.09396	-17.37403	11.57999
C	76.96330	-16.19430	11.30511
C	77.28954	-15.12581	12.09027
N	77.88362	-16.20546	10.26554
C	78.74613	-15.21481	10.44212
N	78.40556	-14.53183	11.53659
C	83.68521	-18.81104	13.37994
C	84.19684	-18.44806	14.78306
C	84.05076	-16.94034	14.94641
O	84.94872	-16.22253	14.43651
O	82.99393	-16.52542	15.50261
C	86.42501	-17.05309	8.35900
C	86.74096	-18.15091	9.41510
C	86.81969	-17.52087	10.79931
C	85.68481	-19.24500	9.37561
C	88.10399	-10.68801	10.14100
C	89.03501	-11.60998	10.93399
C	88.25513	-12.25181	12.05487
C	87.90863	-11.50852	13.18939
C	87.72947	-13.54071	11.94841
C	87.05584	-12.01424	14.16091

C	86.88093	-14.07376	12.91829
C	86.52053	-13.30172	14.03025
O	85.66712	-13.73014	14.97711
C	81.77300	-16.25000	0.53700
C	82.22301	-15.85900	1.94500
C	81.15325	-15.19807	2.80424
C	81.65724	-15.06401	4.22968
N	80.81057	-14.15729	5.02060
C	80.94484	-13.97885	6.34118
N	80.71321	-12.75544	6.85426
N	81.31585	-14.97959	7.12594
O	81.92277	-19.29699	8.36499
H	73.89286	-11.09164	14.93694
H	74.39704	-11.59216	16.55243
H	76.53136	-10.24205	16.29851
H	76.04822	-9.76519	14.69119
H	78.56607	-12.23029	14.05259
H	78.27861	-10.55283	14.38327
H	79.02313	-18.29428	3.96911
H	78.35854	-16.95638	4.92658
H	80.10511	-17.30062	4.96000
H	79.73742	-19.43943	6.15419
H	77.96700	-19.23930	6.06424
H	76.51140	-19.47422	11.97359
H	77.46499	-18.79624	10.64476
H	75.57982	-17.22778	12.53736
H	75.33105	-17.51086	10.80326
H	76.84813	-14.75436	13.00672
H	77.93729	-16.89422	9.44951
H	79.59908	-15.02667	9.80812
H	83.72441	-19.89059	13.19525
H	82.64232	-18.48707	13.25132
H	84.28891	-18.31258	12.61200
H	85.25153	-18.73050	14.87906
H	83.61076	-18.96326	15.55261
H	86.39335	-17.47085	7.34512
H	85.44217	-16.60895	8.57339
H	87.17411	-16.25147	8.38293
H	87.72088	-18.58908	9.16749
H	87.00705	-18.26554	11.58333
H	87.61279	-16.76456	10.86036
H	85.86753	-17.02428	11.04357
H	85.89795	-20.03384	10.10848
H	84.69372	-18.83167	9.60971
H	85.61046	-19.71135	8.38547
H	88.61944	-10.19727	9.30540
H	87.25963	-11.25950	9.73544
H	87.68985	-9.90621	10.78904
H	89.88053	-11.03188	11.33260

H	89.45670	-12.38034	10.27444
H	88.31029	-10.50048	13.30733
H	87.98285	-14.14930	11.07776
H	86.78786	-11.43093	15.03946
H	86.49207	-15.08794	12.83233
H	85.38331	-14.67469	14.81831
H	80.94449	-16.96733	0.57253
H	81.43244	-15.37549	-0.03131
H	83.09219	-15.18785	1.88276
H	82.58023	-16.76110	2.46555
H	80.22168	-15.78324	2.79183
H	80.91043	-14.20536	2.39035
H	82.68568	-14.67130	4.23240
H	81.68617	-16.04459	4.71597
H	80.35429	-13.41250	4.50734
H	80.55335	-12.63108	7.84289
H	80.73041	-11.92939	6.27525
H	81.59634	-14.75511	8.07097
H	80.91309	-15.94901	7.03110
H	81.32362	-18.55387	8.17719
H	81.61778	-19.67154	9.19579
H	79.01363	-13.88409	12.05884
H	74.07782	-9.87451	16.22188
H	77.86034	-18.39228	12.33374
H	82.59242	-16.71259	-0.02093
Cl	80.25608	-16.54312	18.39895
Cl	77.21668	-16.28995	19.38001
C	83.22001	-13.95351	12.75713
C	82.49666	-13.41928	13.98976
C	81.05432	-13.91372	14.00247
O	80.14958	-13.34241	13.36670
N	80.93278	-15.07021	14.66866
C	79.76500	-15.84025	14.82213
C	79.90300	-17.23190	14.78099
C	78.79297	-18.04426	14.95930
C	77.54970	-17.45736	15.18437
C	77.40999	-16.07432	15.27622
C	78.52210	-15.26408	15.09385
S	76.11576	-18.49407	15.37674
O	74.98608	-17.78917	14.78382
O	76.49006	-19.83812	14.96583
N	75.78387	-18.58019	17.00756
S	82.63286	-11.59365	13.92883
C	81.57955	-11.13392	15.24640
N	81.39257	-9.79896	15.42235
C	80.53029	-9.25450	16.39545
O	80.41395	-8.04925	16.49874
C	79.83619	-10.27567	17.16374
C	80.06520	-11.62111	16.90391

N	80.97153	-12.02833	15.97193
C	79.35492	-12.73316	17.56574
C	78.01363	-12.64552	17.95554
C	77.36958	-13.74528	18.50032
C	78.05503	-14.94296	18.67201
C	79.39014	-15.05052	18.27365
C	80.02896	-13.94979	17.71981
C	78.93514	-9.79900	18.15563
N	78.18118	-9.40170	18.94873
H	81.88712	-9.11593	14.85549
H	81.81358	-15.52594	15.02760
H	82.66433	-13.70868	11.84236
H	84.23316	-13.54015	12.68506
H	83.33398	-15.04154	12.84999
H	83.02171	-13.75139	14.89357
H	80.89618	-17.65474	14.63676
H	78.87698	-19.12700	14.90541
H	76.43806	-15.61312	15.45616
H	78.40568	-14.18663	15.17059
H	75.50513	-17.67802	17.38647
H	76.55292	-18.99233	17.53081
H	81.05959	-14.05040	17.38641
H	77.44603	-11.72977	17.81718
H	76.32359	-13.68493	18.78731

Compound **8**

C	81.31031	-14.19270	11.43797
C	81.25116	-15.51482	11.88505
C	81.27208	-16.54265	10.94846
C	81.57824	-16.29937	9.61599
C	81.67958	-14.98649	9.18684
C	81.42568	-13.93937	10.07209
O	81.18032	-12.73189	9.45994
C	81.35895	-11.50971	10.11611
C	80.17101	-11.09380	10.97988
O	79.21588	-11.82042	11.22656
O	80.25697	-9.88146	11.46233
C	81.65059	-10.38763	9.05667
O	81.76627	-9.25029	9.57522
O	81.73653	-10.71697	7.86537
Br	80.81081	-18.30647	11.45897
H	81.20597	-13.38691	12.15923
H	81.16859	-15.73289	12.94943
H	81.67394	-17.11491	8.90278
H	81.88836	-14.76211	8.14485
H	82.24466	-11.54398	10.77324
H	80.96094	-9.39603	10.88768
C	74.49099	-10.79701	15.80501
C	75.96201	-10.58499	15.41896

C	76.38194	-11.26447	14.12518
N	77.41532	-10.66859	13.48071
O	75.84994	-12.29094	13.71374
C	79.10965	-17.75673	4.92000
C	78.92048	-18.70723	6.12401
C	78.89685	-17.82571	7.39656
O	78.62182	-18.38052	8.49365
O	79.13668	-16.58854	7.26189
C	77.03892	-18.57793	11.62994
C	76.09407	-17.37408	11.58009
C	76.87488	-16.18872	11.13046
C	76.97637	-14.91482	11.61398
N	77.79187	-16.29146	10.09697
C	78.42470	-15.13545	9.96862
N	77.94554	-14.27895	10.86421
C	83.68498	-18.81101	13.37999
C	84.19702	-18.44809	14.78301
C	84.21967	-16.90723	14.83320
O	85.37403	-16.37748	14.78502
O	83.11719	-16.32345	14.83571
C	86.42500	-17.05310	8.35899
C	86.74100	-18.15090	9.41511
C	87.20358	-17.51987	10.72002
C	85.51086	-19.02077	9.64645
C	88.10400	-10.68800	10.14100
C	89.03500	-11.61000	10.93400
C	88.30646	-12.27630	12.07341
C	88.14310	-11.62148	13.29853
C	87.68490	-13.52107	11.92797
C	87.39633	-12.17589	14.32959
C	86.93595	-14.09790	12.95003
C	86.77321	-13.42526	14.17308
O	86.06186	-13.90914	15.18682
C	81.77301	-16.25000	0.53700
C	82.22298	-15.85904	1.94500
C	81.10908	-15.40604	2.88576
C	81.66416	-15.14637	4.28545
N	80.65001	-14.81020	5.27540
C	80.65804	-13.76429	6.11655
N	79.67908	-13.70896	7.03565
N	81.54623	-12.77943	6.06326
O	81.92280	-19.29700	8.36500
H	73.82105	-10.33015	15.07484
H	74.25845	-11.86590	15.83001
H	76.61208	-11.00020	16.20319
H	76.19680	-9.51305	15.36850
H	77.85713	-11.11496	12.67936
H	77.87762	-9.85811	13.86323
H	78.97622	-18.28279	3.96432

H	78.40088	-16.92527	4.95686
H	80.13365	-17.37054	4.92645
H	79.73692	-19.43386	6.20867
H	77.98051	-19.26795	6.07610
H	76.52455	-19.45918	12.02934
H	77.41845	-18.84225	10.63651
H	75.66288	-17.15894	12.56406
H	75.25713	-17.56898	10.89493
H	76.45472	-14.40363	12.41422
H	78.06733	-17.13488	9.51901
H	79.24249	-14.97339	9.28176
H	83.69523	-19.89263	13.18086
H	82.66250	-18.44988	13.27301
H	84.29925	-18.31777	12.61234
H	85.20325	-18.84546	14.96167
H	83.50804	-18.83697	15.54421
H	86.08348	-17.49470	7.41403
H	85.63012	-16.39383	8.73573
H	87.30672	-16.43205	8.15610
H	87.54949	-18.78485	9.01522
H	87.41981	-18.27540	11.48556
H	88.10464	-16.90930	10.58294
H	86.41863	-16.86898	11.13135
H	85.71278	-19.82176	10.36939
H	84.69261	-18.41085	10.06206
H	85.15538	-19.47854	8.71341
H	88.62229	-10.19056	9.31033
H	87.26178	-11.25730	9.72859
H	87.68229	-9.91381	10.79406
H	89.88459	-11.02753	11.32098
H	89.45798	-12.37153	10.26229
H	88.61328	-10.64619	13.44507
H	87.78852	-14.05729	10.98096
H	87.27632	-11.66111	15.28097
H	86.46357	-15.07234	12.83477
H	85.69925	-14.84338	15.00628
H	81.06128	-17.08414	0.56904
H	81.27752	-15.41232	0.03012
H	82.97918	-15.06137	1.87592
H	82.73939	-16.71583	2.40460
H	80.32679	-16.17801	2.94055
H	80.62232	-14.49553	2.50666
H	82.40825	-14.34187	4.22975
H	82.21143	-16.03624	4.63368
H	80.04467	-15.57411	5.59427
H	79.84981	-13.08767	7.82413
H	79.20964	-14.59689	7.23163
H	81.57891	-12.04139	6.80015
H	82.30002	-12.80803	5.39732

H	81.02256	-19.28622	8.72548
H	82.48767	-19.43003	9.13478
H	78.34462	-13.34388	11.02125
H	74.28702	-10.36478	16.78953
H	77.90001	-18.36748	12.27390
H	82.62521	-16.55795	-0.07735

Compound **9**

C	74.49146	-10.79681	15.80460
C	75.96154	-10.58508	15.41961
C	76.42890	-11.40372	14.22139
N	77.59204	-10.97520	13.67194
O	75.81162	-12.37728	13.80261
C	79.10958	-17.75671	4.92020
C	78.92070	-18.70767	6.12351
C	78.94689	-17.85035	7.41092
O	78.59108	-18.38411	8.49197
O	79.31000	-16.64105	7.29728
C	77.03888	-18.57828	11.62960
C	76.09411	-17.37374	11.58060
C	76.83633	-16.15733	11.16783
C	76.90347	-14.90316	11.70398
N	77.70439	-16.17232	10.08797
C	78.27472	-14.97664	9.98427
N	77.79959	-14.18757	10.93846
C	83.68545	-18.81054	13.37961
C	84.19655	-18.44868	14.78328
C	84.07996	-16.92976	14.97547
O	85.02801	-16.24814	14.47880
O	83.05181	-16.49380	15.53734
C	86.42501	-17.05323	8.35887
C	86.74108	-18.15075	9.41534
C	86.99831	-17.51205	10.77298
C	85.58783	-19.14024	9.50053
C	88.10400	-10.68809	10.14102
C	89.03510	-11.60991	10.93387
C	88.27867	-12.28084	12.05309
C	88.14994	-11.66406	13.30132
C	87.57180	-13.47214	11.85378
C	87.35208	-12.20202	14.30295
C	86.76784	-14.03043	12.84376
C	86.63928	-13.39295	14.08944
O	85.87322	-13.85562	15.07527
C	81.77300	-16.25040	0.53750
C	82.22299	-15.85860	1.94430
C	81.15175	-15.46468	2.95299
C	81.79315	-15.31785	4.33603
N	80.86371	-15.02850	5.41063
C	80.76619	-13.90970	6.14025

N	79.79067	-13.83590	7.03322
N	81.58409	-12.85511	5.95883
O	81.92254	-19.29673	8.36507
H	73.82552	-10.48861	14.99163
H	74.29605	-11.85507	16.00217
H	76.61150	-10.86167	16.26296
H	76.16020	-9.52182	15.22451
H	78.05799	-11.48585	12.92290
H	78.10691	-10.21153	14.08197
H	78.86253	-18.25718	3.97331
H	78.48666	-16.86327	5.01056
H	80.16149	-17.46494	4.84899
H	79.71757	-19.45867	6.17776
H	77.96587	-19.24398	6.09027
H	76.53168	-19.45711	12.04238
H	77.40450	-18.84501	10.63100
H	75.64429	-17.18321	12.56236
H	75.26526	-17.56933	10.88482
H	76.39392	-14.44773	12.54485
H	77.99751	-16.99433	9.50853
H	79.03986	-14.70073	9.27909
H	83.81529	-19.87785	13.15648
H	82.62032	-18.57465	13.26652
H	84.23724	-18.23456	12.62496
H	85.24823	-18.74776	14.88162
H	83.60251	-18.96270	15.55021
H	86.25815	-17.49058	7.36608
H	85.51382	-16.51169	8.65131
H	87.24219	-16.32406	8.28704
H	87.64790	-18.68707	9.09033
H	87.18132	-18.26227	11.55258
H	87.85913	-16.83210	10.75105
H	86.12159	-16.92894	11.09192
H	85.79188	-19.93982	10.22388
H	84.67950	-18.62305	9.84254
H	85.36457	-19.60291	8.53079
H	88.62380	-10.17736	9.31895
H	87.27086	-11.26189	9.71632
H	87.67068	-9.92535	10.80018
H	89.87478	-11.02769	11.34093
H	89.46939	-12.36375	10.26093
H	88.68651	-10.73128	13.48980
H	87.64630	-13.97812	10.88735
H	87.25768	-11.71698	15.27261
H	86.22623	-14.96189	12.68358
H	85.45127	-14.75062	14.85657
H	81.09764	-17.11451	0.56434
H	81.23902	-15.43019	0.04099
H	82.95186	-15.03570	1.86791

H	82.78990	-16.70368	2.36675
H	80.36344	-16.23006	2.99677
H	80.66027	-14.52278	2.66839
H	82.57059	-14.54337	4.28864
H	82.32199	-16.24862	4.58962
H	80.31316	-15.80510	5.80171
H	79.27819	-14.70377	7.20192
H	81.61983	-12.14412	6.69570
H	82.45510	-13.00582	5.47478
H	80.98226	-19.22527	8.58409
H	82.36494	-18.78601	9.05166
H	78.17698	-13.23746	11.11697
H	74.24231	-10.21704	16.69918
H	77.91733	-18.35947	12.25058
H	82.63411	-16.51569	-0.08434
H	79.77450	-13.10786	7.77113
C	81.38208	-15.52611	10.05066
C	80.91223	-16.60869	10.78695
C	80.97342	-16.57982	12.18252
C	81.58827	-15.50227	12.82883
C	82.04500	-14.42958	12.07037
C	81.91597	-14.39697	10.67959
C	82.31142	-13.18387	9.88023
C	81.58473	-11.88732	10.28703
C	80.03871	-12.07521	10.33969
O	79.47446	-12.31930	9.24417
O	79.47878	-12.00580	11.45610
C	81.85788	-10.79429	9.29980
O	81.78661	-9.57467	9.85558
O	82.08742	-10.92385	8.10904
H	81.28437	-15.55762	8.96211
H	80.42993	-17.45428	10.29328
H	81.75850	-15.50976	13.90481
H	82.51489	-13.59598	12.59237
H	81.90321	-11.54852	11.27887
O	80.41913	-17.63884	12.82774
C	80.24250	-17.53244	14.23447
H	79.73706	-18.45296	14.53919
H	81.19821	-17.42945	14.77141
H	79.60285	-16.66866	14.47306
H	83.39351	-12.99892	9.96459
H	82.11303	-13.37519	8.81706
H	81.91690	-8.93183	9.14082

Compound **10**

C	74.49149	-10.79681	15.80463
C	75.96151	-10.58509	15.41956
C	76.38677	-11.32648	14.15693
N	77.52389	-10.85878	13.58209

O	75.76477	-12.28392	13.71106
C	79.10936	-17.75643	4.92011
C	78.92095	-18.70794	6.12358
C	78.82304	-17.88177	7.41884
O	78.87574	-18.49143	8.52258
O	78.67746	-16.63536	7.30497
C	77.03887	-18.57826	11.62961
C	76.09413	-17.37372	11.58059
C	76.85986	-16.17423	11.14056
C	76.88551	-14.88501	11.59200
N	77.80983	-16.25109	10.13471
C	78.38494	-15.06216	9.98925
N	77.83634	-14.21585	10.85089
C	83.68541	-18.81049	13.37961
C	84.19649	-18.44873	14.78329
C	84.39560	-16.93733	14.91715
O	85.44893	-16.47946	14.36789
O	83.52859	-16.27849	15.52244
C	86.42500	-17.05320	8.35891
C	86.74109	-18.15069	9.41529
C	86.98884	-17.51646	10.77730
C	85.59132	-19.14584	9.49241
C	88.10399	-10.68810	10.14100
C	89.03511	-11.60989	10.93390
C	88.31522	-12.30782	12.05196
C	88.17593	-11.70675	13.30602
C	87.69464	-13.54556	11.85809
C	87.45405	-12.31216	14.32581
C	86.97039	-14.17243	12.86474
C	86.83676	-13.55708	14.12258
O	86.15440	-14.09902	15.12576
C	81.77297	-16.25040	0.53749
C	82.22306	-15.85863	1.94432
C	81.07421	-15.35051	2.81365
C	81.51267	-14.85928	4.19292
N	80.34335	-14.62444	5.03143
C	80.23485	-13.84330	6.12370
N	79.13124	-13.94881	6.86161
N	81.14932	-12.92487	6.44786
O	81.92246	-19.29670	8.36512
H	73.82242	-10.39105	15.03835
H	74.27414	-11.86510	15.89600
H	76.61521	-10.94358	16.22831
H	76.18351	-9.51510	15.30433
H	77.93981	-11.31811	12.77509
H	78.03812	-10.09186	13.98664
H	79.09954	-18.30285	3.96754
H	78.31398	-17.00408	4.89850
H	80.08485	-17.26534	5.01060

H	79.75151	-19.41750	6.21521
H	78.00137	-19.29934	6.03020
H	76.52932	-19.45885	12.03631
H	77.40501	-18.84582	10.63070
H	75.66229	-17.16661	12.56632
H	75.25609	-17.56768	10.89605
H	76.32230	-14.38564	12.37091
H	78.11516	-17.07867	9.58323
H	79.20267	-14.83972	9.31745
H	83.56645	-19.89466	13.24865
H	82.70828	-18.33548	13.20652
H	84.38319	-18.44197	12.61576
H	85.15906	-18.94740	14.96220
H	83.47618	-18.78338	15.53997
H	86.26128	-17.49009	7.36522
H	85.51292	-16.51281	8.65014
H	87.24071	-16.32214	8.28995
H	87.65141	-18.68270	9.09292
H	87.19364	-18.26658	11.55123
H	87.83418	-16.81717	10.75803
H	86.10188	-16.95631	11.11140
H	85.79458	-19.94519	10.21630
H	84.67868	-18.63211	9.83117
H	85.37323	-19.60787	8.52104
H	88.62750	-10.17596	9.32233
H	87.27215	-11.26197	9.71265
H	87.66689	-9.92652	10.79924
H	89.87231	-11.01970	11.33642
H	89.47836	-12.35168	10.25277
H	88.64800	-10.73794	13.48558
H	87.78310	-14.03605	10.88469
H	87.35114	-11.84394	15.30286
H	86.50107	-15.14308	12.71233
H	85.79293	-15.01484	14.86569
H	81.01350	-17.04144	0.57490
H	81.33303	-15.39385	0.01167
H	83.00151	-15.08271	1.87703
H	82.69640	-16.71915	2.43896
H	80.34038	-16.16209	2.94165
H	80.54074	-14.53617	2.30063
H	82.07500	-13.92222	4.08215
H	82.18671	-15.59312	4.66513
H	79.62344	-15.33934	4.98189
H	78.70655	-14.88404	6.92185
H	81.05153	-12.47296	7.36867
H	82.00974	-12.83198	5.93422
H	80.97093	-19.17789	8.52416
H	82.36488	-18.75354	9.02548
H	78.17890	-13.23583	10.95471

H	74.26950	-10.30527	16.75719
H	77.90514	-18.35502	12.26323
H	82.61107	-16.61917	-0.06258
H	79.10706	-13.36078	7.70330
C	81.57461	-11.73640	10.61842
H	81.53639	-11.48942	11.68391
C	82.07467	-10.49702	9.93139
C	80.12139	-12.01350	10.16598
O	82.08521	-9.38580	10.40879
O	79.22400	-11.89909	11.03292
O	82.50858	-10.71478	8.66300
O	79.96649	-12.37544	8.96880
C	82.47689	-12.96101	10.36699
H	82.66936	-13.04354	9.29058
H	83.44807	-12.76937	10.84711
C	81.90438	-14.26364	10.86050
C	81.55914	-14.43561	12.21041
C	81.70558	-15.32239	9.98401
C	81.01695	-15.63103	12.67651
H	81.73454	-13.62508	12.91411
C	81.17504	-16.53642	10.43661
H	81.95440	-15.21258	8.92757
C	80.83308	-16.70392	11.76992
H	80.95806	-17.32264	9.71836
O	80.62902	-15.86416	13.93862
O	80.30483	-17.84005	12.29313
C	80.93487	-14.88690	14.92121
H	80.41354	-13.94219	14.70258
H	80.57246	-15.29666	15.86551
H	82.02094	-14.75276	15.00522
C	80.47455	-19.03471	11.55918
H	81.53816	-19.20435	11.33137
H	80.12355	-19.84190	12.20776
H	79.88783	-19.03616	10.62992
H	82.78517	-9.84440	8.33633

Compound **11**

C	74.49106	-10.79710	15.80488
C	74.62831	-10.73085	14.29408
C	75.37773	-11.89997	13.68615
N	75.65325	-11.76490	12.35230
O	75.73433	-12.88201	14.32329
C	79.10980	-17.75682	4.91974
C	78.92038	-18.70704	6.12457
C	78.91094	-17.82759	7.35575
O	79.84725	-17.07599	7.61861
O	77.80393	-17.88684	8.05688
C	77.03899	-18.57801	11.63007
C	76.09400	-17.37399	11.57990

C	76.87950	-16.14680	11.25704
C	77.08614	-15.01176	11.99497
N	77.61985	-16.07992	10.09232
C	78.25586	-14.93047	10.12046
N	77.96185	-14.24250	11.24954
C	83.68497	-18.81096	13.37998
C	84.19704	-18.44811	14.78302
C	84.38632	-16.94757	15.04023
O	84.96411	-16.29579	14.10699
O	84.01248	-16.49900	16.13553
C	86.42516	-17.05310	8.35903
C	86.74042	-18.15094	9.41507
C	87.16654	-17.51635	10.73097
C	85.52648	-19.04704	9.61843
C	88.10398	-10.68800	10.14099
C	89.03503	-11.60999	10.93400
C	88.28916	-12.31725	12.03101
C	88.14122	-11.73457	13.29288
C	87.61954	-13.52293	11.79744
C	87.35630	-12.31987	14.27714
C	86.82925	-14.12771	12.76764
C	86.67516	-13.52382	14.02908
O	85.91958	-14.03289	14.99325
O	81.92317	-19.29701	8.36476
H	73.93545	-11.69232	16.10427
H	75.47144	-10.84702	16.28939
H	75.13168	-9.80474	13.98170
H	73.63629	-10.70722	13.81429
H	75.91434	-12.61681	11.86675
H	75.11280	-11.11784	11.78848
H	79.03254	-18.30343	3.97305
H	78.35369	-16.96314	4.92255
H	80.10182	-17.29310	4.96154
H	79.75975	-19.40856	6.20109
H	77.98497	-19.26869	6.05511
H	76.50162	-19.49993	11.88071
H	77.53002	-18.72676	10.66339
H	75.57640	-17.23607	12.53817
H	75.32259	-17.53804	10.81149
H	76.71170	-14.67978	12.95886
H	77.79394	-17.18828	8.79511
H	78.92596	-14.56514	9.35151
H	83.63233	-19.89842	13.23440
H	82.68337	-18.39525	13.20918
H	84.35272	-18.38286	12.62228
H	85.18084	-18.91841	14.93563
H	83.52894	-18.84590	15.55703
H	86.11516	-17.49480	7.40324
H	85.60802	-16.41391	8.72192

H	87.29796	-16.41221	8.18116
H	87.56975	-18.76523	9.02659
H	87.38956	-18.27199	11.49462
H	88.05533	-16.88398	10.61203
H	86.36101	-16.88792	11.13743
H	85.73184	-19.84612	10.34224
H	84.69218	-18.45356	10.02221
H	85.19453	-19.50846	8.67911
H	88.62901	-10.16278	9.33121
H	87.28127	-11.26526	9.70072
H	87.65512	-9.93738	10.80379
H	89.86160	-11.01979	11.35746
H	89.49144	-12.34266	10.25147
H	88.65214	-10.79237	13.50542
H	87.71568	-14.00250	10.81911
H	87.24335	-11.86327	15.25856
H	86.31321	-15.06835	12.58264
H	85.47819	-14.90433	14.70448
H	81.47154	-18.44367	8.29132
H	82.43681	-19.24761	9.17680
H	78.37292	-13.36537	11.53862
H	73.95944	-9.91710	16.18155
H	77.82057	-18.42277	12.38225
C	72.68388	-12.89530	11.52933
C	71.70687	-11.89391	11.50057
C	70.87496	-11.68850	12.59610
C	71.02439	-12.46358	13.74568
C	72.01000	-13.44670	13.79163
C	72.82920	-13.66605	12.68865
C	73.59709	-13.08852	10.38213
N	74.00629	-11.97700	9.74332
C	74.91468	-12.11024	8.77550
C	75.46790	-13.33167	8.38509
C	74.99732	-14.48103	9.01426
C	74.05076	-14.36114	10.02252
C	76.57074	-13.40071	7.36047
O	76.96005	-12.30505	6.87223
O	77.03333	-14.54112	7.09740
H	71.61443	-11.28060	10.60716
H	70.11037	-10.91554	12.55566
H	70.38296	-12.29263	14.60746
H	72.16049	-14.03217	14.69593
H	73.63142	-14.40141	12.75180
H	75.25240	-11.19950	8.28226
H	75.40305	-15.44493	8.71203
H	73.66847	-15.24072	10.53660
C	81.78766	-16.54636	0.42440
C	82.16473	-16.06857	1.82558
C	81.18265	-15.08832	2.45202

C	81.62381	-14.67528	3.85382
N	80.89509	-13.52492	4.37023
C	79.76865	-13.54778	5.12774
N	78.94979	-12.49922	5.08635
N	79.47393	-14.56616	5.91756
H	81.71263	-15.70324	-0.27423
H	83.16064	-15.60063	1.79637
H	82.26654	-16.94081	2.49046
H	80.17207	-15.52438	2.50337
H	81.10357	-14.18906	1.81970
H	82.69184	-14.41957	3.85471
H	81.51848	-15.51203	4.55469
H	81.07858	-12.64551	3.90672
H	78.15163	-12.40792	5.77790
H	79.03598	-11.83133	4.33719
H	78.53122	-14.58412	6.38565
H	80.15256	-15.26500	6.19593
H	80.81743	-17.05850	0.42960
H	82.53254	-17.24445	0.02932

Compound **12**

C	83.71003	-10.32843	12.12307
C	82.32075	-10.23937	12.26492
C	81.71117	-10.99761	13.26799
C	81.53109	-9.32110	11.33842
C	84.46756	-11.15577	12.94470
C	82.46800	-11.82895	14.09297
C	83.84673	-11.91366	13.93761
N	81.99698	-9.38219	9.95346
C	81.71826	-10.47803	9.17571
C	80.63574	-11.33239	9.58797
C	79.77603	-10.97511	10.64995
C	80.04332	-9.62230	11.28891
O	78.80807	-11.64933	11.07931
O	82.41248	-10.64856	8.13804
S	80.37520	-12.82407	8.69298
C	81.47397	-14.00241	9.49205
C	82.11568	-13.74871	10.70895
C	82.92481	-14.71161	11.30535
C	83.11113	-15.94943	10.69512
C	82.48978	-16.22911	9.48027
C	81.68686	-15.25292	8.90250
Cl	80.90315	-15.63456	7.35467
H	81.97293	-12.43444	14.84873
H	83.72952	-16.70007	11.18657
H	82.59727	-17.19776	8.98812
H	83.40126	-14.51290	12.26553
H	81.97234	-12.78643	11.19767
H	79.54683	-8.84986	10.68401

H	79.58973	-9.60127	12.28394
H	84.21744	-9.76109	11.34288
H	80.63143	-10.98165	13.40244
H	85.54663	-11.22347	12.80689
H	82.87777	-8.94580	9.71251
H	84.42829	-12.57981	14.57308
H	81.66999	-8.28012	11.66625
C	74.49098	-10.79700	15.80501
C	75.96212	-10.58501	15.41889
C	76.36836	-11.31930	14.15222
N	77.26804	-10.66480	13.37677
O	75.93464	-12.43160	13.87646
C	79.10960	-17.75691	4.92001
C	78.92050	-18.70709	6.12399
C	78.57216	-18.06854	7.46365
O	79.25898	-18.36826	8.46675
O	77.55200	-17.31086	7.47703
C	77.03899	-18.57800	11.62999
C	76.09411	-17.37400	11.58001
C	76.77907	-16.16136	11.04771
C	77.07925	-14.95931	11.63090
N	77.31341	-16.12160	9.77503
C	77.91581	-14.95647	9.59987
N	77.79297	-14.22512	10.70556
C	83.68500	-18.81103	13.37993
C	84.19701	-18.44797	14.78306
C	84.31016	-16.94572	15.05758
O	84.66899	-16.21755	14.06704
O	84.09991	-16.55149	16.21432
C	86.42492	-17.05311	8.35911
C	86.74107	-18.15099	9.41499
C	87.14831	-17.51441	10.73668
C	85.52864	-19.05471	9.60331
C	88.10401	-10.68799	10.14100
C	88.85958	-11.87901	10.72570
C	88.13083	-12.53907	11.85895
C	88.24824	-12.05346	13.16479
C	87.28220	-13.62963	11.64674
C	87.54511	-12.62472	14.21730
C	86.57266	-14.21935	12.68548
C	86.69210	-13.71619	13.99206
O	86.00901	-14.20628	15.02426
C	81.77309	-16.25000	0.53687
C	82.22291	-15.85900	1.94513
C	81.48111	-14.66828	2.53306
C	81.93996	-14.37849	3.95392
N	81.33704	-13.14091	4.43986
C	81.77993	-12.42358	5.48477
N	81.31961	-11.19390	5.69828

N	82.73863	-12.90161	6.28396
O	81.92281	-19.29700	8.36501
H	73.82080	-10.35874	15.05708
H	74.27053	-11.86716	15.86147
H	76.61113	-10.97188	16.21761
H	76.18655	-9.51318	15.33108
H	77.70276	-11.11138	12.56174
H	77.61767	-9.76414	13.66433
H	79.26780	-18.32720	3.99685
H	78.22826	-17.11675	4.79619
H	79.98489	-17.10791	5.07065
H	79.82160	-19.31968	6.25445
H	78.09436	-19.39531	5.89249
H	76.51198	-19.47497	11.97332
H	77.47047	-18.78594	10.64246
H	75.70735	-17.13892	12.57917
H	75.22330	-17.60834	10.95112
H	76.83024	-14.55384	12.60352
H	77.33010	-16.81525	8.94870
H	78.43262	-14.65936	8.69775
H	83.61164	-19.89818	13.24372
H	82.69481	-18.37418	13.19649
H	84.36474	-18.40960	12.61786
H	85.20347	-18.86988	14.92607
H	83.56082	-18.88688	15.56155
H	86.12006	-17.49713	7.40295
H	85.59960	-16.42070	8.71812
H	87.29509	-16.40721	8.18431
H	87.58013	-18.75729	9.03498
H	87.39359	-18.27023	11.49380
H	88.01588	-16.85091	10.62548
H	86.32531	-16.91076	11.14876
H	85.73254	-19.85897	10.32242
H	84.68049	-18.47374	9.99708
H	85.19606	-19.50702	8.66007
H	88.64839	-10.22205	9.30934
H	87.11755	-11.00197	9.77401
H	87.93537	-9.92266	10.91088
H	89.85084	-11.54344	11.06720
H	89.04364	-12.61553	9.92947
H	88.90954	-11.20596	13.35870
H	87.17203	-14.03568	10.63751
H	87.63454	-12.24457	15.23325
H	85.91784	-15.07250	12.51669
H	85.41876	-14.98259	14.72922
H	80.71082	-16.52396	0.52474
H	81.91172	-15.42142	-0.16945
H	83.30028	-15.63614	1.93656
H	82.10067	-16.72110	2.61784

H	80.39695	-14.86691	2.53141
H	81.64725	-13.77776	1.90628
H	83.03169	-14.25457	3.98164
H	81.68620	-15.22125	4.61556
H	80.47391	-12.84107	4.00718
H	81.55994	-10.75826	6.60598
H	80.68967	-10.75455	5.04785
H	82.90179	-12.33207	7.12284
H	82.74024	-13.90494	6.44375
H	80.98270	-19.00267	8.39324
H	82.07995	-19.71534	9.21622
H	78.20719	-13.27984	10.82398
H	74.27466	-10.33775	16.77487
H	77.87376	-18.38621	12.31310
H	82.34332	-17.10707	0.16524

Malonate

C	75.68460	-7.43309	12.10940
N	75.94930	-8.06200	10.79938
C	75.72891	-9.38393	10.64809
C	75.95080	-10.00810	9.43617
C	75.70024	-11.48077	9.19977
O	75.65707	-11.89278	8.05272
N	75.52838	-12.24985	10.29599
C	76.40324	-9.23915	8.36596
C	76.65240	-7.88169	8.54750
C	76.41886	-7.31233	9.77999
H	75.41810	-13.24440	10.13990
H	75.64192	-11.93148	11.25729
H	76.63960	-7.23868	12.60646
H	75.14278	-6.49715	11.95878
H	75.08585	-8.11643	12.71381
H	76.56408	-9.73521	7.41234
H	77.02232	-7.26088	7.73855
H	76.58487	-6.26046	9.99203
H	75.39696	-9.90806	11.54162
C	79.47070	-11.62905	9.10217
O	79.70256	-12.65033	8.43291
O	78.99690	-10.55281	8.43150
C	74.49067	-10.79611	15.80459
C	75.96234	-10.58599	15.41952
C	76.34754	-11.10042	14.05631
N	77.60540	-11.56059	13.92952
O	75.56667	-11.05512	13.09525
C	79.10939	-17.75691	4.92001
C	78.92072	-18.70709	6.12399
C	78.88291	-17.86229	7.36587
O	79.80847	-17.10697	7.66496
O	77.76563	-17.95785	8.03737

C	77.03899	-18.57786	11.63003
C	76.09400	-17.37415	11.57996
C	76.84580	-16.15856	11.14682
C	77.13954	-15.00379	11.82714
N	77.48846	-16.13112	9.92582
C	78.15109	-14.99456	9.87043
N	77.97325	-14.27759	10.99840
C	83.68550	-18.81120	13.37980
C	84.19640	-18.44770	14.78320
C	84.22582	-16.91691	14.91419
O	85.30226	-16.36662	14.51198
O	83.20203	-16.35203	15.33853
C	86.42510	-17.05310	8.35890
C	86.74100	-18.15080	9.41520
C	87.18084	-17.51430	10.72600
C	85.52582	-19.04085	9.62926
C	88.10510	-10.68890	10.14340
C	89.03410	-11.60910	10.93160
C	88.29753	-12.28670	12.05656
C	88.08342	-11.62785	13.27148
C	87.71253	-13.54691	11.90064
C	87.31517	-12.19191	14.28087
C	86.94458	-14.13480	12.90083
C	86.72190	-13.45456	14.11145
O	85.98068	-13.94395	15.09905
O	81.92270	-19.29710	8.36500
H	73.82539	-10.35075	15.05839
H	74.25134	-11.86157	15.87210
H	76.62364	-11.01778	16.18158
H	76.19333	-9.50906	15.40377
H	78.01744	-11.65832	13.00745
H	78.25508	-11.55011	14.70350
H	79.07719	-18.30815	3.97438
H	78.32924	-16.98604	4.89364
H	80.08383	-17.26184	4.98659
H	79.77130	-19.39607	6.19892
H	77.99922	-19.28821	6.03625
H	76.51457	-19.48136	11.95953
H	77.46651	-18.78063	10.64275
H	75.64272	-17.19328	12.56341
H	75.27155	-17.57244	10.87837
H	76.86967	-14.66855	12.81979
H	77.70628	-17.26872	8.79626
H	78.77213	-14.63871	9.05795
H	83.63748	-19.89710	13.22114
H	82.68117	-18.39478	13.22641
H	84.35154	-18.38330	12.61877
H	85.20541	-18.85371	14.92938
H	83.52441	-18.86294	15.54477

H	86.11850	-17.49544	7.40232
H	85.60543	-16.41612	8.72066
H	87.29654	-16.41009	8.18286
H	87.56530	-18.76902	9.02340
H	87.38017	-18.26623	11.49951
H	88.08851	-16.91080	10.60228
H	86.39342	-16.85502	11.12009
H	85.73604	-19.84222	10.34911
H	84.69794	-18.44392	10.03981
H	85.18230	-19.49795	8.69228
H	88.62296	-10.18354	9.31673
H	87.26623	-11.26028	9.72584
H	87.67869	-9.91996	10.80019
H	89.87821	-11.02519	11.32831
H	89.46594	-12.36308	10.25732
H	88.53091	-10.64324	13.42740
H	87.86234	-14.08688	10.96194
H	87.15592	-11.67632	15.22612
H	86.50520	-15.12375	12.77764
H	85.62298	-14.87646	14.88513
H	81.45135	-18.45415	8.41264
H	82.30284	-19.43211	9.23821
H	78.39518	-13.36579	11.15788
H	74.28717	-10.33680	16.77557
H	77.86737	-18.39295	12.32302
C	81.41799	-16.76101	-0.10102
C	81.99401	-16.37198	1.26602
C	80.94687	-15.67789	2.13755
C	81.43371	-15.26152	3.52077
N	80.41773	-14.39648	4.13984
C	80.35928	-13.97287	5.42014
N	79.80055	-12.79569	5.69245
N	80.84283	-14.70515	6.42504
H	80.57200	-17.44961	0.01155
H	81.06011	-15.87685	-0.64294
H	82.38887	-14.71905	3.45341
H	81.60526	-16.14011	4.15301
H	80.06464	-16.32665	2.25398
H	80.59802	-14.77844	1.60130
H	82.85917	-15.70658	1.13458
H	82.36899	-17.26714	1.78252
H	79.90642	-13.81841	3.48433
H	79.62881	-12.54353	6.68501
H	79.67245	-12.10702	4.96833
H	80.76614	-14.29883	7.35611
H	80.79634	-15.72392	6.41144
H	82.16984	-17.25389	-0.72462
C	79.66978	-11.50553	10.50934
C	79.46918	-10.27993	11.17084

O	79.90641	-10.25783	12.45850
H	79.82063	-9.34166	12.75829
O	78.92364	-9.24467	10.71541
H	80.29367	-12.25723	10.98676
H	78.94668	-9.80797	9.08114

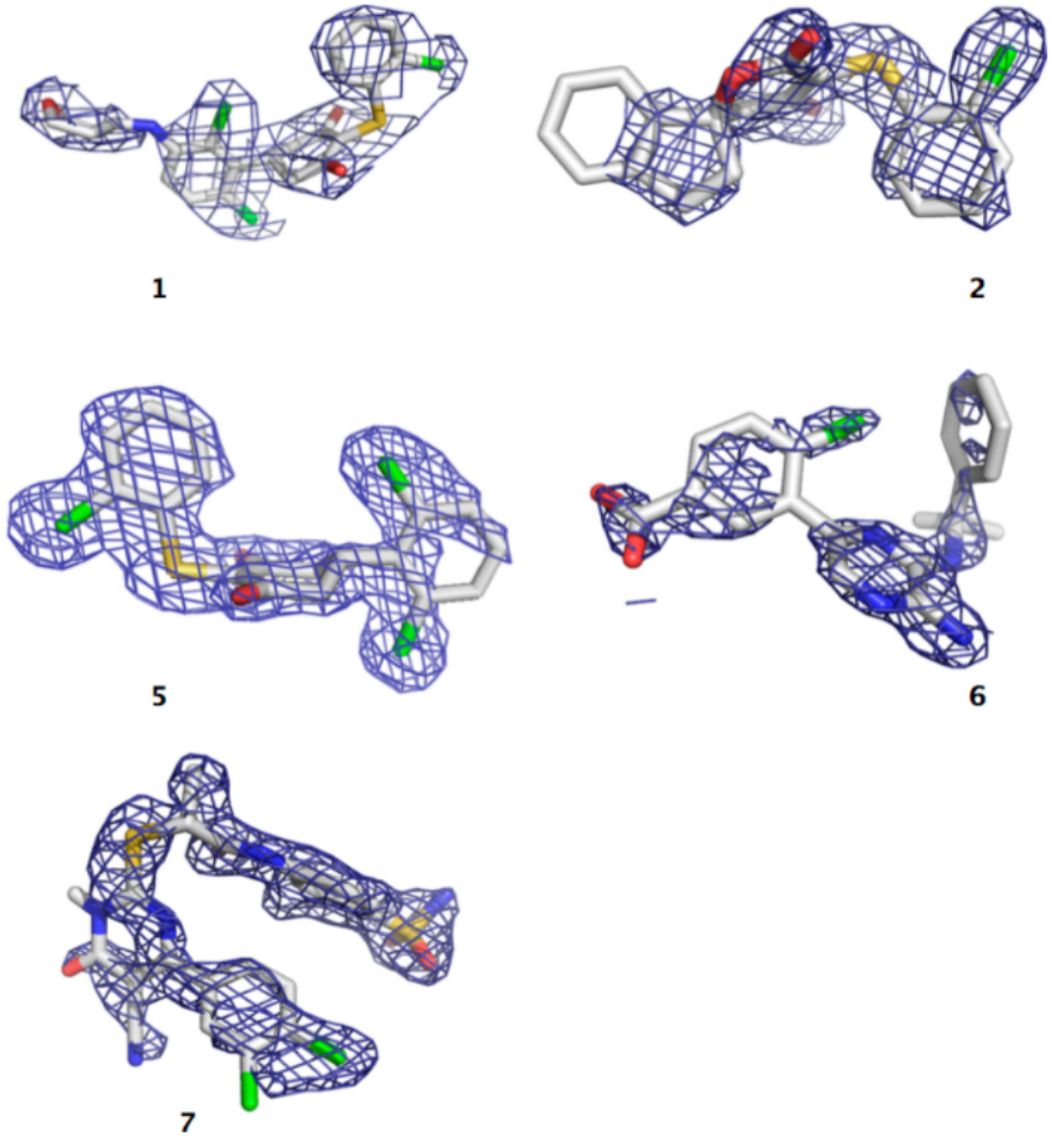
Oxamate

C	74.49074	-10.79610	15.80454
C	75.96232	-10.58599	15.41961
C	76.29531	-10.93435	13.98623
N	77.60616	-11.08566	13.71077
O	75.42619	-11.01198	13.10808
C	79.10940	-17.75695	4.91994
C	78.92065	-18.70693	6.12416
C	78.82598	-17.87240	7.36749
O	79.73860	-17.11323	7.70343
O	77.68720	-17.98296	7.99047
C	77.03909	-18.57786	11.63009
C	76.09386	-17.37418	11.57986
C	76.82159	-16.17489	11.06869
C	77.15912	-14.99980	11.69107
N	77.38115	-16.17887	9.80898
C	78.03298	-15.03981	9.67637
N	77.93060	-14.29340	10.78900
C	83.68548	-18.81119	13.37979
C	84.19639	-18.44771	14.78320
C	84.26875	-16.92137	14.91463
O	85.30738	-16.38455	14.40682
O	83.31342	-16.33361	15.45230
C	86.42506	-17.05310	8.35889
C	86.74101	-18.15083	9.41519
C	87.18592	-17.51903	10.72664
C	85.52439	-19.03875	9.63100
C	88.10510	-10.68890	10.14340
C	89.03409	-11.60910	10.93160
C	88.29107	-12.29450	12.04584
C	88.06904	-11.64404	13.26485
C	87.70593	-13.55319	11.87261
C	87.29247	-12.21456	14.26278
C	86.92958	-14.14769	12.85996
C	86.69943	-13.47641	14.07614
O	85.95114	-13.97490	15.05035
O	81.92279	-19.29711	8.36501
H	73.82968	-10.20447	15.16403
H	74.20273	-11.84597	15.69465
H	76.62238	-11.15322	16.08935
H	76.24270	-9.53022	15.55793
H	77.93817	-11.28484	12.76312
H	78.28733	-11.12061	14.45606

H	79.08399	-18.31206	3.97626
H	78.32595	-16.98978	4.88785
H	80.08171	-17.25784	4.98616
H	79.78674	-19.37435	6.21449
H	78.01780	-19.31313	6.01253
H	76.53089	-19.46799	12.01659
H	77.41949	-18.81565	10.63095
H	75.69006	-17.15730	12.57696
H	75.23824	-17.59594	10.92707
H	76.95292	-14.63650	12.68882
H	77.58133	-17.28153	8.75958
H	78.58621	-14.70964	8.80677
H	83.61209	-19.89722	13.23558
H	82.69173	-18.37484	13.21358
H	84.36582	-18.40872	12.61854
H	85.19650	-18.87364	14.93520
H	83.51600	-18.84407	15.54665
H	86.11082	-17.49571	7.40514
H	85.61034	-16.41137	8.72343
H	87.29906	-16.41525	8.17645
H	87.56319	-18.77051	9.02131
H	87.40082	-18.27610	11.49108
H	88.08715	-16.90645	10.59912
H	86.39608	-16.87233	11.13692
H	85.73341	-19.83874	10.35283
H	84.69676	-18.43967	10.03873
H	85.18017	-19.49819	8.69555
H	88.62564	-10.17770	9.32245
H	87.27146	-11.26170	9.71762
H	87.67261	-9.92465	10.80172
H	89.87240	-11.02395	11.33796
H	89.47306	-12.35738	10.25607
H	88.51793	-10.66216	13.43152
H	87.86221	-14.08407	10.93013
H	87.12731	-11.70870	15.21204
H	86.48816	-15.13380	12.72516
H	85.60663	-14.91228	14.82178
H	81.41120	-18.47752	8.40887
H	82.29040	-19.42075	9.24512
H	78.33665	-13.35966	10.89247
H	74.32796	-10.50075	16.84460
H	77.89942	-18.36820	12.27542
C	81.41801	-16.76108	-0.10086
C	81.99403	-16.37194	1.26577
C	80.94632	-15.68430	2.14411
C	81.43533	-15.26923	3.52843
N	80.41732	-14.41728	4.16091
C	80.34386	-14.01981	5.45023
N	79.77473	-12.85301	5.73947

N	80.81542	-14.76778	6.44992
H	80.57647	-17.45524	0.01105
H	81.05351	-15.87780	-0.63991
H	82.38572	-14.71853	3.45700
H	81.62018	-16.14966	4.15445
H	80.06767	-16.33750	2.26161
H	80.59047	-14.78516	1.61209
H	82.85583	-15.70223	1.13364
H	82.37487	-17.26657	1.77904
H	79.90435	-13.82795	3.51659
H	79.62416	-12.60396	6.73294
H	79.71449	-12.11964	5.05014
H	80.73230	-14.36305	7.38084
H	80.75169	-15.78614	6.44210
H	82.17177	-17.24768	-0.72729
C	75.76811	-7.52525	12.13543
N	76.21426	-8.12348	10.85238
C	75.97592	-9.43707	10.64194
C	76.40979	-10.06658	9.49304
C	76.18581	-11.53803	9.23894
O	76.48749	-12.00096	8.15025
N	75.62514	-12.25155	10.24097
C	77.08326	-9.31205	8.52916
C	77.32583	-7.95787	8.76690
C	76.88893	-7.38042	9.93743
H	75.59057	-13.25355	10.09068
H	75.59439	-11.93928	11.21043
H	77.86778	-7.35509	8.04578
H	77.04825	-6.33630	10.18942
H	75.45317	-9.95090	11.44639
H	77.42471	-9.80710	7.62407
H	76.63513	-7.37831	12.78584
H	75.28139	-6.56717	11.93972
H	75.06407	-8.20994	12.61155
C	79.51165	-10.96434	10.23033
N	80.16495	-9.82538	10.52287
O	78.80741	-11.55859	11.05537
C	79.66464	-11.42121	8.75610
O	79.68870	-12.65576	8.56261
O	79.73449	-10.49008	7.92737
H	80.71709	-9.38795	9.79679
H	80.27720	-9.54302	11.48641

S5. Density maps (2mFo-DFc) of ligands 1, 2, 5, 6 and 7 contoured at 1 σ.



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