Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Full Theoretical Protocol for the Design of Metal-Free Organic Electron Donor-Spacer-Acceptor Systems

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S1 – Input geometries of the 140 compounds on Table 1 (in the paper)

S2 – Input geometries of the 34 compounds on Table 2 (in the paper)

S3 – Input geometries of the 10 compounds on Figure 5 (in the paper)

S4 – Input geometries of the compounds 10 to 12 on Figure 7 (in the paper)

S5 – Input geometries of the compounds 18 to 20 on Figure 8 (in the paper)

S6 – Input geometries of the 12 systems on Table 4 (in the paper)

S7 – Input geometries of the compounds on Figure 11 (in the paper)

S1 – Input geometries of the 140 compounds on Table 1 (in the paper)

Tetramethylphenilenodiamine

C	-6.3336	3.9638	-0.2111
C	-6.3988	2.5698	-0.1078
C	-5.2598	1.7612	0.0951
C	-3.9684	2.2897	0.1907
C	-3.9027	3.6850	0.1324
C	-5.0441	4.4927	-0.0652
H	-7.3383	2.0377	-0.2055
H	-5.4323	0.6918	0.1571
N	-2.8363	1.4859	0.3697
H	-2.9538	4.2039	0.2283
H	-4.8654	5.5614	-0.1092
C	-1.5190	2.0640	0.1064
C	-2.9497	0.0492	0.1212
H	-3.6576	-0.4182	0.8140
H	-1.9921	-0.4585	0.2842
H	-3.2570	-0.1510	-0.9115
H	-1.3020	2.8885	0.7936
H	-1.4411	2.4155	-0.9285
H	-0.7239	1.3262	0.2644
N	-7.4436	4.7517	-0.5134
C	-7.3503	6.2118	-0.4727
C	-8.8045	4.2500	-0.3169
H	-6.4440	6.5996	-0.9460
H	-7.4096	6.5738	0.5597
H	-8.1818	6.6573	-1.0319
H	-8.9310	3.1845	-0.5161
H	-9.4853	4.7557	-1.0121
H	-9.1463	4.4614	0.7022

p-fluoroacetophenone

C	-6.9869	2.4414	0.0167
C	-7.0370	1.0400	0.0025
C	-5.7521	3.0968	0.0463
C	-5.8392	0.3072	0.0179
C	-4.6081	0.9659	0.0475
C	-4.5763	2.3545	0.0615
H	-7.8894	3.0454	0.0053
H	-5.6991	4.1814	0.0577
H	-5.8610	-0.7816	0.0070
H	-3.6792	0.4042	0.0596
C	-8.3282	0.2891	-0.0287
O	-8.3203	-0.9400	-0.0444
C	-9.6220	1.0602	-0.0406
F	-3.3973	2.9884	0.0899
H	-10.4597	0.3559	-0.0584
H	-9.6839	1.6826	-0.9370
H	-9.7099	1.6671	0.8642

4-cyanobenzaldehyde

C	-7.0821	2.4425	0.0090
C	-7.1233	1.0454	-0.0042
C	-5.8468	3.0973	0.0422
C	-5.9387	0.3024	0.0095
C	-4.7058	0.9596	0.0426
C	-4.6566	2.3584	0.0621
H	-7.9972	3.0299	-0.0034
H	-5.8183	4.1861	0.0553
H	-5.9731	-0.7859	-0.0027
H	-3.7887	0.3726	0.0559
C	-8.4301	0.3576	-0.0272
O	-8.5199	-0.8634	-0.0352
H	-9.3267	0.9998	-0.0346
C	-3.3921	3.0338	0.1081
N	-2.3720	3.5850	0.1487

Fumaronitrile

C	-13.8765	2.3078	0.0035
C	-12.5473	2.4770	0.0035
C	-11.6574	1.3715	0.0024

C	-14.7664	3.4133	0.0045
N	-15.4839	4.3233	0.0053
N	-10.9398	0.4615	0.0016
H	-14.3213	1.3175	0.0027
H	-12.1025	3.4673	0.0042

Tetracyanoethylene

C	-13.8815	2.3076	0.0035
C	-12.5429	2.4767	0.0035
C	-11.9580	3.7748	0.0045
C	-11.6529	1.3655	0.0024
C	-14.7709	3.4193	0.0045
C	-14.4670	1.0099	0.0024
N	-15.4850	4.3317	0.0053
N	-11.4933	4.8362	0.0053
N	-10.9375	0.4541	0.0016
N	-14.9332	-0.0509	0.0016

Tetracyanobenzene

C	-6.5510	2.2503	0.0000
C	-6.6127	0.8504	-0.0002
C	-5.2999	2.8895	-0.0001
C	-4.1100	2.1428	-0.0003
C	-4.1716	0.7428	-0.0004
C	-5.4227	0.1037	-0.0004
H	-5.4708	-0.9879	-0.0005
H	-5.2518	3.9810	0.0000
C	-2.8560	2.8424	-0.0003
C	-2.9841	-0.0645	-0.0007
C	-7.7386	3.0576	0.0001
C	-7.8666	0.1506	-0.0001
N	-8.6824	3.7300	0.0002
N	-8.8659	-0.4363	0.0000
N	-1.8566	3.4291	-0.0003
N	-2.0403	-0.7370	-0.0009

4-nitrobenzaldehyde

C	-7.1027	2.4332	0.0000
C	-7.1435	1.0348	0.0000
C	-5.8685	3.0912	0.0000
C	-5.9590	0.2886	0.0000
C	-4.7227	0.9404	0.0000
C	-4.6817	2.3418	0.0000
H	-8.0190	3.0196	0.0000
H	-5.8475	4.1798	0.0000
H	-5.9970	-0.8001	0.0000
H	-3.8108	0.3459	0.0000
C	-8.4514	0.3478	0.0000
N	-3.3851	3.0328	0.0000
O	-8.5407	-0.8732	0.0000
H	-9.3480	0.9901	0.0000
O	-3.3947	4.2719	0.0000
O	-2.3606	2.3364	0.0000

4-trifluoride-benzophenone

C	-6.3902	3.9616	-0.2165
C	-6.4431	2.5844	-0.0674
C	-5.2574	1.8704	0.0955
C	-4.0278	2.5187	0.1076
C	-3.9831	3.9007	-0.0330
C	-5.1627	4.6285	-0.1926
H	-7.3951	2.0661	-0.0803
C	-5.3107	0.3884	0.3258
H	-3.0211	4.3988	-0.0201
H	-7.2997	4.5352	-0.3464
H	-3.1110	1.9537	0.2231
F	-5.0633	0.0630	1.6346
F	-4.3594	-0.2893	-0.4481
F	-6.4566	-0.0770	0.1666
C	-5.1588	6.1260	-0.3419
O	-6.1883	6.7129	-0.5936
C	-3.8560	6.8602	-0.1628

H	-3.1403	6.5576	-0.9313
H	-3.4125	6.6263	0.8078
H	-4.0366	7.9302	-0.2382

Benzotrifluoride

C	-6.3277	4.0861	-0.1503
C	-6.3821	2.6990	-0.0745
C	-5.1993	1.9748	0.0488
C	-3.9663	2.6191	0.0894
C	-3.9196	4.0069	0.0130
C	-5.0982	4.7389	-0.1023
H	-7.3349	2.1832	-0.1147
C	-5.2618	0.4875	0.2148
H	-2.9635	4.5159	0.0454
H	-5.0587	5.8210	-0.1559
H	-7.2446	4.6557	-0.2447
H	-3.0518	2.0441	0.1757
F	-5.8020	0.1157	1.2709
F	-4.0772	-0.0447	0.2844
F	-6.0949	-0.1138	-0.7418

Benzoyl fluoride

C	-6.3357	4.0826	-0.1711
C	-6.4535	2.6949	-0.0789
C	-5.3039	1.9114	0.0625
C	-4.0408	2.5102	0.1119
C	-3.9296	3.8979	0.0192
C	-5.0758	4.6818	-0.1220
H	-7.4388	2.2362	-0.1180
C	-5.4286	0.4445	0.1599
H	-2.9499	4.3686	0.0571
H	-4.9866	5.7635	-0.1940
H	-7.2252	4.6987	-0.2812
H	-3.1455	1.9014	0.2219
O	-4.4871	-0.3212	0.2847
F	-6.6582	-0.0869	0.1082

4-cyano-N,N, dimethylaniline

C	-6.3677	4.0326	-0.1857
C	-6.5036	2.6506	-0.0915
C	-5.3695	1.8392	0.0656
C	-4.0665	2.3678	0.1245
C	-3.9697	3.7694	0.0405
C	-5.0952	4.5925	-0.1169
C	-7.5214	4.8673	-0.3447
H	-7.4868	2.1861	-0.1335
H	-5.5421	0.7699	0.1457
N	-2.9426	1.5546	0.3008
H	-3.0060	4.2669	0.0992
H	-4.9598	5.6704	-0.1793
C	-1.6106	2.1162	0.0812
C	-3.0632	0.1125	0.0917
H	-3.7658	-0.3335	0.8037
H	-2.1065	-0.3960	0.2563
H	-3.3836	-0.1110	-0.9319
H	-1.4044	2.9326	0.7816
H	-1.5004	2.4761	-0.9477
H	-0.8288	1.3681	0.2548
N	-8.4559	5.5433	-0.4749

4-fluoro-N,N-dimethylaniline

C	-6.3497	4.0133	-0.2150
C	-6.5000	2.6415	-0.1162
C	-5.3690	1.8322	0.0547
C	-4.0658	2.3654	0.1204
C	-3.9681	3.7687	0.0304
C	-5.0928	4.5867	-0.1406
F	-7.4277	4.7911	-0.3770
H	-7.4907	2.2024	-0.1664
H	-5.5415	0.7638	0.1394
N	-2.9412	1.5539	0.3089
H	-3.0065	4.2682	0.0949

H	-4.9865	5.6641	-0.2100
C	-1.6102	2.1169	0.0885
C	-3.0603	0.1116	0.1015
H	-3.7665	-0.3335	0.8105
H	-2.1043	-0.3960	0.2725
H	-3.3747	-0.1141	-0.9235
H	-1.4065	2.9369	0.7855
H	-1.4987	2.4721	-0.9419
H	-0.8274	1.3710	0.2670

Benzene

C	-7.3903	2.8850	0.0000
C	-7.3809	1.4879	0.0000
C	-6.1878	3.5831	0.0000
C	-6.1591	0.8184	0.0000
C	-4.9566	1.5165	0.0000
C	-4.9660	2.9136	0.0000
H	-8.3171	3.4443	0.0000
H	-6.1863	4.6676	0.0000
H	-6.1605	-0.2661	0.0000
H	-4.0298	0.9572	0.0000
H	-8.2671	0.9590	0.0000
H	-4.0798	3.4425	0.0000

1,2,4-trimethoxybenzene

C	-7.3454	2.7946	0.0000
C	-7.3465	1.3982	0.0000
C	-6.1345	3.5035	0.0000
C	-6.1320	0.7129	0.0000
C	-4.9199	1.4065	0.0000
C	-4.9107	2.8032	0.0000
H	-8.2841	3.3314	0.0000
O	-6.0385	4.8747	0.0000
O	-8.4518	0.5919	0.0000
H	-6.1285	-0.3747	0.0000
H	-4.0045	0.8253	0.0000
O	-3.7735	3.5723	0.0000
C	-2.5233	2.8986	0.0000
H	-1.7346	3.6572	0.0000
H	-2.4007	2.2927	-0.9037
H	-2.4007	2.2927	0.9037
C	-9.7214	1.2320	0.0000
H	-10.4890	0.4522	0.0000
H	-9.8594	1.8349	-0.9036
H	-9.8594	1.8349	0.9036
C	-7.2433	5.6255	0.0000
H	-6.9763	6.6867	0.0000
H	-7.8301	5.4312	0.9038
H	-7.8301	5.4312	-0.9038

1,4-dimethoxybenzene

C	-7.3865	2.8933	0.0000
C	-7.3936	1.5001	0.0000
C	-6.1705	3.5863	0.0000
C	-6.1764	0.8151	0.0000
C	-4.9604	1.5080	0.0000
C	-4.9533	2.9013	0.0000
H	-8.3027	3.4734	0.0000
H	-6.1729	4.6738	0.0000
O	-8.5016	0.6991	0.0000
H	-6.1740	-0.2724	0.0000
H	-4.0442	0.9280	0.0000
O	-3.8453	3.7023	0.0000
C	-2.5819	3.0496	0.0000
H	-1.8068	3.8219	0.0000
H	-2.4497	2.4453	-0.9036
H	-2.4497	2.4453	0.9036
C	-9.7649	1.3520	0.0000
H	-10.5402	0.5798	0.0000
H	-9.8971	1.9563	-0.9036
H	-9.8971	1.9563	0.9036

Anisole

C	-7.5268	2.8606	0.0000
C	-7.5262	1.4680	0.0000
C	-6.3164	3.5561	0.0000
C	-6.3165	0.7755	0.0000
C	-5.1043	1.4734	0.0000
C	-5.0992	2.8692	0.0000
H	-8.4661	3.4068	0.0000
H	-6.3201	4.6432	0.0000
H	-8.4665	0.9230	0.0000
H	-6.3151	-0.3115	0.0000
H	-4.1852	0.8978	0.0000
O	-3.9907	3.6707	0.0000
C	-2.7274	3.0185	0.0000
H	-1.9524	3.7911	0.0000
H	-2.5948	2.4143	-0.9036
H	-2.5948	2.4143	0.9036

Isopropylidenemalonitrile

C	-6.4669	3.1386	-0.0637
C	-5.6808	1.8462	-0.0894
H	-7.1175	3.1630	0.8171
H	-7.0946	3.2122	-0.9583
H	-5.8425	4.0350	-0.0306
C	-6.5777	0.6285	-0.1301
H	-7.2263	0.6123	0.7524
H	-6.0346	-0.3197	-0.1512
H	-7.2110	0.6603	-1.0232
C	-4.3251	1.7861	-0.0773
C	-3.5199	2.9635	-0.0391
C	-3.6267	0.5419	-0.1024
N	-2.8748	3.9279	-0.0080
N	-3.0691	-0.4758	-0.1229

N,N-dimethylaniline

C	-6.3536	4.0157	-0.2060
C	-6.4798	2.6325	-0.1156
C	-5.3658	1.8178	0.0449
C	-4.0698	2.3694	0.1327
C	-3.9528	3.7707	0.0221
C	-5.0785	4.5698	-0.1382
H	-7.2264	4.6451	-0.3333
H	-7.4603	2.1720	-0.1790
H	-5.5103	0.7472	0.1019
N	-2.9583	1.5668	0.3302
H	-2.9810	4.2448	0.0625
H	-4.9484	5.6443	-0.2163
C	-1.6460	2.1446	0.0902
C	-3.0989	0.1369	0.1067
H	-3.8009	-0.3004	0.8189
H	-2.1337	-0.3408	0.2597
H	-3.4493	-0.0955	-0.9081
H	-1.4472	2.9600	0.7883
H	-1.5393	2.5332	-0.9314
H	-0.8874	1.3819	0.2534

o-xylene

C	-6.1558	3.8703	-0.0792
C	-6.3121	2.4884	-0.0635
C	-5.1845	1.6740	-0.0171
C	-3.9229	2.2573	0.0143
C	-3.7549	3.6444	0.0011
C	-4.8917	4.4669	-0.0505
C	-4.7786	5.9721	-0.0635
H	-7.0352	4.5065	-0.1171
H	-7.3049	2.0531	-0.0917
H	-5.2855	0.5942	-0.0078
H	-3.0396	1.6251	0.0486
C	-2.3532	4.2047	0.0724
H	-4.1016	6.3210	-0.8464
H	-4.3931	6.3530	0.8866
H	-5.7548	6.4264	-0.2376

H	-1.3616	3.6361	-0.0071
H	-2.2567	4.9414	0.9244
H	-2.8548	4.7202	-0.8290

2-methylphenanthrene

C	-7.2336	3.5484	-0.0018
C	-5.8224	3.5108	-0.0008
C	-7.9712	2.3869	-0.0022
C	-7.3117	1.1454	-0.0016
C	-5.9345	1.0861	-0.0006
C	-5.1521	2.2627	-0.0002
H	-7.8893	0.2276	-0.0018
C	-2.9405	1.0486	0.0013
C	-3.6959	2.2433	0.0008
H	-5.4566	0.1142	-0.0001
H	-9.0547	2.4264	-0.0030
C	-1.5644	1.0754	0.0023
H	-3.4392	0.0871	0.0011
C	-0.8529	2.2946	0.0030
C	-1.5772	3.4670	0.0027
C	-2.9893	3.4687	0.0014
H	-1.0106	0.1411	0.0029
C	0.6527	2.2907	0.0027
H	-7.7286	4.5146	-0.0023
H	-1.0590	4.4223	0.0035
C	-5.0637	4.7319	-0.0002
C	-3.7111	4.7118	0.0009
H	-5.6058	5.6723	-0.0007
H	-3.1418	5.6361	0.0014
H	1.0851	3.1338	-0.7438
H	1.0531	1.1986	-0.0152
H	0.9922	2.7632	1.0295

3-3-dimethylbiphenyl

C	-7.2112	3.5678	0.0000
C	-5.8188	3.5254	0.0000
C	-7.9194	2.3638	0.0000
C	-7.2353	1.1555	0.0000
C	-5.8440	1.1297	0.0000
C	-5.1032	2.3181	0.0000
C	-7.9487	4.8832	0.0000
H	-7.7863	0.2211	0.0000
H	-5.2928	4.4725	0.0000
C	-2.8918	1.0935	0.0000
C	-3.6063	2.3017	0.0000
H	-5.3516	0.1660	0.0000
H	-9.0053	2.3770	0.0000
H	-7.4799	5.4949	-0.7740
H	-7.9153	5.7458	0.8812
H	-8.9518	4.5261	0.0460
C	-1.5033	1.0869	0.0000
H	-3.4074	0.1422	0.0000
C	-0.7887	2.2815	0.0000
C	-1.4673	3.4982	0.0000
C	-2.8637	3.4884	0.0000
C	-0.7251	4.8107	0.0000
H	-3.3649	4.4495	0.0000
H	-0.9736	0.1403	0.0000
H	0.2967	2.2680	0.0000
H	0.3541	4.6538	0.0000
H	-0.9827	5.4053	0.8800
H	-0.9827	5.4053	-0.8800

2-methylnaphthalene

C	-7.1327	3.6380	0.0083
C	-5.7651	3.5939	0.0032
C	-7.9102	2.4450	0.0123
C	-7.2625	1.2349	0.0106
C	-5.8438	1.1507	0.0050
C	-5.0794	2.3491	0.0017
H	-7.6452	4.5956	0.0100
C	-9.4125	2.5425	0.0174

H	-7.8367	0.3120	0.0138
H	-5.1836	4.5110	0.0010
C	-5.1658	-0.0966	0.0032
C	-3.7951	-0.1479	-0.0014
C	-3.0345	1.0469	-0.0041
C	-3.6629	2.2663	-0.0027
H	-3.0849	3.1856	-0.0047
H	-5.7531	-1.0098	0.0054
H	-3.2853	-1.1051	-0.0028
H	-9.7632	3.6837	-0.5580
H	-9.7247	2.2621	1.3312
H	-9.9139	1.9271	-0.9918
H	-1.9515	0.9922	-0.0074

4,4’dimethylbiphenyl

C	-7.1519	3.6377	0.0000
C	-5.7609	3.6129	0.0000
C	-7.8986	2.4611	0.0000
C	-7.1961	1.2538	0.0000
C	-5.8083	1.2250	0.0000
C	-5.0501	2.4064	0.0000
H	-7.6636	4.5955	0.0000
C	-9.4047	2.4781	0.0000
H	-7.7460	0.3169	0.0000
H	-5.2394	4.5618	0.0000
C	-2.8441	1.1694	0.0000
C	-3.5566	2.3785	0.0000
C	-1.4560	1.1455	0.0000
H	-9.7545	3.0290	-1.0744
H	-9.8178	3.1383	1.0068
H	-9.8180	1.3218	0.0470
H	-5.3230	0.2571	0.0000
H	-3.3663	0.2209	0.0000
C	-2.8004	3.5574	0.0000
C	-1.4095	3.5295	0.0000
C	-0.7082	2.3254	0.0000
C	0.7975	2.2861	0.0000
H	-0.9423	0.1884	0.0000
H	-3.2851	4.5255	0.0000
H	-0.8615	4.4670	0.0000
H	1.1721	3.1168	1.0581
H	1.2043	3.1425	-0.9188
H	1.1924	0.9660	0.0462

2,6-dimethylnaphthalene

C	-7.1384	3.6333	0.0000
C	-5.7683	3.5898	0.0000
C	-7.9163	2.4436	0.0000
C	-7.2649	1.2327	0.0000
C	-5.8492	1.1499	0.0000
C	-5.0821	2.3475	0.0000
H	-7.6478	4.5922	0.0000
C	-9.4231	2.5149	0.0000
H	-7.8392	0.3091	0.0000
H	-5.1889	4.5083	0.0000
C	-5.1631	-0.0924	0.0000
C	-3.7930	-0.1360	0.0000
C	-3.0151	1.0537	0.0000
C	-3.6665	2.2646	0.0000
C	-1.5082	0.9824	0.0000
H	-3.0922	3.1883	0.0000
H	-5.7424	-1.0109	0.0000
H	-3.2836	-1.0949	0.0000
H	-1.2574	0.1221	-0.9014
H	-1.0303	0.6139	1.0356
H	-1.0546	1.9485	-0.2133
H	-9.7528	3.3082	0.7862
H	-9.9102	1.4483	0.0260
H	-9.7789	2.9766	-0.9105

3-biphenyl-carboxylic acid

C	-7.2743	3.0898	-0.7636

C	-7.9409	1.9968	-0.2161
C	-7.2087	0.9565	0.3497
C	-5.8188	1.0090	0.3694
C	-5.1400	2.1036	-0.1758
C	-5.8849	3.1427	-0.7435
C	-3.6569	2.1655	-0.1509
C	-3.0015	3.3768	0.0674
C	-1.6100	3.4400	0.1078
C	-0.8492	2.2887	-0.0985
C	-1.4940	1.0793	-0.3320
C	-2.8821	1.0164	-0.3499
H	-3.3705	0.0679	-0.5458
H	-3.5689	4.2856	0.2331
H	-0.9105	0.1846	-0.5138
H	-5.2582	0.2037	0.8325
H	-5.3736	3.9879	-1.1921
H	-7.7195	0.1054	0.7858
C	-0.9925	4.7831	0.3335
H	-7.8352	3.9004	-1.2154
H	-9.0243	1.9555	-0.2309
H	0.2353	2.3225	-0.1166
O	-1.0743	5.7139	-0.4640
O	-0.1954	4.9568	1.2223
H	-0.2584	4.1338	2.0026

4-acetate-biphenyl

C	-7.2137	3.1394	-0.6528
C	-7.8536	1.9955	-0.1828
C	-7.0944	0.9358	0.3066
C	-5.7060	1.0194	0.3263
C	-5.0524	2.1635	-0.1448
C	-5.8254	3.2221	-0.6346
C	-3.5704	2.2534	-0.1313
C	-2.9304	3.4627	0.1663
C	-1.5451	3.5568	0.1720
C	-0.7909	2.4295	-0.1218
C	-1.3946	1.2176	-0.4182
C	-2.7825	1.1340	-0.4172
H	-3.2558	0.1907	-0.6665
H	-3.5205	4.3375	0.4164
H	-0.7801	0.3554	-0.6503
H	-5.1256	0.1965	0.7304
H	-5.3362	4.1086	-1.0248
H	-7.5832	0.0437	0.6823
H	-1.0489	4.4902	0.4118
O	0.5990	2.4795	-0.0724
H	-7.7953	3.9675	-1.0427
H	-8.9357	1.9302	-0.1981
C	1.2493	3.1708	-1.0485
C	2.7310	3.0942	-0.8421
H	3.0275	2.1166	-0.0622
H	3.2839	4.0786	-0.5364
H	2.9590	2.6171	-2.0385
O	0.6787	3.7372	-1.9373

4-methylbiphenyl

C	-7.2827	3.0567	-0.6564
C	-7.8821	1.9782	-0.0111
C	-7.0848	0.9826	0.5474
C	-5.6990	1.0669	0.4646
C	-5.0843	2.1469	-0.1800
C	-5.8970	3.1392	-0.7407
C	-3.6049	2.2408	-0.2644
C	-2.9563	3.4741	-0.1597
C	-1.5700	3.5618	-0.2398
C	-0.7854	2.4243	-0.4284
C	-1.4352	1.1908	-0.5326
C	-2.8179	1.0977	-0.4516
H	-3.2944	0.1284	-0.5580
H	-3.5377	4.3746	0.0089
H	-0.8477	0.2906	-0.6879
H	-5.0866	0.2970	0.9226

H	-5.4402	3.9728	-1.2638
H	-7.5433	0.1418	1.0559
H	-1.0914	4.5317	-0.1452
C	0.7160	2.5097	-0.5159
H	-7.8952	3.8327	-1.1023
H	-8.9623	1.9129	0.0552
H	0.9810	3.4242	-1.4452
H	1.1766	1.2853	-0.7790
H	1.1503	2.9059	0.4537

3,4,4’-trimethoxybiphenyl

C	-6.6818	2.3605	-1.8263
C	-8.0618	2.3930	-1.8003
C	-8.7231	2.6901	-0.5974
C	-7.9736	2.9378	0.5677
C	-6.6025	2.8815	0.5335
C	-5.9110	2.5982	-0.6695
H	-8.6144	2.1785	-2.7050
O	-10.0484	2.7556	-0.4627
H	-8.5053	3.1792	1.4802
H	-6.0539	3.1041	1.4402
C	-4.4649	2.5546	-0.7080
C	-3.7184	2.2720	0.4797
C	-3.7601	2.7710	-1.9069
C	-2.3812	2.7171	-1.9603
C	-1.6423	2.4194	-0.7525
C	-2.3596	2.1988	0.4489
H	-4.3066	3.0317	-2.8019
O	-1.6565	2.9351	-3.0514
O	-0.3438	2.3305	-0.6403
H	-1.7806	1.9595	1.3323
H	-6.1955	2.1001	-2.7589
H	-4.2335	2.0676	1.4089
C	0.6133	2.4923	-1.7091
H	1.5736	2.3392	-1.2275
H	0.5402	3.4944	-2.1224
H	0.4389	1.7439	-2.4778
C	-2.3302	3.2245	-4.2798
H	-1.5442	3.3536	-5.0168
H	-2.9114	4.1425	-4.1832
H	-2.9772	2.3906	-4.5567
C	-10.8653	2.5527	-1.6160
H	-11.8888	2.6673	-1.2719
H	-10.7188	1.5494	-2.0196
H	-10.6423	3.3010	-2.3787

4-biphenyl-carboxylate

C	-7.0656	3.0406	-0.7745
C	-7.6568	2.1066	0.0722
C	-6.8598	1.2072	0.7756
C	-5.4701	1.2422	0.6312
C	-4.8525	2.1766	-0.2172
C	-5.6757	3.0749	-0.9170
C	-3.3883	2.2129	-0.3686
C	-2.6699	3.4046	-0.1749
C	-1.2776	3.4440	-0.3185
C	-0.5725	2.2851	-0.6619
C	-1.2759	1.0910	-0.8571
C	-2.6673	1.0576	-0.7114
H	-3.1896	0.1177	-0.8816
H	-3.1940	4.3172	0.1044
H	-0.7461	0.1792	-1.1271
H	-4.8665	0.5371	1.1994
H	-5.2364	3.8052	-1.5936
H	-7.3176	0.4785	1.4395
H	-0.7609	4.3865	-0.1557
H	-7.6847	3.7418	-1.3279
H	-8.7375	2.0793	0.1835
C	0.9063	2.2667	-0.8297
O	1.5410	1.2615	-1.1088
O	1.4269	3.5042	-0.6339
C	2.8459	3.5659	-0.7834

H	3.3374	2.9285	-0.0416
H	3.1595	4.5996	-0.6138
H	3.1380	3.2777	-1.7981

Biphenyl

C	-7.2177	2.9535	-0.8182
C	-7.8111	1.9802	-0.0184
C	-7.0136	1.0933	0.7003
C	-5.6211	1.1800	0.6178
C	-5.0016	2.1546	-0.1823
C	-5.8250	3.0396	-0.8983
C	-3.5346	2.2456	-0.2679
C	-2.8672	3.4525	0.0002
C	-1.4746	3.5397	-0.0802
C	-0.7252	2.4200	-0.4319
C	-1.3666	1.2140	-0.7025
C	-2.7592	1.1283	-0.6202
H	-3.2415	0.1796	-0.8468
H	-3.4333	4.3362	0.2879
H	-0.7855	0.3387	-0.9805
H	-5.0162	0.4847	1.1964
H	-5.3815	3.8000	-1.5381
H	-7.4729	0.3344	1.3281
H	-0.9775	4.4819	0.1349
H	0.3577	2.4872	-0.4951
H	-7.8366	3.6455	-1.3831
H	-8.8939	1.9131	0.0448

3,3’,4,4’-tetramethoxybiphenyl

C	-7.1390	3.2908	-0.2880
C	-7.7343	2.2532	0.4339
C	-6.9278	1.2791	1.0191
C	-5.5423	1.3035	0.8287
C	-4.9333	2.3071	0.0562
C	-5.7567	3.2992	-0.5015
C	-3.4753	2.3222	-0.1549
C	-2.7143	3.4755	0.1189
C	-1.3246	3.5113	-0.0811
C	-0.6766	2.3507	-0.5335
C	-1.4254	1.2090	-0.8337
C	-2.8072	1.1918	-0.6418
H	-3.3602	0.2877	-0.8880
H	-3.2382	4.3456	0.5032
O	-0.5570	4.6263	0.1305
O	0.6644	2.2113	-0.7877
H	-0.9241	0.3231	-1.2159
H	-4.9367	0.5287	1.2954
H	-5.3257	4.0913	-1.1096
O	-7.8618	4.3149	-0.8425
O	-9.0789	2.1354	0.6633
H	-7.3786	0.4886	1.6133
C	-8.2018	5.2712	0.1639
C	-9.8470	2.1543	-0.5401
C	-1.2260	5.8588	0.3624
C	1.5365	2.8500	0.1386
H	-7.3060	5.6557	0.6647
H	-8.8978	4.8522	0.8978
H	-8.6993	6.1114	-0.3298
H	-10.7584	1.5759	-0.3596
H	-9.3210	1.6927	-1.3839
H	-10.1486	3.1766	-0.7850
H	-0.4688	6.6482	0.3936
H	-1.7361	5.8509	1.3309
H	-1.9198	6.0964	-0.4510
H	2.4818	2.2980	0.1356
H	1.1491	2.8311	1.1634
H	1.7558	3.8713	-0.1857

4-methoxy-4’-methylbiphenyl

C	-6.6752	2.1650	-1.8888
C	-8.0638	2.2588	-1.8783
C	-8.7427	2.7983	-0.7859

C	-7.9841	3.2441	0.3003
C	-6.5985	3.1547	0.2939
C	-5.9171	2.6128	-0.8033
H	-8.6288	1.8988	-2.7329
C	-10.2455	2.9042	-0.7673
H	-8.4874	3.6774	1.1598
H	-6.0354	3.5291	1.1429
C	-4.4369	2.5185	-0.8111
C	-3.7262	2.1963	0.3549
C	-3.7037	2.7476	-1.9756
C	-2.3130	2.6619	-1.9973
C	-1.6264	2.3371	-0.8272
C	-2.3455	2.1055	0.3501
H	-4.2218	3.0201	-2.8894
H	-1.7862	2.8577	-2.9223
O	-0.2785	2.2240	-0.7324
H	-1.7971	1.8456	1.2488
H	-6.1772	1.7186	-2.7435
H	-4.2648	1.9921	1.2743
C	0.4866	2.4304	-1.9105
H	1.5245	2.2839	-1.6228
H	0.3519	3.4449	-2.2942
H	0.2150	1.7079	-2.6844
H	-10.7375	1.6948	-1.2138
H	-10.5818	3.4302	-1.9552
H	-10.5967	3.4804	0.2498

4-methoxyacetanilide

C	-6.1740	4.6944	0.5110
C	-7.4810	4.2586	0.2617
C	-7.7214	2.9428	-0.1289
C	-6.6318	2.0733	-0.2647
C	-5.3239	2.5106	-0.0151
C	-5.0896	3.8273	0.3737
H	-6.0053	5.7250	0.8146
H	-8.2849	4.9777	0.3825
H	-6.7802	1.0399	-0.5669
H	-4.5156	1.7972	-0.1339
N	-9.0017	2.4203	-0.4043
C	-10.2148	3.0808	-0.3290
C	-11.3730	2.1890	-0.7031
H	-11.1010	1.5159	-1.5212
H	-12.2124	2.8055	-1.0375
H	-11.6761	1.6043	0.1693
O	-10.4060	4.2397	0.0205
O	-3.8713	4.3836	0.6459
C	-2.7327	3.5455	0.4971
H	-2.7693	2.7026	1.1951
H	-1.8461	4.1396	0.7389
H	-2.6294	3.1991	-0.5366
H	-9.0310	1.4479	-0.6824

4-cyanoacetanilide

C	-6.3433	4.5527	0.1431
C	-7.6392	4.0833	-0.0078
C	-7.8657	2.7082	-0.1600
C	-6.7746	1.8243	-0.1585
C	-5.4854	2.2953	-0.0089
C	-5.2623	3.6685	0.1442
H	-6.1705	5.6157	0.2626
H	-8.4688	4.7714	-0.0082
H	-6.9489	0.7606	-0.2790
H	-4.6493	1.6062	-0.0104
N	-9.1341	2.1440	-0.3112
C	-10.3526	2.7768	-0.3762
C	-11.5268	1.8315	-0.4626
H	-11.7268	1.8032	-1.5595
H	-12.4697	2.2429	0.2313
H	-11.2754	0.7738	-0.0611
O	-10.4837	3.9849	-0.3430
C	-3.9280	4.1654	0.3009
N	-2.8557	4.5652	0.4266

H	-9.1540	1.1346	-0.3648

3-methylindole

C	-6.2226	4.1952	0.0000
C	-7.3843	3.4439	0.0000
C	-7.3432	2.0339	0.0000
C	-6.1376	1.3548	0.0000
C	-4.9384	2.0885	0.0000
C	-5.0048	3.5049	0.0000
H	-6.2500	5.2797	0.0000
H	-8.3439	3.9492	0.0000
H	-8.2734	1.4763	0.0000
H	-6.1198	0.2693	0.0000
C	-3.5451	1.7246	0.0000
C	-2.8491	2.9043	0.0000
N	-3.7178	3.9720	0.0000
C	-2.9802	0.3332	0.0000
H	-3.4453	4.9425	0.0000
H	-1.7821	3.0748	0.0000
H	-3.5027	-0.1372	-0.9983
H	-3.0951	-0.5318	0.8330
H	-1.8287	0.6310	-0.1042

3,4-dimethoxy-4’-methylbiphenyl

C	-6.7282	1.9437	-1.7265
C	-8.1229	2.0505	-1.7174
C	-8.7694	2.7971	-0.7284
C	-8.0006	3.4260	0.2558
C	-6.6064	3.3160	0.2455
C	-5.9461	2.5749	-0.7465
H	-8.6972	1.5422	-2.4885
C	-10.2645	2.9116	-0.6995
H	-8.4816	4.0087	1.0384
H	-6.0340	3.8258	1.0180
C	-4.4788	2.4622	-0.7582
C	-3.7855	1.9796	0.3549
C	-3.7326	2.8383	-1.8910
C	-2.3291	2.7414	-1.9290
C	-1.6542	2.2509	-0.7980
C	-2.3946	1.8757	0.3319
H	-4.2849	3.2231	-2.7434
O	-1.5888	3.1045	-3.0227
O	-0.3089	2.0690	-0.6081
H	-1.8751	1.4933	1.2080
H	-6.2533	1.3469	-2.5027
H	-4.3235	1.6678	1.2476
C	0.5881	2.4057	-1.6541
H	1.6014	2.1897	-1.3004
H	0.5494	3.4751	-1.8834
H	0.4182	1.7854	-2.5396
H	-10.7191	2.4560	-1.5852
H	-10.5633	3.9647	-0.6776
H	-10.6631	2.4056	0.1855
C	-2.2674	3.6212	-4.1597
H	-1.5142	3.8589	-4.9171
H	-2.7968	4.5483	-3.9171
H	-2.9440	2.8750	-4.5889

4,4’-dimethoxybiphenyl

C	-6.6909	2.0298	-1.7705
C	-8.0879	2.1397	-1.7480
C	-8.7183	2.8469	-0.7264
C	-7.9400	3.4397	0.2683
C	-6.5459	3.3282	0.2462
C	-5.8959	2.6208	-0.7755
H	-8.6483	1.6581	-2.5419
O	-10.0657	3.0311	-0.5855
H	-8.4214	3.9963	1.0687
H	-5.9688	3.8117	1.0317
C	-4.4293	2.5012	-0.8032
C	-3.7209	2.0148	0.3051
C	-3.6927	2.8709	-1.9399

C	-2.2959	2.7603	-1.9710
C	-1.6071	2.2744	-0.8616
C	-2.3271	1.9026	0.2741
H	-4.2055	3.2652	-2.8154
H	-1.7821	3.0657	-2.8760
O	-0.2530	2.1157	-0.7591
H	-1.7999	1.5195	1.1444
H	-6.2241	1.4614	-2.5729
H	-4.2518	1.7060	1.2032
C	0.5249	2.4880	-1.8895
H	1.5761	2.3041	-1.6472
H	0.4159	3.5551	-2.1099
H	0.2723	1.8757	-2.7616
C	-10.9016	2.4402	-1.5723
H	-11.9390	2.6763	-1.3166
H	-10.7993	1.3499	-1.5751
H	-10.6994	2.8594	-2.5635

3,4-dimethoxybiphenyl

C	-6.7316	1.9484	-1.7229
C	-8.1250	2.0538	-1.7090
C	-8.7589	2.7847	-0.7074
C	-8.0012	3.4089	0.2803
C	-6.6079	3.3017	0.2657
C	-5.9484	2.5706	-0.7363
H	-8.7138	1.5614	-2.4785
H	-8.4924	3.9816	1.0627
H	-6.0340	3.8054	1.0412
C	-4.4807	2.4600	-0.7519
C	-3.7840	1.9756	0.3585
C	-3.7374	2.8398	-1.8854
C	-2.3339	2.7444	-1.9270
C	-1.6556	2.2526	-0.7985
C	-2.3929	1.8739	0.3321
H	-4.2918	3.2268	-2.7354
O	-1.5965	3.1111	-3.0215
O	-0.3097	2.0722	-0.6121
H	-1.8709	1.4903	1.2062
H	-6.2572	1.3615	-2.5069
H	-4.3192	1.6607	1.2517
C	0.5844	2.4107	-1.6600
H	1.5987	2.1946	-1.3093
H	0.5447	3.4804	-1.8877
H	0.4124	1.7915	-2.5459
H	-9.8425	2.8668	-0.6956
C	-2.2791	3.6186	-4.1602
H	-1.5282	3.8549	-4.9204
H	-2.8115	4.5451	-3.9217
H	-2.9538	2.8675	-4.5839

4-methoxy-1,1’-biphenyl

C	-6.7641	2.0085	-1.8083
C	-8.1577	2.1135	-1.7943
C	-8.7934	2.8199	-0.7765
C	-8.0373	3.4201	0.2270
C	-6.6439	3.3129	0.2122
C	-5.9819	2.6059	-0.8056
H	-8.7447	1.6404	-2.5771
H	-9.8770	2.9020	-0.7650
H	-8.5296	3.9745	1.0217
H	-6.0716	3.7989	0.9999
C	-4.5142	2.4947	-0.8208
C	-3.8120	2.0148	0.2943
C	-3.7703	2.8664	-1.9521
C	-2.3726	2.7641	-1.9714
C	-1.6901	2.2847	-0.8553
C	-2.4173	1.9110	0.2753
H	-4.2786	3.2551	-2.8327
H	-1.8533	3.0705	-2.8729
O	-0.3360	2.1345	-0.7411
H	-1.8952	1.5326	1.1506
H	-6.2884	1.4415	-2.6060

H	-4.3489	1.7041	1.1882
C	0.4484	2.5033	-1.8683
H	1.4985	2.3246	-1.6177
H	0.3370	3.5688	-2.0953
H	0.2041	1.8853	-2.7386

2,2’-dimethoxybiphenyl

C	-6.7115	1.8639	-1.7819
C	-8.1012	2.0394	-1.7341
C	-8.6794	2.8817	-0.7817
C	-7.8776	3.5550	0.1322
C	-6.4938	3.3889	0.0922
C	-5.8858	2.5478	-0.8597
O	-6.0708	1.0409	-2.6761
H	-8.7659	1.5314	-2.4245
H	-9.7586	3.0089	-0.7533
H	-8.3241	4.2083	0.8769
H	-5.8761	3.9203	0.8144
C	-4.4138	2.4162	-0.8667
C	-3.6994	1.8502	0.2057
C	-3.6709	2.8890	-1.9639
C	-2.2748	2.8135	-1.9823
C	-1.5904	2.2717	-0.8971
C	-2.3018	1.7960	0.2018
O	-4.3471	1.3901	1.3271
H	-4.1875	3.3274	-2.8157
H	-1.7249	3.1870	-2.8422
H	-0.5050	2.2241	-0.9052
H	-1.7729	1.3834	1.0559
C	-6.8707	0.3270	-3.6078
C	-4.6718	0.0088	1.1649
H	-6.2011	-0.2720	-4.2326
H	-7.4154	1.0110	-4.2667
H	-7.5525	-0.3614	-3.0978
H	-3.7654	-0.6008	1.0808
H	-5.3217	-0.1572	0.2993
H	-5.2134	-0.3136	2.0593

N,3,3-trimethyl-2-oxindole

C	-6.0574	4.1938	0.1006
C	-7.2526	3.4701	0.0883
C	-7.2408	2.0658	0.0410
C	-6.0341	1.3626	0.0052
C	-4.8527	2.0878	0.0176
C	-4.8720	3.4831	0.0646
H	-6.0745	5.2767	0.1371
H	-8.2034	3.9977	0.1157
H	-8.1827	1.5214	0.0323
H	-6.0299	0.2778	-0.0313
C	-3.4215	1.6018	-0.0132
C	-2.6299	2.9319	0.0237
N	-3.5625	3.9709	0.0677
C	-3.2215	5.3675	0.1117
H	-3.6227	5.8096	1.0285
H	-3.6459	5.8720	-0.7612
H	-2.1358	5.4984	0.1023
C	-3.1049	0.8521	-1.3065
C	-3.0796	0.7671	1.2202
O	-1.4123	3.0405	0.0154
H	-3.2721	1.3220	2.1463
H	-2.0198	0.4877	1.2253
H	-3.6707	-0.1549	1.2574
H	-3.3155	1.4680	-2.1891
H	-3.6973	-0.0656	-1.3937
H	-2.0457	0.5744	-1.3516

N-methyl-2-oxindole

C	-6.0173	4.1263	0.0974
C	-7.2122	3.4012	0.0852
C	-7.2001	1.9958	0.0380
C	-5.9936	1.2919	0.0023
C	-4.8177	2.0205	0.0148

C	-4.8335	3.4145	0.0615
H	-6.0336	5.2092	0.1337
H	-8.1633	3.9282	0.1124
H	-8.1422	1.4517	0.0294
H	-5.9854	0.2073	-0.0340
C	-3.4009	1.5349	-0.0156
C	-2.6004	2.8408	0.0204
N	-3.5199	3.8916	0.0640
C	-3.1656	5.2845	0.1086
H	-3.5580	5.7286	1.0281
H	-3.5897	5.7948	-0.7612
H	-2.0787	5.4043	0.0938
H	-3.1846	0.9979	-0.9426
H	-3.1667	0.9371	0.8688
O	-1.3816	2.9246	0.0119

N-methylindole

C	-6.0593	4.1283	0.0000
C	-7.2344	3.3960	0.0000
C	-7.2167	1.9861	0.0000
C	-6.0231	1.2848	0.0000
C	-4.8124	1.9970	0.0000
C	-4.8554	3.4146	0.0000
H	-6.0719	5.2131	0.0000
H	-8.1852	3.9174	0.0000
H	-8.1563	1.4445	0.0000
H	-6.0210	0.1995	0.0000
C	-3.4247	1.6302	0.0000
C	-2.7124	2.7992	0.0000
N	-3.5640	3.8779	0.0000
H	-3.0119	0.6327	0.0000
H	-1.6442	2.9629	0.0000
C	-3.1836	5.2774	0.0000
H	-2.5829	5.2119	1.0755
H	-4.1565	6.0662	-0.0733
H	-2.3621	5.5468	-0.7418

1,2-dimethoxy-4-methylbenzene

C	-10.1729	1.1225	0.6458
C	-10.0871	-0.2292	0.3092
C	-11.1800	-0.9023	-0.2252
C	-12.3894	-0.2450	-0.4276
C	-12.4945	1.1066	-0.0732
C	-11.3912	1.7729	0.4492
H	-11.1138	-1.9481	-0.5053
O	-13.4382	-0.9596	-0.9379
C	-8.9958	1.8520	1.2416
H	-9.1503	-0.7590	0.4501
H	-11.5091	2.8218	0.7048
C	-14.0921	-0.4144	-2.0864
O	-13.6680	1.7963	-0.2488
C	-14.7004	1.3933	0.6543
H	-14.3997	1.5973	1.6851
H	-14.9244	0.3299	0.5425
H	-15.5798	1.9826	0.4033
H	-13.7245	-1.0471	-2.9914
H	-14.0279	0.7655	-2.0260
H	-15.3326	-0.7815	-2.0392
H	-8.2109	1.1130	1.5750
H	-9.4216	2.7246	1.8143
H	-8.3051	2.3629	0.2735

2-oxoindole

C	-6.3062	4.7380	0.2242
C	-7.5379	4.1918	-0.0634
C	-7.7262	2.8246	-0.2555
C	-6.6636	1.9458	-0.1631
C	-5.4022	2.4750	0.1280
C	-5.2248	3.8587	0.3200
H	-6.1729	5.8032	0.3714
H	-6.7972	0.8791	-0.3106
H	-4.5447	1.8098	0.2076

H	-4.2333	4.2450	0.5454
C	-9.1720	2.5583	-0.5499
C	-9.7756	3.9671	-0.4975
H	-9.6277	1.9343	0.2227
H	-9.3043	2.1387	-1.5502
N	-8.7460	4.8543	-0.2074
O	-10.9446	4.2659	-0.6763
H	-8.8893	5.8486	-0.1188

4-methoxy-N-methylacetanilide

C	-6.2206	4.5940	0.6095
C	-7.5067	4.0816	0.3883
C	-7.7031	2.7664	-0.0505
C	-6.5507	1.9850	-0.2483
C	-5.2612	2.4969	-0.0293
C	-5.0911	3.8076	0.4016
H	-6.1089	5.6200	0.9525
H	-8.3411	4.7423	0.6038
H	-6.6151	0.9628	-0.6093
H	-4.4163	1.8415	-0.2115
N	-9.0230	2.2150	-0.2641
C	-10.1292	3.0353	-0.5502
C	-11.4611	2.3419	-0.7315
H	-11.4088	1.6130	-1.5444
H	-12.2205	3.0840	-0.9992
H	-11.7724	1.8699	0.2039
O	-10.0967	4.2590	-0.6912
C	-9.1360	0.7545	-0.2850
H	-8.4976	0.3099	0.4855
H	-8.8515	0.3926	-1.2780
H	-10.1501	0.4127	-0.0725
O	-3.9008	4.4280	0.6550
C	-2.7195	3.6671	0.4388
H	-2.6831	2.7977	1.1035
H	-1.8627	4.3045	0.6774
H	-2.6293	3.3669	-0.6105

Acetanilide

C	-6.3108	4.6165	0.2144
C	-7.6216	4.1531	0.0590
C	-7.8689	2.8052	-0.2060
C	-6.7813	1.9278	-0.3142
C	-5.4717	2.3906	-0.1590
C	-5.2368	3.7367	0.1058
H	-6.1343	5.6692	0.4208
H	-8.4274	4.8744	0.1510
H	-6.9352	0.8720	-0.5203
H	-4.6367	1.7003	-0.2447
N	-9.1572	2.2571	-0.3768
C	-10.3705	2.9173	-0.3053
C	-11.5370	1.9894	-0.5389
H	-11.3041	1.2568	-1.3170
H	-12.4030	2.5703	-0.8693
H	-11.7807	1.4724	0.3929
O	-10.5553	4.1031	-0.0564
H	-4.2202	4.1011	0.2274
H	-9.1907	1.2637	-0.5659

N-methylacetanilide

C	-6.3756	4.5856	0.2946
C	-7.6541	4.0213	0.1970
C	-7.8373	2.6703	-0.1328
C	-6.6773	1.9035	-0.3502
C	-5.3976	2.4647	-0.2547
C	-5.2470	3.8077	0.0675
H	-6.2715	5.6363	0.5534
H	-8.4954	4.6710	0.4192
H	-6.7333	0.8565	-0.6319
H	-4.5208	1.8495	-0.4397
N	-9.1516	2.0718	-0.2197
C	-10.2974	2.8399	-0.4941
C	-11.6148	2.0987	-0.5491

H	-11.5832	1.3113	-1.3066
H	-12.4101	2.7971	-0.8297
H	-11.8610	1.6914	0.4350
O	-10.3128	4.0515	-0.7185
C	-9.2215	0.6114	-0.1263
H	-8.5203	0.2415	0.6290
H	-8.9935	0.1834	-1.1075
H	-10.2086	0.2621	0.1805
H	-4.2562	4.2472	0.1411

4-cyano-N-methylacetanilide

C	-6.3852	4.5058	0.2274
C	-7.6624	3.9320	0.1473
C	-7.8401	2.5538	-0.0488
C	-6.6778	1.7671	-0.1474
C	-5.3977	2.3346	-0.0692
C	-5.2484	3.7081	0.1173
H	-6.2976	5.5801	0.3808
H	-8.5096	4.6008	0.2752
H	-6.7304	0.6959	-0.3202
H	-4.5236	1.6924	-0.1617
N	-9.1533	1.9528	-0.1179
C	-9.2378	0.5092	0.1196
H	-8.9727	-0.0162	-0.8032
H	-10.2389	0.1946	0.4181
H	-8.5696	0.2164	0.9361
C	-10.2826	2.6923	-0.5139
C	-11.6078	1.9637	-0.5176
H	-11.5727	1.1043	-1.1921
H	-12.3897	2.6394	-0.8793
H	-11.8752	1.6592	0.4976
O	-10.2719	3.8688	-0.8804
C	-3.9414	4.2905	0.1993
N	-2.8798	4.7545	0.2684

N-methylaniline

C	-6.3621	4.4589	-0.0567
C	-7.6083	3.8319	0.0375
C	-7.7232	2.4345	0.0897
C	-6.5389	1.6886	0.1179
C	-5.2881	2.3098	0.0229
C	-5.2000	3.6952	-0.0716
H	-6.3035	5.5426	-0.1070
H	-8.5010	4.4514	0.0727
H	-6.5622	0.6081	0.2167
H	-4.3838	1.7072	0.0348
H	-4.2291	4.1779	-0.1398
N	-8.9963	1.8766	0.2523
C	-9.1985	0.4667	-0.0267
H	-8.8845	0.2118	-1.0443
H	-10.2643	0.2330	0.0626
H	-8.6679	-0.1642	0.6935
H	-9.7177	2.4668	-0.1545

1,3-benzodioxole

C	-10.0602	0.9770	0.7525
C	-9.7907	-0.1757	0.0265
C	-10.7945	-0.8227	-0.7137
C	-12.0487	-0.2575	-0.6847
C	-12.3167	0.8997	0.0374
C	-11.3460	1.5427	0.7699
H	-10.5962	-1.7222	-1.2832
O	-13.1875	-0.6828	-1.3069
H	-9.2671	1.4547	1.3155
H	-8.7889	-0.5888	0.0273
H	-11.5709	2.4405	1.3323
C	-14.2131	0.2554	-0.9698
O	-13.6300	1.2416	-0.1142
H	-15.0121	-0.2599	-0.4367
H	-14.5758	0.7350	-1.8792

N-methyl-N-phenylaniline

C	-5.9014	4.2124	0.6723
C	-7.1992	3.7602	0.4182
C	-7.4139	2.7446	-0.5101
C	-6.3322	2.1795	-1.1805
C	-5.0353	2.6324	-0.9231
C	-4.7974	3.6596	0.0039
H	-5.7504	4.9866	1.4201
H	-8.0390	4.1969	0.9518
H	-6.4934	1.3860	-1.9052
H	-4.2052	2.1861	-1.4654
N	-3.4818	4.1285	0.2719
C	-2.3259	3.3089	0.3100
C	-3.3047	5.5323	-0.1192
H	-4.1849	6.1487	0.0972
H	-3.1009	5.6158	-1.1934
H	-2.4812	5.9941	0.4385
H	-8.4223	2.3909	-0.7076
C	-2.3988	2.0364	0.9095
C	-1.2871	1.1915	0.9864
C	-0.0657	1.6036	0.4671
C	0.0405	2.8589	-0.1227
C	-1.0761	3.7017	-0.1959
H	-0.9414	4.6651	-0.6772
H	0.8010	0.9511	0.5251
H	0.9929	3.1879	-0.5301
H	-3.3378	1.6980	1.3429
H	-1.3811	0.2170	1.4576

4-methylcarboxy-N,N-dimethylaniline

C	-5.8705	4.4893	0.0672
C	-7.1883	4.0053	0.0895
C	-7.4458	2.6539	-0.1419
C	-6.3720	1.8017	-0.3995
C	-5.0604	2.2982	-0.4158
C	-4.7664	3.6517	-0.1701
H	-5.7366	5.5504	0.2561
H	-7.9971	4.7038	0.2880
H	-6.5430	0.7454	-0.5983
H	-4.2692	1.5922	-0.6509
N	-3.4508	4.1300	-0.2081
C	-2.3892	3.2176	0.2214
C	-3.1930	5.5472	0.0362
H	-3.7750	6.1807	-0.6423
H	-2.1413	5.7893	-0.1543
H	-3.4165	5.8160	1.0744
H	-2.2628	2.3911	-0.4853
H	-2.5935	2.8177	1.2211
H	-1.4206	3.7287	0.2645
C	-8.8191	2.0817	-0.1328
O	-9.7375	3.0440	0.1357
C	-11.0836	2.5678	0.1626
H	-11.7378	3.4147	0.3872
H	-11.2090	1.8157	0.9479
H	-11.3662	2.1613	-0.8136
O	-9.0608	0.9028	-0.3388

2-methylindole

C	-6.1551	4.1166	0.0000
C	-7.3430	3.3787	0.0000
C	-7.3235	1.9854	0.0000
C	-6.1094	1.2885	0.0000
C	-4.9005	2.0104	0.0000
C	-4.9503	3.4035	0.0000
H	-6.1738	5.2012	0.0000
H	-8.2966	3.9016	0.0000
H	-8.2590	1.4317	0.0000
H	-6.1015	0.2028	0.0000
C	-3.5271	1.6413	0.0000
C	-2.7732	2.7970	0.0000
N	-3.6499	3.8545	0.0000
H	-3.1353	0.6325	0.0000
C	-1.3047	3.0004	0.0000

H	-3.3860	4.8297	0.0000
H	-0.7756	2.0421	0.0000
H	-0.9938	3.5594	0.8884
H	-0.9938	3.5594	-0.8884

4-trifluoromethyl-N,N-dimethylaniline

C	-5.9629	4.1708	0.0000
C	-7.1977	3.4989	0.0000
C	-7.3086	2.0963	0.0000
C	-6.0786	1.4129	0.0000
C	-4.8349	2.0692	0.0000
C	-4.7634	3.4605	0.0000
H	-5.9541	5.2599	0.0000
H	-8.0731	4.1380	0.0000
H	-6.0307	0.3301	0.0000
H	-3.9251	1.4706	0.0000
C	-3.4444	4.1870	0.0000
F	-2.3628	3.3579	0.0000
F	-3.2926	4.9945	1.0869
F	-3.2926	4.9945	-1.0869
N	-8.5305	1.4408	0.0000
C	-9.8213	2.1318	0.0000
C	-8.6689	-0.0168	0.0000
H	-9.7815	3.2206	0.0000
H	-10.3961	1.8379	0.8858
H	-10.3961	1.8379	-0.8858
H	-7.7397	-0.5859	0.0000
H	-9.2316	-0.3331	-0.8858
H	-9.2316	-0.3331	0.8858

indole

C	-6.0526	4.1986	0.0000
C	-7.2288	3.4424	0.0000
C	-7.1881	2.0495	0.0000
C	-5.9637	1.3710	0.0000
C	-4.7656	2.1109	0.0000
C	-4.8369	3.5043	0.0000
H	-6.0883	5.2828	0.0000
H	-8.1905	3.9506	0.0000
H	-8.1152	1.4818	0.0000
H	-5.9398	0.2855	0.0000
C	-3.3867	1.7620	0.0000
C	-2.6581	2.9296	0.0000
N	-3.5432	3.9752	0.0000
H	-2.9752	0.7614	0.0000
H	-1.5910	3.1059	0.0000
H	-3.2906	4.9535	0.0000

1,3,5-trimethoxybenzene

C	-9.9735	0.9574	0.8105
C	-9.7267	-0.2003	0.0727
O	-8.5364	-0.8739	0.0086
C	-10.7558	-0.7645	-0.6879
C	-12.0213	-0.1784	-0.7123
C	-12.2570	0.9822	0.0314
C	-11.2383	1.5538	0.7937
H	-13.2510	1.4151	-0.0073
O	-11.3453	2.6833	1.5602
H	-10.5338	-1.6648	-1.2511
O	-13.1045	-0.6343	-1.4147
H	-9.2014	1.4248	1.4125
C	-7.4558	-0.3410	0.7649
H	-6.5873	-0.9878	0.6076
H	-7.6838	-0.3447	1.8359
H	-7.1896	0.6634	0.4193
C	-12.9178	-1.8131	-2.1887
H	-13.8670	-2.0419	-2.6828
H	-12.6597	-2.6663	-1.5526
H	-12.1655	-1.6580	-2.9691
C	-12.6125	3.3294	1.5777
H	-12.5318	4.2050	2.2289
H	-13.3841	2.6741	1.9953

H	-12.8897	3.6821	0.5787

1,3-dimethoxybenzene

C	-10.0224	1.0538	0.8636
C	-9.7791	-0.1042	0.1244
O	-8.5898	-0.7796	0.0595
C	-10.8106	-0.6683	-0.6375
C	-12.0778	-0.0838	-0.6647
C	-12.3090	1.0745	0.0787
C	-11.2879	1.6425	0.8401
H	-13.2929	1.5368	0.0637
H	-11.4799	2.5447	1.4150
H	-10.5883	-1.5686	-1.2005
O	-13.1605	-0.5383	-1.3668
H	-9.2524	1.5227	1.4666
C	-7.5066	-0.2483	0.8122
H	-6.6394	-0.8963	0.6528
H	-7.7316	-0.2510	1.8838
H	-7.2399	0.7557	0.4656
C	-12.9734	-1.7171	-2.1402
H	-13.9222	-1.9459	-2.6350
H	-12.7159	-2.5702	-1.5039
H	-12.2204	-1.5624	-2.9200

Diphenyl ether

C	-10.0660	1.0154	0.8203
C	-9.7853	-0.1294	0.0699
O	-8.5594	-0.7549	0.0971
C	-10.7880	-0.7349	-0.6883
C	-12.0642	-0.1727	-0.7294
C	-12.3401	0.9844	0.0000
C	-11.3434	1.5760	0.7772
H	-13.3353	1.4208	-0.0302
H	-11.5628	2.4700	1.3550
H	-10.5730	-1.6403	-1.2489
H	-12.8440	-0.6391	-1.3258
H	-9.3006	1.4707	1.4423
C	-7.4425	0.0358	-0.0514
C	-6.3744	-0.2092	0.8122
C	-5.1984	0.5318	0.6916
C	-5.0864	1.5049	-0.3021
C	-6.1462	1.7328	-1.1809
C	-7.3235	0.9927	-1.0626
H	-8.1371	1.1626	-1.7622
H	-6.4609	-0.9730	1.5799
H	-4.3686	0.3472	1.3687
H	-4.1690	2.0803	-0.3975
H	-6.0532	2.4822	-1.9626

Quinoxaline

C	-7.3878	-0.2547	0.0488
C	-7.4267	1.1141	-0.1203
N	-8.5879	1.7962	-0.2175
C	-9.7188	1.0659	-0.1405
C	-9.6788	-0.3412	0.0333
N	-8.5083	-1.0039	0.1282
C	-10.8746	-1.0456	0.1064
C	-12.1076	-0.3979	0.0126
C	-12.1467	0.9799	-0.1575
C	-10.9527	1.6989	-0.2325
H	-13.0996	1.4976	-0.2322
H	-10.9812	2.7776	-0.3656
H	-10.8418	-2.1242	0.2396
H	-13.0295	-0.9708	0.0726
H	-6.4495	-0.7916	0.1256
H	-6.5205	1.7052	-0.1827

Phenazine

C	-7.3802	-0.2710	0.0505
C	-7.4198	1.1307	-0.1218
N	-8.5882	1.7910	-0.2166
C	-9.7173	1.0634	-0.1403

C	-9.6775	-0.3382	0.0326
N	-8.5093	-0.9985	0.1269
C	-6.1472	-0.9059	0.1426
C	-6.2242	1.8361	-0.1939
C	-4.9910	1.1892	-0.1000
C	-4.9523	-0.1885	0.0688
H	-3.9999	-0.7071	0.1435
H	-6.1198	-1.9848	0.2748
H	-6.2572	2.9148	-0.3262
H	-4.0691	1.7622	-0.1590
C	-10.8727	-1.0440	0.1063
C	-12.1061	-0.3977	0.0129
C	-12.1454	0.9797	-0.1576
C	-10.9508	1.6976	-0.2326
H	-13.0981	1.4977	-0.2323
H	-10.9788	2.7764	-0.3660
H	-10.8390	-2.1226	0.2398
H	-13.0277	-0.9711	0.0734

Pyrazine

C	-7.5020	-0.2937	0.0494
C	-7.6073	1.0816	-0.0783
N	-8.8008	1.7134	-0.1571
C	-9.8841	0.9051	-0.1023
C	-9.7788	-0.4702	0.0253
N	-8.5853	-1.1020	0.1042
H	-6.5379	-0.7850	0.1113
H	-6.7293	1.7157	-0.1208
H	-10.8482	1.3964	-0.1642
H	-10.6568	-1.1043	0.0679

Acridine

C	-7.4837	-0.2990	0.0502
C	-7.5381	1.1020	-0.0790
C	-8.7999	1.7014	-0.1559
C	-9.9555	0.9146	-0.1044
C	-9.7961	-0.4783	0.0258
N	-8.5882	-1.0642	0.1007
H	-8.8825	2.7808	-0.2561
C	-10.9391	-1.2652	0.0773
C	-12.2203	-0.7099	0.0038
C	-12.3715	0.6658	-0.1245
C	-11.2418	1.4792	-0.1788
H	-13.3645	1.1039	-0.1822
H	-11.3679	2.5547	-0.2793
H	-10.8282	-2.3424	0.1777
H	-13.0934	-1.3558	0.0472
C	-6.2344	-0.9005	0.1272
C	-6.3530	1.8582	-0.1274
C	-5.1128	1.2285	-0.0481
C	-5.0528	-0.1543	0.0795
H	-4.0918	-0.6579	0.1425
H	-6.1801	-1.9820	0.2271
H	-6.3921	2.9404	-0.2272
H	-4.1982	1.8145	-0.0858

Quinoline

C	-7.7205	-0.3552	0.0669
C	-7.7449	1.0224	-0.0397
C	-8.9830	1.6480	-0.1179
C	-10.1546	0.8799	-0.0872
C	-10.0250	-0.5214	0.0245
N	-8.8273	-1.1296	0.1002
H	-9.0307	2.7303	-0.2023
H	-6.7797	-0.8946	0.1307
H	-6.8244	1.5941	-0.0614
C	-11.1840	-1.2855	0.0562
C	-12.4526	-0.7023	-0.0199
C	-12.5747	0.6782	-0.1306
C	-11.4287	1.4701	-0.1643
H	-13.5582	1.1369	-0.1905
H	-11.5326	2.5491	-0.2510

H	-11.0956	-2.3658	0.1425
H	-13.3392	-1.3304	0.0078

Pyridine

C	-7.6016	-0.3733	0.0000
C	-7.6723	1.0107	0.0000
C	-8.9298	1.6053	0.0000
C	-10.0640	0.8000	0.0000
C	-9.8916	-0.5751	0.0000
N	-8.6843	-1.1811	0.0000
H	-10.7458	-1.2461	0.0000
H	-11.0580	1.2323	0.0000
H	-9.0252	2.6872	0.0000
H	-6.6433	-0.8846	0.0000
H	-6.7692	1.6102	0.0000

p-phenanthroline

C	-6.3987	1.7681	0.0000
C	-5.1625	1.0847	0.0000
C	-5.1685	-0.2957	0.0000
C	-6.3608	-1.0217	0.0000
C	-7.5899	-0.3935	0.0000
C	-7.6297	1.0185	0.0000
H	-4.2207	-0.8291	0.0000
H	-6.3219	-2.1086	0.0000
C	-8.9218	1.5939	0.0000
C	-10.0632	0.7985	0.0000
C	-9.8944	-0.5681	0.0000
N	-8.6879	-1.1685	0.0000
H	-10.7470	-1.2410	0.0000
H	-11.0544	1.2371	0.0000
C	-6.3169	3.1802	0.0000
C	-5.0863	3.8292	0.0000
C	-3.9496	3.0519	0.0000
N	-3.9699	1.7045	0.0000
H	-2.9605	3.5006	0.0000
H	-5.0209	4.9111	0.0000
H	-9.0576	2.6710	0.0000
H	-7.2114	3.7953	0.0000

m-phenanthroline

C	-6.3671	1.7394	0.0000
C	-5.1493	1.0247	0.0000
C	-5.1496	-0.3734	0.0000
C	-6.3555	-1.0698	0.0000
C	-7.5688	-0.4076	0.0000
C	-7.5718	1.0045	0.0000
H	-4.2173	-0.9332	0.0000
H	-6.3489	-2.1574	0.0000
C	-8.8323	1.6327	0.0000
C	-10.0004	0.8802	0.0000
C	-9.8790	-0.4937	0.0000
N	-8.6949	-1.1430	0.0000
H	-10.7567	-1.1336	0.0000
H	-10.9740	1.3560	0.0000
N	-6.3687	3.0952	0.0000
C	-5.1891	3.7539	0.0000
C	-3.9611	3.1275	0.0000
C	-3.9440	1.7403	0.0000
H	-3.0423	3.7022	0.0000
H	-2.9888	1.2209	0.0000
H	-5.2660	4.8375	0.0000
H	-8.8987	2.7193	0.0000

o-phenanthroline

C	-6.3369	1.5580	0.0000
C	-5.1378	0.9297	0.0000
C	-5.1665	-0.4187	0.0000
C	-6.3324	-1.1685	0.0000
C	-7.5631	-0.5011	0.0000
C	-7.5738	0.9078	0.0000
H	-4.1932	-0.9015	0.0000

H	-6.2759	-2.2516	0.0000
N	-8.8000	1.5965	0.0000
C	-10.0048	0.8927	0.0000
C	-9.9970	-0.5003	0.0000
C	-8.7850	-1.1943	0.0000
H	-10.9357	-1.0487	0.0000
H	-8.8013	-2.2820	0.0000
H	-10.9491	1.4312	0.0000
N	-6.2955	3.2450	0.0000
C	-5.0699	3.8123	0.0000
C	-4.1207	3.1726	0.0000
C	-3.9525	1.8810	0.0000
H	-3.2428	3.7152	0.0000
H	-2.9950	1.4959	0.0000
H	-4.9877	4.8410	0.0000

Isoquinoline

C	-6.3369	1.5580	0.0000
N	-5.1378	0.9297	0.0000
C	-5.1665	-0.4187	0.0000
C	-6.3324	-1.1685	0.0000
C	-7.5631	-0.5011	0.0000
C	-7.5738	0.9078	0.0000
H	-4.1932	-0.9015	0.0000
H	-6.2759	-2.2516	0.0000
C	-8.8000	1.5965	0.0000
C	-10.0048	0.8927	0.0000
C	-9.9970	-0.5003	0.0000
C	-8.7850	-1.1943	0.0000
H	-10.9357	-1.0487	0.0000
H	-8.8013	-2.2820	0.0000
H	-8.8211	2.6839	0.0000
H	-10.9491	1.4312	0.0000
H	-6.2736	2.6430	0.0000

Benzo[h]quinoline

C	-5.1389	3.6627	0.0000
N	-6.3249	3.0167	0.0000
C	-6.3395	1.6603	0.0000
C	-5.1275	0.9319	0.0000
C	-3.9156	1.6365	0.0000
C	-3.9178	3.0238	0.0000
H	-2.9931	3.5887	0.0000
H	-5.2049	4.7468	0.0000
C	-5.1333	-0.4688	0.0000
C	-6.3361	-1.1677	0.0000
C	-7.5520	-0.4795	0.0000
C	-7.5538	0.9388	0.0000
H	-4.1999	-1.0272	0.0000
H	-6.3145	-2.2553	0.0000
C	-8.8041	1.5936	0.0000
C	-10.0059	0.8824	0.0000
C	-9.9873	-0.5065	0.0000
C	-8.7682	-1.1835	0.0000
H	-10.9201	-1.0640	0.0000
H	-8.7754	-2.2714	0.0000
H	-8.8415	2.6825	0.0000
H	-10.9515	1.4180	0.0000
H	-2.9655	1.1079	0.0000

Benzo[f]quinoline

C	-5.0266	3.7448	0.0000
C	-6.2644	3.1095	0.0000
C	-6.3650	1.6986	0.0000
C	-5.1343	1.0010	0.0000
N	-3.9342	1.6080	0.0000
C	-3.8991	2.9549	0.0000
H	-7.1511	3.7356	0.0000
H	-2.9052	3.3926	0.0000
H	-4.9498	4.8258	0.0000
C	-5.1470	-0.3805	0.0000
C	-6.3378	-1.1050	0.0000

C	-7.5691	-0.4480	0.0000
C	-7.6073	0.9681	0.0000
H	-4.1992	-0.9143	0.0000
H	-6.2861	-2.1917	0.0000
C	-8.8905	1.5714	0.0000
C	-10.0674	0.8167	0.0000
C	-10.0009	-0.5684	0.0000
C	-8.7583	-1.1964	0.0000
H	-10.9119	-1.1608	0.0000
H	-8.7245	-2.2842	0.0000
H	-8.9976	2.6525	0.0000
H	-11.0328	1.3163	0.0000

Pyrimidine

N	-4.9659	3.8693	0.0000
C	-6.1335	3.1994	0.0000
C	-6.2223	1.8264	0.0000
C	-5.0227	1.1525	0.0000
N	-3.8247	1.7662	0.0000
C	-3.8602	3.1081	0.0000
H	-7.0246	3.8202	0.0000
H	-7.1720	1.3110	0.0000
H	-4.9880	0.0670	0.0000
H	-2.9072	3.6253	0.0000

Pyridazine

C	-15.6600	-0.5057	-0.3623
C	-15.5643	0.8632	-0.2028
C	-14.2979	1.4215	-0.1139
C	-13.2088	0.5749	-0.1902
N	-13.3343	-0.7589	-0.3463
N	-14.5774	-1.3069	-0.4335
H	-16.6168	-1.0090	-0.4388
H	-16.4547	1.4787	-0.1492
H	-14.1621	2.4894	0.0117
H	-12.1911	0.9421	-0.1282

Phenanthridine

C	-8.6153	1.2445	0.0000
N	-7.2666	1.2814	0.0000
C	-9.3781	0.0829	0.0000
C	-8.6948	-1.1511	0.0000
C	-7.2589	-1.1414	0.0000
C	-6.6084	0.1156	0.0000
C	-9.4964	-2.3212	0.0000
C	-10.7847	0.1350	0.0000
C	-11.5387	-1.0348	0.0000
C	-10.8942	-2.2639	0.0000
H	-11.4743	-3.1833	0.0000
H	-9.0410	-3.3076	0.0000
H	-11.3009	1.0929	0.0000
H	-12.6243	-0.9859	0.0000
C	-6.4474	-2.3060	0.0000
C	-5.0540	-2.2299	0.0000
C	-4.4381	-0.9891	0.0000
C	-5.2208	0.1654	0.0000
H	-3.3544	-0.9114	0.0000
H	-4.7330	1.1379	0.0000
H	-6.8935	-3.2963	0.0000
H	-4.4570	-3.1382	0.0000
H	-9.0845	2.2254	0.0000

Phthalazine

C	-8.6029	1.2612	0.0000
N	-7.2518	1.2346	0.0000
C	-9.3920	0.1142	0.0000
C	-8.7293	-1.1227	0.0000
C	-7.3373	-1.1011	0.0000
N	-6.6109	0.0385	0.0000
C	-9.4799	-2.3126	0.0000
C	-10.7984	0.1484	0.0000
C	-11.5333	-1.0386	0.0000

C	-10.8752	-2.2669	0.0000
H	-11.4491	-3.1905	0.0000
H	-8.9820	-3.2799	0.0000
H	-11.3280	1.0987	0.0000
H	-12.6202	-1.0048	0.0000
H	-6.7480	-2.0115	0.0000
H	-9.0345	2.2561	0.0000

Cinnoline

N	-8.6542	1.2699	0.0000
N	-7.2837	1.2460	0.0000
C	-9.3639	0.1286	0.0000
C	-8.7161	-1.1200	0.0000
C	-7.3190	-1.1390	0.0000
C	-6.6445	0.0641	0.0000
C	-9.4719	-2.3064	0.0000
C	-10.7545	0.1548	0.0000
C	-11.5083	-1.0221	0.0000
C	-10.8650	-2.2548	0.0000
H	-11.4457	-3.1739	0.0000
H	-8.9791	-3.2761	0.0000
H	-11.2613	1.1171	0.0000
H	-12.5942	-0.9708	0.0000
H	-6.7638	-2.0704	0.0000
H	-5.5622	0.1169	0.0000

Benzo[c]cinnoline

N	-8.6715	1.2442	0.0000
N	-7.3006	1.2501	0.0000
C	-9.3532	0.0955	0.0000
C	-8.6920	-1.1468	0.0000
C	-7.2595	-1.1406	0.0000
C	-6.6090	0.1074	0.0000
C	-9.4946	-2.3185	0.0000
C	-10.7434	0.1410	0.0000
C	-11.5168	-1.0188	0.0000
C	-10.8892	-2.2541	0.0000
H	-11.4785	-3.1678	0.0000
H	-9.0414	-3.3060	0.0000
H	-11.2365	1.1110	0.0000
H	-12.6015	-0.9513	0.0000
C	-6.4468	-2.3053	0.0000
C	-5.0527	-2.2289	0.0000
C	-4.4358	-0.9882	0.0000
C	-5.2192	0.1649	0.0000
H	-3.3518	-0.9113	0.0000
H	-4.7345	1.1390	0.0000
H	-6.8914	-3.2967	0.0000
H	-4.4556	-3.1375	0.0000

Phenanthrene

C	-8.6823	1.3099	0.0000
C	-7.2903	1.3159	0.0000
C	-9.3937	0.1075	0.0000
C	-8.6964	-1.1282	0.0000
C	-7.2552	-1.1220	0.0000
C	-6.5686	0.1197	0.0000
H	-9.2070	2.2630	0.0000
H	-6.7739	2.2735	0.0000
C	-9.4893	-2.3042	0.0000
C	-10.7989	0.1361	0.0000
C	-11.5422	-1.0410	0.0000
C	-10.8870	-2.2626	0.0000
H	-11.4571	-3.1879	0.0000
H	-9.0265	-3.2867	0.0000
H	-11.3298	1.0861	0.0000
H	-12.6279	-1.0014	0.0000
C	-6.4522	-2.2910	0.0000
C	-5.0549	-2.2374	0.0000
C	-4.4103	-1.0102	0.0000
C	-5.1637	0.1605	0.0000
H	-3.3250	-0.9612	0.0000

H	-4.6410	1.1149	0.0000
H	-6.9065	-3.2776	0.0000
H	-4.4768	-3.1578	0.0000

Anthracene

C	-5.5755	3.0705	0.0000
C	-6.8082	2.4159	0.0000
C	-6.8563	1.0254	0.0000
C	-5.6718	0.2872	0.0000
C	-4.4233	0.9312	0.0000
C	-4.3745	2.3418	0.0000
C	-3.1263	2.9865	0.0000
C	-3.2226	0.2018	0.0000
C	-1.9744	0.8465	0.0000
C	-1.9256	2.2571	0.0000
H	-3.2602	-0.8859	0.0000
H	-7.8151	0.5136	0.0000
H	-5.7299	-0.7989	0.0000
H	-7.7293	2.9927	0.0000
H	-3.0887	4.0742	0.0000
H	-5.5585	4.1580	0.0000
C	-0.6771	2.9011	0.0000
C	-0.7734	0.1178	0.0000
C	0.4593	0.7724	0.0000
C	0.5074	2.1629	0.0000
H	1.4662	2.6747	0.0000
H	-0.6190	3.9872	0.0000
H	-0.7904	-0.9697	0.0000
H	1.3804	0.1955	0.0000

Acenaphthylene

C	-6.0835	3.2049	0.0000
C	-7.3543	2.6444	0.0000
C	-7.4201	1.2359	0.0000
C	-6.2618	0.4279	0.0000
C	-4.9856	1.0211	0.0000
C	-4.9629	2.3855	0.0000
C	-3.8157	3.1672	0.0000
C	-3.7298	0.3858	0.0000
C	-2.5453	1.1548	0.0000
C	-2.5643	2.5648	0.0000
H	-1.5847	0.6426	0.0000
H	-1.6542	3.1522	0.0000
H	-3.6651	-0.6990	0.0000
H	-8.3973	0.7559	0.0000
H	-6.3627	-0.6541	0.0000
H	-8.2443	3.2618	0.0000
C	-5.6039	4.6363	0.0000
C	-4.2474	4.6138	0.0000
H	-6.2434	5.5048	0.0000
H	-3.5795	5.4605	0.0000

4-methylacetophenone

C	-5.1156	3.3507	-0.0283
C	-6.3674	2.7510	-0.0332
C	-6.4948	1.3594	-0.0218
C	-5.3304	0.5854	-0.0058
C	-4.0755	1.1798	-0.0006
C	-3.9558	2.5731	-0.0112
H	-5.0233	4.4307	-0.0367
H	-7.2598	3.3687	-0.0450
H	-5.4114	-0.4973	0.0040
H	-3.1924	0.5507	0.0122
C	-7.8473	0.6975	-0.0305
H	-8.5279	1.3763	0.9765
H	-7.6987	-0.7099	-0.0236
H	-8.5457	1.3528	-1.1037
C	-2.6269	3.2616	-0.0025
C	-1.3783	2.4149	0.0147
H	-1.3610	1.7754	0.9005
H	-0.5055	3.0646	0.0173
H	-1.3459	1.7617	-0.8607

O	-2.5611	4.4742	-0.0083

Trans-stilbene

C	-6.5054	0.4371	-0.0763
C	-7.7051	-0.2577	0.0630
C	-7.7010	-1.6505	0.0911
C	-6.4954	-2.3488	-0.0151
C	-5.2807	-1.6616	-0.1382
C	-5.2996	-0.2613	-0.1816
H	-8.6427	0.2859	0.1440
H	-8.6358	-2.1952	0.1943
H	-6.5069	1.5234	-0.1090
H	-6.5126	-3.4360	0.0086
C	-4.0384	-2.4348	-0.2779
H	-4.3782	0.3010	-0.3100
C	-2.8691	-2.0767	0.2775
H	-4.1198	-3.3445	-0.8677
C	-1.6268	-2.8498	0.1378
H	-2.7878	-1.1670	0.8673
C	-1.6079	-4.2501	0.1809
C	-0.4020	-4.9485	0.0756
C	0.7976	-4.2537	-0.0633
C	0.7935	-2.8609	-0.0911
C	-0.4121	-2.1626	0.0151
H	-2.5293	-4.8126	0.3090
H	-0.4005	-6.0348	0.1080
H	1.7353	-4.7972	-0.1443
H	1.7283	-2.3162	-0.1940
H	-0.3949	-1.0754	-0.0084

2,3,5-trimethylcyclohexa-2,5-diene-1,4-dione

C	-5.1674	3.4319	0.0487
C	-5.2741	2.0937	0.0031
C	-4.0450	1.2469	-0.0439
C	-2.7005	1.8966	-0.0884
C	-2.5932	3.2346	-0.0374
C	-3.8227	4.0817	0.0089
C	-6.3615	4.3362	0.1038
C	-1.5097	0.9885	-0.1491
C	-1.2693	3.9405	-0.0458
O	-3.7324	5.2941	0.0109
O	-4.1344	0.0344	-0.0415
H	-0.5934	3.5073	0.6943
H	-1.3951	4.9994	0.1661
H	-0.7887	3.8419	-1.0235
H	-6.8134	4.4282	-0.8892
H	-6.0773	5.3324	0.4352
H	-7.1237	3.9372	0.7745
H	-1.7894	0.0101	-0.5345
H	-1.0908	0.8450	0.8524
H	-0.7241	1.4123	-0.7763
H	-6.2060	1.6505	0.0006

2,3,5,6-tetramethylcyclohexa-2,5-diene-1,4-dione

C	-5.1430	3.4361	0.0153
C	-5.2329	2.0964	-0.0104
C	-3.9977	1.2572	-0.0408
C	-2.6489	1.9037	-0.0416
C	-2.5591	3.2432	-0.0104
C	-3.7940	4.0824	0.0185
C	-6.3337	4.3508	0.0499
C	-6.5226	1.3341	-0.0039
C	-1.4572	0.9906	-0.0803
C	-1.2688	4.0045	-0.0104
O	-3.6925	5.2938	0.0388
O	-4.0992	0.0457	-0.0601
H	-0.6363	3.5249	0.7861
H	-1.6573	5.1783	0.0433
H	-1.1852	3.6537	-0.9424
H	-6.7022	4.5228	-1.0212
H	-5.9736	5.4708	0.5205
H	-7.1793	3.9527	0.9141

H	-1.8117	-0.0861	-0.5677
H	-1.1112	0.6804	0.8808
H	-0.6396	1.3865	-0.9431
H	-7.3751	1.8019	-0.8405
H	-7.0269	1.5447	0.9983
H	-6.3858	0.2592	-0.1288

Naphthalene

C	-7.5703	3.1927	0.0000
C	-7.5576	1.8010	0.0000
C	-6.3422	1.1143	0.0000
C	-5.1234	1.8121	0.0000
C	-5.1364	3.2262	0.0000
C	-6.3678	3.9015	0.0000
C	-3.9176	3.9240	0.0000
C	-3.8920	1.1368	0.0000
C	-2.6895	1.8456	0.0000
C	-2.7023	3.2374	0.0000
H	-1.7666	3.7903	0.0000
H	-3.9073	5.0115	0.0000
H	-3.8618	0.0497	0.0000
H	-1.7439	1.3099	0.0000
H	-6.3525	0.0268	0.0000
H	-8.5159	3.7284	0.0000
H	-8.4932	1.2480	0.0000
H	-6.3980	4.9887	0.0000

Ethyl benzoate

C	-5.2498	3.3765	-0.0172
C	-6.4762	2.7090	-0.0069
C	-6.5109	1.3154	0.0128
C	-5.3219	0.5867	0.0222
C	-4.0927	1.2509	0.0118
C	-4.0496	2.6520	-0.0080
H	-5.2333	4.4648	-0.0325
H	-7.4032	3.2771	-0.0142
H	-5.3514	-0.5001	0.0376
H	-3.1782	0.6632	0.0195
C	-2.7702	3.4125	-0.0200
O	-1.7098	2.5662	-0.0142
C	-0.4360	3.2217	-0.0263
O	-2.7092	4.6319	-0.0336
H	-7.4664	0.7963	0.0208
H	-0.3368	3.8538	0.8633
H	-0.3446	3.8364	-0.9288
C	0.6432	2.1567	-0.0207
H	0.5520	1.5202	0.8657
H	1.6385	2.6096	-0.0297
H	0.5440	1.5030	-0.8936

Methyl benzoate

C	-5.1689	3.3611	-0.0174
C	-6.4102	2.7216	-0.0085
C	-6.4765	1.3292	0.0114
C	-5.3044	0.5738	0.0225
C	-4.0603	1.2099	0.0135
C	-3.9854	2.6096	-0.0067
H	-5.1278	4.4487	-0.0330
H	-7.3240	3.3107	-0.0171
H	-5.3585	-0.5121	0.0381
H	-3.1594	0.6015	0.0225
C	-2.6891	3.3411	-0.0175
O	-1.6470	2.4721	-0.0137
C	-0.3662	3.1038	-0.0258
O	-2.6015	4.5591	-0.0293
H	-7.4436	0.8319	0.0183
H	-0.2341	3.7205	0.8687
H	-0.2428	3.7035	-0.9331
H	0.3974	2.3210	-0.0222

Propiophenone

C	-5.1910	3.3239	-0.0166

C	-6.4544	2.7295	-0.0104
C	-6.5701	1.3413	0.0095
C	-5.4246	0.5469	0.0233
C	-4.1578	1.1386	0.0171
C	-4.0327	2.5336	-0.0032
H	-5.1144	4.4099	-0.0321
H	-7.3459	3.3517	-0.0211
H	-5.5183	-0.5365	0.0391
H	-3.2893	0.4874	0.0287
C	-2.7032	3.2193	-0.0112
C	-1.4457	2.3663	-0.0088
H	-1.4412	1.7466	0.8941
C	-0.1787	3.2067	-0.0305
H	-1.4543	1.7215	-0.8939
O	-2.6614	4.4482	-0.0194
H	-7.5540	0.8784	0.0143
H	-0.1257	3.8614	0.8458
H	-0.1407	3.8381	-0.9243
H	0.7057	2.5621	-0.0295

Acetophenone

C	-5.1109	3.3521	-0.0174
C	-6.3727	2.7546	-0.0121
C	-6.4851	1.3659	0.0077
C	-5.3378	0.5738	0.0224
C	-4.0725	1.1683	0.0170
C	-3.9520	2.5635	-0.0032
H	-5.0356	4.4381	-0.0329
H	-7.2659	3.3745	-0.0234
H	-5.4291	-0.5098	0.0382
H	-3.2011	0.5207	0.0294
C	-2.6252	3.2492	-0.0100
C	-1.3720	2.4132	-0.0095
H	-1.3200	1.8090	0.8998
H	-0.4995	3.0739	-0.0280
H	-1.3364	1.7823	-0.9014
O	-2.5680	4.4774	-0.0157
H	-7.4680	0.9007	0.0119

Benzophenone

C	-6.2855	0.2826	-0.0002
C	-7.6240	-0.1235	0.0000
C	-7.9334	-1.4752	0.0001
C	-6.9036	-2.4088	0.0000
C	-5.5606	-1.9964	-0.0002
C	-5.2174	-0.6429	-0.0003
H	-8.4156	0.6214	0.0001
H	-8.9702	-1.8004	0.0002
H	-6.0837	1.3539	-0.0002
H	-7.1413	-3.4706	0.0001
H	-4.8409	-2.7941	-0.0003
C	-3.8357	-0.0485	-0.0005
C	-2.4943	-0.7290	-0.0003
C	-2.2372	-2.1014	-0.0002
C	-0.9229	-2.5979	0.0000
C	0.1637	-1.7312	0.0001
C	-0.0597	-0.3626	0.0001
C	-1.3699	0.1272	-0.0001
H	-3.0058	-2.8521	-0.0004
H	-0.7528	-3.6725	0.0000
H	1.1780	-2.1212	0.0002
H	0.7775	0.3308	0.0001
H	-1.5036	1.2091	-0.0002
O	-3.7965	1.1896	-0.0010

Diethyl terephthalate

C	-4.6604	3.0959	0.3001
C	-6.0547	3.1029	0.1792
C	-6.7456	1.9108	-0.0756
C	-6.0259	0.7147	-0.2052
C	-4.6315	0.7079	-0.0855
C	-3.9404	1.9003	0.1671

H	-4.1376	4.0308	0.4979
H	-6.5854	4.0462	0.2868
H	-6.5488	-0.2204	-0.4020
H	-4.1010	-0.2357	-0.1919
C	-2.4586	1.9536	0.3018
C	-8.2269	1.8585	-0.2160
O	-1.8417	2.9775	0.5493
O	-1.9165	0.7262	0.1070
O	-8.8491	0.8250	-0.4032
O	-8.7608	3.1005	-0.1138
C	-10.1870	3.1396	-0.2475
C	-10.6321	4.5849	-0.1394
H	-10.6485	2.5487	0.5517
H	-10.4794	2.7347	-1.2228
H	-10.3279	5.0111	0.8224
H	-11.7183	4.6670	-0.2348
H	-10.1615	5.1922	-0.9197
C	-0.4878	0.6919	0.2118
C	-0.0293	-0.7299	-0.0478
H	-0.1840	1.0014	1.2180
H	-0.0454	1.3646	-0.5315
H	-0.4803	-1.4183	0.6745
H	1.0593	-0.8077	0.0218
H	-0.3448	-1.0608	-1.0428

Diethyl fumarate

C	-3.5764	0.6573	0.0375
C	-2.6031	1.5497	0.2619
C	-4.9698	1.0203	0.3413
H	-3.3854	-0.3324	-0.3611
C	-1.2095	1.1860	-0.0404
H	-2.7940	2.5391	0.6613
O	-0.8490	0.1147	-0.4981
O	-0.4194	2.2392	0.2787
O	-5.3319	2.0966	0.7861
O	-5.7575	-0.0407	0.0428
C	0.9747	2.0175	0.0342
C	1.7319	3.2654	0.4445
H	1.1360	1.8203	-1.0316
H	1.3230	1.1626	0.6247
H	1.3804	4.1337	-0.1226
H	2.8054	3.1438	0.2753
H	1.5637	3.4875	1.5035
C	-7.1506	0.1779	0.2954
C	-7.9027	-1.0865	-0.0715
H	-7.5103	1.0132	-0.3160
H	-7.3035	0.4045	1.3566
H	-7.7429	-1.3382	-1.1251
H	-8.9754	-0.9676	0.1047
H	-7.5395	-1.9355	0.5172

3,6-dioxocyclohexa-1,4-diene-1,2,4,5-tetracarbonitrile

C	-5.1461	3.4164	0.0374
C	-5.2494	2.0815	-0.0313
C	-4.0372	1.2323	-0.0882
C	-2.7087	1.8868	-0.0673
C	-2.6055	3.2217	0.0015
C	-3.8176	4.0709	0.0579
O	-3.7233	5.2900	0.1204
O	-4.1315	0.0133	-0.1513
C	-6.2924	4.2614	0.0934
C	-6.5121	1.4211	-0.0528
C	-1.5624	1.0418	-0.1229
C	-1.3427	3.8820	0.0234
N	-0.2968	4.3800	0.0390
N	-0.6054	0.3904	-0.1664
N	-7.2494	4.9128	0.1374
N	-7.5581	0.9232	-0.0680

3,6-dioxocyclohexa-1,4-diene-1,2-dicarbonitrile

C	-5.1186	3.4282	0.0211
C	-5.2247	2.1008	-0.0288

C	-4.0293	1.2399	-0.0717
C	-2.6989	1.8942	-0.0580
C	-2.5919	3.2330	-0.0076
C	-3.8014	4.0893	0.0354
O	-3.7440	5.3108	0.0817
O	-4.1667	0.0247	-0.1169
H	-5.9883	4.0759	0.0531
H	-6.1864	1.5988	-0.0400
C	-1.5577	1.0442	-0.1002
C	-1.3300	3.8919	0.0069
N	-0.2829	4.3896	0.0171
N	-0.6029	0.3873	-0.1335

2,3,5,6-tetrafluorocyclohexa-2,5-diene-1,4-dione

C	-5.0970	3.4242	0.0041
C	-5.1924	2.0983	-0.0161
C	-4.0015	1.2253	-0.0380
C	-2.6978	1.9192	-0.0362
C	-2.6024	3.2451	-0.0161
C	-3.7934	4.1181	0.0059
O	-3.7056	5.3385	0.0245
O	-4.0892	0.0049	-0.0565
F	-6.1919	4.2092	0.0240
F	-6.3884	1.4778	-0.0175
F	-1.6029	1.1341	-0.0562
F	-1.4064	3.8656	-0.0147

2,6-dimethylcyclohexa-2,5-diene-1,4-dione

C	-5.1043	3.3439	-0.0001
C	-5.1645	2.0058	0.0000
C	-3.9515	1.1705	0.0000
C	-2.6510	1.8617	0.0000
C	-2.5578	3.1978	-0.0001
C	-3.7870	4.0390	-0.0001
C	-6.3198	4.2169	-0.0001
H	-6.1047	1.4662	0.0000
H	-1.7787	1.2180	0.0000
C	-1.2504	3.9261	-0.0001
O	-3.7168	5.2629	-0.0002
O	-4.0216	-0.0510	0.0001
H	-0.3998	3.2361	-0.0001
H	-1.1632	4.5590	0.8892
H	-1.1632	4.5590	-0.8894
H	-7.2438	3.6287	-0.0001
H	-6.3341	4.8556	-0.8894
H	-6.3341	4.8557	0.8892

2-methylcyclohexa-2,5-diene-1,4-dione

C	-5.1663	3.4094	-0.0001
C	-5.2601	2.0773	0.0000
C	-4.0549	1.2294	0.0000
C	-2.7452	1.9096	0.0000
C	-2.6354	3.2455	-0.0001
C	-3.8574	4.0943	-0.0001
H	-6.0419	4.0476	-0.0001
H	-6.2141	1.5643	0.0000
H	-1.8801	1.2560	0.0000
C	-1.3227	3.9629	-0.0001
O	-3.8014	5.3176	-0.0002
O	-4.1371	0.0088	0.0001
H	-0.4779	3.2658	-0.0001
H	-1.2306	4.5952	0.8891
H	-1.2306	4.5951	-0.8893

Benzoquinone

C	-5.0663	3.4652	-0.0001
C	-5.1523	2.1315	0.0000
C	-3.9427	1.2848	0.0000
C	-2.6345	1.9692	0.0000
C	-2.5485	3.3029	-0.0001
C	-3.7581	4.1495	-0.0001
H	-5.9436	4.1007	-0.0001

H	-6.1039	1.6138	0.0000
H	-1.7572	1.3337	0.0000
H	-1.5969	3.8205	-0.0001
O	-3.6794	5.3702	-0.0002
O	-4.0214	0.0641	0.0000

4-methyl-1-naphthonitrile

C	-6.7874	3.5668	0.0000
C	-7.9855	2.9032	0.0000
C	-8.0105	1.4909	0.0000
C	-6.8416	0.7756	0.0000
C	-5.5754	1.4250	0.0000
C	-5.5627	2.8517	0.0000
C	-4.3042	3.5247	0.0000
C	-4.3352	0.7082	0.0000
C	-3.1510	1.4143	0.0000
C	-3.1229	2.8173	0.0000
C	-4.2612	4.9572	0.0000
C	-4.2511	-0.7980	0.0000
H	-2.2120	0.8706	0.0000
H	-8.9602	0.9682	0.0000
H	-6.8950	-0.3046	0.0000
H	-6.7678	4.6517	0.0000
H	-8.9140	3.4627	0.0000
H	-2.1759	3.3444	0.0000
N	-4.2238	6.1080	0.0000
H	-4.2607	-1.3700	1.1318
H	-3.1091	-0.9480	-0.6463
H	-5.2674	-1.2271	-0.7500

Anthracene-9,10-dicarbonitrile

C	-6.7672	3.5668	-0.0094
C	-8.0126	2.9407	-0.0338
C	-8.0817	1.5600	-0.0318
C	-6.9050	0.8128	-0.0053
C	-5.6211	1.4207	0.0200
C	-5.5504	2.8338	0.0179
C	-4.2717	3.4589	0.0431
C	-4.4112	0.6711	0.0472
C	-3.1326	1.2962	0.0725
C	-3.0618	2.7093	0.0704
C	-4.1996	4.8995	0.0408
H	-9.0465	1.0589	-0.0507
H	-7.0137	-0.2721	-0.0048
H	-6.7669	4.6571	-0.0121
H	-8.9226	3.5356	-0.0543
N	-4.1415	6.0592	0.0390
C	-1.7779	3.3172	0.0958
C	-1.9158	0.5632	0.0999
C	-0.6703	1.1893	0.1245
C	-0.6012	2.5700	0.1225
H	0.3636	3.0711	0.1415
H	-1.6693	4.4021	0.0954
H	-1.9160	-0.5271	0.1027
H	0.2396	0.5944	0.1452
C	-4.4834	-0.7696	0.0492
N	-4.5414	-1.9292	0.0508

1-naphthonitrile

C	-6.7891	3.5490	-0.0105
C	-8.0089	2.8695	-0.0327
C	-8.0285	1.4810	-0.0272
C	-6.8293	0.7705	0.0004
C	-5.5933	1.4373	0.0230
C	-5.5550	2.8544	0.0177
C	-4.2872	3.4921	0.0410
C	-4.3958	0.7046	0.0507
C	-3.1600	1.3476	0.0733
C	-3.1050	2.7371	0.0685
C	-4.1679	4.9236	0.0372
H	-8.9762	0.9489	-0.0444
H	-6.8685	-0.3171	0.0042

H	-6.8174	4.6379	-0.0157
H	-8.9413	3.4283	-0.0541
N	-4.0650	6.0800	0.0343
H	-4.4180	-0.3840	0.0549
H	-2.2429	0.7639	0.0947
H	-2.1350	3.2316	0.0863

Anthracene-9-carbonitrile

C	-6.7776	3.5481	-0.0102
C	-8.0002	2.8734	-0.0321
C	-8.0233	1.4863	-0.0270
C	-6.8247	0.7762	0.0000
C	-5.5870	1.4417	0.0226
C	-5.5409	2.8532	0.0177
C	-4.2651	3.4879	0.0413
C	-4.3942	0.7060	0.0502
C	-3.1385	1.3283	0.0742
C	-3.0536	2.7380	0.0702
C	-4.1984	4.9261	0.0358
H	-8.9716	0.9554	-0.0439
H	-6.8658	-0.3116	0.0036
H	-6.8075	4.6372	-0.0152
H	-8.9307	3.4354	-0.0530
N	-4.1445	6.0863	0.0312
C	-1.7579	3.3156	0.0957
C	-1.9677	0.5512	0.1025
C	-0.7085	1.1474	0.1274
C	-0.6031	2.5307	0.1240
H	0.3754	3.0042	0.1435
H	-1.6273	4.3972	0.0942
H	-2.0275	-0.5357	0.1056
H	0.1865	0.5311	0.1494
H	-4.4447	-0.3828	0.0535

Naphthalene-1,4-dicarbonitrile

C	-6.7947	3.5411	0.0000
C	-8.0178	2.8709	0.0000
C	-8.0429	1.4861	0.0000
C	-6.8449	0.7720	0.0000
C	-5.5860	1.4224	0.0000
C	-5.5602	2.8455	0.0000
C	-4.3055	3.5104	0.0000
C	-4.3562	0.7124	0.0000
C	-3.1330	1.3945	0.0000
C	-3.1078	2.7844	0.0000
C	-4.2120	4.9452	0.0000
C	-4.3148	-0.7248	0.0000
H	-2.1929	0.8437	0.0000
H	-8.9927	0.9565	0.0000
H	-6.9144	-0.3158	0.0000
H	-6.8247	4.6308	0.0000
H	-8.9477	3.4347	0.0000
H	-2.1483	3.3008	0.0000
N	-4.1292	6.1029	0.0000
N	-4.2740	-1.8847	0.0000

2-naphthonitrile

C	-6.7364	3.5098	0.0000
C	-7.9559	2.8310	0.0000
C	-7.9780	1.4395	0.0000
C	-6.7806	0.7224	0.0000
C	-5.5453	1.3893	0.0000
C	-5.5226	2.8038	0.0000
C	-4.2873	3.4728	0.0000
C	-4.3330	0.6812	0.0000
C	-3.1113	1.3586	0.0000
C	-3.0861	2.7548	0.0000
C	-1.8333	3.4514	0.0000
H	-4.2614	4.5617	0.0000
H	-4.3322	-0.4071	0.0000
H	-2.1844	0.7881	0.0000
H	-8.9277	0.9105	0.0000

H	-6.8203	-0.3648	0.0000
H	-6.7424	4.5978	0.0000
H	-8.8884	3.3898	0.0000
N	-0.8191	4.0157	0.0000

2,3,5,6-tetrafluoroterephthalonitrile

C	-6.1481	4.1743	-0.1788
C	-7.4836	3.7722	-0.1449
C	-7.8174	2.4390	0.0723
C	-6.7937	1.5146	0.2550
C	-5.4582	1.9167	0.2211
C	-5.1244	3.2499	0.0039
C	-9.1825	2.0279	0.1070
C	-3.7593	3.6609	-0.0309
N	-2.6490	3.9952	-0.0591
N	-10.2928	1.6936	0.1353
F	-5.8613	5.4664	-0.3903
F	-8.4454	4.6884	-0.3246
F	-7.0805	0.2224	0.4665
F	-4.4964	1.0005	0.4008

Terephthalonitrile

C	-6.1501	4.1871	-0.1811
C	-7.4892	3.7839	-0.1470
C	-7.8134	2.4402	0.0722
C	-6.7917	1.5018	0.2572
C	-5.4526	1.9050	0.2232
C	-5.1284	3.2487	0.0039
C	-9.1863	2.0268	0.1071
C	-3.7555	3.6621	-0.0310
N	-2.6448	3.9965	-0.0592
N	-10.2970	1.6924	0.1354
H	-5.9117	5.2359	-0.3526
H	-8.2744	4.5245	-0.2925
H	-7.0301	0.4529	0.4287
H	-4.6674	1.1644	0.3686

2,3,5,6-methylterephthalonitrile

C	-6.1471	4.2059	-0.2129
C	-7.5049	3.8069	-0.1225
C	-7.8189	2.4417	0.0904
C	-6.7947	1.4830	0.2891
C	-5.4369	1.8819	0.1987
C	-5.1229	3.2471	-0.0143
C	-5.7971	5.6577	-0.4699
C	-8.6106	4.8273	-0.3035
C	-7.1447	0.0311	0.5461
C	-4.3312	0.8616	0.3798
H	-6.4983	6.1150	-1.1754
H	-4.8128	5.7751	-0.9324
H	-5.8134	6.2164	0.4710
H	-8.3420	5.7867	0.1503
H	-9.5394	4.5297	0.1918
H	-8.8106	4.9738	-1.3694
C	-9.1988	2.0199	0.0898
H	-8.1292	-0.0864	1.0081
H	-6.4437	-0.4259	1.2520
H	-7.1277	-0.5276	-0.3948
H	-4.5998	-0.0979	-0.0737
H	-4.1310	0.7153	1.4457
H	-3.4025	1.1591	-0.1157
C	-3.7430	3.6690	-0.0136
N	-2.6329	4.0090	-0.0090
N	-10.3089	1.6799	0.0852

p-dinitrobenzene

C	-6.2070	4.1904	-0.1537
C	-7.5360	3.7527	-0.1439
C	-7.8199	2.3967	0.0806
C	-6.7830	1.4757	0.2953
C	-5.4539	1.9134	0.2855
C	-5.1700	3.2693	0.0610

H	-5.9982	5.2449	-0.3288
N	-3.7739	3.7291	0.0507
H	-8.3328	4.4761	-0.3116
N	-9.2161	1.9370	0.0909
H	-6.9918	0.4211	0.4704
H	-4.6571	1.1899	0.4532
O	-10.1006	2.7820	-0.1037
O	-9.4228	0.7326	0.2934
O	-3.5672	4.9338	-0.1495
O	-2.8892	2.8837	0.2430

1-nitro-4-(trifluoromethyl)benzene

C	-6.2552	4.1179	-0.1731
C	-7.5910	3.7059	-0.1625
C	-7.8967	2.3613	0.0833
C	-6.8756	1.4309	0.3157
C	-5.5423	1.8520	0.3027
C	-5.2187	3.1984	0.0645
H	-6.0214	5.1651	-0.3671
C	-3.7780	3.6582	0.0326
H	-8.3740	4.4394	-0.3472
N	-9.2984	1.9232	0.0956
H	-7.0987	0.3824	0.5058
H	-4.7528	1.1217	0.4815
O	-10.1706	2.7767	-0.1193
O	-9.5257	0.7260	0.3204
F	-3.5843	4.8199	0.7157
F	-3.3393	3.8890	-1.2346
F	-2.9113	2.7579	0.5732

4-nitrobenzonitrile

C	-6.3718	4.1540	-0.2568
C	-7.6936	3.7054	-0.1637
C	-7.9476	2.3581	0.1291
C	-6.8885	1.4615	0.3281
C	-5.5698	1.9190	0.2331
C	-5.3081	3.2640	-0.0589
H	-6.1785	5.2019	-0.4844
C	-3.9543	3.7288	-0.1546
H	-8.5063	4.4128	-0.3207
N	-9.3341	1.8824	0.2285
H	-7.0709	0.4125	0.5560
H	-4.7494	1.2191	0.3885
O	-10.2397	2.7082	0.0479
O	-9.5138	0.6842	0.4870
N	-2.8594	4.1048	-0.2319

Methyl 4-nitrobenzoate

C	-6.3813	4.1279	-0.2644
C	-7.7065	3.6915	-0.1640
C	-7.9697	2.3479	0.1325
C	-6.9171	1.4434	0.3286
C	-5.5938	1.8881	0.2262
C	-5.3181	3.2317	-0.0711
H	-6.1799	5.1737	-0.4954
C	-3.9288	3.7551	-0.1925
H	-8.5125	4.4067	-0.3191
N	-9.3591	1.8831	0.2383
H	-7.1069	0.3967	0.5599
H	-4.7873	1.1740	0.3812
O	-10.2600	2.7150	0.0610
O	-9.5472	0.6863	0.4985
O	-3.0251	2.7635	0.0025
C	-1.6655	3.1894	-0.1036
H	-1.0243	2.3200	0.0657
H	-1.4389	3.9411	0.6591
H	-1.4629	3.5794	-1.1060
O	-3.6705	4.9225	-0.4374

1-methoxy-4-nitrobenzene

C	-3.2135	3.6398	-0.0595
C	-4.4353	3.0022	-0.0244

C	-4.4642	1.6087	0.0072
C	-3.3005	0.8543	0.0076
C	-2.0707	1.4962	-0.0279
C	-2.0227	2.8951	-0.0649
H	-3.1485	4.7207	-0.0881
H	-5.3578	3.5674	-0.0234
N	-5.7540	0.9255	0.0382
H	-3.3542	-0.2259	0.0357
H	-1.1677	0.9010	-0.0271
O	-0.8892	3.6120	-0.1095
O	-6.7625	1.6045	0.0400
O	-5.7600	-0.2905	0.0605
C	0.3535	2.9149	-0.1493
H	1.1189	3.6827	-0.2135
H	0.4041	2.2686	-1.0282
H	0.4936	2.3236	0.7578

1-methyl-4-nitro-benzene

C	-3.2755	3.6296	-0.0664
C	-4.4993	2.9816	-0.0224
C	-4.5090	1.5920	0.0095
C	-3.3411	0.8441	0.0008
C	-2.1259	1.5158	-0.0437
C	-2.0735	2.9112	-0.0797
H	-3.2496	4.7140	-0.0932
H	-5.4287	3.5353	-0.0137
N	-5.7998	0.8928	0.0520
H	-3.3842	-0.2365	0.0285
H	-1.2051	0.9429	-0.0514
C	-0.7607	3.6431	-0.1346
O	-6.8125	1.5626	0.0575
O	-5.7913	-0.3214	0.0796
H	-0.1154	3.1076	-1.0563
H	-0.0696	3.2130	0.8211
H	-0.9351	4.8235	-0.1093

1-(4-nitrophenyl)ethan-1-one

C	-3.3526	3.5699	-0.1209
C	-4.6001	2.9419	-0.0470
C	-4.6628	1.5480	0.0628
C	-3.4874	0.7851	0.0992
C	-2.2422	1.4216	0.0243
C	-2.1679	2.8170	-0.0868
H	-3.3086	4.6557	-0.2062
H	-5.5017	3.5511	-0.0763
N	-5.9686	0.8796	0.1406
H	-3.5229	-0.2999	0.1852
H	-1.3478	0.8049	0.0562
O	-6.9831	1.5894	0.1004
O	-5.9764	-0.3554	0.2416
C	-0.8640	3.5420	-0.1704
C	0.4163	2.7487	-0.1712
O	-0.8532	4.7693	-0.2362
H	0.4372	2.0626	-1.0219
H	0.5260	2.2066	0.7715
H	1.2636	3.4345	-0.2702

4-nitrobenzamide

C	-3.2940	3.5599	-0.0701
C	-4.5497	2.9450	-0.0891
C	-4.6343	1.5505	0.0080
C	-3.4733	0.7733	0.1291
C	-2.2199	1.3966	0.1465
C	-2.1249	2.7912	0.0366
H	-3.2271	4.6454	-0.1399
H	-5.4408	3.5639	-0.1759
N	-5.9495	0.8964	-0.0111
H	-3.5274	-0.3103	0.2198
H	-1.3335	0.7812	0.2739
O	-6.9519	1.6190	-0.0998
O	-5.9769	-0.3406	0.0589
C	-0.8178	3.5022	0.0568

N	0.2983	2.7911	-0.2845
O	-0.7423	4.6916	0.3363
H	0.2663	1.8918	-0.7414
H	1.1585	3.3207	-0.3576

1-fluoro-4-nitrobenzene

C	-3.2914	3.6354	-0.0703
C	-4.5213	2.9748	-0.0247
C	-4.5491	1.5718	0.0096
C	-3.3562	0.8321	-0.0016
C	-2.1327	1.5046	-0.0473
C	-2.1115	2.8963	-0.0812
H	-3.2444	4.7203	-0.0975
H	-5.4386	3.5604	-0.0165
N	-5.8393	0.8708	0.0577
H	-3.3635	-0.2558	0.0247
H	-1.1965	0.9540	-0.0568
O	-6.8690	1.5599	0.0665
O	-5.8208	-0.3678	0.0865
F	-0.9358	3.5352	-0.1250

Nitrobenzene

C	-3.2754	3.6422	-0.0709
C	-4.5044	2.9817	-0.0253
C	-4.5325	1.5809	0.0090
C	-3.3412	0.8426	-0.0022
C	-2.1183	1.5143	-0.0479
C	-2.0869	2.9097	-0.0821
H	-3.2430	4.7293	-0.0977
H	-5.4214	3.5670	-0.0171
N	-5.8216	0.8804	0.0570
H	-3.3486	-0.2450	0.0241
H	-1.1881	0.9503	-0.0569
O	-6.8526	1.5685	0.0660
O	-5.8047	-0.3587	0.0858
H	-1.1313	3.4289	-0.1177

4-nitroaniline

C	-3.0998	3.6214	-0.0401
C	-4.3511	2.9974	-0.0103
C	-4.4217	1.6002	0.0127
C	-3.2524	0.8321	-0.0103
C	-2.0100	1.4734	-0.0401
C	-1.9211	2.8690	-0.0030
H	-3.0527	4.7067	-0.0933
H	-5.2492	3.6110	-0.0209
N	-5.7304	0.9362	0.0397
H	-3.2877	-0.2551	-0.0209
H	-1.1063	0.8704	-0.0933
N	-0.6827	3.4973	-0.1645
H	0.1071	2.9535	0.1701
H	-0.6552	4.4558	0.1701
O	-6.7412	1.6534	0.0523
O	-5.7485	-0.3031	0.0523

Tetracyanoquinodimethane

C	-3.6421	3.4622	0.0476
C	-4.8116	2.7977	0.0408
C	-4.8593	1.3227	0.0763
C	-3.5677	0.6095	0.1136
C	-2.3978	1.2732	0.1204
C	-2.3506	2.7484	0.0907
H	-3.6703	4.5495	0.0200
H	-5.7310	3.3785	0.0082
H	-3.5394	-0.4779	0.1365
H	-1.4785	0.6922	0.1483
C	-1.1681	3.4208	0.1016
C	-6.0419	0.6504	0.0736
C	-7.2975	1.3258	0.0376
C	-6.1040	-0.7740	0.1074
C	-1.1060	4.8453	0.0732
C	0.0874	2.7455	0.1430

N	-8.3089	1.8940	0.0079
N	-6.1332	-1.9338	0.1353
N	-1.0767	6.0052	0.0495
N	1.0987	2.1774	0.1768

1,2,3,5-tetramethylbenzene

C	-2.4131	3.0887	-0.0003
C	-3.6330	2.3918	-0.0648
C	-3.6607	1.0554	0.3265
C	-2.5119	0.4063	0.7739
C	-1.2971	1.0839	0.8389
C	-1.2729	2.4252	0.4473
C	-2.3452	4.5383	-0.4049
C	-4.8836	3.0830	-0.5420
H	-2.5637	-0.6355	1.0762
H	-0.3341	2.9722	0.4967
C	-0.0361	0.3942	1.2941
H	-2.6603	4.6765	-1.4433
H	-1.3318	4.9273	-0.3026
H	-3.0091	5.1523	0.2106
H	0.5797	0.1046	0.4378
H	-0.2632	-0.5106	1.8599
H	0.5694	1.0497	1.9231
H	-4.5994	0.5104	0.2845
H	-5.1313	3.9414	0.0894
H	-5.7348	2.4011	-0.5345
H	-4.7635	3.4651	-1.5601

1,2,4-trimethylbenzene

C	-2.4107	3.0890	0.0035
C	-3.6237	2.3824	-0.0747
C	-3.6356	1.0338	0.2757
C	-2.4783	0.3836	0.6977
C	-1.2710	1.0730	0.7831
C	-1.2615	2.4244	0.4281
C	-2.3561	4.5474	-0.3691
C	-4.8822	3.0719	-0.5322
H	-2.5161	-0.6694	0.9614
H	-0.3266	2.9776	0.4819
C	-0.0159	0.3948	1.2705
H	-2.6810	4.7065	-1.4015
H	-1.3450	4.9421	-0.2659
H	-3.0199	5.1429	0.2646
H	0.2159	-0.2250	0.3432
H	-0.5025	-0.2470	2.2496
H	1.0141	1.2388	1.8359
H	-4.5680	0.4798	0.2153
H	-5.1316	3.9179	0.1152
H	-5.7287	2.3843	-0.5316
H	-4.7714	3.4728	-1.5442

m-xylene

C	-2.5109	2.9336	0.0231
C	-3.7709	2.2214	0.0675
C	-3.8255	0.8270	0.0595
C	-2.6482	0.1243	0.0058
C	-1.3722	0.8104	-0.0400
C	-1.3394	2.2090	-0.0310
C	-2.5425	4.4192	0.0397
H	-4.6857	2.8032	0.1039
H	-4.7793	0.3171	0.0939
H	-2.6455	-0.9604	-0.0034
C	-0.1392	-0.0056	-0.0941
H	-0.3841	2.7201	-0.0660
H	-3.1558	4.7857	-0.7898
H	-1.5444	4.8466	-0.0289
H	-3.0253	4.7667	0.9593
H	-0.1145	-0.6853	0.7655
H	0.7606	0.6048	-0.1080
H	-0.1659	-0.6466	-0.9834

1,2,4,5-tetramethoxybenzene

C	-5.4787	2.8555	0.1162
C	-4.2869	3.4546	-0.2380
C	-5.5132	1.4175	0.3069
C	-4.3429	0.6768	0.1180
C	-3.1531	1.2750	-0.2439
C	-3.1142	2.7152	-0.4154
O	-6.6155	3.5044	0.3017
O	-2.0560	3.4239	-0.7403
H	-4.2134	4.5237	-0.3822
O	-2.0227	0.6231	-0.4570
C	-0.7155	2.9136	-0.8880
C	-1.9946	-0.7975	-0.2765
H	-0.1167	3.7991	-1.0764
H	-0.6653	2.2302	-1.7316
H	-0.3979	2.4206	0.0272
H	-0.9741	-1.0930	-0.4967
H	-2.6878	-1.2753	-0.9698
H	-2.2496	-1.0472	0.7542
O	-6.5682	0.7099	0.6439
C	-6.6494	4.9213	0.0963
H	-7.6744	5.2146	0.2981
H	-6.3823	5.1545	-0.9352
H	-5.9682	5.4156	0.7897
H	-4.4168	-0.3925	0.2605
C	-7.8855	1.2341	0.9050
H	-8.4727	0.3569	1.1579
H	-8.2798	1.7192	0.0159
H	-7.8538	1.9286	1.7404

1,2,3,5-tetramethoxybenzene

C	-5.5500	2.5017	0.0056
C	-4.2908	3.0507	-0.2093
C	-5.7014	1.1297	0.2450
C	-4.5855	0.3034	0.2670
C	-3.3025	0.8463	0.0639
C	-3.1781	2.2051	-0.1890
O	-6.7038	3.2164	0.0043
O	-1.9418	2.7341	-0.4536
H	-4.1292	4.1022	-0.4058
O	-4.6256	-1.0331	0.4711
O	-2.1980	0.0363	0.1087
C	-1.1319	2.9029	0.7121
C	-1.8537	-0.4960	-1.1712
H	-0.9648	1.9439	1.2051
H	-1.6086	3.6011	1.4050
H	-0.1834	3.3131	0.3713
H	-0.6963	-0.4531	-1.2789
H	-2.4407	-0.0022	-2.0184
H	-2.2185	-1.6726	-1.0765
C	-5.9042	-1.6318	0.6346
H	-5.7218	-2.6959	0.7568
H	-6.5285	-1.4620	-0.2459
H	-6.4062	-1.2390	1.5220
H	-6.7020	0.7487	0.4011
C	-6.6097	4.6126	-0.2355
H	-7.6274	4.9917	-0.1971
H	-6.1802	4.8121	-1.2207
H	-6.0059	5.1019	0.5331

1,2,3,4-tetramethoxybenzene

C	-5.6224	2.6312	-0.0348
C	-4.3752	3.2774	-0.0969
C	-5.7257	1.2202	0.0422
C	-4.5979	0.4469	0.0081
C	-3.3036	1.0811	-0.1365
C	-3.2253	2.5252	-0.1151
O	-6.7729	3.2688	-0.0140
O	-2.0671	3.1694	-0.2176
H	-4.2795	4.3538	-0.1203
O	-4.5723	-0.8783	0.0914
O	-2.1685	0.4726	-0.3177
C	-0.8770	2.7099	0.4553

C	-1.9733	-0.9456	-0.5283
H	-0.2884	2.0835	-0.2097
H	-1.1349	2.1653	1.3625
H	-0.3293	3.6140	0.7074
H	-0.9163	-1.0295	-0.7583
H	-2.5854	-1.2752	-1.3636
H	-2.2243	-1.4879	0.3780
C	-5.8137	-1.5697	0.2539
H	-5.5542	-2.6223	0.3025
H	-6.4642	-1.3776	-0.6007
H	-6.2970	-1.2531	1.1796
H	-6.7148	0.7940	0.1349
C	-6.7902	4.7022	-0.0932
H	-7.8398	4.9762	-0.0820
H	-6.3226	5.0304	-1.0218
H	-6.2776	5.1300	0.7686

1,2,3-trimethoxybenzene

C	-5.8310	2.6245	0.2499
C	-4.5730	3.2201	0.2319
C	-5.9402	1.2772	0.0132
C	-4.7490	0.5017	-0.2363
C	-3.4616	1.0898	-0.2348
C	-3.3719	2.4559	-0.0143
H	-6.7103	3.2230	0.4457
H	-6.9073	0.7926	0.0121
O	-2.2895	3.2043	-0.0043
H	-4.4446	4.2816	0.4044
O	-4.7780	-0.7791	-0.4763
O	-2.3811	0.3038	-0.4764
C	-0.9831	2.6932	-0.3309
C	-1.9585	-0.4664	0.6628
H	-0.3437	3.5704	-0.3293
H	-1.0008	2.2278	-1.3131
H	-0.6552	1.9844	0.4270
H	-1.0766	-1.0163	0.3447
H	-2.7421	-1.1611	0.9667
H	-1.7084	0.1986	1.4928
C	-6.0239	-1.5071	-0.4945
H	-5.7442	-2.5319	-0.7110
H	-6.6681	-1.1137	-1.2793
H	-6.5027	-1.4388	0.4812

Aniline

C	-2.3287	3.1535	0.0735
C	-3.5138	2.4269	-0.0699
C	-3.5309	1.0612	0.2031
C	-2.3590	0.4216	0.5999
C	-1.1769	1.1533	0.7415
C	-1.1627	2.5348	0.5320
N	0.0477	3.2394	0.5547
H	-2.3247	4.2109	-0.1764
H	-2.3589	-0.6492	0.7846
H	-4.4174	2.9257	-0.4093
H	-4.4496	0.4930	0.0857
H	-0.2643	0.6329	1.0186
H	0.7408	2.8336	1.1754
H	-0.0670	4.2364	0.7069

Durene

C	-2.3611	3.1347	0.1089
C	-3.5518	2.4169	-0.0861
C	-3.5636	1.0316	0.1512
C	-2.3874	0.4017	0.5879
C	-1.1967	1.1195	0.7829
C	-1.1848	2.5048	0.5456
C	0.0624	3.3239	0.7353
C	0.0328	0.3924	1.2541
H	-0.1372	-0.6878	1.3166
H	0.3203	0.7418	2.2507
H	0.8620	0.5513	0.5574
C	-4.8108	0.2125	-0.0384

H	0.4437	3.2099	1.7550
H	-0.1283	4.3906	0.5765
H	0.8311	3.0137	0.0205
H	-5.5795	0.5227	0.6763
H	-4.6201	-0.8542	0.1203
H	-5.1921	0.3265	-1.0581
C	-4.7812	3.1440	-0.5573
H	-4.6112	4.2241	-0.6197
H	-5.6104	2.9850	0.1394
H	-5.0687	2.7946	-1.5539
H	-2.3501	4.2068	-0.0813
H	-2.3983	-0.6704	0.7781

Hexamethylbenzene

C	-2.3161	3.1245	-0.0581
C	-3.5391	2.4120	-0.1383
C	-3.5791	1.0364	0.2027
C	-2.4324	0.4119	0.7550
C	-1.2094	1.1244	0.8352
C	-1.1694	2.4999	0.4941
C	-2.2433	4.5606	-0.5306
C	-2.5052	-1.0242	1.2276
C	0.1056	3.2922	0.6881
C	0.0445	0.4262	1.3160
H	-2.9232	4.7461	-1.3680
H	-1.2515	4.8084	-0.9213
H	-2.4883	5.2397	0.2915
H	0.0520	-0.6316	1.0347
H	0.1291	0.5119	2.4035
H	0.9432	0.8414	0.8493
C	-4.8540	0.2442	0.0085
H	0.6800	2.9308	1.5469
H	-0.1013	4.3421	0.9176
H	0.7251	3.2338	-0.2118
H	-5.4737	0.3026	0.9083
H	-4.6470	-0.8058	-0.2208
H	-5.4282	0.6054	-0.8504
C	-4.7930	3.1103	-0.6191
H	-4.8006	4.1678	-0.3372
H	-5.6917	2.6947	-0.1528
H	-4.8772	3.0251	-1.7066
H	-3.4971	-1.2721	1.6180
H	-1.8256	-1.2094	2.0654
H	-2.2598	-1.7034	0.4057

Pentamethylbenzene

C	-2.3195	3.0795	-0.0357
C	-3.5494	2.3701	-0.1095
C	-3.5856	1.0046	0.2415
C	-2.4229	0.3854	0.7183
C	-1.2155	1.0836	0.8493
C	-1.1638	2.4497	0.5020
C	-2.2531	4.5240	-0.4825
H	-2.4592	-0.6670	0.9965
C	0.1253	3.2236	0.6527
C	-0.0156	0.3430	1.3777
H	-2.9450	4.7259	-1.3059
H	-1.2649	4.7820	-0.8752
H	-2.4902	5.1854	0.3563
H	-0.2036	-0.7341	1.4446
H	0.2372	0.6997	2.3811
H	0.8423	0.4754	0.7105
C	-4.8428	0.1820	0.1399
H	0.7982	2.7756	1.3891
H	-0.0668	4.2386	1.0158
H	0.6461	3.2721	-0.3085
H	-5.5682	0.5053	0.8930
H	-4.6429	-0.8823	0.3052
H	-5.2812	0.2719	-0.8593
C	-4.7979	3.0594	-0.6092
H	-4.8676	4.0786	-0.2151
H	-5.7123	2.5586	-0.2793

H	-4.7948	3.0903	-1.7031

1,2,3,4-tetramethylbenzene

C	-2.4604	3.0859	-0.0044
C	-3.6701	2.3607	-0.1099
C	-3.6833	0.9954	0.1985
C	-2.5261	0.3496	0.6227
C	-1.3232	1.0519	0.7620
C	-1.2910	2.4381	0.4831
C	-2.4242	4.5559	-0.3536
C	-4.9523	3.0022	-0.5696
H	-2.5724	-0.7137	0.8477
C	-0.0061	3.2163	0.6484
C	-0.1064	0.2995	1.2309
H	-3.2068	4.8323	-1.0657
H	-1.4811	4.8237	-0.8407
H	-2.5480	5.1570	0.5524
H	-0.2809	-0.7819	1.2401
H	0.1573	0.6036	2.2487
H	0.7396	0.4799	0.5598
H	-4.6013	0.4190	0.1077
H	-5.1587	3.9079	0.0098
H	-5.8087	2.3334	-0.4311
H	-4.8907	3.2500	-1.6339
H	0.6727	2.7497	1.3678
H	-0.2001	4.2198	1.0408
H	0.5075	3.2961	-0.3146

Mesitylene

C	-2.4976	3.1470	0.0505
C	-3.6585	2.4019	-0.1893
C	-3.6847	1.0220	0.0476
C	-2.5322	0.3877	0.5299
C	-1.3627	1.1166	0.7753
C	-1.3549	2.4959	0.5326
C	-2.4639	4.6253	-0.2016
H	-4.5501	2.9005	-0.5638
C	-4.9262	0.2194	-0.2079
H	-2.5501	-0.6845	0.7147
H	-0.4492	3.0694	0.7210
C	-0.1266	0.4419	1.2916
H	-3.4256	4.9920	-0.5751
H	-1.7008	4.8629	-0.9497
H	-2.2382	5.1608	0.7263
H	-0.2836	-0.6326	1.4322
H	0.1599	0.8684	2.2582
H	0.6973	0.5705	0.5823
H	-5.7419	0.8474	-0.5810
H	-5.2653	-0.2554	0.7185
H	-4.7279	-0.5533	-0.9575

Toluene

C	-2.4992	3.0653	0.0645
C	-3.6570	2.3152	-0.1735
C	-3.6696	0.9400	0.0670
C	-2.5261	0.3038	0.5467
C	-1.3688	1.0421	0.7866
C	-1.3548	2.4170	0.5466
C	-2.4708	4.5432	-0.1892
H	-4.5578	2.7959	-0.5477
H	-4.5726	0.3651	-0.1204
H	-2.5370	-0.7666	0.7335
H	-0.4454	2.9820	0.7378
H	-0.4764	0.5475	1.1606
H	-3.4342	4.9056	-0.5625
H	-1.7090	4.7827	-0.9381
H	-2.2464	5.0806	0.7379

tert-butylbenzene

C	-2.5081	3.0804	0.0589
C	-3.6576	2.3057	-0.1719
C	-3.6663	0.9276	0.0703

C	-2.5259	0.2917	0.5489
C	-1.3749	1.0338	0.7861
C	-1.3671	2.4103	0.5439
C	-2.4625	4.5972	-0.1961
H	-4.5755	2.7508	-0.5454
H	-4.5694	0.3523	-0.1170
H	-2.5348	-0.7783	0.7363
H	-0.4477	2.9572	0.7415
C	-3.7911	5.1819	-0.7266
H	-0.4795	0.5445	1.1602
H	-4.0770	4.7306	-1.6838
H	-3.7087	6.2629	-0.8924
H	-4.6121	5.0271	-0.0168
C	-2.1324	5.3351	1.1194
H	-2.1281	6.4215	0.9728
H	-1.1471	5.0614	1.5124
H	-2.8717	5.1062	1.8962
C	-1.3738	4.9151	-1.2438
H	-1.3440	5.9874	-1.4700
H	-1.5621	4.3812	-2.1828
H	-0.3726	4.6328	-0.9002

1,2-dimethoxybenzene

C	-5.7792	2.5124	0.0791
C	-4.5659	3.1502	-0.1807
C	-5.8103	1.1297	0.1860
C	-4.6454	0.3771	0.0255
C	-3.4342	1.0122	-0.2418
C	-3.4031	2.4160	-0.3482
H	-6.6838	3.0962	0.2003
H	-6.7439	0.6178	0.3890
O	-2.2380	3.0676	-0.6560
H	-4.5026	4.2295	-0.2684
H	-4.6944	-0.7015	0.1033
O	-2.2506	0.3773	-0.4216
C	-1.2722	3.0823	0.3965
C	-2.2426	-1.0408	-0.3405
H	-0.4750	3.7496	0.0737
H	-0.8689	2.0837	0.5697
H	-1.7200	3.4667	1.3170
H	-1.2111	-1.3412	-0.5060
H	-2.8799	-1.4770	-1.1137
H	-2.5748	-1.3800	0.6435

p-xylene

C	-6.8120	1.0150	-0.9078
C	-5.9828	2.1381	-0.8225
C	-6.2415	-0.2591	-0.8076
C	-4.8643	-0.4083	-0.6252
C	-4.0351	0.7148	-0.5400
C	-4.6057	1.9889	-0.6402
C	-8.2918	1.1596	-1.1034
H	-6.4013	3.1390	-0.8973
H	-6.8684	-1.1457	-0.8713
H	-4.4459	-1.4092	-0.5504
C	-2.5554	0.5702	-0.3444
H	-3.9788	2.8755	-0.5765
H	-2.2587	-0.4821	-0.2844
H	-2.2485	1.0589	0.5859
H	-2.0180	1.0230	-1.1838
H	-8.5885	2.2119	-1.1634
H	-8.8292	0.7067	-0.2640
H	-8.5987	0.6709	-2.0337

Pentamethoxybenzene

C	-5.5261	2.8146	0.0042
C	-4.2682	3.3547	0.0694
C	-5.6737	1.4124	-0.3293
C	-4.5034	0.6044	-0.4821
C	-3.2435	1.1569	-0.3954
C	-3.1196	2.5613	-0.1370
O	-6.6535	3.4819	0.2064

O	-1.9906	3.2198	-0.0460
H	-4.1051	4.4006	0.2885
O	-2.1455	0.3906	-0.5701
C	-0.6842	2.6565	-0.2870
C	-1.8698	-0.5190	0.5111
H	-0.0156	3.5089	-0.2202
H	-0.6446	2.2087	-1.2757
H	-0.4465	1.9241	0.4813
H	-0.9271	-0.9992	0.2627
H	-2.6595	-1.2648	0.5959
H	-1.7742	0.0369	1.4462
O	-6.7925	0.7774	-0.5359
C	-6.5717	4.8714	0.5417
H	-7.5986	5.1987	0.6671
H	-6.0922	5.4238	-0.2676
H	-6.0155	4.9965	1.4717
O	-4.6031	-0.6941	-0.8043
C	-8.1208	1.3474	-0.4790
H	-8.7702	0.5180	-0.7387
H	-8.2063	2.1533	-1.2026
H	-8.3233	1.7052	0.5265
C	-5.4152	-1.5519	0.0248
H	-4.8911	-2.5043	0.0655
H	-6.3982	-1.6789	-0.4217
H	-5.5077	-1.1379	1.0296

Hexamethoxybenzene

C	-5.3752	2.8589	-0.2066
C	-4.0767	3.2785	-0.5523
C	-5.6093	1.5787	0.3263
C	-4.5216	0.7226	0.5513
C	-3.2232	1.1422	0.2055
C	-2.9890	2.4223	-0.3274
O	-6.4277	3.7241	-0.4104
O	-1.7402	2.8301	-0.7286
O	-3.9767	4.5150	-1.1452
O	-2.1706	0.2770	0.4092
C	-0.7589	2.7494	0.3061
C	-1.9706	-0.5254	-0.7554
H	-0.0581	3.5776	0.1615
H	-0.1916	1.8188	0.2163
H	-1.1877	2.8482	1.3101
H	-1.1249	-1.1914	-0.5599
H	-1.7207	0.0910	-1.6258
H	-2.8470	-1.1465	-0.9694
O	-6.8583	1.1711	0.7273
C	-6.6283	4.5259	0.7546
H	-7.4735	5.1924	0.5587
H	-5.7518	5.1463	0.9699
H	-6.8795	3.9090	1.6243
O	-4.6212	-0.5139	1.1444
C	-7.8391	1.2512	-0.3079
H	-8.5399	0.4230	-0.1632
H	-7.4097	1.1519	-1.3117
H	-8.4064	2.1818	-0.2189
C	-5.6193	-1.3616	0.5858
H	-5.2724	-2.3945	0.6901
H	-5.7849	-1.1750	-0.4814
H	-6.5525	-1.2708	1.1487
C	-2.9804	5.3632	-0.5839
H	-3.3280	6.3958	-0.6880
H	-2.0460	5.2735	-1.1452
H	-2.8165	5.1757	0.4833

S2 – Input geometries of the 34 compounds on Table 2 (in the paper)

Benzene

C	-3.0563	2.6825	0.0000
C	-3.0480	1.2902	0.0000
C	-1.8382	0.6012	0.0000
C	-0.6367	1.3045	0.0000
C	-0.6449	2.6967	0.0000
C	-1.8547	3.3857	0.0000
H	-3.9986	3.2191	0.0000
H	-1.8612	4.4701	0.0000
H	-3.9839	0.7424	0.0000
H	-1.8318	-0.4832	0.0000
H	0.3056	0.7679	0.0000
H	0.2910	3.2445	0.0000

Toluene

C	-3.0564	2.8069	-0.0602
C	-3.0424	1.4143	-0.0308
C	-1.8403	0.7105	0.0358
C	-0.6469	1.4373	0.0716
C	-0.6547	2.8267	0.0425
C	-1.8625	3.5180	-0.0237
H	-4.0024	3.3348	-0.1132
H	-1.8707	4.6019	-0.0478
H	-3.9791	0.8663	-0.0614
C	-1.8158	-0.7961	0.0777
H	0.2983	0.9045	0.1223
H	0.2824	3.3720	0.0702
H	-2.8131	-1.2139	-0.0653
H	-1.4363	-1.1535	1.0384
H	-1.1640	-1.2002	-0.7002

Phenol

C	-3.0932	2.7045	0.0000
C	-3.0808	1.3142	0.0000
C	-1.8763	0.6170	0.0000
C	-0.6720	1.3184	0.0000
C	-0.6755	2.7128	0.0000
C	-1.8834	3.3968	0.0000
H	-4.0328	3.2438	0.0000
H	-1.8786	4.4811	0.0000
H	-4.0134	0.7609	0.0000
H	-1.8685	-0.4693	0.0000
O	0.5377	0.6955	0.0000
H	0.2734	3.2366	0.0000
H	0.4170	-0.2598	0.0000

Anisole

C	-2.9988	2.8900	0.0000
C	-3.0039	1.4944	0.0000
C	-1.7912	0.8056	0.0000
C	-0.5872	1.5177	0.0000
C	-0.5989	2.9027	0.0000
C	-1.8075	3.6012	0.0000
H	-3.9461	3.4179	0.0000
H	-1.8150	4.6846	0.0000
H	-3.9485	0.9662	0.0000
O	-1.6777	-0.5475	0.0000
H	0.3413	0.9583	0.0000
H	0.3415	3.4427	0.0000
C	-2.8706	-1.3073	0.0000
H	-2.5623	-2.3498	0.0000
H	-3.4690	-1.1035	-0.8928
H	-3.4690	-1.1035	0.8928

Benzonitrile

C	-3.0205	3.0146	0.0000
C	-3.1086	1.6290	0.0000
C	-1.9369	0.8675	0.0000
C	-0.6839	1.4865	0.0000
C	-0.6092	2.8728	0.0000

C	-1.7741	3.6355	0.0000
H	-3.9258	3.6099	0.0000
H	-1.7106	4.7175	0.0000
H	-4.0720	1.1335	0.0000
C	-2.0208	-0.5669	0.0000
H	0.2148	0.8816	0.0000
H	0.3596	3.3579	0.0000
N	-2.0874	-1.7152	0.0000

Aniline

C	-3.0120	3.0015	-0.0037
C	-3.0986	1.6164	0.0477
C	-1.9385	0.8322	0.0738
C	-0.6947	1.4755	0.0476
C	-0.6190	2.8612	-0.0037
C	-1.7740	3.6380	-0.0296
H	-3.9240	3.5885	-0.0251
H	-1.7107	4.7188	-0.0701
H	-4.0695	1.1309	0.0714
N	-2.0203	-0.5567	0.1882
H	0.2128	0.8799	0.0714
H	0.3554	3.3376	-0.0249
H	-2.8775	-0.9521	-0.1713
H	-1.2160	-1.0508	-0.1718

N,N-Dimethyl-aniline

C	-3.0012	3.1156	-0.0251
C	-3.0920	1.7303	0.0164
C	-1.9327	0.9298	0.0536
C	-0.6879	1.5896	0.0174
C	-0.6166	2.9760	-0.0241
C	-1.7672	3.7570	-0.0428
H	-3.9160	3.6984	-0.0498
H	-1.7040	4.8380	-0.0775
H	-4.0736	1.2760	0.0203
N	-2.0139	-0.4534	0.1336
H	0.2339	1.0238	0.0222
H	0.3600	3.4481	-0.0478
C	-3.2894	-1.0810	-0.1591
C	-0.8212	-1.2266	-0.1604
H	-0.0321	-1.0130	0.5631
H	-0.4276	-1.0292	-1.1669
H	-1.0578	-2.2859	-0.0809
H	-4.0473	-0.7757	0.5649
H	-3.1789	-2.1606	-0.0792
H	-3.6578	-0.8393	-1.1655

Chlorobenzene

C	-3.0103	3.1725	-0.0248
C	-3.1061	1.7851	0.0121
C	-1.9392	1.0330	0.0302
C	-0.6866	1.6319	0.0121
C	-0.6069	3.0204	-0.0248
C	-1.7645	3.7924	-0.0433
H	-3.9162	3.7674	-0.0391
H	-1.6961	4.8734	-0.0723
H	-4.0700	1.2913	0.0269
H	0.2073	1.0206	0.0267
H	0.3668	3.4962	-0.0392
Cl	-2.0498	-0.7121	0.0764

Styrene

C	-2.9660	2.9871	0.0270
C	-3.0168	1.5973	0.0028
C	-1.8459	0.8328	-0.0167
C	-0.6154	1.5018	-0.0309
C	-0.5624	2.8886	-0.0079
C	-1.7372	3.6380	0.0241
H	-3.8861	3.5603	0.0461
H	-1.6924	4.7211	0.0395
H	-3.9781	1.0928	0.0045
H	0.3082	0.9351	-0.0758

H	0.3992	3.3894	-0.0225
C	-1.9514	-0.6385	-0.0239
C	-0.9676	-1.5025	0.2177
H	-2.9455	-1.0272	-0.2341
H	0.0413	-1.1850	0.4601
H	-1.1466	-2.5707	0.1899

Phenylboronic acid

C	-2.9702	3.1571	0.0611
C	-2.9691	1.7825	0.2739
C	-1.7777	1.0489	0.2371
C	-0.5835	1.7321	-0.0201
C	-0.5768	3.1065	-0.2340
C	-1.7721	3.8200	-0.1931
H	-3.9012	3.7124	0.0934
H	-1.7699	4.8920	-0.3591
H	-3.9026	1.2658	0.4722
H	0.3480	1.1763	-0.0521
H	0.3565	3.6223	-0.4321
B	-1.7803	-0.4958	0.4800
O	-2.9774	-1.1075	0.7253
O	-0.5849	-1.1562	0.4362
H	-0.6254	-2.1038	0.5926
H	-2.9399	-2.0572	0.8698

N-Phenylbenzylamine

C	-2.8447	2.9884	0.9713
C	-2.1039	1.8311	1.1433
C	-1.3279	1.3110	0.0931
C	-1.3295	1.9871	-1.1343
C	-2.0727	3.1549	-1.2906
C	-2.8346	3.6663	-0.2481
H	-3.4358	3.3669	1.7984
H	-3.4128	4.5730	-0.3796
H	-2.1100	1.3156	2.0990
H	-0.7549	1.6089	-1.9707
H	-2.0556	3.6629	-2.2490
N	-0.5603	0.1725	0.3161
H	-0.9270	-0.4293	1.0418
C	0.0015	-0.5626	-0.8062
C	0.7304	-1.7902	-0.3161
H	0.7098	0.0911	-1.3261
H	-0.7672	-0.8491	-1.5379
C	1.7056	-1.6730	0.6778
C	0.4531	-3.0484	-0.8458
C	1.1428	-4.1734	-0.3991
C	2.1135	-4.0484	0.5882
C	2.3925	-2.7940	1.1276
H	3.1488	-2.6903	1.8976
H	1.9188	-0.6949	1.0968
H	0.9170	-5.1468	-0.8201
H	2.6497	-4.9232	0.9386
H	-0.3085	-3.1504	-1.6126

Biphenyl

C	-2.6858	2.9245	1.0549
C	-1.8479	1.8177	1.1303
C	-1.2481	1.2951	-0.0201
C	-1.5109	1.9096	-1.2489
C	-2.3492	3.0161	-1.3254
C	-2.9393	3.5279	-0.1735
H	-3.1356	3.3213	1.9582
H	-3.5927	4.3909	-0.2325
H	-1.6363	1.3670	2.0944
H	-1.0729	1.5021	-2.1541
H	-2.5478	3.4747	-2.2877
C	-0.3514	0.1149	0.0604
C	0.8179	0.0535	-0.7048
C	-0.6566	-0.9603	0.9014
C	0.1824	-2.0667	0.9737
C	1.3427	-2.1164	0.2068
C	1.6578	-1.0519	-0.6326

H	2.5641	-1.0786	-1.2273
H	1.0818	0.8895	-1.3440
H	-0.0744	-2.8948	1.6248
H	1.9971	-2.9789	0.2630
H	-1.5712	-0.9388	1.4848

Naphthalene

C	-7.0237	2.1282	0.0000
C	-7.0911	0.7131	0.0000
C	-5.9428	-0.0328	0.0000
C	-4.6694	0.5953	0.0000
C	-4.6017	2.0152	0.0000
C	-5.8097	2.7616	0.0000
C	-3.4614	-0.1511	0.0000
C	-2.2474	0.4823	0.0000
C	-2.1800	1.8974	0.0000
C	-3.3283	2.6433	0.0000
H	-3.2815	3.7279	0.0000
H	-3.5181	-1.2351	0.0000
H	-1.3313	-0.0975	0.0000
H	-1.2128	2.3874	0.0000
H	-5.7530	3.8457	0.0000
H	-7.9398	2.7081	0.0000
H	-8.0583	0.2232	0.0000
H	-5.9896	-1.1173	0.0000

o-Xylene

C	-2.9399	2.8650	-0.0352
C	-2.9680	1.4713	-0.0341
C	-1.7551	0.7624	0.0074
C	-0.5557	1.4717	0.0470
C	-0.5381	2.8636	0.0458
C	-1.7368	3.5642	0.0042
H	-3.8775	3.4117	-0.0679
H	-1.7390	4.6485	0.0023
C	-4.2795	0.7312	-0.0762
C	-1.7550	-0.7442	0.0092
H	0.3807	0.9229	0.0797
H	0.4070	3.3942	0.0773
H	-2.2971	-1.1412	0.8725
H	-0.7382	-1.1368	0.0393
H	-2.2452	-1.1428	-0.8835
H	-5.1208	1.4241	-0.1060
H	-4.4018	0.0886	0.8006
H	-4.3435	0.0833	-0.9551

m-Xylene

C	-2.8554	2.8202	-0.0626
C	-2.8420	1.4281	-0.0619
C	-1.6515	0.7006	0.0333
C	-0.4514	1.4000	0.1326
C	-0.4449	2.7937	0.1334
C	-1.6365	3.4987	0.0363
C	-4.1476	3.5899	-0.1642
H	-1.6274	4.5847	0.0394
C	-1.6787	-0.8064	0.0083
H	0.4834	0.8538	0.2117
H	0.4952	3.3289	0.2131
H	-0.7238	-1.2257	0.3276
H	-1.8847	-1.1746	-1.0005
H	-2.4595	-1.1983	0.6635
H	-5.0053	2.9198	-0.2341
H	-4.1501	4.2354	-1.0459
H	-4.2905	4.2317	0.7086
H	-3.7838	0.8894	-0.1362

p-Xylene

C	-2.7949	2.7179	-0.2407
C	-2.8124	1.3255	-0.2452
C	-1.6605	0.5905	0.0287
C	-0.4888	1.2959	0.3140
C	-0.4714	2.6847	0.3185

C	-1.6251	3.4215	0.0391
C	-1.5919	4.9285	0.0360
C	-1.6694	-0.9163	-0.0067
H	0.4216	0.7478	0.5391
H	0.4525	3.2086	0.5474
H	-1.3866	-1.2839	-0.9971
H	-2.6604	-1.3124	0.2204
H	-0.9621	-1.3341	0.7120
H	-3.7397	0.8033	-0.4619
H	-1.1468	5.3153	0.9556
H	-2.5953	5.3463	-0.0563
H	-0.9944	5.3051	-0.7984
H	-3.7086	3.2646	-0.4537

Mesitylene

C	-2.9464	2.7762	-0.0259
C	-2.9404	1.3835	-0.0247
C	-1.7451	0.6617	-0.0008
C	-0.5427	1.3635	0.0242
C	-0.5149	2.7597	0.0235
C	-1.7235	3.4505	-0.0021
C	-4.2388	3.5523	-0.0467
H	-1.7167	4.5379	-0.0015
C	-1.7476	-0.8462	-0.0155
H	0.3953	0.8130	0.0460
C	0.8032	3.4913	0.0510
H	-2.7525	-1.2435	0.1320
H	-1.1042	-1.2488	0.7703
H	-1.3737	-1.2269	-0.9696
H	-5.1014	2.8867	-0.0968
H	-4.2789	4.2239	-0.9077
H	-4.3397	4.1680	0.8506
H	-3.8853	0.8467	-0.0422
H	0.6579	4.5721	0.0618
H	1.4083	3.2406	-0.8238
H	1.3833	3.2192	0.9361

Durene

C	-2.8467	2.7180	-0.0638
C	-2.8878	1.3251	-0.0403
C	-1.6803	0.6163	0.0236
C	-0.4845	1.3311	0.0620
C	-0.4435	2.7240	0.0398
C	-1.6508	3.4329	-0.0253
C	-1.6542	4.9393	-0.0501
C	-1.6775	-0.8901	0.0496
H	0.4519	0.7806	0.1112
C	0.8727	3.4561	0.0841
H	-2.2291	-1.2752	0.9122
H	-0.6606	-1.2808	0.0988
H	-2.1556	-1.3052	-0.8424
C	-4.2039	0.5932	-0.0832
H	0.9209	4.1381	0.9377
H	1.0214	4.0626	-0.8143
H	1.7081	2.7597	0.1617
H	-5.0408	1.2908	-0.1292
H	-4.3386	-0.0374	0.8005
H	-4.2655	-0.0657	-0.9543
H	-2.6696	5.3291	-0.1278
H	-1.0779	5.3263	-0.8954
H	-1.2027	5.3535	0.8564
H	-3.7833	3.2681	-0.1146

Pentamethylbenzene

C	-2.8962	2.7574	-0.0261
C	-2.9341	1.3661	0.0005
C	-1.7252	0.6573	0.0303
C	-0.5100	1.3608	0.0144
C	-0.4919	2.7648	0.0219
C	-1.7016	3.4718	-0.0089
C	-1.7402	4.9812	-0.0296
C	-1.7197	-0.8535	0.0763

C	0.7957	0.5987	0.0018
C	0.8286	3.4991	0.0598
H	-2.7014	-1.2557	0.3189
H	-1.0180	-1.2252	0.8262
H	-1.4186	-1.2823	-0.8851
C	-4.2696	0.6615	-0.0091
H	0.7016	4.5507	0.3103
H	1.3409	3.4523	-0.9069
H	1.5033	3.0644	0.8004
H	-5.0822	1.3823	-0.1050
H	-4.4352	0.0960	0.9122
H	-4.3486	-0.0445	-0.8396
H	-2.7662	5.3370	-0.1281
H	-1.1631	5.3889	-0.8635
H	-1.3274	5.4090	0.8883
H	-3.8339	3.3061	-0.0572
H	0.6934	-0.3680	-0.4900
H	1.1564	0.4100	1.0193
H	1.5770	1.1497	-0.5211

Hexamethylbenzene

C	-2.8799	2.7361	0.0068
C	-2.8883	1.3342	-0.0160
C	-1.6789	0.6257	0.0225
C	-0.4602	1.3192	0.0103
C	-0.4519	2.7212	0.0330
C	-1.6613	3.4297	-0.0054
C	-1.6507	4.9413	-0.0866
C	-1.6892	-0.8860	0.1038
C	0.8453	0.5555	-0.0545
C	0.8613	3.4687	0.1258
H	-2.5725	-1.2486	0.6287
H	-0.8208	-1.2600	0.6452
H	-1.6830	-1.3510	-0.8884
C	-4.2014	0.5866	-0.1092
H	0.7433	4.4143	0.6539
H	1.2763	3.6945	-0.8629
H	1.6086	2.8913	0.6692
H	-4.9488	1.1643	-0.6522
H	-4.6164	0.3601	0.8793
H	-4.0833	-0.3586	-0.6381
H	-2.5201	5.3157	-0.6261
H	-0.7684	5.3036	-0.6134
H	-1.6546	5.4062	0.9056
C	-4.1853	3.5000	0.0719
H	0.7274	-0.3873	-0.5878
H	1.2348	0.3221	0.9427
H	1.6118	1.1246	-0.5794
H	-4.9523	2.9303	0.5957
H	-4.5744	3.7349	-0.9251
H	-4.0675	4.4420	0.6065

1,2,4,5-Tetracyanobenzene

C	-3.2976	1.9459	-0.0036
C	-3.3045	0.5419	-0.0038
C	-2.1065	-0.1650	-0.0014
C	-0.9014	0.5301	0.0012
C	-0.8945	1.9341	0.0014
C	-2.0926	2.6409	-0.0009
C	-4.5329	2.6759	-0.0060
H	-2.0871	3.7238	-0.0007
C	-4.5472	-0.1756	-0.0066
H	-2.1119	-1.2478	-0.0016
C	0.3339	-0.1999	0.0037
C	0.3481	2.6516	0.0041
N	-5.5203	3.2626	-0.0079
N	-5.5404	-0.7522	-0.0088
N	1.3414	3.2282	0.0063
N	1.3213	-0.7866	0.0057

p-Phenylenediamine

C	-2.4302	2.3939	0.0790

C	-3.5700	1.5838	0.0786
C	-1.1823	1.7629	0.0787
C	-1.0780	0.3767	0.0786
C	-2.2178	-0.4334	0.0790
C	-3.4657	0.1975	0.0787
H	-4.3675	-0.4078	0.0763
H	-4.5523	2.0472	0.0758
N	-2.5358	3.7964	0.1487
H	-0.2805	2.3682	0.0763
H	-0.0958	-0.0867	0.0758
N	-2.1122	-1.8359	0.1487
H	-3.3918	4.1443	-0.2644
H	-1.7466	4.2701	-0.2727
H	-1.2563	-2.1839	-0.2644
H	-2.9014	-2.3096	-0.2727

1,4-Diethynylbenzene

C	-2.4270	2.3645	0.0841
C	-3.5748	1.5616	0.0852
C	-1.1637	1.7594	0.0851
C	-1.0503	0.3785	0.0872
C	-2.1980	-0.4244	0.0883
C	-3.4614	0.1807	0.0873
H	-4.3505	-0.4386	0.0882
H	-4.5529	2.0277	0.0844
C	-2.5436	3.7931	0.0819
H	-0.2746	2.3787	0.0842
H	-0.0721	-0.0876	0.0879
C	-2.0814	-1.8531	0.0906
C	-2.6409	4.9919	0.0806
H	-2.7274	6.0554	0.0796
C	-1.9840	-3.0518	0.0931
H	-1.8974	-4.1153	0.0954

Hydroquinone

C	-2.0047	0.3991	0.0000
C	-1.9198	-0.9887	0.0000
C	-0.6751	-1.6164	0.0000
C	0.4820	-0.8422	0.0000
C	0.3971	0.5455	0.0000
C	-0.8475	1.1732	0.0000
H	-2.9698	0.8931	0.0000
H	1.4471	-1.3363	0.0000
H	1.3035	1.1438	0.0000
H	-2.8261	-1.5870	0.0000
O	-0.9921	2.5313	0.0000
O	-0.5306	-2.9744	0.0000
H	-0.1280	2.9589	0.0000
H	-1.3947	-3.4021	0.0000

7-Hydroxy-4-(trifluoromethyl)coumarin

C	-0.4968	0.6270	-0.0408
C	-0.5322	-0.7769	-0.0602
C	0.6481	-1.5108	-0.0473
C	1.8539	-0.8313	-0.0162
C	1.9242	0.5693	0.0041
C	0.7141	1.2845	-0.0083
C	3.2465	1.1495	0.0342
C	4.3475	0.3808	0.0397
C	4.2434	-1.0748	0.0182
O	2.9807	-1.6004	-0.0063
H	0.6294	-2.5934	-0.0618
H	-1.4259	1.1865	-0.0520
H	0.7202	2.3670	0.0069
H	5.3495	0.7864	0.0604
O	5.1724	-1.8358	0.0217
O	-1.6861	-1.4690	-0.0916
H	-2.4469	-0.8748	-0.0987
C	3.3889	2.6502	0.0658
F	2.8071	3.1658	1.1571
F	2.8008	3.2150	-0.9972
F	4.6625	3.0416	0.0707

Acridine

C	-4.2114	2.4432	0.0000
C	-4.2130	1.0142	0.0000
C	-3.0454	0.3133	0.0000
C	-1.7869	0.9955	0.0000
C	-1.7884	2.4301	0.0000
C	-3.0356	3.1294	0.0000
H	-3.0298	-0.7707	0.0000
H	-5.1557	2.9751	0.0000
H	-5.1608	0.4876	0.0000
H	-3.0201	4.2147	0.0000
C	-0.5576	3.0825	0.0000
N	-0.6628	0.2679	0.0000
C	0.5127	0.9096	0.0000
C	0.6211	2.3402	0.0000
H	-0.5169	4.1688	0.0000
C	1.7169	0.1359	0.0000
C	2.9336	0.7480	0.0000
C	3.0384	2.1731	0.0000
C	1.9167	2.9447	0.0000
H	4.0197	2.6332	0.0000
H	1.9822	4.0281	0.0000
H	1.6214	-0.9440	0.0000
H	3.8394	0.1521	0.0000

Acridone

C	-4.2374	2.4576	-0.0425
C	-4.2423	1.0513	-0.0080
C	-3.0638	0.3387	0.0084
C	-1.8319	1.0221	-0.0094
C	-1.8156	2.4280	-0.0434
C	-3.0345	3.1281	-0.0597
H	-3.0670	-0.7459	0.0350
H	-5.1729	3.0036	-0.0554
H	-5.1853	0.5162	0.0060
H	-2.9951	4.2110	-0.0863
C	-0.5416	3.1627	-0.0619
N	-0.6542	0.3190	0.0062
C	0.5756	0.9266	-0.0089
C	0.6702	2.3294	-0.0419
C	1.7495	0.1479	0.0084
C	2.9806	0.7659	-0.0063
C	3.0864	2.1684	-0.0386
C	1.9402	2.9317	-0.0561
H	4.0621	2.6388	-0.0495
H	1.9854	4.0144	-0.0815
H	1.6671	-0.9335	0.0335
H	3.8786	0.1584	0.0073
H	-0.6945	-0.6917	0.0314
O	-0.4925	4.3882	-0.0924

Coumarin 151.0000

C	-4.7551	2.0310	0.0438
C	-4.8365	0.6194	0.0553
C	-3.6525	-0.1251	0.0437
C	-2.4329	0.5321	0.0247
C	-2.3293	1.9294	0.0150
C	-3.5314	2.6605	0.0240
O	-1.3201	-0.2575	0.0131
C	-0.0477	0.2623	-0.0054
C	0.0706	1.7051	-0.0148
C	-1.0099	2.5204	-0.0057
N	-6.0592	-0.0024	0.1327
C	-0.8611	4.0116	-0.0164
H	0.1894	4.2977	-0.0306
H	-1.3337	4.4502	0.8660
H	-1.3541	4.4392	-0.8931
H	-6.8578	0.5359	-0.1696
H	-6.0982	-0.9690	-0.1560
O	0.8660	-0.5265	-0.0123
H	-3.6733	-1.2091	0.0498

H	-3.4946	3.7440	0.0135
H	-5.6710	2.6117	0.0519
H	1.0811	2.0937	-0.0294
Coumarin	314.0000		
C	-3.8996	1.1645	0.0653
C	-2.6816	1.7889	0.0105
C	-1.4726	1.0638	-0.0026
C	-1.5551	-0.3367	0.0307
C	-2.7536	-1.0261	0.0647
C	-3.9551	-0.2714	0.0828
H	-2.6371	2.8744	-0.0104
C	-0.1891	1.6454	-0.0393
O	-0.4144	-1.0808	0.0304
C	0.8668	-0.5581	-0.0015
C	0.9557	0.8968	-0.0368
H	-0.0991	2.7272	-0.0680
C	2.2428	1.6330	-0.0692
O	2.3024	2.8422	-0.1284
O	3.3218	0.8588	-0.0218
C	4.5921	1.5407	-0.0449
C	5.6640	0.4792	0.0314
H	4.6337	2.2285	0.8014
H	4.6568	2.1255	-0.9641
H	5.5686	-0.0979	0.9524
H	6.6491	0.9480	0.0171
H	5.5925	-0.2019	-0.8180
O	1.7582	-1.3653	-0.0005
C	-5.1764	1.9690	0.1291
C	-6.3422	1.1731	-0.4415
H	-5.0406	2.9118	-0.4047
H	-5.3947	2.2224	1.1727
C	-6.4118	-0.1733	0.2574
H	-6.2047	1.0165	-1.5154
H	-7.2844	1.7044	-0.2978
N	-5.1583	-0.9088	0.1076
H	-7.2026	-0.7897	-0.1731
H	-6.6415	-0.0374	1.3229
C	-5.2262	-2.3482	0.3457
C	-4.1097	-3.0679	-0.3912
H	-6.2015	-2.6914	-0.0014
H	-5.1658	-2.5518	1.4235
C	-2.7623	-2.5355	0.0785
H	-4.2276	-2.9006	-1.4656
H	-4.1837	-4.1414	-0.2101
H	-1.9558	-2.9117	-0.5533
H	-2.5549	-2.8943	1.0928
Coumarin	343.0000		
C	-3.9036	1.1693	0.0701
C	-2.6898	1.7987	0.0180
C	-1.4758	1.0792	0.0076
C	-1.5563	-0.3241	0.0400
C	-2.7481	-1.0193	0.0720
C	-3.9543	-0.2682	0.0893
H	-2.6489	2.8841	-0.0041
C	-0.1992	1.6691	-0.0295
O	-0.4100	-1.0704	0.0408
C	0.8382	-0.5307	0.0068
C	0.9414	0.9113	-0.0305
H	-0.1070	2.7508	-0.0581
C	2.2618	1.5916	-0.0697
O	2.3690	2.7941	-0.1056
O	3.3479	0.8179	-0.0641
O	1.7700	-1.3156	0.0114
C	-5.1840	1.9680	0.1280
C	-6.3425	1.1662	-0.4492
H	-5.0495	2.9114	-0.4047
H	-5.4080	2.2191	1.1708
C	-6.4113	-0.1787	0.2521
H	-6.1974	1.0082	-1.5218
H	-7.2878	1.6938	-0.3127

N	-5.1518	-0.9086	0.1168
H	-7.1941	-0.8011	-0.1839
H	-6.6501	-0.0426	1.3152
C	-5.2169	-2.3504	0.3459
C	-4.0962	-3.0637	-0.3901
H	-6.1900	-2.6934	-0.0071
H	-5.1607	-2.5579	1.4228
C	-2.7515	-2.5289	0.0846
H	-4.2115	-2.8947	-1.4644
H	-4.1671	-4.1377	-0.2112
H	-1.9431	-2.9024	-0.5461
H	-2.5461	-2.8871	1.0994
H	3.0986	-0.1276	-0.0338

Coumarin 1.0000

C	-4.6559	1.2535	-0.1869
C	-3.4320	1.8705	-0.0596
C	-4.7661	-0.1657	-0.2096
C	-3.5679	-0.9033	-0.1128
C	-2.3531	-0.2532	0.0098
C	-2.2356	1.1416	0.0456
C	-0.9199	1.7217	0.1750
C	0.1506	0.8968	0.2630
C	0.0205	-0.5446	0.2298
O	-1.2497	-1.0535	0.1048
H	-5.5299	1.8774	-0.3021
H	-3.3952	2.9544	-0.0567
H	-3.5561	-1.9843	-0.1066
C	-0.7624	3.2119	0.2092
H	1.1604	1.2749	0.3612
H	-1.1592	3.6597	-0.7055
H	0.2853	3.4909	0.3107
H	-1.3229	3.6370	1.0456
N	-5.9700	-0.8078	-0.3259
C	-7.2349	-0.0750	-0.3669
C	-6.0070	-2.2019	-0.7702
C	-6.0132	-3.2159	0.3720
H	-5.1587	-2.3834	-1.4343
H	-6.9006	-2.3277	-1.3850
H	-5.1500	-3.0815	1.0267
H	-5.9810	-4.2315	-0.0291
H	-6.9134	-3.1164	0.9797
C	-8.3728	-0.8166	0.3272
H	-7.5067	0.1479	-1.4072
H	-7.1034	0.8741	0.1467
H	-8.6163	-1.7631	-0.1575
H	-9.2684	-0.1933	0.3041
H	-8.1199	-1.0163	1.3703
O	0.9247	-1.3422	0.3007

7-Benzylamino-4-nitrobenz-2-oxa-1,3-diazole

C	-3.4563	-0.9914	-0.6196
C	-4.1010	-2.0175	0.0354
C	-3.2962	-2.9868	0.7083
C	-1.8726	-2.8317	0.6628
C	-1.2117	-1.7426	-0.0277
C	-2.0612	-0.8380	-0.6647
N	-3.5566	-4.0622	1.4107
N	-1.3250	-3.8070	1.3302
O	-2.3426	-4.5477	1.7791
H	-4.0705	-0.2605	-1.1318
H	-1.6517	0.0001	-1.2113
N	0.1164	-1.6706	-0.0109
C	0.8660	-0.6033	-0.6709
C	2.3346	-0.7405	-0.3645
H	0.4886	0.3584	-0.3085
H	0.6890	-0.6492	-1.7497
C	2.8096	-0.4240	0.9103
C	4.1592	-0.5673	1.2123
C	5.0457	-1.0268	0.2398
C	4.5776	-1.3447	-1.0315
C	3.2243	-1.2049	-1.3311

H	2.8576	-1.4542	-2.3218
H	2.1172	-0.0602	1.6637
H	4.5210	-0.3160	2.2030
H	6.0990	-1.1349	0.4735
H	5.2640	-1.7021	-1.7908
H	0.6383	-2.3971	0.4618
N	-5.5280	-2.1025	0.0339
O	-6.1685	-1.2502	-0.5614
O	-6.0386	-3.0332	0.6353

L-Phenylalanine

C	-3.6839	1.0407	0.6691
C	-4.8544	0.3545	0.9850
C	-5.2039	-0.7920	0.2769
C	-4.3768	-1.2477	-0.7479
C	-3.2084	-0.5592	-1.0594
C	-2.8482	0.5930	-0.3556
H	-3.4176	1.9377	1.2206
H	-5.4940	0.7172	1.7822
H	-2.5671	-0.9158	-1.8607
H	-6.1157	-1.3263	0.5195
H	-4.6444	-2.1376	-1.3072
C	-1.5548	1.3010	-0.6672
C	-0.3755	0.6567	0.0755
H	-1.6165	2.3546	-0.3758
H	-1.3484	1.2664	-1.7383
C	0.9528	1.2742	-0.3731
H	-0.3093	-0.3973	-0.2175
N	-0.4436	0.7019	1.5351
O	1.1837	1.6235	-1.5026
O	1.8607	1.3670	0.5918
H	-1.0033	-0.0607	1.8972
H	-0.8788	1.5661	1.8472
H	1.4207	1.0554	1.4139

7-Methoxycoumarin-4-acetic acid

C	-3.7958	1.9544	-0.0530
C	-3.7748	0.5511	-0.0080
C	-2.5601	-0.1268	0.0915
C	-1.3842	0.5982	0.1400
C	-1.3691	2.0000	0.0919
C	-2.6036	2.6547	-0.0036
O	-0.2298	-0.1221	0.2378
C	1.0028	0.4733	0.2882
C	1.0391	1.9260	0.2304
C	-0.0829	2.6693	0.1376
C	-0.0651	4.1780	0.1015
C	1.3299	4.7633	0.1630
H	-0.6265	4.5664	0.9528
H	-0.5665	4.5222	-0.8096
O	1.7963	5.2792	1.1399
O	2.0648	4.6656	-0.9545
H	2.0331	2.3541	0.2701
O	1.9638	-0.2460	0.3783
O	-4.8746	-0.2237	-0.0550
C	-6.1428	0.4156	-0.1566
H	-6.3246	1.0583	0.7075
H	-6.8756	-0.3861	-0.1776
H	-6.2102	1.0008	-1.0763
H	-4.7276	2.4978	-0.1270
H	-2.6365	3.7374	-0.0393
H	-2.5385	-1.2089	0.1291
H	1.5797	4.2614	-1.6866

S3 – Input geometries of the 10 compounds on Figure 5 (in the paper)

Compound 1

C	-4.14037	2.50423	0.33630
C	-3.79972	3.34707	1.57013
C	-2.46895	4.08339	1.39500
H	-3.77258	2.72007	2.46855
H	-4.59327	4.08584	1.73845
C	-1.27631	3.14398	1.06460
H	-2.61654	4.80246	0.58069
H	-2.25495	4.66605	2.29936
C	-2.98880	1.56213	-0.03887
H	-4.30824	3.18759	-0.50720
C	-5.43080	1.71751	0.55981
C	-1.65386	2.31449	-0.19097
H	-2.89611	0.76199	0.70526
H	-3.23144	1.06492	-0.98723
C	0.06292	3.94304	0.82837
C	-0.53774	1.34453	-0.57993
H	-1.78543	3.01652	-1.02809
C	0.73512	2.10547	-0.90441
H	-0.35035	0.60901	0.20972
H	-0.83683	0.77002	-1.46563
C	1.21143	3.07605	0.19716
H	0.55553	2.65953	-1.83547
H	1.53319	1.38691	-1.12815
C	-0.04097	5.29789	0.09249
H	0.38455	4.22161	1.83888
C	1.25828	6.13972	0.19358
H	-0.84350	5.91957	0.49973
H	-0.28401	5.12329	-0.96285
C	2.54355	5.29395	0.30686
H	1.29631	6.79438	-0.68590
H	1.17840	6.81399	1.05571
C	2.30840	3.96932	-0.42139
H	1.65016	2.47452	1.00385
C	3.74826	5.85408	-0.48376
C	3.70807	3.38333	-0.55423
H	1.98684	4.22256	-1.44579
C	4.55920	4.61033	-0.97286
H	4.02612	2.95095	0.40012
H	3.75669	2.59173	-1.30952
H	4.33287	6.55373	0.12328
H	3.40864	6.41016	-1.36713
C	6.02413	4.60246	-0.57862
H	4.55466	4.63843	-2.07299
C	6.79538	5.76363	-0.74410
C	8.15767	5.78495	-0.42202
C	8.80551	4.63984	0.05847
C	8.04334	3.47179	0.19471
C	6.67935	3.45035	-0.12640
H	6.15111	2.50708	-0.01748
H	8.50767	2.55854	0.56207
H	6.34510	6.67247	-1.13825
H	8.71658	6.70697	-0.56911
C	10.23805	4.66024	0.39646
C	10.75806	5.61467	1.28679
C	12.11793	5.63534	1.60885
C	12.98237	4.70119	1.04399
C	12.48830	3.74681	0.15855
C	11.12788	3.72691	-0.16132
H	10.76460	2.98026	-0.86465
H	13.16026	3.01808	-0.28702
H	12.49902	6.37985	2.30280
H	14.03994	4.71697	1.29352
H	10.09770	6.34627	1.74818
C	-1.03528	2.22666	2.30202
H	-1.86880	1.54777	2.49885
H	-0.89483	2.83034	3.20683
H	-0.13993	1.60763	2.19372
C	2.98706	5.15847	1.78391
H	2.28196	4.60255	2.40224

H	3.10559	6.14965	2.23783
H	3.95439	4.65475	1.88235
H	-5.32888	1.01346	1.39264
H	-5.69756	1.14649	-0.33573
H	-6.26270	2.39251	0.78678

Donor moiety of compound 1

C	-6.88010	1.29451	-0.00073
C	-6.17719	2.49057	-0.00031
C	-6.17900	0.09739	-0.00048
C	-4.77659	0.10000	0.00020
C	-4.02167	1.29235	0.00069
C	-4.77479	2.48583	0.00038
C	-2.51997	1.29124	0.00155
C	-1.76493	2.48186	0.00199
C	-1.76655	0.09938	0.00206
C	-0.36269	0.09335	0.00303
C	0.35195	1.28812	0.00353
C	-0.36143	2.48453	0.00297
H	-2.24386	3.45577	0.00161
C	1.85028	1.30091	0.00468
H	0.16576	3.43623	0.00331
H	0.15937	-0.86098	0.00342
H	-2.24738	-0.87365	0.00176
H	-4.29351	3.45861	0.00071
H	-7.96626	1.29533	-0.00123
H	-6.71347	3.43614	-0.00049
H	-6.71671	-0.84737	-0.00080
H	-4.29680	-0.87351	0.00036
H	2.26091	0.28582	0.00511
H	2.22267	1.81373	0.89733
H	2.22405	1.81357	-0.88748

Compound 2

C	-9.55161	2.08083	-0.00000
C	-9.49182	0.69044	-0.00000
C	-8.25379	0.04580	-0.00000
C	-7.05947	0.78495	-0.00000
C	-7.11964	2.19652	0.00000
C	-8.37351	2.82959	0.00000
H	-8.44040	3.91509	0.00000
H	-10.51467	2.58440	-0.00000
H	-10.40805	0.10602	-0.00000
H	-8.22676	-1.04141	-0.00000
C	-5.92415	2.93556	0.00000
C	-5.80668	0.15280	0.00000
C	-4.62696	0.90135	0.00000
C	-4.67582	2.29741	0.00000
H	-5.73949	-0.93272	0.00000
H	-3.67117	0.38253	0.00000
C	-3.41831	3.11489	0.00000
H	-5.96336	4.02332	0.00000
H	-2.52609	2.48015	-0.00000
H	-3.38002	3.74765	0.89253
H	-3.38002	3.74765	-0.89252

Compound 3

C	-4.30448	3.82460	0.00000
C	-5.54782	3.22084	0.00000
C	-5.63869	1.82763	-0.00000
C	-4.49642	0.98495	0.00000
C	-3.22075	1.61839	0.00000
C	-3.15858	3.03222	0.00000
H	-4.21957	4.90763	0.00000
H	-6.45082	3.82517	-0.00000
H	-6.64041	1.40800	-0.00000
H	-2.19992	3.54569	0.00000
C	-4.58214	-0.45372	-0.00000
C	-3.39003	-1.21586	0.00000
C	-2.15154	-0.57108	0.00000
C	-2.04836	0.82600	0.00000
H	-1.24060	-1.16817	0.00000

C	-0.66789	1.43342	0.00000
C	-5.79829	-1.18730	-0.00000
C	-5.83224	-2.58541	-0.00000
C	-4.64789	-3.30375	-0.00000
C	-3.43497	-2.62155	0.00000
H	-6.75684	-0.67695	-0.00000
H	-6.78669	-3.10509	-0.00000
H	-4.66445	-4.38993	-0.00000
H	-2.51393	-3.20119	0.00000
H	0.11303	0.66522	-0.00000
H	-0.52084	2.04527	0.89587
H	-0.52084	2.04527	-0.89587

Compound 4

C	-5.25054	2.61680	-0.00000
C	-6.45444	1.91954	-0.00000
C	-6.46282	0.52349	-0.00000
C	-5.23636	-0.18468	-0.00000
C	-3.99925	0.51733	0.00000
C	-4.01933	1.93968	-0.00000
C	-5.26563	-1.60685	0.00000
C	-2.81789	-0.25552	0.00000
C	-7.67574	-0.17765	-0.00000
C	-7.69509	-1.57211	-0.00000
C	-2.84628	-1.65356	0.00000
C	-4.06019	-2.34196	0.00000
C	-6.50088	-2.29977	-0.00000
C	-6.51068	-3.70252	-0.00000
C	-5.31688	-4.42069	0.00000
C	-4.09887	-3.74450	0.00000
C	-2.78652	2.80717	0.00000
H	-5.27422	3.70514	0.00000
H	-7.38638	2.48011	-0.00000
H	-1.83872	0.21305	0.00000
H	-1.90365	-2.19638	0.00000
H	-8.62253	0.35814	-0.00000
H	-8.65452	-2.08425	-0.00000
H	-5.33579	-5.50727	-0.00000
H	-3.17676	-4.32139	0.00000
H	-7.45210	-4.24734	-0.00000
H	-1.84872	2.25122	-0.00000
H	-2.78373	3.44463	0.89100
H	-2.78373	3.44463	-0.89100

Compound 5

C	-9.41088	0.05791	-2.73906
H	-8.76752	0.34452	-3.57785
C	-10.77106	-0.36330	-3.20000
C	-11.75038	-0.74337	-2.13934
C	-11.13516	-0.38375	-4.48870
C	-13.20136	-0.94183	-2.52970
C	-13.32325	-1.59515	-3.90843
C	-12.46496	-0.86649	-4.93025
O	-11.39005	-0.81394	-0.96621
O	-12.75960	-0.75565	-6.11673
C	-13.92563	0.40974	-2.43235
H	-13.64035	-1.63468	-1.79775
C	-15.23884	0.43507	-3.15190
H	-13.30428	1.22400	-2.82568
H	-14.09651	0.64276	-1.37374
C	-15.63182	-0.52427	-4.00001
C	-14.78924	-1.71578	-4.34972
H	-14.85890	-1.89578	-5.42852
H	-15.23799	-2.58975	-3.86057
H	-12.90313	-2.61058	-3.86486
H	-9.48259	0.91945	-2.06711
H	-8.91554	-0.76067	-2.20664
H	-10.46482	-0.07776	-5.28495
H	-16.60715	-0.45194	-4.47689
H	-15.89516	1.28158	-2.96074

Compound 6

C	-9.30999	-0.08307	-2.78390
H	-8.53667	-0.33277	-3.51826
C	-10.68741	-0.28661	-3.33421
C	-11.81940	0.01914	-2.41814
C	-10.91886	-0.71957	-4.57992
C	-13.19412	-0.16798	-2.92562
C	-13.41641	-0.61902	-4.22538
C	-12.27973	-0.91692	-5.11415
O	-11.62068	0.41495	-1.27565
O	-12.44058	-1.31542	-6.26034
C	-14.28353	0.11185	-2.08974
C	-15.58742	-0.06063	-2.55838
C	-15.80797	-0.51190	-3.85947
C	-14.72511	-0.79175	-4.69454
H	-16.43132	0.15750	-1.90733
H	-16.82401	-0.64610	-4.22444
H	-9.16396	0.96205	-2.49171
H	-9.14957	-0.71724	-1.90580
H	-14.12018	0.46460	-1.07266
H	-14.90383	-1.14376	-5.70922
H	-10.11309	-0.95012	-5.26881

Compound 7

C	-8.90511	3.24494	-0.00117
C	-8.91818	1.90962	-0.00061
C	-7.66386	1.13619	-0.00005
C	-6.39768	1.89432	-0.00010
C	-6.36892	3.23446	-0.00066
C	-7.64003	4.00781	-0.00126
H	-9.81769	3.82901	-0.00159
H	-9.83937	1.33986	-0.00054
H	-5.49465	1.29433	0.00034
C	-5.10204	4.02993	-0.00072
H	-4.21665	3.38519	-0.00032
H	-5.04856	4.66697	0.88824
H	-5.04822	4.66632	-0.89012
O	-7.65819	5.23221	-0.00181
O	-7.67206	-0.08714	0.00044

Compound 8

C	-8.87100	3.26819	-0.00120
C	-8.88392	1.93379	-0.00065
C	-7.62587	1.14605	-0.00002
C	-6.36193	1.91365	-0.00009
C	-6.33536	3.25297	-0.00064
C	-7.60632	4.02329	-0.00122
H	-9.77869	3.85994	-0.00166
Cl	-10.37539	1.07110	-0.00064
H	-5.45629	1.31658	0.00035
C	-5.06870	4.04987	-0.00072
H	-4.18272	3.40595	-0.00033
H	-5.01584	4.68692	0.88826
H	-5.01553	4.68625	-0.89018
O	-7.62220	5.24765	-0.00171
O	-7.59147	-0.07818	0.00052

Compound 9

C	-8.85269	3.23965	-0.00120
C	-8.85831	1.90120	-0.00064
C	-7.58790	1.13316	0.00002
C	-6.32916	1.90154	-0.00006
C	-6.30584	3.23862	-0.00062
C	-7.57804	4.01029	-0.00118
Cl	-10.30558	4.18549	-0.00198
Cl	-10.31166	0.95947	-0.00064
H	-5.42106	1.30710	0.00036
C	-5.03670	4.03372	-0.00073
H	-4.15179	3.38827	-0.00037
H	-4.98224	4.67039	0.88847
H	-4.98198	4.66973	-0.89037
O	-7.55083	5.23647	-0.00161
O	-7.53744	-0.09108	0.00061

S4 – Input geometries of the compounds 10 to 12 on Figure 7 (in the paper)

Compound 10

C	-8.34609	4.88147	0.00126
C	-6.95556	4.83721	0.00233
C	-9.09096	3.70071	0.00088
C	-8.42398	2.45137	0.00158
C	-7.00274	2.39359	0.00267
C	-6.26814	3.61172	0.00305
C	-4.76309	3.69669	0.00420
H	-8.84103	5.84986	0.00073
H	-6.40052	5.77368	0.00261
C	-10.49120	3.74644	-0.00019
C	-11.24454	2.57281	-0.00058
C	-10.61524	1.32398	0.00010
C	-9.20037	1.25947	0.00118
H	-11.01185	4.70164	-0.00074
H	-12.32970	2.64504	-0.00141
C	-8.56547	-0.00163	0.00186
C	-7.17112	-0.05870	0.00292
C	-6.40823	1.11318	0.00332
H	-6.65772	-1.01767	0.00346
H	-5.32933	0.99353	0.00415
C	-11.36484	0.13827	-0.00028
C	-10.73086	-1.10230	0.00040
C	-9.33948	-1.17190	0.00146
H	-8.86151	-2.14894	0.00198
H	-12.45198	0.17323	-0.00110
H	-11.32112	-2.01477	0.00010
H	-4.26074	2.72913	0.00473
H	-4.42455	4.23652	0.89539
H	-4.42317	4.23627	-0.88661

Compound 11

C	-4.01302	3.77124	-0.00000
C	-4.73505	2.57391	-0.00000
C	-4.10025	1.32688	-0.00000
C	-2.68698	1.24866	0.00000
C	-1.93472	2.46881	0.00000
C	-2.60136	3.73814	0.00000
H	-5.82346	2.61406	-0.00000
C	-0.41967	2.46255	0.00000
C	-4.88284	0.15857	-0.00000
C	-4.29557	-1.10287	0.00000
C	-2.91461	-1.20962	0.00000
C	-2.12569	-0.05460	0.00000
H	-2.44264	-2.18862	0.00000
H	-1.05113	-0.20579	0.00000
H	-5.96915	0.22428	-0.00000
H	-4.91546	-1.99492	-0.00000
C	-4.69701	5.00004	-0.00000
C	-1.93004	4.98651	0.00000
C	-2.61945	6.20227	0.00000
C	-4.00567	6.20876	0.00000
H	-4.54968	7.14913	0.00000
H	-5.78492	5.02350	-0.00000
H	-0.84374	5.03195	0.00000
H	-2.06852	7.13897	0.00000
H	0.02871	1.46961	-0.00000
H	-0.04480	2.97088	0.89506
H	-0.04480	2.97088	-0.89506

Compound 12

C	-5.83323	1.90873	-0.02439
C	-5.08070	3.07678	0.07571
C	-5.16217	0.68800	-0.00670
C	-3.76200	0.64325	0.07638
C	-2.97306	1.80515	0.14425
C	-3.68094	3.02006	0.15810
H	-3.16025	3.96868	0.24215
H	-5.57100	4.04720	0.09550
C	-7.32964	1.96081	-0.07493

H	-5.71768	-0.24570	-0.05320
H	-3.30764	-0.34233	0.09146
H	-7.67290	2.88043	-0.56045
H	-7.74053	1.92190	0.93858
H	-7.72988	1.12058	-0.65206
N	-1.57627	1.75514	0.24245
C	-0.80783	2.97109	-0.01685
H	-0.99539	3.34811	-1.02835
H	0.26894	2.78753	0.07208
H	-1.03941	3.75086	0.71653
C	-0.89051	0.49929	-0.05456
H	0.19446	0.60266	0.06024
H	-1.08460	0.17780	-1.08381
H	-1.19023	-0.29114	0.64188

S5 – Input geometries of the compounds 18 to 20 on Figure 8 (in the paper)

Compound 18

C	-3.10686	2.66068	-0.09936
C	-3.08649	1.26172	0.03239
C	-1.84786	0.57647	0.01624
C	-0.65466	1.30405	-0.13131
C	-0.67859	2.69877	-0.26241
C	-1.91535	3.38298	-0.24630
H	-4.05368	3.18889	-0.08744
C	-1.93770	4.78088	-0.37782
C	-4.38734	0.51774	0.18859
C	-1.78403	-0.92250	0.15463
H	0.29589	0.78258	-0.14412
C	0.51477	3.42410	-0.40976
H	-2.22678	-1.23102	1.12461
H	-0.73853	-1.29631	0.12154
H	-2.34490	-1.40214	-0.67449
H	-5.25993	1.20507	0.18050
H	-4.39415	-0.03193	1.15290
H	-4.51229	-0.20309	-0.64620
C	-0.74306	5.49158	-0.52386
C	0.47936	4.81531	-0.53978
H	1.40156	5.37050	-0.65314
H	1.47216	2.91691	-0.42437
H	-2.87611	5.32250	-0.36773
H	-0.76483	6.56901	-0.62492

Compound 19

C	-3.20594	2.36046	-0.44085
C	-3.19850	1.02297	-0.12787
C	-1.96867	0.39240	0.23917
C	-0.81303	1.13402	0.27590
C	-0.80166	2.52129	-0.04097
C	-2.01940	3.14529	-0.40761
O	-4.37655	2.98813	-0.80591
C	-2.01884	4.52396	-0.73913
C	-4.46880	0.21669	-0.17761
C	-1.95201	-1.07151	0.58982
O	0.38311	0.55059	0.63094
C	0.38509	3.29569	0.01089
H	-2.73960	-1.31062	1.30800
H	-0.99515	-1.35332	1.02520
H	-2.12557	-1.69310	-0.29405
H	-5.26724	0.78314	-0.65324
H	-4.79763	-0.06653	0.82710
H	-4.32324	-0.70905	-0.73882
C	-0.85591	5.24808	-0.69003
C	0.35679	4.62919	-0.30568
H	1.26748	5.21584	-0.26164
H	1.30722	2.81559	0.31646
H	-2.95038	4.98742	-1.04181
H	-0.86255	6.30155	-0.94612
C	-5.10647	3.48697	0.30946
C	1.06885	-0.02093	-0.47742
H	-5.98880	3.98475	-0.08897
H	-4.50384	4.20214	0.87740

H	-5.41158	2.66942	0.96976
H	2.00663	-0.42069	-0.09549
H	1.27386	0.73800	-1.23852
H	0.47919	-0.82758	-0.92354

Compound 20

C	-2.42086	1.89139	-0.00000
C	-1.06385	1.88584	0.00000
C	-0.30641	3.09520	0.00000
C	-0.31589	0.67059	-0.00000
C	-3.25794	3.15164	0.00000
H	-2.66966	4.07277	-0.00000
H	-3.89855	3.17496	0.88813
H	-3.89855	3.17496	-0.88813
C	-3.26871	0.63838	-0.00000
H	-2.68838	-0.28777	0.00000
H	-3.90958	0.62062	-0.88809
H	-3.90958	0.62062	0.88809
N	0.29959	4.08514	0.00000
N	0.28292	-0.32368	-0.00000

S6 – Input geometries of the 12 systems on Table 4 (in the paper)

System 11-13-12

C	-2.55033	0.34115	0.21101
C	-1.77414	1.12791	1.07150
C	-2.23980	0.32206	-1.15593
C	-1.17453	1.07596	-1.65274
C	-0.39604	1.86158	-0.79273
C	-0.70874	1.88197	0.57365
H	-0.11685	2.48312	1.26104
H	-1.99407	1.16183	2.13622
H	-2.83456	-0.27698	-1.84276
H	-0.95845	1.04499	-2.71826
C	0.74837	2.68880	-1.33555
C	2.10938	2.31875	-0.79302
H	0.79095	2.61076	-2.42984
H	0.52651	3.74334	-1.12489
C	2.90939	3.27263	-0.16317
C	2.61599	1.02534	-0.93028
C	3.88966	0.69749	-0.44103
C	4.72141	1.64206	0.18392
C	4.18322	2.93402	0.31816
H	2.55362	4.29175	-0.03125
H	2.02241	0.25136	-1.41208
H	4.21134	-0.33042	-0.57530
H	4.74157	3.71896	0.81873
N	5.98917	1.31566	0.68357
C	6.97224	2.38951	0.82215
H	7.11679	2.91767	-0.12706
H	7.94826	1.99835	1.13116
H	6.67482	3.10240	1.59820
C	6.53944	-0.01228	0.42354
H	7.49738	-0.14800	0.93836
H	6.71216	-0.16498	-0.64747
H	5.88006	-0.79853	0.80712
C	-3.71302	-0.47249	0.74262
C	-5.11368	0.02743	0.40636
H	-3.63766	-0.55658	1.83440
H	-3.57015	-1.48219	0.33904
C	-5.32388	1.38963	0.12770
C	-6.59167	1.87886	-0.17733
C	-7.69610	1.02645	-0.19581
C	-7.52590	-0.34328	0.11417
C	-6.23666	-0.85365	0.42996
H	-4.49585	2.09585	0.13608
H	-6.70382	2.93758	-0.40026
C	-6.14907	-2.22473	0.75714
C	-7.26844	-3.06252	0.75314
C	-8.53023	-2.56368	0.42673
C	-8.66521	-1.19492	0.10799
H	-5.19932	-2.67650	1.03065

H	-7.13896	-4.11151	1.01029
C	-8.96872	1.52035	-0.51116
C	-10.07936	0.67707	-0.52343
C	-9.94452	-0.68028	-0.21517
H	-9.10791	2.57226	-0.75127
H	-11.05244	1.09340	-0.77354
C	-11.05637	-1.53554	-0.22018
C	-10.91459	-2.88578	0.09243
C	-9.65928	-3.39661	0.41521
H	-12.04443	-1.15392	-0.46771
H	-11.78268	-3.53956	0.08594
H	-9.56782	-4.45278	0.65867

System 10-14-12

C	-2.59292	-0.03834	0.50532
C	-1.66440	0.45934	1.42604
C	-2.31719	0.08949	-0.86160
C	-1.13871	0.70621	-1.29524
C	-0.19138	1.19737	-0.38132
C	-0.48155	1.06541	0.98680
H	0.23045	1.41430	1.73240
H	-1.84277	0.36662	2.49512
H	-3.02075	-0.29007	-1.60026
H	-0.96676	0.80051	-2.36563
C	4.83369	3.55150	-2.17219
C	6.02854	3.09575	-1.36945
C	6.60780	3.92492	-0.40845
C	6.57909	1.82686	-1.55930
C	7.69063	1.40652	-0.81374
C	8.31067	2.23293	0.13745
C	7.72377	3.49658	0.32668
H	6.19801	4.91284	-0.21303
H	6.14861	1.14425	-2.28776
H	8.06265	0.40688	-1.01475
H	8.11173	4.17902	1.07673
N	9.41843	1.82005	0.89165
C	10.38139	2.84983	1.28367
H	10.73204	3.41497	0.41263
H	11.26191	2.40625	1.76256
H	9.95340	3.53824	2.01931
C	9.98261	0.49248	0.66106
H	10.76138	0.26799	1.39884
H	10.43454	0.42190	-0.33445
H	9.22357	-0.28893	0.77805
C	-3.84381	-0.75110	0.97951
C	-5.18819	-0.14888	0.58908
H	-3.82911	-0.84019	2.07337
H	-3.75812	-1.76714	0.57622
C	-5.29206	1.23029	0.33794
C	-6.50742	1.80948	-0.01957
C	-7.66446	1.03411	-0.11368
C	-7.60271	-0.34948	0.17463
C	-6.36801	-0.95189	0.54015
H	-4.41952	1.87716	0.40930
H	-6.53808	2.87781	-0.22234
C	-6.38954	-2.33138	0.84354
C	-7.56128	-3.09048	0.77136
C	-8.76894	-2.50127	0.39620
C	-8.79532	-1.12141	0.09749
H	-5.48756	-2.85226	1.15314
H	-7.51540	-4.14980	1.01446
C	-8.88407	1.61792	-0.48118
C	-10.04706	0.85230	-0.56423
C	-10.01971	-0.51589	-0.27573
H	-8.94067	2.68076	-0.70656
H	-10.97642	1.33783	-0.85288
C	-11.18541	-1.29314	-0.34869
C	-11.15064	-2.65452	-0.05425
C	-9.94972	-3.25485	0.31709
H	-12.13247	-0.84122	-0.63494
H	-12.05972	-3.24717	-0.11271
H	-9.94157	-4.31831	0.54551

C	1.07297	1.80712	-0.84138
C	1.57110	2.98824	-0.26697
C	2.78051	3.55144	-0.69251
C	3.52252	2.95411	-1.71735
C	3.03626	1.77782	-2.29812
C	1.83220	1.21389	-1.86368
H	1.49920	0.28584	-2.32402
H	3.59497	1.28300	-3.08896
H	1.01473	3.48967	0.52226
H	3.13789	4.46082	-0.21481
H	5.00296	3.31317	-3.23099
H	4.75830	4.64693	-2.14508

System 11-13-12

C	-2.60148	0.96710	0.57142
C	-1.52947	1.67966	1.12784
C	-2.48641	0.51683	-0.74975
C	-1.34599	0.80450	-1.50625
C	-0.28274	1.53136	-0.95471
C	-0.39136	1.97064	0.37077
H	0.41280	2.54237	0.82932
H	-1.57443	2.02615	2.15815
H	-3.28981	-0.04974	-1.21519
H	-1.30116	0.45962	-2.53705
C	0.91277	1.88934	-1.81106
C	2.25989	1.68449	-1.15800
H	0.90361	1.29915	-2.73719
H	0.79933	2.93507	-2.12544
C	3.06320	2.77298	-0.81639
C	2.73270	0.40299	-0.87451
C	3.98580	0.22083	-0.27020
C	4.82410	1.29820	0.06817
C	4.31352	2.57789	-0.21047
H	2.72653	3.78872	-1.01067
H	2.12675	-0.46922	-1.11008
H	4.28086	-0.80242	-0.06004
H	4.87953	3.47119	0.03400
N	6.06711	1.10518	0.68535
C	6.96467	2.24539	0.85497
H	7.26698	2.65697	-0.11429
H	7.87527	1.95490	1.39112
H	6.49955	3.03071	1.46069
C	6.71908	-0.19593	0.54417
H	7.70938	-0.19813	1.01366
H	6.85597	-0.45632	-0.51135
H	6.14729	-0.98299	1.04686
C	-3.81748	0.66394	1.42357
C	-5.16855	0.78092	0.71784
H	-3.84053	1.33267	2.29502
H	-3.67631	-0.32102	1.87830
C	-5.72648	2.08408	0.48475
C	-6.99135	2.18248	-0.13703
C	-7.67218	1.02270	-0.51956
C	-7.13359	-0.25264	-0.32064
C	-5.86798	-0.39971	0.29312
C	-5.38273	-1.72642	0.43252
C	-6.11442	-2.83988	0.00803
C	-7.35812	-2.66631	-0.57646
C	-7.86164	-1.37965	-0.74148
H	-4.40734	-1.92579	0.86714
H	-5.70506	-3.83866	0.13507
H	-8.64737	1.11644	-0.99575
H	-7.93377	-3.52566	-0.90857
H	-8.83715	-1.26094	-1.20925
C	-7.57438	3.43948	-0.37816
C	-6.92421	4.61652	-0.01856
C	-5.68027	4.54899	0.58743
C	-5.09380	3.30445	0.83440
H	-5.15737	5.45960	0.86722
H	-4.11296	3.31010	1.30172
H	-8.54897	3.51091	-0.85694
H	-7.38687	5.57934	-0.21574

System 11-14-12

C	-2.62019	0.93530	0.69653
C	-1.45986	1.34407	1.36953
C	-2.54501	0.73731	-0.68644
C	-1.35307	0.97952	-1.38038
C	-0.19274	1.40906	-0.71687
C	-0.26834	1.58001	0.67331
H	0.61115	1.89096	1.23377
H	-1.47237	1.48457	2.44855
H	-3.41306	0.40620	-1.25242
H	-1.34669	0.84292	-2.46012
C	4.65393	2.53202	-3.74975
C	5.95792	2.34146	-3.01449
C	6.74216	3.43606	-2.64939
C	6.42373	1.06574	-2.69526
C	7.65660	0.89419	-2.04740
C	8.48339	1.97702	-1.69995
C	7.97381	3.25186	-2.00166
H	6.41100	4.44868	-2.86722
H	5.83380	0.18695	-2.94463
H	7.94768	-0.12585	-1.81718
H	8.52800	4.14975	-1.74719
N	9.71522	1.79385	-1.05646
C	10.61568	2.93515	-0.90794
H	10.92577	3.32269	-1.88472
H	11.52215	2.65418	-0.35973
H	10.14989	3.73598	-0.32363
C	10.36714	0.48912	-1.16476
H	11.34790	0.49240	-0.67562
H	10.52462	0.21219	-2.21327
H	9.78403	-0.28914	-0.66137
C	-3.87943	0.67477	1.49928
C	-5.20587	0.79149	0.74975
H	-3.91660	1.36661	2.35200
H	-3.78057	-0.30290	1.98178
C	-5.76615	2.09172	0.51250
C	-7.01945	2.18573	-0.13297
C	-7.68329	1.02397	-0.53985
C	-7.13461	-0.24837	-0.34799
C	-5.88015	-0.38944	0.28891
C	-5.37657	-1.71027	0.41340
C	-6.08470	-2.82639	-0.04256
C	-7.32091	-2.66044	-0.64532
C	-7.83957	-1.37825	-0.79944
H	-4.40396	-1.90097	0.85849
H	-5.66263	-3.82122	0.07362
H	-8.64997	1.11396	-1.03371
H	-7.87815	-3.52222	-1.00176
H	-8.80758	-1.26536	-1.28382
C	-7.60649	3.44057	-0.37459
C	-6.96937	4.61880	0.00438
C	-5.73412	4.55490	0.62895
C	-5.14390	3.31258	0.87799
H	-5.22084	5.46720	0.92095
H	-4.16766	3.31994	1.35599
H	-8.57291	3.50956	-0.86999
H	-7.43460	5.58020	-0.19412
C	1.05485	1.67677	-1.45814
C	1.54338	0.76896	-2.41166
C	2.70716	1.03656	-3.14104
C	3.41926	2.22366	-2.93572
C	2.95574	3.12545	-1.97138
C	1.78880	2.85563	-1.24708
H	1.44420	3.59176	-0.52365
H	3.49395	4.05175	-1.78328
H	1.01780	-0.16629	-2.59398
H	3.04750	0.31049	-3.87570
H	4.67219	1.91163	-4.65596
H	4.57594	3.56272	-4.12140

System 10-15-12

C	-2.40337	0.21370	-0.68419
C	-1.89870	1.07609	0.32809
C	-1.80584	0.22744	-1.95047
C	-0.74033	1.07321	-2.23242
C	-0.21911	1.93721	-1.25868
C	-0.80464	1.94783	0.03779
H	-2.16866	-0.42211	-2.73771
H	-0.31385	1.04367	-3.22772
C	0.95913	2.81471	-1.65460
C	2.22202	2.43857	-0.91541
H	1.18303	2.69794	-2.73748
H	0.68955	3.88169	-1.49915
C	2.91227	3.38281	-0.14400
C	2.73060	1.13635	-1.00921
C	3.90079	0.77886	-0.33505
C	4.60444	1.71811	0.45355
C	4.08303	3.03009	0.53205
H	2.54514	4.39854	-0.06331
H	2.21749	0.39232	-1.60622
H	4.24345	-0.24030	-0.44206
H	4.57090	3.79912	1.11355
N	5.81433	1.35114	1.15194
C	6.53032	2.32907	1.96044
H	6.85612	3.17891	1.32404
H	7.43851	1.90198	2.43508
H	5.87239	2.69965	2.77481
C	6.34144	-0.00410	1.06166
H	7.27359	-0.13553	1.65016
H	6.57874	-0.24707	0.00428
H	5.59507	-0.72626	1.45512
C	-3.56539	-0.74123	-0.45050
C	-4.93101	-0.09767	-0.20929
H	-3.28792	-1.38221	0.41341
H	-3.68794	-1.40879	-1.33130
C	-5.10555	1.30166	-0.29457
C	-6.34832	1.89266	-0.07837
C	-7.46221	1.10895	0.22636
C	-7.32610	-0.29366	0.31239
C	-6.06378	-0.90709	0.09384
H	-4.28428	1.96070	-0.53489
H	-6.43728	2.97030	-0.15250
C	-5.97635	-2.31445	0.18812
C	-7.09874	-3.08897	0.48956
C	-8.34168	-2.48589	0.70613
C	-8.45996	-1.08238	0.61781
H	-5.04413	-2.83818	0.03099
H	-6.99249	-4.16560	0.55346
C	-8.71250	1.70773	0.44370
C	-9.82964	0.92629	0.74608
C	-9.71517	-0.46725	0.83525
H	-8.82676	2.78344	0.37937
H	-10.78410	1.41252	0.90964
C	-10.83311	-1.25902	1.13773
C	-10.70843	-2.64813	1.22374
C	-9.47107	-3.26118	1.00957
H	-11.80209	-0.80470	1.30728
H	-11.57526	-3.25276	1.45741
H	-9.39749	-4.33987	1.08110
C	-2.45804	1.08909	1.62612
C	-1.96583	1.94480	2.60876
C	-0.91158	2.80368	2.32257
C	-0.33552	2.80864	1.05372
H	-3.28094	0.44363	1.89833
H	-2.40781	1.94422	3.59693
H	-0.53697	3.47059	3.08859
H	0.47333	3.49844	0.88564

System 11-15-12

C	-2.47973	0.79236	0.28547
C	-1.57232	1.73867	0.78470
C	-2.27460	0.28558	-1.03168
C	-1.18412	0.77151	-1.82833

C	-0.30137	1.75140	-1.28616
C	-0.51767	2.20852	0.01889
H	0.14391	2.94811	0.45477
H	-1.68104	2.13128	1.78863
C	0.88782	2.35734	-2.01905
C	2.18008	2.01643	-1.31903
H	0.99632	2.03345	-3.06528
H	0.73726	3.45857	-2.05855
C	2.98609	3.02373	-0.77463
C	2.58952	0.68157	-1.20992
C	3.78457	0.35580	-0.56386
C	4.60976	1.36001	-0.00644
C	4.18226	2.70280	-0.12743
H	2.68957	4.06277	-0.84824
H	1.97958	-0.11072	-1.62701
H	4.04973	-0.69023	-0.50879
H	4.76353	3.52015	0.27461
N	5.84567	1.02612	0.66239
C	6.68682	2.07034	1.23226
H	7.01447	2.76887	0.43347
H	7.60081	1.66225	1.71246
H	6.12255	2.62677	2.01031
C	6.27458	-0.36127	0.78005
H	7.24080	-0.46122	1.31757
H	6.40915	-0.80166	-0.23056
H	5.51721	-0.94366	1.34628
C	-3.61129	0.34591	1.21959
C	-5.04454	0.57512	0.69044
H	-3.54257	0.87238	2.19614
H	-3.38226	-0.69985	1.45349
C	-5.50134	1.90464	0.39701
C	-6.80827	2.11077	-0.12086
C	-7.66207	1.03420	-0.32870
C	-7.26510	-0.26273	-0.02017
C	-5.96365	-0.52050	0.49690
C	-5.64826	-1.87627	0.79558
C	-6.57080	-2.90258	0.58284
C	-7.83055	-2.62214	0.07127
C	-8.17848	-1.31074	-0.22874
H	-4.70513	-2.19966	1.19291
H	-6.30392	-3.92547	0.81716
H	-8.65850	1.21048	-0.72253
H	-8.54043	-3.42298	-0.09139
H	-9.16859	-1.11438	-0.62402
C	-7.26431	3.40573	-0.42446
C	-6.44572	4.51013	-0.21208
C	-5.17018	4.33422	0.31024
C	-4.70361	3.05375	0.61294
H	-4.53772	5.19522	0.48578
H	-3.72055	2.99907	1.02808
H	-8.25974	3.56499	-0.82284
H	-6.80413	5.50459	-0.44495
C	-1.01551	0.24824	-3.13413
C	-1.88069	-0.71856	-3.63937
C	-2.92793	-1.19211	-2.86412
C	-3.12262	-0.69953	-1.57801
H	-0.22519	0.55436	-3.79543
H	-1.73344	-1.10722	-4.63914
H	-3.59341	-1.94855	-3.26043
H	-3.94039	-1.11138	-1.02643

System 10-16-12

C	-1.98222	0.61816	-0.58432
C	-1.00761	1.28434	0.22428
C	-1.98924	0.85050	-1.97320
C	-1.07525	1.71426	-2.56377
C	-0.13034	2.36355	-1.78370
C	-0.07389	2.16914	-0.39854
H	-2.71389	0.35203	-2.60629
H	-1.09561	1.88094	-3.63243
C	1.92209	3.79589	-0.23128
C	3.32728	3.29282	-0.01357

C	4.24483	4.03869	0.73638
C	3.73115	2.07035	-0.56512
C	5.03082	1.59717	-0.36849
C	5.96969	2.33638	0.38790
C	5.54592	3.56949	0.93585
H	3.95485	4.98718	1.17141
H	3.03569	1.48053	-1.14999
H	5.28635	0.64772	-0.81659
H	6.21086	4.18584	1.52369
N	7.31394	1.84942	0.59321
C	8.27159	2.62084	1.37454
H	8.43340	3.61229	0.90103
H	9.26029	2.12085	1.44518
H	7.89247	2.75578	2.40965
C	7.73770	0.57739	0.02309
H	8.79405	0.33634	0.26500
H	7.64944	0.61169	-1.08344
H	7.10852	-0.24468	0.42525
C	-3.02374	-0.36473	-0.05990
C	-4.48135	0.08201	-0.17784
H	-2.86561	-0.62909	0.99661
H	-2.88213	-1.30185	-0.64108
C	-4.81545	1.38178	-0.62001
C	-6.14182	1.79481	-0.72432
C	-7.18264	0.92824	-0.38782
C	-6.88621	-0.37574	0.06471
C	-5.53753	-0.80805	0.17526
H	-4.05652	2.10286	-0.88588
H	-6.35295	2.80064	-1.06856
C	-5.29014	-2.12142	0.63549
C	-6.34000	-2.97814	0.97347
C	-7.66776	-2.55368	0.86375
C	-7.94620	-1.24745	0.40801
H	-4.28653	-2.50777	0.74207
H	-6.11055	-3.97820	1.32241
C	-8.51730	1.34827	-0.49438
C	-9.56125	0.48488	-0.15577
C	-9.28778	-0.81279	0.29604
H	-8.75442	2.34750	-0.84030
H	-10.58337	0.83293	-0.24674
C	-10.33125	-1.68557	0.63900
C	-10.04790	-2.97766	1.08926
C	-8.72463	-3.41226	1.20223
H	-11.36455	-1.36931	0.55931
H	-10.85800	-3.64563	1.35222
H	-8.52808	-4.41818	1.55378
C	-0.92836	1.11326	1.62515
C	0.03492	1.78370	2.37545
C	0.94115	2.63871	1.76043
C	0.90458	2.84519	0.37459
H	-1.59368	0.47518	2.17937
H	0.07823	1.63950	3.44765
H	1.67807	3.14724	2.37042
H	1.78052	3.93046	-1.32307
H	1.78100	4.79497	0.23596

System 10-17-12

C	-2.40434	0.46410	-0.26442
C	-1.50082	1.13297	0.71412
C	-2.20324	0.65476	-1.58783
C	-1.10622	1.53088	-2.06437
C	-0.29704	2.13777	-1.17674
C	-0.50353	1.92737	0.28062
H	-2.84369	0.16879	-2.31819
H	-0.96655	1.67333	-3.13191
C	2.74236	4.51319	-1.14837
C	4.07374	3.96831	-0.69708
C	4.88620	4.70233	0.17584
C	4.51548	2.71894	-1.15100
C	5.74822	2.20794	-0.73740
C	6.58019	2.93491	0.14536
C	6.11999	4.19534	0.59236

H	4.56583	5.67109	0.53898
H	3.90186	2.13743	-1.82841
H	6.03701	1.23912	-1.11888
H	6.70430	4.80433	1.26712
N	7.85503	2.40895	0.57486
C	8.70277	3.16823	1.48453
H	8.97515	4.14101	1.02315
H	9.64808	2.63761	1.72400
H	8.16766	3.34275	2.44192
C	8.31738	1.10906	0.10670
H	9.31152	0.83938	0.52078
H	8.40927	1.11737	-1.00004
H	7.60175	0.31919	0.41875
C	-3.51681	-0.43936	0.22647
C	-4.94534	0.01605	-0.06922
H	-3.43271	-0.55096	1.32903
H	-3.34611	-1.43524	-0.23682
C	-5.20702	1.25681	-0.69213
C	-6.50904	1.67474	-0.95912
C	-7.59659	0.87221	-0.61143
C	-7.37287	-0.37110	0.01869
C	-6.04986	-0.80740	0.29606
H	-4.41084	1.92799	-0.97715
H	-6.66455	2.63403	-1.43907
C	-5.87530	-2.05814	0.93074
C	-6.97136	-2.85101	1.27793
C	-8.27406	-2.42281	1.00403
C	-8.47985	-1.17789	0.37202
H	-4.89380	-2.44299	1.16880
H	-6.79760	-3.80430	1.76328
C	-8.90640	1.29665	-0.88225
C	-9.99693	0.49729	-0.53319
C	-9.79572	-0.73955	0.09348
H	-9.08793	2.24964	-1.36516
H	-10.99857	0.84734	-0.75305
C	-10.88629	-1.54773	0.44799
C	-10.67487	-2.77935	1.07328
C	-9.37727	-3.21722	1.35124
H	-11.90083	-1.22773	0.24216
H	-11.52102	-3.39764	1.34407
H	-9.23673	-4.17554	1.83698
H	-1.65166	0.97924	1.77903
C	0.81036	3.01943	-1.61256
C	1.61245	3.61409	-0.70209
C	0.40971	2.61015	1.22304
C	1.39548	3.39691	0.76041
H	0.28800	2.47981	2.29469
H	2.05229	3.88794	1.47242
H	0.97273	3.18158	-2.67503
H	2.76668	4.61521	-2.25553
H	2.56384	5.52572	-0.72581

System 18-21

C	5.94756	1.21438	-1.63389
C	6.29953	0.79393	-2.86104
C	6.52129	1.72646	-3.91320
C	6.46501	-0.59300	-3.13464
C	5.71222	2.60528	-1.08401
C	5.65988	0.44835	-0.36000
N	6.70264	2.50194	-4.75746
N	6.60001	-1.72773	-3.33771
C	4.24514	2.40578	-0.63882
C	4.20957	0.93967	-0.14669
C	6.72535	1.10447	0.52097
H	5.74548	-0.63879	-0.40757
C	6.76085	2.56747	0.02988
H	5.84442	3.43880	-1.77629
H	7.70543	0.64180	0.34252
H	6.52835	0.99692	1.58968
H	6.58438	3.30620	0.81452
H	7.75745	2.78566	-0.37711
C	3.57994	1.06371	1.25735

H	3.58933	0.32910	-0.80731
C	2.03408	1.40959	1.17467
C	2.07080	2.92313	0.66661
C	3.63131	3.18112	0.54659
H	3.64251	2.52078	-1.54299
C	4.10396	2.40514	1.78026
H	3.78979	0.20369	1.89849
H	5.16412	2.44799	1.98454
H	3.61514	2.72732	2.70474
H	3.88780	4.24363	0.54239
C	-1.02039	2.33135	-3.29004
C	-1.08595	-0.37040	-2.38310
C	-1.39611	-0.06208	-3.71947
C	-1.36322	1.29337	-4.17447
C	-1.67439	1.57018	-5.51402
C	-2.01432	0.54315	-6.39642
C	-2.04633	-0.77611	-5.95356
C	-1.73862	-1.07682	-4.62546
H	-2.31101	-1.57417	-6.64238
H	-1.76992	-2.11500	-4.30253
H	-1.65568	2.59320	-5.88301
H	-2.25401	0.77494	-7.43094
C	-0.35429	0.69331	-0.07864
C	-0.76875	0.66845	-1.53592
C	-0.73642	2.00097	-1.98323
C	-0.30216	2.84194	-0.79990
C	-1.01905	2.02776	0.28574
H	-0.81753	2.36255	1.29764
H	-2.11121	2.01220	0.16044
H	-1.09436	-1.39321	-2.02157
H	-0.97892	3.36441	-3.61864
C	1.38190	1.03915	2.51057
H	1.95065	1.42325	3.36324
H	1.33227	-0.05045	2.61538
H	0.36901	1.42298	2.62113
C	1.45500	4.05223	1.49915
H	2.01888	4.23570	2.41916
H	0.42806	3.85732	1.80398
H	1.45444	4.98547	0.92493
C	1.16512	1.02224	-0.08563
H	-0.65643	-0.17429	0.50887
C	1.20121	2.50950	-0.58488
H	-0.55757	3.90045	-0.85896
H	1.65489	0.29228	-0.73689
H	1.71275	2.67682	-1.53734

System 19-21

C	5.93533	1.21134	-1.64382
C	6.28560	0.79079	-2.87133
C	6.50587	1.72291	-3.92425
C	6.44960	-0.59613	-3.14578
C	5.69976	2.60224	-1.09397
C	5.64743	0.44531	-0.36995
N	6.68654	2.49604	-4.77081
N	6.58401	-1.73045	-3.35213
C	4.23249	2.40241	-0.64981
C	4.19691	0.93627	-0.15767
C	6.71230	1.10167	0.51159
H	5.73339	-0.64181	-0.41746
C	6.74779	2.56463	0.02051
H	5.83232	3.43575	-1.78619
H	7.69258	0.63920	0.33373
H	6.51474	0.99417	1.58020
H	6.57076	3.30329	0.80509
H	7.74460	2.78300	-0.38589
C	3.56619	1.06020	1.24582
H	3.57729	0.32551	-0.81869
C	2.02036	1.40567	1.16158
C	2.05708	2.91896	0.65360
C	3.61755	3.17756	0.53508
H	3.63047	2.51728	-1.55442
C	4.08946	2.40176	1.76912

H	3.77569	0.20026	1.88718
H	5.14949	2.44487	1.97415
H	3.59986	2.72383	2.69322
H	3.87369	4.24016	0.53109
C	-1.01904	2.34366	-3.31249
C	-1.08545	-0.39381	-2.39356
C	-1.40181	-0.09051	-3.75568
C	-1.36821	1.29444	-4.22058
C	-1.69537	1.51964	-5.58569
C	-2.03539	0.50580	-6.48040
C	-2.06696	-0.79608	-6.04338
C	-1.75840	-1.07887	-4.71342
H	-2.33215	-1.59920	-6.72565
H	-1.81714	-2.12681	-4.46241
H	-1.70471	2.50826	-6.01832
H	-2.27527	0.74560	-7.51276
C	-0.36674	0.69347	-0.09512
C	-0.77998	0.66469	-1.55992
C	-0.74783	1.98998	-2.00480
C	-0.31485	2.83241	-0.81312
C	-1.03361	2.02266	0.26952
H	-0.83417	2.35761	1.28176
H	-2.12526	2.00615	0.14143
O	-1.01731	-1.56584	-1.70099
O	-0.88977	3.69188	-3.46592
C	1.36676	1.03514	2.49668
H	1.93353	1.42089	3.34990
H	1.31873	-0.05445	2.60221
H	0.35305	1.41739	2.60528
C	1.43984	4.04770	1.48543
H	2.00168	4.23029	2.40685
H	0.41213	3.85291	1.78772
H	1.44090	4.98131	0.91181
C	1.15288	1.01889	-0.09983
H	-0.66897	-0.16822	0.50119
C	1.18891	2.50414	-0.59840
H	-0.57048	3.89153	-0.86160
H	1.64253	0.28820	-0.75029
H	1.70038	2.67253	-1.55067
C	-1.25801	-2.83146	-2.27153
C	-1.08335	4.36637	-4.68774
H	-1.10301	-3.58065	-1.48809
H	-0.54026	-3.05391	-3.06603
H	-2.29859	-2.92726	-2.59420
H	-0.88438	5.42881	-4.51244
H	-2.12337	4.29347	-5.01811
H	-0.36829	4.03312	-5.44503

System 19-22

C	-0.13716	2.26818	-1.70483
C	-0.33351	3.65509	-1.64613
C	-0.66763	3.98443	-0.21640
C	-0.38845	1.72044	-0.31999
C	0.69233	2.15945	0.69929
C	0.52953	3.72225	0.74410
C	-1.51139	2.71631	0.07295
H	-0.67841	0.66971	-0.27652
H	-1.19361	4.92843	-0.06603
H	-2.40508	2.63424	-0.56074
H	-1.81635	2.63169	1.12268
C	2.18770	2.03343	0.42645
C	1.96127	4.22893	0.43278
C	2.86576	3.93872	1.65916
C	2.99641	2.39638	1.67081
H	4.04072	2.08030	1.57351
H	2.58110	1.95724	2.58296
H	2.43386	4.31523	2.59271
H	3.85464	4.39955	1.53909
C	2.52419	3.15597	-0.45670
C	3.20342	3.17397	-1.61459
C	3.70543	1.97530	-2.19798
C	3.49684	4.41097	-2.25006

N	4.15688	1.01450	-2.66848
N	3.74312	5.44137	-2.72576
C	-0.25350	4.43906	-2.78002
C	0.09370	3.83285	-4.01232
C	0.36624	2.42864	-4.05620
C	0.19762	1.64709	-2.88926
O	-0.64207	5.74963	-2.70423
O	0.42279	0.29779	-2.88482
C	0.18566	4.57047	-5.21109
C	0.58747	3.97480	-6.40729
C	0.90069	2.62294	-6.43634
C	0.78752	1.85898	-5.27508
H	1.22770	2.15735	-7.36240
H	1.03690	0.80023	-5.32519
H	-0.04936	5.63292	-5.21885
H	0.66331	4.57219	-7.31211
C	0.47006	6.61673	-2.49303
C	-0.78121	-0.40386	-3.20042
H	-0.56719	-1.47531	-3.14400
H	-1.11881	-0.17954	-4.21778
H	-1.57673	-0.17981	-2.48141
H	0.09580	7.64489	-2.50244
H	1.21413	6.52549	-3.28906
H	0.92464	6.43666	-1.51588
H	0.22884	4.03502	1.75378
H	2.01860	5.26091	0.08889
H	0.44828	1.72921	1.67982

System 19-23

C	-0.25784	2.27690	-1.45816
C	-0.45504	3.66893	-1.45865
C	-1.37791	3.97818	-0.31504
C	-1.04760	1.69618	-0.31297
C	-0.67041	2.13039	1.10542
C	0.54725	1.90698	2.00551
C	1.96307	2.40351	1.69549
C	-0.85363	3.66891	1.09095
C	0.31690	4.17955	1.93830
C	1.81038	3.94058	1.63840
C	-2.24984	2.68688	-0.50388
H	-1.32986	0.64708	-0.41687
H	-1.95735	4.89826	-0.40842
H	-2.72953	2.61701	-1.49145
H	-3.03305	2.57728	0.25693
C	0.20675	3.05015	3.03269
H	0.54940	0.91252	2.46077
H	-0.78764	2.95878	3.48760
H	0.93182	3.14873	3.85057
H	0.13136	5.17962	2.34011
H	-1.49764	1.71505	1.71131
H	-1.73632	3.89347	1.71877
C	2.89611	2.06943	0.53046
H	2.52740	2.14424	2.60729
C	2.68374	4.34819	0.44805
H	2.30998	4.36985	2.52350
C	4.16026	4.13543	0.91992
C	4.30615	2.57764	0.97092
H	5.08799	2.25036	0.27347
H	4.59634	2.23212	1.96895
H	4.37097	4.59136	1.89327
H	4.87594	4.55583	0.20174
C	2.71210	3.16596	-0.48081
H	2.87804	1.03262	0.19504
C	3.05277	3.14138	-1.79063
C	3.48039	1.92709	-2.40962
C	3.26822	4.35723	-2.50522
N	3.87730	0.94496	-2.88518
N	3.48311	5.36719	-3.03758
C	-0.20419	4.42486	-2.59516
C	0.26982	3.78017	-3.76538
C	0.49046	2.36836	-3.76202
C	0.18186	1.62300	-2.59853

H	2.49087	5.33965	0.04175
O	-0.58174	5.74114	-2.67504
O	0.28841	0.25936	-2.54966
C	0.53764	4.49965	-4.94823
C	1.03884	3.87191	-6.08880
C	1.28220	2.50602	-6.07553
C	1.00929	1.76394	-4.92685
H	1.68811	2.01444	-6.95585
H	1.22811	0.69756	-4.93921
H	0.37273	5.57555	-4.98109
H	1.24946	4.45649	-6.98054
C	0.12220	6.57364	-1.75731
C	-0.83057	-0.37072	-3.17855
H	-1.13860	-1.21198	-2.55028
H	-0.52421	-0.76753	-4.15079
H	-1.69431	0.29299	-3.30660
H	0.05967	7.60200	-2.12595
H	1.17990	6.30963	-1.68643
H	-0.34276	6.54545	-0.76813

S7 – Input geometries of the compounds on Figure 11 (in the paper)

Compound 24

C	-4.78458	1.67219	0.02970
C	-5.98139	1.07252	0.48184
C	-6.17609	-0.30917	0.41907
C	-5.18167	-1.13014	-0.10445
C	-3.99502	-0.56807	-0.56884
C	-3.79346	0.81550	-0.50848
N	-4.69590	3.10941	0.13073
H	-6.77628	1.68185	0.89401
H	-7.10147	-0.74226	0.77659
H	-5.33196	-2.20085	-0.15488
H	-2.86223	1.15280	-0.90025
H	-3.22575	-1.20782	-0.98271
C	-3.65438	3.98860	-0.05505
H	-5.58501	3.56756	0.39058
C	-2.20357	3.61702	-0.35379
O	-3.91180	5.18157	0.05058
C	-1.58129	2.87353	0.84288
H	-2.13556	1.95819	1.11823
H	-1.57308	3.53046	1.73950
H	-0.53522	2.58091	0.60988
C	-1.33873	4.85952	-0.64488
H	-2.16008	3.02902	-1.28775
H	-0.29851	4.55608	-0.89185
H	-1.30787	5.54129	0.23282
H	-1.74711	5.41572	-1.51614

Compound 25

C	-7.95152	2.75378	-0.52101
C	-8.35857	1.46223	-0.33020
C	-7.20026	0.68957	-0.09929
C	-6.08480	1.54755	-0.15434
N	-6.56906	2.85172	-0.37511
C	-5.91836	4.11157	-0.45196
O	-6.58664	5.09126	-0.77748
C	-4.44733	4.19708	-0.11928
C	-4.13433	5.56703	0.49466
H	-4.33258	6.38282	-0.20960
H	-3.08202	5.62617	0.79231
H	-4.74869	5.74223	1.38481
C	-3.62035	4.00367	-1.38760
H	-4.19141	3.47130	0.65355
H	-3.79504	4.81751	-2.10092
H	-3.87343	3.07219	-1.90293
H	-2.55093	3.98417	-1.15345
C	-7.02034	-0.68964	0.13872
C	-5.73812	-1.20922	0.30234
C	-4.63769	-0.37173	0.22181
C	-4.79045	1.00128	-0.00949
H	-3.88753	1.59335	-0.08195

H	-5.60381	-2.27275	0.48141
H	-3.63826	-0.78682	0.33545
H	-7.88203	-1.35046	0.18556
H	-8.53185	3.64518	-0.72716
H	-9.38108	1.10943	-0.36630

Compound 26

C	-4.53810	3.35240	-0.19911
C	-5.14664	2.13475	0.17483
C	-4.31147	1.02093	0.39757
C	-2.92517	1.11679	0.25470
C	-2.32446	2.33139	-0.11699
C	-3.15033	3.44635	-0.34172
H	-5.10520	4.24852	-0.38950
H	-2.72239	4.39828	-0.63010
H	-4.72824	0.06384	0.68554
H	-2.32253	0.23584	0.43613
N	-0.90590	2.43066	-0.26364
C	-6.63152	1.97852	0.34128
N	-7.50576	3.01590	0.16306
C	-8.95054	2.87226	0.32347
C	-9.63326	4.24431	0.23287
H	-9.23469	4.91779	1.02136
H	-10.72901	4.14185	0.38564
H	-9.45097	4.70944	-0.76001
C	-9.53681	1.94251	-0.75167
H	-9.16696	2.45752	1.33304
H	-9.10804	0.92283	-0.69065
H	-9.33429	2.34914	-1.76577
H	-10.63561	1.84885	-0.61687
H	-7.14916	3.95063	-0.06900
O	-7.06499	0.88052	0.66426
O	-0.40042	3.46556	-0.57996
O	-0.20894	1.47990	-0.07159

Compound 27

N	-4.27884	1.49133	0.52578
C	-3.31843	2.45553	0.50152
O	-3.63796	3.55464	0.97153
C	-1.89622	2.20709	0.00874
C	-1.10785	3.52772	-0.05170
C	0.30079	3.33804	-0.62001
H	-1.03052	3.95664	0.95676
H	-1.64225	4.27144	-0.65594
C	0.91394	1.97236	-0.28063
H	0.93238	4.15831	-0.25547
H	0.27512	3.44672	-1.71191
C	0.33906	1.42502	1.02728
C	-1.17197	1.19740	0.92017
H	0.54843	2.12828	1.84431
H	0.82589	0.48352	1.30912
H	-1.59815	1.20311	1.93142
H	-1.33579	0.18448	0.53730
H	-1.94330	1.84803	-1.02148
N	2.36566	2.06191	-0.22285
H	0.65926	1.26981	-1.08555
C	3.15859	0.95666	-0.46052
O	2.71813	-0.13626	-0.79684
C	4.62265	1.13373	-0.24999
C	5.25232	2.37610	-0.41341
C	6.63265	2.49566	-0.21546
C	7.38396	1.36575	0.13923
C	6.76512	0.11826	0.29014
C	5.38588	0.00672	0.08976
H	4.90358	-0.96420	0.19924
H	4.68991	3.25316	-0.72383
H	7.10530	3.46702	-0.35120
H	7.33483	-0.77023	0.55612
N	8.83288	1.49062	0.34652
O	9.33831	2.61368	0.20895
O	9.46233	0.46770	0.65018
C	-4.41597	0.18891	0.01562

C	-3.58767	-0.41256	-0.92899
C	-5.52321	-0.53780	0.48269
C	-5.77379	-1.84107	0.04449
C	-4.92456	-2.43486	-0.88112
C	-3.83608	-1.71928	-1.37006
H	-6.63104	-2.38859	0.42760
H	-5.11309	-3.44771	-1.22719
H	-3.17721	-2.17381	-2.10668
H	-2.74979	0.09450	-1.38270
H	-6.20455	-0.10277	1.21082
H	-5.08556	1.84039	1.03288
H	2.76274	2.83866	0.28832

Compound 28

N	-4.39013	1.51516	0.25621
C	-3.39053	2.51100	0.42469
O	-3.71462	3.57325	0.95393
C	-1.97178	2.22006	-0.00919
C	-1.21125	3.53964	-0.23780
C	0.20884	3.30231	-0.75991
H	-1.15340	4.10126	0.70467
H	-1.75425	4.18439	-0.94012
C	0.82080	1.98150	-0.27150
H	0.83124	4.15848	-0.46969
H	0.20230	3.29877	-1.85746
C	0.26690	1.59914	1.10298
C	-1.24963	1.38356	1.06301
H	0.50390	2.39191	1.82520
H	0.74991	0.69181	1.48545
H	-1.65575	1.59302	2.06125
H	-1.44587	0.32009	0.89170
H	-1.98229	1.73160	-0.98408
N	2.27327	2.06427	-0.25091
H	0.54650	1.19003	-0.98193
C	3.05155	0.92865	-0.36254
O	2.59281	-0.19109	-0.55620
C	4.52026	1.11131	-0.19361
C	5.16136	2.31697	-0.51292
C	6.54529	2.44249	-0.34595
C	7.28862	1.35453	0.13452
C	6.65814	0.14204	0.44151
C	5.27538	0.02413	0.27116
H	4.78417	-0.92050	0.50278
H	4.60502	3.15727	-0.92057
H	7.02691	3.38450	-0.60296
H	7.22143	-0.71475	0.80676
N	8.74115	1.48599	0.31019
O	9.25665	2.57845	0.03378
O	9.36317	0.49935	0.72773
C	-4.37024	0.23144	-0.32546
C	-3.37444	-0.53665	-0.96859
C	-5.66382	-0.31113	-0.18741
C	-5.94659	-1.60479	-0.67574
C	-4.95020	-2.35016	-1.30068
C	-3.68011	-1.81838	-1.44489
H	-6.94461	-2.02120	-0.56598
H	-5.17190	-3.34610	-1.67490
H	-2.90502	-2.40471	-1.93493
H	-2.35997	-0.19331	-1.11821
H	2.68684	2.89295	0.15517
C	-6.47310	0.64272	0.46477
C	-5.68904	1.73439	0.71312
H	-7.51971	0.54338	0.72181
H	-5.93583	2.67359	1.19361