Supporting Information for

Fuel selection for a regenerative organic fuel cell/flow battery: thermodynamic considerations

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Static bomb combustion calorimetry

The heat capacity of the calorimeter vessel was determined using the following setup: a quartz crucible combustion vessel (C 5010), combustion crucible support (C 5010.4), cotton thread igniter (C 710.4), benzoic acid pellet (CAS 65-85-0, standard reference material (SRM 309j) supplied by National Institute of Standards, C 723, $Q_{standard}$ value = 26434 J/g) and 1 ml deionized water to absorb any acid formed. The calorimeter vessel is purged with pure oxygen three times prior to filling the vessel to the reaction pressure of 35 psi of oxygen. Following the combustion experiment the calorimeter vessel gaseous contents were purged into approximately 15 mL of deionized water and the interior of the vessel, including crucible and ignition apparatus, were rinsed with deionized water. The total amount of deionized rinse/purge water was not allowed to exceed 50 mL as a precaution for unnecessary dilution of acidic species formed during combustion. To this solution is added approximately 1 mL of a 1% w/v aqueous methyl red indicator and is then titrated using the following titration setup: 1) a 10 mL capacity Kimax automatic buret with 0.05 mL subdivisions that is purchased as traceable to standards provided by NIST ; 2) 0.1M NaOH standardized to KHP as the titrant. In the case of benzoic acid, the amount of acid species formed after combustion is negligible relative to the acidity of deionized water. If nitrogen containing organic fuels are used, acid corrections become significant, see above ASTM standard for more details. The heat capacity determination for a calorimeter setup as described above gave the average number of 9974 J/K with a relative standard deviation of 0.07 % (see Supporting Information, Table S1).

The internal calorific values assigned as constant during the calorimetric experiments is 100 J for the ignition wire and 50 J for the cotton thread primary combustor. In the cases of very high and

very low vapour pressure liquids it was found that Scotch Brand tape, #610, was adequate in providing, in conjunction with the cotton thread, a secondary, non-absorbing ignition source for low volatility organic fuels and a combustion crucible cover for high volatility liquids. The acid corrected calorific value for Scotch brand #610 tape used in determining the calorific values of organic fuels was measured with a relative standard deviation 0.36 % (see Supporting Information, Table S2).

Table S1. Heat capacity determination of the calorimeter vessel.

Calibration run	Heat capacity of the calorimeter vessel , W (J/K)
1	9978
2	9986
3	9976
4	9968
5	9967
6	9971
Average	9974
Standard deviation	±7

Table S2. Calorific values for Scotch brand #610 tape.

Tape calibration run	Calorific value Q of the tape (J/g)
1	25032
2	24948
3	25130
Average	25037
Standard deviation	±91

Table S3. Combustion enthalpy of select organic fuels.

Compound	$-\Delta H_{c,298K}$ (MJ/mol)*	$-\Delta H_{c,298K}$ literature (MJ/mol)	% deviation from literature
cyclohexane	3.891±0.002	3.920	0.7
benzene	3.242±0.009	3.267	0.7
decalin	6.266±0.006	6.280	0.2
naphthalene	5.156±0.003	5.154	0.04
piperidine	3.442±0.002	3.448	0.17
pyridine	2.777±0.005	2.782	0.18
pyrrolidine	2.796±0.001	2.819	0.8
pyrrole	2.350±0.001	2.352	0.09
Indoline**	4.489±0.001	4.492	0.07
indole	4.243±0.007	4.273	0.7
2,3-dihydrobenzofuran	4.164±0.003	4.192	0.7
2,3-benzofuran	3.954±0.0001	3.971	0.4
decahydroquinoline	5.741±0.003	5.822	1.4
quinoline	4.630±0.005	4.698	1.5
N-ethyldodecahydrocarbazole**	8.806±0.02	NA	NA
N-ethylcarbazole	7.345±0.02	7.438	1.3

* - Values for the enthalpy of combustion for fuels/spent fuels have been corrected to 298K if the enthalpy value has a correction factor associated with it (see ASTM D4809-00 page 845).[1]

** - The dehydrogenation thermodynamic data for these fuels is based on combustion data from 4 combustion measurements (2 runs for each substrate). All other fuels are based on six experiments (3 runs per substrate).

Table S4. Thermodynamic parameters of tabulated organic compounds.

Organic compounds	$\Delta_f H°$ (kJ/mol)	S° (J/mol*K)	C_p (J/mol*K)
Hydrogenated form			
ethylbenzene	-12.5	255.0	184.8
cyclooctane	-169.4	262.0	215.8
cyclohexane	-156.2	204.35	156
cyclohexene	-38.2	214.6	148.8
cyclopentane	-105.9	204.1	126.7
indane	10.7	234.4	190.3
cycloheptane	-156.8	242.6	123.1
tetrahydrofuran	-216.1	203.9	124.1
tetrahydrothiophene	-72.8	207.82	140.2
2,3-dihydrobenzofuran	-99.8	226.4	188.6
n-propylamine	-101.5	324.0	162.5
cyclohexanethiol	-140.4	255.6	192.6
cyclohexanol	-352	203.9	214.1
N-methylpyrrolidine	-50.0	236.4	161.1
trans-Decalin	-228.7	264.9	229.2
tetralin	-32.6	251.5	217.4
tetrahydroquinoline	16.7	240.4	236.0
piperidine	-86.4	209.9	179.9
cyclohexylamine	-147.6	241.0	n/a
2-methylpiperidine	-124.9	243.8	213.0
isopropanol	-318.2	180.6	161.2
2-butanol	-342.6	213.1	198.3
piperazine	-41.8	301.2	237.0
pyrrolidine	-49.5	204.1	160.2
1,4-cyclohexadiene	66.1	189.4	142.2
1,3-cyclohexadiene	71.4	197.3	141.3
Dehydrogenated form			
phenylacetylene	284.3	221.2	180.1
styrene	103.4	240.5	183.2
cyclooctatetraene	255.0	220.3	180.0
cyclopentene	4.3	201.3	122.4
cyclopentadiene	24.0	250.0	198.9
1H-Indene	110.4	214.2	187.0
cycloheptatriene	143.2	214.7	162.8
furan	-62.3	176.7	114.6
thiophene	80.96	181.2	122.4
benzofuran	-34.8	215.6	178.7

propionitrile	15.5	189.33	119.5
benzene	49.0	173.3	135.9
thiophenol	63.7	222.8	173.2
toluene	12.0	221.0	157.1
phenol	-165.1	144.0	127.2
N-methylpyrrole	62.4	200.5	150.1
Naphtalene	75.4	167.4	165.7
quinoline	141.2	219.7	194.9
pyridine	100.0	177.7	134.9
aniline	31.3	191.3	194.1
2-methylpyridine	56.5	217.9	158.4
acetone	-249.4	200.4	125.5
2-butanone	-273.3	239.0	159.0
pyrazine	139.8	280.4	180.0

Table S5. Comparison of the electronic energy (E) of the investigated organic molecules computed using Spartan 08 and Gaussian 09 software packages.

Organic compounds	E (Spartan) (Hartree)	E (Gaussian) (Hartree)	Difference (kcal/mol)
ethylbenzene	-310.9921	-310.9919	0.112
cyclooctane	-314.6024	-314.6028	-0.256
cyclohexane	-235.9656	-235.9655	0.098
cyclohexene	-234.7342	-234.7341	0.020
cyclopentane	-196.6292	-196.6292	-0.007
indane	-349.1086	-349.1086	0.011
cycloheptane	-275.2826	-275.2825	0.090
tetrahydrofuran	-232.5380	-232.5379	0.043
tetrahydrothiophene	-555.5294	-555.5293	0.080
2,3-dihydrobenzofuran	-385.0205	-385.0206	-0.013
n-propylamine	-174.5590	-174.5590	-0.018
cyclohexanethiol	-634.1882	-634.1880	0.109
cyclohexanol	-311.2129	-311.2128	0.084
N-methylpyrrolidine	-251.9869	-251.9870	-0.043
trans-Decalin	-392.0697	-392.0694	0.205
tetralin	-388.4404	-388.4403	0.086
tetrahydroquinoline	-404.4830	-404.4829	0.059
piperidine	-251.9991	-251.9989	0.100
cyclohexylamine	-291.3364	-291.3362	0.130
2-methylpiperidine	-291.3308	-291.3307	0.041
isopropanol	-194.4391	-194.4391	0.001

2-butanol	-233.7668	-233.7668	0.018
piperazine	-268.0308	-268.0315	-0.430
pyrrolidine	-212.6632	-212.6630	0.110
1,4-cyclohexadiene	-233.5052	-233.5053	-0.029
1,3-cyclohexadiene	-233.5053	-233.5051	0.110
phenylacetylene	-308.5064	-308.5064	0.031
styrene	-309.7604	-309.7603	0.020
cyclooctatetraene	-309.6811	-309.6811	0.015
cyclopentene	-195.3996	-195.3996	-0.023
cyclopentadiene	-194.1740	-194.1741	-0.072
1H-Indene	-347.8835	-347.8836	-0.036
cycloheptatriene	-271.6093	-271.6094	-0.048
furan	-230.1087	-230.1087	-0.029
thiophene	-553.0982	-553.0982	-0.005
benzofuran	-383.8095	-383.8096	-0.022
propionitrile	-172.1346	-172.1346	0.022
benzene	-232.3334	-232.3334	0.029
thiophenol	-630.5562	-630.5561	0.068
toluene	-271.6645	-271.6645	0.019
phenol	-307.5857	-307.5857	0.027
N-methylpyrrole	-249.5714	-249.5714	-0.011
Naphtalene	-386.0256	-386.0256	0.046
quinoline	-402.0676	-402.0676	0.033
pyridine	-248.3732	-248.3732	0.006
aniline	-287.7129	-287.7129	0.013
2-methylpyridine	-287.7076	-287.7075	0.035
acetone	-193.2332	-193.2332	-0.005
2-butanone	-232.5617	-232.5617	0.016
pyrazine	-264.4095	-264.4095	-0.013
hexahydropyrimidine	-268.0346	-268.0344	0.108
hexahydropyridazine	-268.0068	-268.0067	0.059
hexahydro-1,3,5-triazine			
tetrahydro-1H-imidazole	-228.6997	-228.6997	-0.037
pyrazolidine	-228.6718	-228.6718	0.003
1,2,3-triazolidine	-244.6875	-244.6875	0.009
1,2,4-triazolidine	-244.7181	-244.7181	0.012
perhydroquinoline	-408.1056	-408.1053	0.195
perhydroisoquinoline	-408.1031	-408.1028	0.184
perhydro-4H-quinolizine	-408.1008	-408.1005	0.187
perhydrocinnoline	-424.1160	-424.1158	0.153
perhydrophthalazine	-424.1139	-424.1136	0.177

perhydroquinazoline	-424.1414	-424.1410	0.236
perhydroquinoxaline	-424.1399	-424.1395	0.242
perhydro1,8-naphthyridine	-424.1390	-424.1388	0.167
perhydro1,5-naphthyridine	-424.1412	-424.1409	0.184
perhydropteridine	-456.2148	-456.2144	0.245
perhydropyrazino[2,3-b]pyrazine	-456.2110	-456.2106	0.223
perhydropyrimido[4,5-d]pyrimidine	-456.2056	-456.2053	0.227
perhydro-1H-indene	-352.7322	-352.7319	0.171
perhydrobenzofuran	-388.6431	-388.6429	0.092
perhydrobenzothiophene	-711.6320	-711.6320	0.001
perhydro-1H-indole	-368.7671	-368.7669	0.084
perhydro-2H-isoindole	-368.7643	-368.7641	0.101
perhydroindolizine (delta-coniceine)	-368.7675	-368.7673	0.141
perhydrobenzimidazole	-384.8025	-384.8023	0.113
perhydro-1H-indazole	-384.7732	-384.7731	0.065
octahydro-1H-pyrrolo[2,3-b]pyridine	-384.8030	-384.8029	0.047
perhydroimidazo[1,2-a]pyrazine	-400.8349	-400.8347	0.114
octahydro-1H-purine	-416.8730	-416.8729	0.108
perhydropentalene	-313.3873	-313.3872	0.092
perhydropyrrolizine	-329.4261	-329.4259	0.120
perhydro-1,4-dihydropyrrolo[3,2-b]pyrrole	-345.4509	-345.4509	0.016
perhydro-1,4-dihydroimidazo [4,5-d]imidazole	-377.5179	-377.5181	-0.098
perhydro-N-ethylindole	-447.4185	-447.4184	0.083
perhydro-N-ethylindazole	-463.4295	-463.4291	0.200
octahydro-1Methylpurine	-456.1950	-456.1950	0.013
N-ethylperhydropurine	-495.5134	-495.5134	-0.021
perhydrofluorene	-508.8313	-508.8313	-0.010
perhydro-9-ethylfluorene	-587.4825	-587.4823	0.128
perhydro-9H-carbazole	-524.8675	-524.8675	0.016
perhydro-N-ethylcarbazole	-603.5122	-603.5123	-0.020
perhydro-1,8-diazacarbazole	-556.9379	-556.9379	0.025
perhydro-N-methyl-1,8-diazacarbazole	-596.2537	-596.2534	0.182
perhydro-N-ethyl-1,8-diazacarbazole	-635.5808	-635.5807	0.071
perhydrodibenzoborole	-494.9567	-494.9567	-0.043
perhydro-5Me-dibenzoborole	-534.3038	-534.3038	0.010
perhydro[b,d]dibenzofuran	-544.7452	-544.7451	0.082
perhydrodibenzothiophene	-867.7334	-867.7333	0.035
perhydro-3,6-diazacarbazole	-556.9316	-556.9314	0.081
perhydro-4,5-diazacarbazole	-556.9309	-556.9308	0.019
pyrimidine	-264.4162	-264.4161	0.046
pyridazine	-264.3804	-264.3804	0.038

1,3,5-triazine	-280.4619	-280.4618	0.037
1H-pyrrole	-210.2490	-210.2490	-0.022
1H-imidazole	-226.3014	-226.3013	0.033
1H-pyrazole	-226.2846	-226.2846	0.008
1H-1,2,3-triazole	-242.3125	-242.3125	0.016
1H-1,2,4-triazole	-242.3393	-242.3393	0.009
naphthalene	-386.0256	-386.0256	0.046
isoquinoline	-402.0658	-402.0657	0.056
4H-quinolizine	-403.2206	-403.2205	0.041
cinnoline	-418.0737	-418.0736	0.043
phtalazine	-418.0756	-418.0755	0.059
quinazoline	-418.1112	-418.1111	0.041
quinoxaline	-418.1061	-418.1061	0.018
1,8-naphthyridine	-418.1070	-418.1070	0.009
1,5-naphthyridine	-418.1094	-418.1094	0.011
pteridine	-450.1862	-450.1861	0.004
pyrazino[2,3-b]pyrazine	-450.1815	-450.1816	-0.022
pyrimido[4,5-d]pyrimidine	-450.1912	-450.1912	0.026
benzo[b]thiophene	-706.7969	-706.7969	-0.008
1H-indole	-363.9472	-363.9472	-0.010
2H-isoindole	-363.9327	-363.9327	-0.004
indolizine(delta-coniceine)	-363.9274	-363.9274	-0.006
1H-benzo[d]imidazole	-380.0006	-380.0006	0.005
1H-indazole	-379.9774	-379.9774	-0.006
1H-pyrrolo[2,3-b]pyridine	-379.9951	-379.9951	-0.041
imidazo[1,2-a]pyrazine	-396.0196	-396.0195	0.045
7H-purine	-412.0831	-412.0830	0.006
1,4-dihydropentalene	-309.7163	-309.7164	-0.064
1H-pyrrolizine	-325.7845	-325.7845	-0.039
1,4-dihydropyrrolo [3,2-b]pyrrole	-341.8427	-341.8428	-0.023
1,4-dihydroimidazo[4,5-d]imidazole	-373.9459	-373.9459	-0.010
N-ethylindole	-442.6000	-442.6000	0.005
N-ethylindazole	-458.6315	-458.6314	0.034
N-methylpurine	-451.4074	-451.4074	0.023
N-ethylpurine	-490.7377	-490.7377	0.013
9H-fluorene	-501.5917	-501.5917	0.010
9-ethylfluorene	-580.2458	-580.2458	0.000
N-ethylcarbazole	-596.3012	-596.3011	0.042
N-methyl-1,8-diazacarbazole	-549.7439	-549.7439	0.009
N-ethyl-1,8-diazacarbazole	-589.0684	-589.0683	0.056
5H-dibenzoborole	-628.3990	-628.3989	0.050

dibenzo-5Me-borole	-487.7192	-487.7192	-0.018
dibenzo[b,d]furan	-527.0665	-527.0666	-0.028
dibenzo[b,d]thiophene	-537.5133	-537.5132	0.026
9H-carbazole	-517.6488	-517.6487	0.031
1,8-diazacarbazole	-860.4979	-860.4979	-0.006
3,6-diazacarbazole	-549.7305	-549.7305	0.042
4,5-diazacarbazole	-549.7252	-549.7252	0.003

Table S6. The electronic energy (E), enthalpy (H), Entropy (S) and Gibbs free energy (G) of the investigated organic molecules.

Organic compounds	E (Hartree)	H (Hartree)	S (cal/molK)	G (Hartree)
ethylbenzene	-310.9919	-310.8272	85.279	-310.8678
cyclooctane	-314.6028	-314.3669	87.443	-314.4084
cyclohexane	-235.9655	-235.7891	72.296	-235.8234
cyclohexene	-234.7341	-234.5819	72.508	-234.6164
cyclopentane	-196.6292	-196.4838	66.729	-196.5155
indane	-349.1086	-348.9367	81.817	-348.9756
cycloheptane	-275.2825	-275.0761	80.291	-275.1143
tetrahydrofuran	-232.5379	-232.4165	67.327	-232.4485
tetrahydrothiophene	-555.5293	-555.4097	71.751	-555.4438
2,3-dihydrobenzofuran	-385.0206	-384.8728	81.550	-384.9116
n-propylamine	-174.5590	-174.4315	72.660	-174.4660
cyclohexanethiol	-634.1880	-634.0106	84.225	-634.0506
cyclohexanol	-311.2128	-311.0309	80.510	-311.0692
N-methylpyrrolidine	-251.9870	-251.8231	77.814	-251.8601
trans-Decalin	-392.0694	-391.7965	89.095	-391.8389
tetralin	-388.4403	-388.2382	85.646	-388.2789
tetrahydroquinoline	-404.4829	-404.2924	86.786	-404.3336
piperidine	-251.9989	-251.8339	74.057	-251.8691
cyclohexylamine	-291.3362	-291.1416	81.020	-291.1801
2-methylpiperidine	-291.3307	-291.1366	80.773	-291.1750
isopropanol	-194.4391			-194.3590
2-butanol	-233.7668	-233.6232	78.810	-233.6606
piperazine	-268.0315	-267.8777	71.984	-267.9119
pyrrolidine	-212.6630	-212.5279	74.108	-212.5631
1,4-cyclohexadiene	-233.5053	-233.3772	70.288	-233.4106
1,3-cyclohexadiene	-233.5051	-233.3769	70.917	-233.4106
phenylacetylene	-308.5064	-308.3896	78.134	-308.4267
styrene	-309.7603	-309.6195	82.268	-309.6586
cyclooctatetraene	-309.6811	-309.5407	74.884	-309.5762

cyclopentene	-195.3996	-195.2776	69.503	-195.3107
cyclopentadiene	-194.1741	-194.0767	65.266	-194.1077
1H-Indene	-347.8836	-347.7360	79.504	-347.7738
cycloheptatriene	-271.6094	-271.4750	75.339	-271.5108
furan	-230.1087	-230.0342	63.660	-230.0645
thiophene	-553.0982	-553.0266	66.434	-553.0582
benzofuran	-383.8096	-383.6855	77.884	-383.7225
propionitrile	-172.1346	-172.0548	68.065	-172.0872
benzene	-232.3334	-232.2276	64.037	-232.2581
thiophenol	-630.5561	-630.4497	79.584	-630.4875
toluene	-271.6645	-271.5298	80.458	-271.5680
phenol	-307.5857	-307.4747	74.522	-307.5101
N-methylpyrrole	-249.5714			-249.4905
Naphtalene	-386.0256	-385.8706	79.176	-385.9082
quinoline	-402.0676	-401.9245	81.466	-401.9632
pyridine	-248.3732	-248.2793	67.228	-248.3113
aniline	-287.7129	-287.5893	75.537	-287.6252
2-methylpyridine	-287.7075	-287.5857	73.750	-287.6208
acetone	-193.2332	-193.1436	73.239	-193.1784
2-butanone	-232.5617	-232.4432	74.992	-232.4788
pyrazine	-264.4095	-264.3277	65.533	-264.3588
hexahydropyrimidine	-268.0344	-267.8806	73.417	-267.9155
hexahydropyridazine	-268.0067	-267.8529	73.432	-267.8878
hexahydro-1,3,5-triazine	-284.0603	-283.9185	70.904	-283.9521
tetrahydro-1H-imidazole	-228.6997	-228.5756	70.498	-228.6091
pyrazolidine	-228.6718	-228.5479	71.258	-228.5818
1,2,3-triazolidine	-244.6875	-244.5754	70.204	-244.6087
1,2,4-triazolidine	-244.7181	-244.6053	69.334	-244.6383
perhydroquinoline	-408.1053	-407.8438	89.882	-407.8865
perhydroisoquinoline	-408.1028	-407.8412	89.958	-407.8839
perhydro-4H-quinolizine	-408.1005	-407.8396	90.177	-407.8824
perhydrocinnoline	-424.1158	-423.8659	89.243	-423.9083
perhydrophthalazine	-424.1136	-423.8636	89.245	-423.9060
perhydroquinazoline	-424.1410	-423.8906	89.510	-423.9331
perhydroquinoxaline	-424.1395	-423.8894	89.413	-423.9319
perhydro1,8-naphthyridine	-424.1388	-423.8888	89.560	-423.9313
perhydro1,5-naphthyridine	-424.1409	-423.8907	89.169	-423.9330
perhydropteridine	-456.2144	-455.9866	88.020	-456.0284
perhydropyrazino[2,3-b]pyrazine	-456.2106	-455.9832	88.144	-456.0251
perhydropyrimido[4,5-d]pyrimidine	-456.2053	-455.9779	88.466	-456.0200
perhydro-1H-indene	-352.7319	-352.4891	86.351	-352.5301

perhydrobenzofuran	-388.6429	-388.4241	86.597	-388.4653
perhydrobenzothiophene	-711.6320	-711.4156	88.733	-711.4578
perhydro-1H-indole	-368.7669	-368.5354	87.283	-368.5769
perhydro-2H-isoindole	-368.7641	-368.5325	86.980	-368.5738
perhydroindolizine (delta-coniceine)	-368.7673	-368.5364	87.081	-368.5777
perhydrobenzimidazole	-384.8023	-384.5820	85.843	-384.6227
perhydro-1H-indazole	-384.7731	-384.5530	85.189	-384.5935
octahydro-1H-pyrrolo[2,3-b]pyridine	-384.8029	-384.5824	85.545	-384.6231
perhydroimidazo[1,2-a]pyrazine	-400.8347	-400.6263	85.770	-400.6670
octahydro-1H-purine	-416.8729	-416.6750	84.696	-416.7153
perhydropentalene	-313.3872	-313.1744	82.596	-313.2136
perhydropyrrolizine	-329.4259	-329.2250	83.701	-329.2648
perhydro-1,4-dihydropyrrolo[3,2-b]pyrrole	-345.4509	-345.2606	82.390	-345.2998
perhydro-1,4-dihydroimidazo [4,5-d]imidazole	-377.5181	-377.3504	80.870	-377.3889
perhydro-N-ethylindole	-447.4184	-447.1284	100.652	-447.1763
perhydro-N-ethylindazole	-463.4291	-463.1507	98.855	-463.1977
octahydro-1Methylpurine	-456.1950	-455.9684	91.697	-456.0120
N-ethylperhydropurine	-495.5134	-495.2576	98.861	-495.3046
perhydrofluorene	-508.8313	-508.4917	100.435	-508.5394
perhydro-9-ethylfluorene	-587.4823	-587.0837	116.025	-587.1388
perhydro-9H-carbazole	-524.8675	-524.5393	101.296	-524.5874
perhydro-N-ethylcarbazole	-603.5123	-603.1258	116.157	-603.1810
perhydro-1,8-diazacarbazole	-556.9379	-556.6323	99.882	-556.6797
perhydro-N-methyl-1,8-diazacarbazole	-596.2534	-595.9194	108.035	-595.9707
perhydro-N-ethyl-1,8-diazacarbazole	-635.5807	-635.2170	115.498	-635.2719
perhydrodibenzoborole	-494.9567	-494.6348	101.542	-494.6830
perhydro-5Me-dibenzoborole	-534.3038	-533.9519	113.627	-534.0059
perhydro[b,d]dibenzofuran	-544.7451	-544.4296	99.223	-544.4768
perhydrodibenzothiophene	-867.7333	-867.4203	102.982	-867.4692
perhydro-3,6-diazacarbazole	-556.9314	-556.6259	100.227	-556.6735
perhydro-4,5-diazacarbazole	-556.9308	-556.6257	100.778	-556.6736
pyrimidine	-264.4161	-264.3341	66.960	-264.3659
pyridazine	-264.3804	-264.2991	67.112	-264.3310
1,3,5-triazine	-280.4618	-280.3916	64.582	-280.4222
1H-pyrrole	-210.2490	-210.1618	65.853	-210.1930
1H-imidazole	-226.3013	-226.2256	65.136	-226.2565
1H-pyrazole	-226.2846	-226.2088	65.091	-226.2397
1H-1,2,3-triazole	-242.3125	-242.2490	64.588	-242.2797
1H-1,2,4-triazole	-242.3393	-242.2751	64.475	-242.3057
naphthalene	-386.0256	-385.8706	79.180	-385.9082
isoquinoline	-402.0657	-401.9226	81.603	-401.9613

4H-quinolizine	-403.2205	-403.0549	86.214	-403.0959
cinnoline	-418.0736	-417.9431	81.339	-417.9817
phtalazine	-418.0755	-417.9448	80.224	-417.9830
quinazoline	-418.1111	-417.9798	81.224	-418.0184
quinoxaline	-418.1061	-417.9751	79.656	-418.0129
1,8-naphthyridine	-418.1070	-417.9760	79.753	-418.0139
1,5-naphthyridine	-418.1094	-417.9782	81.003	-418.0167
pteridine	-450.1861	-450.0791	80.428	-450.1173
pyrazino[2,3-b]pyrazine	-450.1816	-450.0748	77.538	-450.1116
pyrimido[4,5-d]pyrimidine	-450.1912	-450.0838	79.319	-450.1215
benzo[b]thiophene	-706.7969	-706.6755	80.858	-706.7139
1H-indole	-363.9472	-363.8105	79.060	-363.8481
2H-isoindole	-363.9327	-363.7961	78.791	-363.8335
indolizine(delta-coniceine)	-363.9274	-363.7913	78.551	-363.8286
1H-benzo[d]imidazole	-380.0006	-379.8755	78.145	-379.9126
1H-indazole	-379.9774	-379.8523	78.433	-379.8896
1H-pyrrolo[2,3-b]pyridine	-379.9951	-379.8701	78.193	-379.9073
imidazo[1,2-a]pyrazine	-396.0195	-395.9068	77.410	-395.9436
7H-purine	-412.0830	-411.9816	77.246	-412.0183
1,4-dihydropentalene	-309.7164	-309.5769	76.387	-309.6132
1H-pyrrolizine	-325.7845	-325.6555	76.560	-325.6919
1,4-dihydropyrrolo [3,2-b]pyrrole	-341.8428	-341.7245	75.867	-341.7606
1,4-dihydroimidazo[4,5-d]imidazole	-373.9459	-373.8507	75.019	-373.8863
N-ethylindole	-442.6000	-442.4042	93.778	-442.4488
N-ethylindazole	-458.6314	-458.4483	88.763	-458.4905
N-methylpurine	-451.4074	-451.2764	85.738	-451.3172
N-ethylpurine	-490.7377	-490.5771	92.578	-490.6211
9H-fluorene	-501.5917	-501.3942	91.063	-501.4374
9-Ethylfluorene	-580.2458	-579.9890	106.396	-580.0395
N-ethylcarbazole	-596.3011	-596.0557	106.452	-596.1063
N-methyl-1,8-diazacarbazole	-589.0683	-588.8770	95.460	-588.9224
N-ethyl-1,8-diazacarbazole	-628.3989	-628.1770	105.661	-628.2272
5H-dibenzoborole	-487.7192	-487.5366	91.777	-487.5802
dibenzo-5Me-borole	-527.0666	-526.8552	99.286	-526.9023
dibenzo[b,d]furan	-537.5132	-537.3396	89.299	-537.3821
dibenzo[b,d]thiophene	-860.4979	-860.3267	92.538	-860.3707
9H-carbazole	-517.6487	-517.4626	90.815	-517.5058
1,8-diazacarbazole	-549.7439	-549.5811	89.097	-549.6235
3,6-diazacarbazole	-549.7305	-549.5678	89.680	-549.6104
4,5-diazacarbazole	-549.7252	-549.5630	89.977	-549.6058

Table S7. The electronic energy (E), enthalpy (H), Entropy (S) and Gibbs free energy (G) of the molecules used for the analysis of correlation with Hammett constant.

Organic compounds	E(Hartree)	H(Hartree)	S(cal/mol-Kelvin)	G(Hartree)
4-aminopiperidine	-307.3692	-307.1859	80.508	-307.2242
4-chloropiperidine	-711.6345	-711.4773	81.278	-711.5160
4-dimethylaminopiperidine	-386.0028	-385.7611	93.938	-385.8057
4-fluoropiperidine	-351.2767	-351.1186	78.595	-351.1559
4-methylpiperidine	-291.3282	-291.1341	80.935	-291.1725
4-trifluoromethylpiperidine	-589.1781	-589.0045	92.858	-589.0486
chlorocyclohexane	-695.6015	-695.4330	81.832	-695.4719
dimethylaminocyclohexane	-369.9697	-369.7168	94.515	-369.7617
fluorocyclohexane	-335.2439	-335.0743	79.064	-335.1119
methylcyclohexane	-275.2947	-275.0892	81.480	-275.1279
trifluoromethylcyclohexane	-573.1449	-572.9599	93.332	-573.0042
aminocyclohexane	-291.3362	-291.1416	81.024	-291.1800
4-aminopyridine	-303.7576	-303.6457	74.985	-303.6814
4-chloropyridine	-708.0049	-707.9195	74.428	-707.9548
4-dimethylaminopyridine	-382.3933	-382.2224	91.170	-382.2657
4-fluoropyridine	-347.6491	-347.5626	71.643	-347.5966
4-methylpyridine	-287.7060	-287.5831	80.498	-287.6213
4-trifluoromethylpyridine	-585.5452	-585.4441	83.596	-585.4839
chlorobenzene	-691.9653	-691.8680	74.798	-691.9035
dimethylaminobenzene	-366.3475	-366.1650	90.705	-366.2081
fluorobenzene	-331.6087	-331.5103	72.016	-331.5446
methylbenzene	-271.6645	-271.5298	80.456	-271.5680
trifluoromethylbenzene	-569.5078	-569.3939	92.463	-569.4378
aminobenzene	-287.7129	-287.5893	75.510	-287.6252

Table S8. Calculated enthalpy and entropy of the dehydrogenation reaction $LQ*nH_2$ -> $LQ + nH_2$. The dissociation temperature is estimated as $T_d = \Delta H / \Delta S$.

$LQ*H_2$	LQ	number of realeased molecules	ΔH (kcal/mol H_2)	ΔS (cal/molK)	T_d (Kelvin)
ethylbenzene	phenylacetylene	2	32.748	27.560	1188.213
ethylbenzene	styrene	1	25.811	28.121	917.861
cyclooctane	cyclooctatetraene	4	25.051	27.993	894.896
cyclohexane	cyclohexene	1	25.431	31.346	811.313
cyclohexene	cyclohexadiene	1	24.051	29.542	814.139
cyclopentane	cyclopentene	1	24.807	33.907	731.611
cyclopentane	cyclopentadiene	2	23.162	30.402	761.878
indane	1H-indene	1	21.364	28.820	741.277
cycloheptane	cycloheptatriene	3	21.187	29.482	718.623
tetrahydrofuran	furan	2	15.381	29.300	524.948

tetrahydrothiophene	thiophene	2	15.624	28.475	548.686
2,3-dihydrobenzofuran	benzofuran	1	12.974	27.467	472.346
n-propylamine	propionitrile	2	13.625	28.836	472.508
chlorocyclohexane	chlorobenzene	3	13.638	28.788	473.743
cyclohexane	benzene	3	12.874	28.380	453.642
cyclohexanethio	thiophenol	3	12.767	29.586	431.524
methylcyclohexane	toluene	3	12.452	30.792	404.380
cyclohexanol	phenol	3	11.779	29.137	404.247
trans-decalin	naphtalene	5	11.651	29.149	399.711
tetralin	naphtalene	2	10.791	27.898	386.811
tetrahydroquinoline	quinoline	2	10.870	28.473	381.771
piperidine	pyridine	3	11.429	28.856	396.073
cyclohexylamine	aniline	3	10.956	29.305	373.845
2-methylpiperidine	2-methylpyridine	3	10.665	28.792	370.408
2-butanol	2-butanone	1	8.387	27.315	307.034
piperazine	pyrazine	3	10.480	28.983	361.603
pyrrolidine	pyrrole	2	10.306	27.006	381.631
cyclohexane	benzene	3	12.874	28.380	453.642
piperidine	pyridine	3	11.429	28.856	396.073
hexahydropyrimidine	pyrimidine	3	9.748	28.981	336.346
hexahydropyridazine	pyridazine	3	11.280	29.026	388.604
hexahydro-1,3,5-triazine	1,3,5-triazine	3	5.650	29.026	194.652
cyclopentane	cyclopentadiene	2	23.162	30.402	761.878
tetrahydrofuran	furan	2	15.381	29.300	524.948
pyrrolidine	1H-pyrrole	2	10.306	27.006	381.631
tetrahydro-1H-imidazole	1H-imidazole	2	5.252	28.452	184.581
pyrazolidine	1H-pyrazole	2	1.836	28.050	65.470
decalin	naphthalene	5	11.651	29.149	399.717
perhydroquinoline	quinoline	5	10.813	29.452	367.142
perhydroisoquinoline	isoquinoline	5	10.731	29.462	364.239
perhydro-4H-quinolizine	4H-quinolizine	4	18.537	30.142	614.993
perhydrocinnoline	cinnoline	5	11.254	29.552	380.803
perhydrophthalazine	phtalazine	5	10.743	29.329	366.285
perhydroquinazoline	quinazoline	5	9.744	29.476	330.588
perhydroquinoxaline	quinoxaline	5	10.184	29.182	348.987
perhydro1,8-naphthyridine	1,8-naphthyridine	5	9.993	29.171	342.551
perhydro1,5-naphthyridine	1,5-naphthyridine	5	9.951	29.500	337.322
perhydropteridine	pteridine	5	9.339	29.615	315.349
perhydropyrazino [2,3-b]pyrazine	pyrazino[2,3-b]pyrazine	5	9.449	29.012	325.708
perhydropyrimido [4,5-d]pyrimidine	pyrimido [4,5-d]pyrimidine	5	7.655	29.304	261.247
perhydro-1H-indene	1H-indene	4	13.577	29.421	461.471
perhydrobenzofuran	benzofuran	4	11.313	28.954	390.725

perhydrobenzothiophene	benzo[b]thiophene	4	11.548	29.164	395.979
perhydro-1H-indole	1H-indole	4	9.156	29.077	314.880
perhydro-2H-isoindole	2H-isoindole	4	10.972	29.086	377.220
perhydroindolizine (delta-coniceine)	indolizine(delta-coniceine)	4	12.328	29.000	425.104
perhydrobenzimidazole	1H-benzo[d]imidazole	4	6.275	29.208	214.834
perhydro-1H-indazole	1H-indazole	4	5.366	29.444	182.228
octahydro-1H-pyrrolo[2,3-b]pyridine	1H-pyrrolo[2,3-b]pyridine	4	7.185	29.295	245.257
perhydroimidazo[1,2-a]pyrazine	imidazo[1,2-a]pyrazine	4	8.301	29.043	285.812
octahydro-1H-purine	7H-purine	4	4.224	29.270	144.307
perhydropentalene	1,4-dihydropentalene	3	20.414	29.063	702.386
perhydropyrrolizine	1H-pyrrolizine	3	14.568	28.753	506.669
perhydro-1,4-dihydropyrrolo [3,2-b]pyrrole	1,4-dihydropyrrolo [3,2-b]pyrrole	3	7.573	28.959	261.509
perhydro-1H-indole	1H-indole	4	9.156	29.077	314.880
perhydro-N-ethylindole	N-ethylindole	4	9.051	29.415	307.690
perhydro-1H-indazole	1H-indazole	4	5.366	29.444	182.228
perhydro-N-ethylindazole	N-ethylindazole	4	5.639	28.610	197.092
octahydro-1H-purine	7H-purine	4	4.224	29.270	144.307
octahydro-1Methylpurine	N-methylpurine	4	4.000	29.643	134.934
N-ethylperhydropurine	N-ethylpurine	4	2.193	29.562	74.187
perhydrofluorene	9H-fluorene	6	10.224	29.571	345.752
perhydro-9-ethylfluorene	9-ethylfluorene	6	9.933	29.528	336.389
perhydro-9H-carbazole	9H-carbazole	6	8.045	29.386	273.758
perhydro-N-ethylcarbazole	N-ethylcarbazole	6	7.355	29.516	249.178
perhydro-1,8-diazacarbazole	1,8-diazacarbazole	6	5.372	29.336	183.115
perhydro-N-methyl-1,8-diazacarbazole	N-methyl-1,8-diazacarbazole	6	4.458	29.037	153.515
perhydro-N-ethyl-1,8-diazacarbazole	N-ethyl-1,8-diazacarbazole	6	4.216	29.493	142.951
perhydrodibenzoborole	5H-dibenzoborole	6	10.298	29.505	349.037
Perhydro-5Me-dibenzoborole	dibenzo-5Me-borole	6	10.146	28.743	352.996
perhydrofluorene	9H-fluorene	6	10.224	29.571	345.752
perhydro[b,d] dibenzofuran	dibenzo[b,d]furan	6	9.439	29.479	320.207
perhydro dibenzothiophene	dibenzo[b,d]thiophene	6	9.815	29.392	333.936
perhydrodibenzoborole	5H-dibenzoborole	6	10.298	29.505	349.037
perhydro-9H-carbazole	9H-carbazole	6	8.045	29.386	273.758
perhydro-1,8-diazacarbazole	1,8-diazacarbazole	6	5.372	29.336	183.115
perhydro-3,6-diazacarbazole	3,6-diazacarbazole	6	6.109	29.375	207.972

perhydro-4,5-diazacarbazole	4,5-diazacarbazole	6	6.579	29.333	224.285
4-aminopiperidine	4-aminopyridine	3	8.434	29.292	287.940
4-chloropiperidine	4-chloropyridine	3	12.134	28.849	420.588
4-dimethyl aminopiperidine	4-dimethyl aminopyridine	3	8.122	30.210	268.856
4-fluoropiperidine	4-fluoropyridine	3	11.740	28.816	407.411
4-methylpiperidine	4-methylpyridine	3	10.693	30.987	345.065
4-trifluoro methylpiperidine	4-trifluoro methylpyridine	3	12.653	28.045	451.149
chlorocyclohexane	chlorobenzene	3	13.638	28.788	473.743
dimethyl aminocyclohexane	Dimethyl aminobenzene	3	10.871	29.863	364.019
fluorocyclohexane	fluorobenzene	3	13.407	28.783	465.801
methylcyclohexane	methylbenzene	3	12.451	30.791	404.382
trifluoro methylcyclohexane	trifluoro methylbenzene	3	13.833	30.843	448.508
aminocyclohexane	aminobenzene	3	10.955	29.295	373.958

Table S9 : Minimum energy geometries of the investigated organic molecules obtained at the DFT/UB3LYP/cc-pVTZ level of theory using Gaussian 09.

ethylbenzene

Atom	x (Å)	y (Å)	z (Å)
H	0.2517881447	-0.2964369076	2.1379612813
C	-0.2731748854	-0.1835491438	1.1970273033
C	-1.6349931385	0.0921227386	-1.2001953284
C	0.4298423456	-0.3238711013	0.0000000000
C	-1.6349931385	0.0921227386	1.2001953284
C	-2.3213077396	0.2321523043	0.0000000000
C	-0.2731748854	-0.1835491438	-1.1970273033
H	-2.1611421810	0.1931553725	2.1403873224
H	-3.3821679504	0.4434031807	0.0000000000
H	0.2517881447	-0.2964369076	-2.1379612813
H	-2.1611421810	0.1931553725	-2.1403873224
C	1.9168420734	-0.5850722901	0.0000000000
H	2.1793185785	-1.1832580765	-0.8753922980
H	2.1793185785	-1.1832580765	0.8753922980
C	2.7532942078	0.7016973358	0.0000000000
H	2.5372029332	1.3083654008	-0.8804392500
H	3.8203241608	0.4729378027	0.0000000000
H	2.5372029332	1.3083654008	0.8804392500

cyclooctane

Atom	x (Å)	y (Å)	z (Å)
C	-1.7240319605	0.7141101673	-0.2817976852
H	-1.6270720850	0.6739520474	-1.3722722916
H	-2.7188518682	1.1263002751	-0.0926845111
C	-0.7140274627	1.7237498069	0.2820222276
H	-0.6735762527	1.6264098356	1.3724545242
H	-1.1261037450	2.7187047399	0.0933947276
C	0.7140274627	1.7237498069	-0.2820222276
H	0.6735762527	1.6264098356	-1.3724545242

Continued on Next Page...

Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	1.1261037450	2.7187047399	-0.0933947276
C	1.7240319605	0.7141101673	0.2817976852
H	1.6270720850	0.6739520474	1.3722722916
H	2.7188518682	1.1263002751	0.0926845111
C	1.7240319605	-0.7141101673	-0.2817976852
H	1.6270720850	-0.6739520474	-1.3722722916
H	2.7188518682	-1.1263002751	-0.0926845111
C	0.7140274627	-1.7237498069	0.2820222276
H	0.6735762527	-1.6264098356	1.3724545242
H	1.1261037450	-2.7187047399	0.0933947276
C	-0.7140274627	-1.7237498069	-0.2820222276
H	-0.6735762527	-1.6264098356	-1.3724545242
H	-1.1261037450	-2.7187047399	-0.0933947276
C	-1.7240319605	-0.7141101673	0.2817976852
H	-2.7188518682	-1.1263002751	0.0926845111
H	-1.6270720850	-0.6739520474	1.3722722916

cyclohexane

Atom	x (Å)	y (Å)	z (Å)
H	2.4886263291	0.0001925385	-0.1501101969
C	1.4634555345	-0.0001452610	0.2273043307
C	-0.7316019676	1.2674623007	0.2273043307
C	-0.7318535669	-1.2673170397	0.2273043307
C	-1.4634555345	0.0001452610	-0.2273043307
C	0.7316019676	-1.2674623007	-0.2273043307
C	0.7318535669	1.2673170397	-0.2273043307
H	-0.7676302445	1.3299228070	1.3203219753
H	-0.7679318137	-1.3297486960	1.3203219753
H	-1.5355620582	0.0001741110	-1.3203219753
H	0.7676302445	-1.3299228070	-1.3203219753
H	0.7679318137	1.3297486960	-1.3203219753
H	1.5355620582	-0.0001741110	1.3203219753
H	-1.2444799078	2.1551173523	-0.1501101969

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-1.2441464214	-2.1553098908	-0.1501101969
H	-2.4886263291	-0.0001925385	0.1501101969
H	1.2444799078	-2.1551173523	0.1501101969
H	1.2441464214	2.1553098908	0.1501101969

cyclohexene

Atom	x (Å)	y (Å)	z (Å)
H	-2.3732234956	0.5362080273	0.1679747349
C	-1.4937295544	-0.1031934276	0.0504195185
C	0.6957285927	-0.3186695774	-1.1881512322
C	0.6628464287	0.0536369824	1.3041731717
C	1.4937295544	0.1031934276	0.0504195185
C	-0.6628464287	-0.0536369824	1.3041731717
C	-0.6957285927	0.3186695774	-1.1881512322
H	0.5892918680	-1.4076120773	-1.1920824261
H	1.8880802310	1.1178568245	-0.0837195085
H	-1.1926309648	-0.1065072781	2.2492055867
H	-0.5892918680	1.4076120773	-1.1920824261
H	-1.8880802310	-1.1178568245	-0.0837195085
H	1.2405246591	-0.0534865033	-2.0962558449
H	1.1926309648	0.1065072781	2.2492055867
H	2.3732234956	-0.5362080273	0.1679747349
H	-1.2405246591	0.0534865033	-2.0962558449

cyclopentane

Atom	x (Å)	y (Å)	z (Å)
H	-0.1866956584	-1.3275244843	-1.8297946401
C	0.2444556836	-0.7259256781	-1.0289735658
C	-0.2444556836	0.7259256781	-1.0289735658
C	0.1384382327	1.2322251124	0.3712623373
C	0.0000000000	0.0000000000	1.3044595533
C	-0.1384382327	-1.2322251124	0.3712623373

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	1.3307411936	-0.7475663053	-1.1538431224
H	-1.3307411936	0.7475663053	-1.1538431224
H	0.1866956584	1.3275244843	-1.8297946401
H	1.1734591176	1.5799725131	0.3621226347
H	-0.4750102386	2.0727519539	0.6955630206
H	-0.8689507626	0.0917842415	1.9561890590
H	0.8689507626	-0.0917842415	1.9561890590
H	-1.1734591176	-1.5799725131	0.3621226347
H	0.4750102386	-2.0727519539	0.6955630206

indane

Atom	x (Å)	y (Å)	z (Å)
H	-1.0558451038	-0.0063366532	2.4834747342
C	-1.0507729386	-0.0094133550	1.4004105961
C	-1.0507729386	-0.0094133550	-1.4004105961
C	0.1460079950	-0.0492258596	0.6981837102
C	-2.2514729510	0.0347257042	0.6959961540
C	-2.2514729510	0.0347257042	-0.6959961540
C	0.1460079950	-0.0492258596	-0.6981837102
H	-3.1898531879	0.0746290766	1.2333744184
H	-3.1898531879	0.0746290766	-1.2333744184
H	-1.0558451038	-0.0063366532	-2.4834747342
C	1.5593681430	-0.1184479173	1.2273576998
H	1.7895178091	-1.1378022423	1.5551019282
H	1.7290883148	0.5335495743	2.0850855431
C	2.4144469968	0.2717697318	0.0000000000
H	3.3960527416	-0.2004572242	0.0000000000
H	2.5713450993	1.3519348269	0.0000000000
C	1.5593681430	-0.1184479173	-1.2273576998
H	1.7895178091	-1.1378022423	-1.5551019282
H	1.7290883148	0.5335495743	-2.0850855431

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)

cycloheptane

Atom	x (Å)	y (Å)	z (Å)
C	-0.3966952997	1.2514098729	0.9698880680
H	-1.4547287465	1.1900976375	0.6990360712
H	-0.3164462257	2.1132555284	1.6366697249
C	0.4018812806	1.5250623647	-0.3134184751
H	1.4647518325	1.3154125268	-0.1545855473
H	0.3387966868	2.5926873890	-0.5382263874
C	-0.1136734595	0.7572411823	-1.5382913572
H	-1.1861864694	0.9574179056	-1.6358738585
H	0.3510574689	1.1701865240	-2.4379986473
C	0.1136734595	-0.7572411823	-1.5382913572
H	1.1861864694	-0.9574179056	-1.6358738585
H	-0.3510574689	-1.1701865240	-2.4379986473
C	-0.4018812806	-1.5250623647	-0.3134184751
H	-0.3387966868	-2.5926873890	-0.5382263874
H	-1.4647518325	-1.3154125268	-0.1545855473
C	0.3966952997	-1.2514098729	0.9698880680
H	1.4547287465	-1.1900976375	0.6990360712
H	0.3164462257	-2.1132555284	1.6366697249
C	0.0000000000	0.0000000000	1.7732710491
H	0.8340970965	0.2506961624	2.4343048840
H	-0.8340970965	-0.2506961624	2.4343048840

tetrahydrofuran

Atom	x (Å)	y (Å)	z (Å)
O	-0.0009684610	-1.1942165994	-0.2248456032
C	-1.1258693343	-0.4416608528	0.2108455906
C	-0.7825007661	1.0163352788	-0.1150544170
C	0.7627778677	1.0462046066	-0.0118592644
C	1.1466311038	-0.4405434765	0.1536385237

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-1.2771662165	-0.5755225958	1.2910504036
H	-2.0040421673	-0.8182778855	-0.3106689664
H	-1.1035853710	1.2603336397	-1.1269512131
H	-1.2649892701	1.7168766419	0.5653861640
H	1.1059437462	1.6378118828	0.8359491181
H	1.2067096977	1.4730814174	-0.9095506647
H	1.4094386504	-0.6590057215	1.1965718502
H	1.9732945207	-0.7539593358	-0.4814945213

tetrahydrothiophene

Atom	x (Å)	y (Å)	z (Å)
H	-0.1178641750	1.2973261063	-2.1146077329
C	0.2679586740	0.7164497694	-1.2747261252
C	-0.1398815463	1.3420792171	0.0584088508
S	0.0000000000	0.0000000000	1.3220527180
C	0.1398815463	-1.3420792171	0.0584088508
C	-0.2679586740	-0.7164497694	-1.2747261252
H	1.3570064016	0.7014731003	-1.3557501153
H	-1.1694058817	1.6965704867	0.0332522692
H	0.5059660533	2.1671954508	0.3499544944
H	-0.5059660533	-2.1671954508	0.3499544944
H	1.1694058817	-1.6965704867	0.0332522692
H	-1.3570064016	-0.7014731003	-1.3557501153
H	0.1178641750	-1.2973261063	-2.1146077329

2,3-dihydrobenzofuran

Atom	x (Å)	y (Å)	z (Å)
H	-1.0250996870	-2.5004169255	0.0133347235
C	-1.0166099391	-1.4177698140	0.0095539178
C	-1.0093019289	1.4002114729	-0.0109365900
C	0.1782243274	-0.7209265546	-0.0155283493
C	-2.2169888688	-0.7051317839	0.0286622791

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-2.2065546202	0.6863844319	0.0151990209
C	0.1677453312	0.6707380252	-0.0237905518
H	-3.1584288190	-1.2363138272	0.0536741621
H	-3.1431286112	1.2279261440	0.0300006146
H	-0.9911373109	2.4806594896	-0.0176937613
C	1.6150671394	-1.1765545811	-0.0926734284
H	1.8431693115	-1.5909194319	-1.0779517712
H	1.8714766860	-1.9329412147	0.6487599650
C	2.3682770927	0.1469652036	0.1559159781
H	3.2055365039	0.3109347047	-0.5182801538
H	2.7227179083	0.2181954081	1.1865441904
O	1.4157874847	1.2198572529	-0.0597842457

n-propylamine

Atom	x (Å)	y (Å)	z (Å)
H	-2.0495192685	-0.6794062047	0.9727495776
C	-1.9237203709	-0.1434408600	0.0296010865
H	-2.0702557640	-0.8619726934	-0.7796003118
H	-2.7220983727	0.5963188997	-0.0382241163
C	-0.5486505000	0.5150266616	-0.0587013700
H	-0.4461587186	1.2558367216	0.7413083438
H	-0.4482877573	1.0628756739	-0.9980316961
C	0.5989412274	-0.4840738259	0.0422458095
H	0.5178108413	-1.2060222105	-0.7747847166
H	0.4937140573	-1.0563482917	0.9763536397
N	1.8934823120	0.1916358536	-0.0889950552
H	2.0469119426	0.8096663727	0.6999488366
H	2.6494793714	-0.4822760972	-0.0759190277

cyclohexanethiol

Atom	x (Å)	y (Å)	z (Å)
C	0.6126501855	-0.0136967204	0.3695118388

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-1.5655470100	1.2603990937	0.2132176816
C	-1.5756112936	-1.2674524401	0.1834156792
C	-2.2698434372	0.0051803489	-0.3089130721
C	-0.0815781043	-1.2661398062	-0.1677956423
C	-0.0714159541	1.2606066082	-0.1335496102
H	-1.6831425721	1.3152599424	1.3003077094
H	-1.6934416949	-1.3469490115	1.2691509788
H	-2.2650573747	0.0178216351	-1.4037247674
H	0.0444603352	-1.2991195831	-1.2534511930
H	0.0510529944	1.3245007984	-1.2193996524
H	0.5781376020	-0.0202535053	1.4606634440
H	-2.0355538449	2.1578824712	-0.1941517197
H	-2.0524898849	-2.1517507987	-0.2444924487
H	-3.3181898033	0.0065978648	-0.0031129256
H	0.4004763858	-2.1612807933	0.2307396055
H	0.4164324168	2.1392426787	0.2919496230
S	2.3965205015	0.0747616826	-0.1071860353
H	2.7788225528	-1.0787724656	0.4714455064

cyclohexanol

Atom	x (Å)	y (Å)	z (Å)
C	1.0322435902	0.0366751246	0.3237494067
C	-1.1901314609	1.2333627163	0.2122224972
C	-1.1180240426	-1.2961848452	0.2071380148
C	-1.8659991049	-0.0507589776	-0.2786230951
C	0.3646674144	-1.2428577496	-0.1798875901
C	0.2934156607	1.2734451324	-0.1700739767
H	-1.2868955182	1.2968168407	1.3011067372
H	-1.2069041878	-1.3678768458	1.2961585895
H	-1.8899903698	-0.0496931019	-1.3731614623
H	0.4693845141	-1.2739753277	-1.2684291443
H	0.3989967975	1.3184971825	-1.2580701362
H	1.0104094900	0.0340500984	1.4232774975

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-1.7005139034	2.1093034685	-0.1927870223
H	-1.5773046960	-2.1995774213	-0.1990791398
H	-2.9054293099	-0.0818768094	0.0551259423
H	0.8920449163	-2.1164108008	0.2159343220
H	0.7763853772	2.1654507884	0.2322428693
O	2.3857235081	0.1458270871	-0.1230110994
H	2.8707823252	-0.6279125597	0.1797507898

N-methylpyrrolidine

Atom	x (Å)	y (Å)	z (Å)
N	0.7131508942	0.3411011254	0.0000000000
C	-0.0218817271	-0.1593387705	-1.1559742785
C	-1.4939232323	0.0563645097	-0.7766565937
C	-1.4939232323	0.0563645097	0.7766565937
C	-0.0218817271	-0.1593387705	1.1559742785
H	0.1774819607	-1.2341489491	-1.3209977525
H	0.2745892229	0.3712127649	-2.0619887434
H	-1.8511515421	1.0116748906	-1.1584445174
H	-2.1327514131	-0.7209773327	-1.1936415317
H	-2.1327514131	-0.7209773327	1.1936415317
H	-1.8511515421	1.0116748906	1.1584445174
H	0.1774819607	-1.2341489491	1.3209977525
H	0.2745892229	0.3712127649	2.0619887434
C	2.1239070300	0.0224596665	0.0000000000
H	2.6034510754	0.4492951897	-0.8818529828
H	2.3156833854	-1.0654493973	0.0000000000
H	2.6034510754	0.4492951897	0.8818529828

trans-Decalin

Atom	x (Å)	y (Å)	z (Å)
C	0.2568879574	-0.7265983644	0.0000000000
C	0.2509200852	-0.7234202294	-2.5436044753

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-0.2568879574	0.7265983644	0.0000000000
C	-0.1747642462	-1.4638216716	-1.2729443040
H	1.3440399454	-0.7248249008	-2.6112005580
H	-1.3551015132	0.6798726483	0.0000000000
H	-1.2650813557	-1.5753296086	-1.2666141339
H	1.3551015132	-0.6798726483	0.0000000000
H	-0.1138532310	-1.2507041545	-3.4281248859
H	0.2374405883	-2.4766021242	-1.2702349602
C	-0.1747642462	-1.4638216716	1.2729443040
H	0.2374405883	-2.4766021242	1.2702349602
H	-1.2650813557	-1.5753296086	1.2666141339
C	0.2509200852	-0.7234202294	2.5436044753
H	1.3440399454	-0.7248249008	2.6112005580
H	-0.1138532310	-1.2507041545	3.4281248859
C	-0.2509200852	0.7234202294	2.5436044753
H	0.1138532310	1.2507041545	3.4281248859
H	-1.3440399454	0.7248249008	2.6112005580
C	0.1747642462	1.4638216716	1.2729443040
H	1.2650813557	1.5753296086	1.2666141339
H	-0.2374405883	2.4766021242	1.2702349602
C	0.1747642462	1.4638216716	-1.2729443040
H	-0.2374405883	2.4766021242	-1.2702349602
H	1.2650813557	1.5753296086	-1.2666141339
C	-0.2509200852	0.7234202294	-2.5436044753
H	-1.3440399454	0.7248249008	-2.6112005580
H	0.1138532310	1.2507041545	-3.4281248859

tetralin

Atom	x (Å)	y (Å)	z (Å)
H	0.0745347705	-2.4604550481	-1.3588140495
C	0.0424667491	-1.3770916121	-1.3606382808
C	-0.0424667491	1.3770916121	-1.3606382808
C	0.0230581948	-0.6999103901	-0.1386251793

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	0.0206321149	-0.6952855265	-2.5672462836
C	-0.0206321149	0.6952855265	-2.5672462836
C	-0.0230581948	0.6999103901	-0.1386251793
H	0.0352078573	-1.2423811689	-3.5006430610
H	-0.0352078573	1.2423811689	-3.5006430610
H	-0.0745347705	2.4604550481	-1.3588140495
C	0.0814330694	-1.4903335976	1.1531780229
H	1.1080336394	-1.8450635245	1.2992402671
H	-0.5328786434	-2.3882799436	1.0568655764
C	-0.3419333747	-0.6831252717	2.3806044810
H	-0.1022509380	-1.2374048500	3.2899996881
H	-1.4274143119	-0.5430525161	2.3749008188
C	0.3419333747	0.6831252717	2.3806044810
H	1.4274143119	0.5430525161	2.3749008188
H	0.1022509380	1.2374048500	3.2899996881
C	-0.0814330694	1.4903335976	1.1531780229
H	0.5328786434	2.3882799436	1.0568655764
H	-1.1080336394	1.8450635245	1.2992402671

tetrahydroquinoline

Atom	x (Å)	y (Å)	z (Å)
C	-1.3430252239	-1.3750787854	-0.0470570175
C	-2.5512005475	0.7058448844	0.0028744186
C	-0.1190919449	0.7141952032	0.0414566398
C	-1.3395402493	1.3834915571	0.0391088986
C	-0.1195458830	-0.6921567891	-0.0092959783
C	-2.5433168092	-0.6847592703	-0.0385427412
H	-3.4842816688	1.2519448415	0.0043258029
H	-1.3342684936	2.4671171595	0.0697124512
H	-1.3404146122	-2.4579903242	-0.0915417331
N	1.0754159765	-1.4023524260	-0.0723540221
C	1.1886536882	1.4748267174	0.1113455046
C	2.3765418034	0.6281368409	-0.3518218779

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	2.3211636935	-0.7507010256	0.2968056735
H	2.4235419150	-0.6437325954	1.3870546546
H	3.1486917332	-1.3721072035	-0.0480198816
H	-3.4748153334	-1.2349077648	-0.0671903201
H	1.3633505307	1.8033202548	1.1415376984
H	1.1182673196	2.3853143575	-0.4872716418
H	2.3490823164	0.5056342096	-1.4367874135
H	3.3177878637	1.1194433856	-0.1012435557
H	1.0012959257	-2.3714212273	0.1894104406

piperidine

Atom	x (Å)	y (Å)	z (Å)
C	0.2307253240	-1.4547154664	0.0000000000
C	0.2031434253	0.7512463561	-1.2149516240
C	0.2031434253	0.7512463561	1.2149516240
N	-0.3149977258	1.3769847122	0.0000000000
C	-0.2236955750	-0.7150337827	1.2627248712
C	-0.2236955750	-0.7150337827	-1.2627248712
H	1.3049158737	0.8022064849	-1.2731078093
H	1.3049158737	0.8022064849	1.2731078093
H	-1.3128602342	-0.7588796704	1.3425218145
H	-1.3128602342	-0.7588796704	-1.3425218145
H	1.3236210251	-1.5259361224	0.0000000000
H	-0.1911640571	1.2898930798	-2.0781491588
H	-0.1911640571	1.2898930798	2.0781491588
H	0.1884073492	-1.1914698627	2.1550302198
H	0.1884073492	-1.1914698627	-2.1550302198
H	-0.1099463841	2.3673897017	0.0000000000
H	-0.1475678029	-2.4789650350	0.0000000000

cyclohexylamine

Atom	x (Å)	y (Å)	z (Å)

Continued on Next Page...

Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	0.8111326387	-0.2098025732	-2.1475837704
C	0.3102684130	0.1834088365	-1.2577860553
C	-1.8849829971	0.2702629104	0.0000000000
C	0.3102684130	0.1834088365	1.2577860553
C	-1.1693697906	-0.2124146056	1.2655616019
C	1.0274340213	-0.3123825421	0.0000000000
C	-1.1693697906	-0.2124146056	-1.2655616019
H	-1.9145966614	1.3647802746	0.0000000000
H	0.4080824746	1.2722616734	1.2984742846
H	-1.2544065176	-1.3019987805	1.3344120432
H	0.9727666330	-1.4134883094	0.0000000000
H	-1.2544065176	-1.3019987805	-1.3344120432
H	0.4080824746	1.2722616734	-1.2984742846
H	-2.9232986390	-0.0688767234	0.0000000000
H	0.8111326387	-0.2098025732	2.1475837704
H	-1.6581485159	0.1910479616	2.1549586092
H	-1.6581485159	0.1910479616	-2.1549586092
N	2.4121618842	0.1722180995	0.0000000000
H	2.9080716774	-0.1767763671	0.8126628644
H	2.9080716774	-0.1767763671	-0.8126628644

2-methylpiperidine

Atom	x (Å)	y (Å)	z (Å)
C	1.2372048972	-1.2271123941	0.2133182893
C	1.0807154320	1.2803631584	0.1787592712
C	-0.9865641619	-0.0171751819	0.3205411592
N	-0.3117384445	1.1532142438	-0.2456023737
C	-0.2515869737	-1.2778430213	-0.1440216293
C	1.8785438533	0.0674079458	-0.2937616175
H	1.1766689398	1.3635068124	1.2757011749
H	-0.9422943128	0.0016144277	1.4253383770
H	-0.3676278749	-1.3625111541	-1.2285834976
H	1.8978668271	0.0649539040	-1.3866276324

Continued on Next Page...

Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	1.3483003841	-1.2808032795	1.3015041988
H	1.4903715508	2.1961636573	-0.2506130930
H	-0.7203109660	-2.1577849111	0.3029334515
H	2.9117892373	0.1456587683	0.0515318967
H	-0.8268872467	1.9934170807	-0.0141306467
H	1.7554747948	-2.0972455606	-0.1948654057
C	-2.4509690250	-0.0168604735	-0.0981341035
H	-2.9730924578	-0.8822048329	0.3123556463
H	-2.5350379341	-0.0423683685	-1.1855107951
H	-2.9632255190	0.8794891790	0.2593713294

isopropanol

Atom	x (Å)	y (Å)	z (Å)
H	-0.8882230642	-1.9377437164	0.3055820827
C	-1.0698471014	-0.9398201020	-0.0975740805
H	-1.0810538773	-1.0016290565	-1.1867292024
H	-2.0608425571	-0.6239971434	0.2366994174
C	0.0015436654	0.0409487739	0.3653059598
H	-0.0094046286	0.0849306902	1.4623720683
C	1.3947598878	-0.3554564241	-0.0915181256
H	1.4343859548	-0.4041004015	-1.1807191974
H	1.6710926640	-1.3307458134	0.3105377373
H	2.1268754848	0.3781466352	0.2442486465
O	-0.2372931499	1.3525025725	-0.1596455705
H	-1.1192392783	1.6314049855	0.1039012644

2-butanol

Atom	x (Å)	y (Å)	z (Å)
H	-1.7482603131	-1.7270975915	0.4464255883
C	-1.7655623487	-0.7271715555	0.0090625292
H	-1.9038016125	-0.8208933921	-1.0690927963
H	-2.6318574739	-0.2020997548	0.4182161032

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-0.4764124566	0.0267185951	0.3151129181
H	-0.3558286122	0.0993958097	1.4051821292
C	0.7546003682	-0.6636011798	-0.2606740777
H	0.6469125567	-0.6912647157	-1.3486013893
H	0.7568031808	-1.7011126421	0.0833046427
C	2.0698712438	0.0143112455	0.1167830583
H	2.9195666258	-0.5024206552	-0.3312286705
H	2.2156888463	0.0145098733	1.1993920234
H	2.0824662196	1.0489952085	-0.2222828780
O	-0.5102335099	1.3460029762	-0.2433101630
H	-1.2573867142	1.8197287783	0.1331089823

piperazine

Atom	x (Å)	y (Å)	z (Å)
C	-0.7360312745	-0.1968461037	1.2105015678
C	-0.7360312745	-0.1968461037	-1.2105015678
N	-1.3688348986	0.3251796456	0.0000000000
C	0.7360312745	0.1968461037	-1.2105015678
C	0.7360312745	0.1968461037	1.2105015678
H	-0.8014820421	-1.2938403583	1.2828866620
H	-0.8014820421	-1.2938403583	-1.2828866620
H	0.8014820421	1.2938403583	-1.2828866620
H	0.8014820421	1.2938403583	1.2828866620
H	-1.2343555841	0.2315090685	2.0815346274
H	-1.2343555841	0.2315090685	-2.0815346274
H	1.2343555841	-0.2315090685	-2.0815346274
H	1.2343555841	-0.2315090685	2.0815346274
H	-2.3581897834	0.1156066265	0.0000000000
N	1.3688348986	-0.3251796456	0.0000000000
H	2.3581897834	-0.1156066265	0.0000000000

pyrrolidine

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
Atom	x (Å)	y (Å)	z (Å)
H	0.6883486848	1.6976095340	-1.1905816149
C	-0.0686484200	1.0321224726	-0.7756494401
C	0.1903525579	-0.4464394852	-1.1587106802
N	-0.1902869122	-1.2632348799	0.0000000000
C	0.1903525579	-0.4464394852	1.1587106802
C	-0.0686484200	1.0321224726	0.7756494401
H	-1.0329765853	1.3646663178	-1.1610538588
H	1.2550831528	-0.6022312414	-1.3523327239
H	-0.3520369333	-0.7648634794	-2.0479875607
H	1.2550831528	-0.6022312414	1.3523327239
H	-0.3520369333	-0.7648634794	2.0479875607
H	0.6883486848	1.6976095340	1.1905816149
H	-1.0329765853	1.3646663178	1.1610538588
H	-1.1968050010	-1.3876403574	0.0000000000

1,4-cyclohexadiene

Atom	x (Å)	y (Å)	z (Å)
H	1.1989887646	-2.1937305513	0.0000000000
C	0.6637668338	-1.2509265536	0.0000000000
C	0.6637668338	1.2509265536	0.0000000000
C	-1.4937173443	0.0000000000	0.0000000000
C	-0.6637668338	1.2509265536	0.0000000000
C	-0.6637668338	-1.2509265536	0.0000000000
C	1.4937173443	0.0000000000	0.0000000000
H	-2.1670178280	0.0000000000	0.8671295391
H	-1.1989887646	2.1937305513	0.0000000000
H	-1.1989887646	-2.1937305513	0.0000000000
H	2.1670178280	0.0000000000	-0.8671295391
H	1.1989887646	2.1937305513	0.0000000000
H	-2.1670178280	0.0000000000	-0.8671295391
H	2.1670178280	0.0000000000	0.8671295391

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)

1,3-cyclohexadiene

Atom	x (Å)	y (Å)	z (Å)
H	0.1411388927	2.4982727723	0.1218285664
C	0.0391099210	1.4202129181	0.1186695850
C	-0.0940240577	-0.7253381423	1.2590092830
C	0.2537220015	-0.7240973772	-1.1853873415
C	-0.0391099210	-1.4202129181	0.1186695850
C	-0.2537220015	0.7240973772	-1.1853873415
C	0.0940240577	0.7253381423	1.2590092830
H	1.3408783371	-0.7336635943	-1.3458447718
H	-0.1411388927	-2.4982727723	0.1218285664
H	-1.3408783371	0.7336635943	-1.3458447718
H	0.2570177693	1.2276904327	2.2041817733
H	-0.2570177693	-1.2276904327	2.2041817733
H	-0.1786760180	-1.2728281368	-2.0233950945
H	0.1786760180	1.2728281368	-2.0233950945

phenylacetylene

Atom	x (Å)	y (Å)	z (Å)
H	-2.1405488515	0.0000000000	0.4241814977
C	-1.2072602094	0.0000000000	-0.1208836474
C	1.2029059614	0.0000000000	-1.5073517745
C	0.0000000000	0.0000000000	0.5903530696
C	-1.2029059614	0.0000000000	-1.5073517745
C	0.0000000000	0.0000000000	-2.2048507426
C	1.2072602094	0.0000000000	-0.1208836474
H	-2.1412475628	0.0000000000	-2.0453594751
H	0.0000000000	0.0000000000	-3.2863903239
H	2.1405488515	0.0000000000	0.4241814977
H	2.1412475628	0.0000000000	-2.0453594751
C	0.0000000000	0.0000000000	2.0160300472

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	0.0000000000	0.0000000000	4.2787393243
C	0.0000000000	0.0000000000	3.2177754335

styrene

Atom	x (Å)	y (Å)	z (Å)
H	-0.0087190604	-2.2938267147	0.0760561603
C	-0.3919172165	-1.2815962439	0.0375772941
C	-1.3782658031	1.3034466323	-0.0606692440
C	0.5118368645	-0.2139879969	-0.0052043009
C	-1.7640158774	-1.0655961769	0.0315448555
C	-2.2636553682	0.2290558952	-0.0176564852
C	-0.0100557683	1.0857497767	-0.0545603572
H	-2.4413571594	-1.9086711207	0.0652706211
H	-3.3313216274	0.4026898211	-0.0225708631
H	0.6595393358	1.9341908636	-0.0884773242
H	-1.7591867298	2.3155576488	-0.0991446319
C	1.9517958152	-0.5022900185	0.0035242051
H	2.1974536505	-1.5589647326	0.0439355797
C	2.9575096192	0.3707643140	-0.0319369118
H	3.9841257205	0.0329150646	-0.0206498006
H	2.8041856050	1.4409329878	-0.0730757968

cyclooctatetraene

Atom	x (Å)	y (Å)	z (Å)
C	1.8363190000	-0.0004380000	0.0000000000
H	2.9200100000	0.0436790000	0.0000000000
C	1.2471120000	1.3478950000	0.0000000000
H	2.0156710000	2.1133910000	0.0000000000
C	0.0004380000	1.8363190000	0.0000000000
H	-0.0436790000	2.9200100000	0.0000000000
C	-1.3478950000	1.2471120000	0.0000000000
H	-2.1133910000	2.0156710000	0.0000000000

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-1.8363190000	0.0004380000	0.0000000000
H	-2.9200100000	-0.0436790000	0.0000000000
C	-1.2471120000	-1.3478950000	0.0000000000
H	-2.0156710000	-2.1133910000	0.0000000000
C	-0.0004380000	-1.8363190000	0.0000000000
H	0.0436790000	-2.9200100000	0.0000000000
C	1.3478950000	-1.2471120000	0.0000000000
H	2.1133910000	-2.0156710000	0.0000000000

cyclopentene

Atom	x (Å)	y (Å)	z (Å)
H	-0.6187220329	-0.5210508503	-2.0343483531
C	0.0956589228	-0.3163542994	-1.2340665788
C	-0.0447743786	1.0729340099	-0.6642592352
C	-0.0447743786	1.0729340099	0.6642592352
C	0.0956589228	-0.3163542994	1.2340665788
C	-0.1240102354	-1.2267728091	0.0000000000
H	1.0914467409	-0.4525662182	-1.6703816681
H	-0.0988870397	1.9580324397	-1.2841287939
H	-0.0988870397	1.9580324397	1.2841287939
H	-0.6187220329	-0.5210508503	2.0343483531
H	1.0914467409	-0.4525662182	1.6703816681
H	-1.1510853857	-1.5936398967	0.0000000000
H	0.5290941941	-2.0983814574	0.0000000000

cyclopentadiene

Atom	x (Å)	y (Å)	z (Å)
H	0.0000000000	-0.8745420000	-1.8740230000
C	0.0000000000	0.0000000000	-1.2131040000
C	-1.1764710000	0.0000000000	-0.2804370000
C	-0.7326670000	0.0000000000	0.9874400000
C	0.7326670000	0.0000000000	0.9874400000

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	1.1764710000	0.0000000000	-0.2804370000
H	0.0000000000	0.8745420000	-1.8740230000
H	-2.2051550000	0.0000000000	-0.6065400000
H	-1.3449970000	0.0000000000	1.8773900000
H	1.3449970000	0.0000000000	1.8773900000
H	2.2051550000	0.0000000000	-0.6065400000

1H-Indene

Atom	x (Å)	y (Å)	z (Å)
H	-1.0173629051	-2.4927465096	0.0000000000
C	-0.9968241556	-1.4104370475	0.0000000000
C	-0.9536835618	1.4044903961	0.0000000000
C	0.2106413356	-0.7200239533	0.0000000000
C	-2.1834073952	-0.6824471737	0.0000000000
C	-2.1642942941	0.7103194196	0.0000000000
C	0.2284599372	0.6865242967	0.0000000000
H	-3.1319783646	-1.2030884901	0.0000000000
H	-3.0970204263	1.2584710609	0.0000000000
H	-0.9482297305	2.4875083584	0.0000000000
C	1.5946639467	-1.1923913392	0.0000000000
H	1.8834703188	-2.2336777016	0.0000000000
C	2.4315747317	-0.1441369522	0.0000000000
H	3.5101673959	-0.1929349395	0.0000000000
C	1.6626474406	1.1518638080	0.0000000000
H	1.8983708634	1.7657423835	-0.8755062363
H	1.8983708634	1.7657423835	0.8755062363

cycloheptatriene

Atom	x (Å)	y (Å)	z (Å)
C	-1.4449098910	-0.5483215419	0.0000000000
H	-1.0407630778	-1.5667321107	0.0000000000
H	-2.5307602285	-0.6232748604	0.0000000000

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-0.9568098003	0.1857129079	-1.2192227614
H	-1.6886180512	0.6423821547	-1.8749166565
C	0.3494809254	0.2726284549	-1.5240019676
H	0.6277876977	0.7203147074	-2.4722742153
C	1.4371663659	-0.1558801029	-0.6792125404
H	2.3769949621	-0.3723473596	-1.1750468874
C	1.4371663659	-0.1558801029	0.6792125404
H	2.3769949621	-0.3723473596	1.1750468874
C	0.3494809254	0.2726284549	1.5240019676
H	0.6277876977	0.7203147074	2.4722742153
C	-0.9568098003	0.1857129079	1.2192227614
H	-1.6886180512	0.6423821547	1.8749166565

furan

Atom	x (Å)	y (Å)	z (Å)
O	0.0000000000	0.0000000000	1.1442281287
C	-1.0924803539	0.0000000000	0.3321217199
C	-0.7157282071	0.0000000000	-0.9688402113
C	0.7157282071	0.0000000000	-0.9688402113
C	1.0924803539	0.0000000000	0.3321217199
H	-2.0460975609	0.0000000000	0.8273893811
H	-1.3692847517	0.0000000000	-1.8235719540
H	1.3692847517	0.0000000000	-1.8235719540
H	2.0460975609	0.0000000000	0.8273893811

thiophene

Atom	x (Å)	y (Å)	z (Å)
C	0.7116343007	0.0000000000	1.2864597402
C	1.2380227027	0.0000000000	0.0296321230
S	0.0000000000	0.0000000000	-1.1733660218
C	-1.2380227027	0.0000000000	0.0296321230
C	-0.7116343007	0.0000000000	1.2864597402

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	1.3141691752	0.0000000000	2.1825696932
H	2.2742672461	0.0000000000	-0.2619375455
H	-2.2742672461	0.0000000000	-0.2619375455
H	-1.3141691752	0.0000000000	2.1825696932

benzofuran

Atom	x (Å)	y (Å)	z (Å)
H	-1.0052439508	-2.5094483084	0.0000000000
C	-0.9695982465	-1.4283013126	0.0000000000
C	-0.9050253856	1.4149592664	0.0000000000
C	0.2533161199	-0.7508832718	0.0000000000
C	-2.1373459588	-0.6818818317	0.0000000000
C	-2.1070006138	0.7199897139	0.0000000000
C	0.2491794420	0.6513109953	0.0000000000
H	-3.0935814466	-1.1873877561	0.0000000000
H	-3.0376970977	1.2707220218	0.0000000000
H	-0.8657993110	2.4947477016	0.0000000000
C	1.6433529460	-1.1287867846	0.0000000000
H	2.0563325604	-2.1227270084	0.0000000000
C	2.3447615523	0.0239003446	0.0000000000
H	3.3998914692	0.2321668705	0.0000000000
O	1.5310389211	1.1272513593	0.0000000000

propionitrile

Atom	x (Å)	y (Å)	z (Å)
H	-1.4484779024	-1.0989818575	0.8819533216
C	-1.5479322770	-0.4683643126	0.0000000000
H	-1.4484779024	-1.0989818575	-0.8819533216
H	-2.5453619971	-0.0306972945	0.0000000000
C	-0.4920979986	0.6461376351	0.0000000000
H	-0.6117159341	1.2865615391	0.8760658444
H	-0.6117159341	1.2865615391	-0.8760658444

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	0.8737429985	0.1295866427	0.0000000000
N	1.9434119471	-0.2934160337	0.0000000000

benzene

Atom	x (Å)	y (Å)	z (Å)
H	2.4722869898	0.0000000050	0.0000000000
C	1.3903488329	0.0000000028	0.0000000000
C	-1.3903488329	-0.0000000028	0.0000000000
C	0.6951744140	1.2040774108	0.0000000000
C	0.6951744189	-1.2040774080	0.0000000000
C	-0.6951744140	-1.2040774108	0.0000000000
C	-0.6951744189	1.2040774080	0.0000000000
H	1.2361434906	2.1410633411	0.0000000000
H	1.2361434992	-2.1410633361	0.0000000000
H	-1.2361434906	-2.1410633411	0.0000000000
H	-1.2361434992	2.1410633361	0.0000000000
H	-2.4722869898	-0.0000000050	0.0000000000

thiophenol

Atom	x (Å)	y (Å)	z (Å)
H	0.3359707659	-2.1435163359	0.0000000000
C	-0.2001056255	-1.2036478289	0.0000000000
C	-1.5853045039	1.2021633295	0.0000000000
C	0.5049198886	0.0006982957	0.0000000000
C	-1.5883171488	-1.1972430756	0.0000000000
C	-2.2887649100	0.0036931902	0.0000000000
C	-0.1960577026	1.2061312161	0.0000000000
H	-2.1230618597	-2.1377859058	0.0000000000
H	-3.3699592342	0.0053542939	0.0000000000
H	0.3378930972	2.1468819764	0.0000000000
H	-2.1174961017	2.1442634344	0.0000000000
S	2.2846558396	-0.0830870120	0.0000000000

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	2.5114154949	1.2415094219	0.0000000000

toluene

Atom	x (Å)	y (Å)	z (Å)
H	0.7270783779	0.0214702041	2.1380684607
C	0.1903262312	0.0112647374	1.1971773779
C	-1.1994107665	-0.0023802006	-1.2000835751
C	0.9073434211	0.0152270143	0.0000000000
C	-1.1994107665	-0.0023802006	1.2000835751
C	-1.9005219792	-0.0103258574	0.0000000000
C	0.1903262312	0.0112647374	-1.1971773779
H	-1.7347267409	-0.0029950331	2.1406363647
H	-2.9822732756	-0.0181556282	0.0000000000
H	0.7270783779	0.0214702041	-2.1380684607
H	-1.7347267409	-0.0029950331	-2.1406363647
C	2.4142023062	-0.0021686660	0.0000000000
H	2.7944906683	-1.0270718370	0.0000000000
H	2.8182543279	0.4938877793	0.8825663818
H	2.8182543279	0.4938877793	-0.8825663818

phenol

Atom	x (Å)	y (Å)	z (Å)
H	0.7421868417	-2.1589962596	0.0000000000
C	0.2075281219	-1.2194963767	0.0000000000
C	-1.1228987899	1.2224937282	0.0000000000
C	0.9330851076	-0.0303533250	0.0000000000
C	-1.1791040678	-1.1763956598	0.0000000000
C	-1.8535935064	0.0411681646	0.0000000000
C	0.2669396896	1.1926977729	0.0000000000
H	-1.7373883270	-2.1032597897	0.0000000000
H	-2.9342705209	0.0674439626	0.0000000000
H	0.8331809236	2.1170580165	0.0000000000

Continued on Next Page...

Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-1.6328312703	2.1767607135	0.0000000000
O	2.2970757943	-0.1240260662	0.0000000000
H	2.6783770037	0.7595021185	0.0000000000

N-methylpyrrole

Atom	x (Å)	y (Å)	z (Å)
N	0.6229332789	0.0344213123	0.0000000000
C	-0.1742341251	0.0121562035	-1.1157170913
C	-1.4870612565	-0.0143102931	-0.7093426876
C	-1.4870612565	-0.0143102931	0.7093426876
C	-0.1742341251	0.0121562035	1.1157170913
H	0.2580677877	0.0205749960	-2.1013534040
H	-2.3470865861	-0.0202389974	-1.3569518857
H	-2.3470865861	-0.0202389974	1.3569518857
H	0.2580677877	0.0205749960	2.1013534040
C	2.0696170322	-0.0262879142	0.0000000000
H	2.4576314929	0.4793681763	-0.8824761073
H	2.4302990625	-1.0573145631	0.0000000000
H	2.4576314929	0.4793681763	0.8824761073

Naphtalene

Atom	x (Å)	y (Å)	z (Å)
H	3.3645215766	-1.2402275820	0.0000000000
C	2.4238428070	-0.7058025573	0.0000000000
H	1.2392614266	-2.4798275384	0.0000000000
C	1.2406174149	-1.3969645822	0.0000000000
C	1.2406174149	1.3969645822	0.0000000000
C	0.0000000000	-0.7139541915	0.0000000000
C	2.4238428070	0.7058025573	0.0000000000
C	0.0000000000	0.7139541915	0.0000000000
C	-1.2406174149	-1.3969645822	0.0000000000
H	3.3645215766	1.2402275820	0.0000000000

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-1.2392614266	2.4798275384	0.0000000000
H	1.2392614266	2.4798275384	0.0000000000
C	-2.4238428070	-0.7058025573	0.0000000000
H	-1.2392614266	-2.4798275384	0.0000000000
H	-3.3645215766	-1.2402275820	0.0000000000
C	-2.4238428070	0.7058025573	0.0000000000
H	-3.3645215766	1.2402275820	0.0000000000
C	-1.2406174149	1.3969645822	0.0000000000

quinoline

Atom	x (Å)	y (Å)	z (Å)
H	3.3873072013	-1.1179926599	0.0000000000
C	2.4143649698	-0.6463802819	0.0000000000
H	1.2920685416	-2.4676109287	0.0000000000
C	1.2628296026	-1.3849404065	0.0000000000
N	1.1842448776	1.4227266132	0.0000000000
C	0.0148341359	-0.7223225077	0.0000000000
C	2.3177610657	0.7630979763	0.0000000000
C	0.0276884848	0.7040505525	0.0000000000
C	-1.2264167478	-1.4016900451	0.0000000000
H	3.2240431270	1.3605712145	0.0000000000
H	-1.1714050850	2.4801686399	0.0000000000
C	-2.4029573656	-0.6994172037	0.0000000000
H	-1.2313343094	-2.4846283466	0.0000000000
H	-3.3485105341	-1.2248441822	0.0000000000
C	-2.3901776781	0.7127741445	0.0000000000
H	-3.3277285981	1.2526849728	0.0000000000
C	-1.2044236881	1.3996914485	0.0000000000

pyridine

Atom	x (Å)	y (Å)	z (Å)
H	0.0000000000	0.0000000000	2.4619988193

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	0.0000000000	0.0000000000	1.3801000078
N	0.0000000000	0.0000000000	-1.4122818073
C	-1.1929662580	0.0000000000	0.6709682817
C	1.1929662580	0.0000000000	0.6709682817
C	1.1386362604	0.0000000000	-0.7178839481
C	-1.1386362604	0.0000000000	-0.7178839481
H	2.1476133087	0.0000000000	1.1787001075
H	2.0526762455	0.0000000000	-1.3011004510
H	-2.0526762455	0.0000000000	-1.3011004510
H	-2.1476133087	0.0000000000	1.1787001075

aniline

Atom	x (Å)	y (Å)	z (Å)
H	0.7554882075	-0.0201250997	2.1429252173
C	0.2171898734	-0.0123285244	1.2028579787
C	-1.1701110877	-0.0050361554	-1.1974416586
C	0.9328981934	-0.0158433343	0.0000000000
C	-1.1701110877	-0.0050361554	1.1974416586
C	-1.8772114457	-0.0014958664	0.0000000000
C	0.2171898734	-0.0123285244	-1.2028579787
H	-1.7023017738	-0.0011792137	2.1398843622
H	-2.9581497564	0.0048514909	0.0000000000
H	0.7554882075	-0.0201250997	-2.1429252173
H	-1.7023017738	-0.0011792137	-2.1398843622
N	2.3258806105	-0.0830209295	0.0000000000
H	2.7724569798	0.2611973130	-0.8344684103
H	2.7724569798	0.2611973130	0.8344684103

2-methylpyridine

Atom	x (Å)	y (Å)	z (Å)
H	-1.5635436207	-2.1690155812	0.0000000000
C	-1.0931657851	-1.1917634217	0.0000000000

Continued on Next Page...

Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	0.1728658810	1.2010354079	0.0000000000
N	0.2417092133	-1.1871029506	0.0000000000
C	-1.8668177866	-0.0409343189	0.0000000000
C	-1.2116752650	1.1847821236	0.0000000000
C	0.8732666343	-0.0091274593	0.0000000000
H	-2.9459888967	-0.1045839513	0.0000000000
H	-1.7717961683	2.1107245015	0.0000000000
H	0.7141698946	2.1381049553	0.0000000000
C	2.3781072528	-0.0360071334	0.0000000000
H	2.7811036470	0.4714184269	-0.8789017473
H	2.7261493525	-1.0656500258	0.0000000000
H	2.7811036470	0.4714184269	0.8789017473

acetone

Atom	x (Å)	y (Å)	z (Å)
C	0.0000000000	0.0000000000	0.1918834177
C	-1.2878322568	0.0000000000	-0.6045693086
H	-1.3313963417	0.8770948024	-1.2542217104
H	-2.1405331971	0.0000000000	0.0689793627
H	-1.3313963417	-0.8770948024	-1.2542217104
C	1.2878322568	0.0000000000	-0.6045693086
H	1.3313963417	0.8770948024	-1.2542217104
H	1.3313963417	-0.8770948024	-1.2542217104
H	2.1405331971	0.0000000000	0.0689793627
O	0.0000000000	0.0000000000	1.4011933159

2-butanone

Atom	x (Å)	y (Å)	z (Å)
H	-1.9843732517	-1.1501657752	0.8770907045
C	-1.8812017858	-0.5075658654	0.0000000000
H	-1.9843732517	-1.1501657752	-0.8770907045
H	-2.6703210328	0.2396057625	0.0000000000

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-0.5271451792	0.1718627988	0.0000000000
C	0.6877834794	-0.7418499481	0.0000000000
H	0.6028176872	-1.4043252250	-0.8680762356
H	0.6028176872	-1.4043252250	0.8680762356
C	2.0202389644	-0.0053925020	0.0000000000
H	2.8503196806	-0.7120076641	0.0000000000
H	2.1128110118	0.6341616267	0.8767039111
H	2.1128110118	0.6341616267	-0.8767039111
O	-0.4228310212	1.3770171653	0.0000000000

pyrazine

Atom	x (Å)	y (Å)	z (Å)
N	0.0000000000	-1.4008270976	0.0000000000
N	0.0000000000	1.4008270976	0.0000000000
C	-1.1295929741	-0.6952812212	0.0000000000
C	1.1295929741	-0.6952812212	0.0000000000
C	1.1295929741	0.6952812212	0.0000000000
C	-1.1295929741	0.6952812212	0.0000000000
H	-2.0598784152	-1.2512162047	0.0000000000
H	2.0598784152	-1.2512162047	0.0000000000
H	2.0598784152	1.2512162047	0.0000000000
H	-2.0598784152	1.2512162047	0.0000000000

hexahydropyrimidine

Atom	x (Å)	y (Å)	z (Å)
H	-2.0048906344	-1.3853422897	0.1592098004
C	-1.1705843229	-0.8010501278	-0.2307808003
C	-0.0154769723	1.4286834301	-0.2089708244
C	1.2310369916	-0.6438683682	-0.2054508822
N	1.1577154249	0.7258467973	0.3122542142
N	0.0832472111	-1.4375355850	0.1859691904
C	-1.2770725668	0.6673464712	0.2010707767

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	0.0062017848	1.5145521948	-1.3093949699
H	1.2747555065	-0.6650802055	-1.3067480493
H	-1.3852038072	0.7208185385	1.2873301874
H	-1.2240402888	-0.8639994671	-1.3224957889
H	-0.0299681752	2.4422981667	0.1939078385
H	2.1396594569	-1.1113219745	0.1746736735
H	-2.1602876695	1.1334994069	-0.2430034450
H	0.0881362529	-1.5359448320	1.1953996263
H	2.0061848084	1.2323558443	0.0899514526

hexahydropyridazine

Atom	x (Å)	y (Å)	z (Å)
C	1.2392610334	-0.6975447202	0.1688187533
N	0.0564938977	1.3548492316	0.3222647784
N	1.1741859296	0.6715028385	-0.3537273895
C	-1.1915219699	0.7678917724	-0.1776563837
C	-0.0254058148	-1.4522566239	-0.2331559667
H	1.3367993039	-0.7069895119	1.2639779284
H	-1.2572378340	0.8325334829	-1.2733359273
H	-0.0489949820	-1.5428590362	-1.3222106376
H	2.1251464295	-1.1694408117	-0.2592440240
H	-2.0163741670	1.3398672988	0.2503578235
H	-0.0036738039	-2.4629872161	0.1789938748
H	2.0009385633	1.1615019089	-0.0278613706
C	-1.2677861736	-0.6963766729	0.2482459862
H	-2.1766113838	-1.1533911906	-0.1479836663
H	-1.3263018001	-0.7422730133	1.3388102850
H	0.1025097718	2.3090242638	-0.0201190638

hexahydro-1,3,5-triazine

Atom	x (Å)	y (Å)	z (Å)
N	1.3626676559	-0.0000001582	0.3089233473

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
N	-0.6813334722	1.1801047597	0.3089233473
C	0.6923522953	1.1991887782	-0.1770086770
C	-1.3847038747	0.0000001607	-0.1770086770
C	0.6923520169	-1.1991889389	-0.1770086770
H	0.7247323414	1.2552726480	-1.2876250550
H	0.7247320499	-1.2552728163	-1.2876250550
H	-2.3993106527	0.0000002785	0.2214355852
H	2.3291381430	-0.0000002704	0.0087947995
H	-1.1645686186	2.0170928096	0.0087947995
H	1.1996553039	-2.0778642424	0.2214355852
H	-1.4494639538	0.0000001683	-1.2876250550
H	1.1996557863	2.0778639639	0.2214355852
N	-0.6813337462	-1.1801046015	0.3089233473
H	-1.1645690869	-2.0170925393	0.0087947995

tetrahydro-1H-imidazole

Atom	x (Å)	y (Å)	z (Å)
H	-1.3412486099	1.0308090814	-1.1614194496
C	-0.9813989481	0.0723890958	-0.7837101642
N	0.4220679449	-0.1261558826	-1.1884976608
C	1.1884501458	0.2645860673	0.0000000000
N	0.4220679449	-0.1261558826	1.1884976608
C	-0.9813989481	0.0723890958	0.7837101642
H	-1.6134263534	-0.7067345871	-1.2075252712
H	2.1825568029	-0.1787637923	0.0000000000
H	1.2953349735	1.3527463307	0.0000000000
H	-1.3412486099	1.0308090814	1.1614194496
H	-1.6134263534	-0.7067345871	1.2075252712
H	0.5786035053	-1.1122455114	-1.3617754947
H	0.5786035053	-1.1122455114	1.3617754947

pyrazolidine

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
Atom	x (Å)	y (Å)	z (Å)
N	0.6809042857	-0.9497872594	-0.3194670559
N	-0.6438353248	-0.9730138607	0.3378330096
C	-1.2162099033	0.3115595766	-0.0964449731
C	-0.0286504141	1.2911309358	-0.0068701808
C	1.1987026918	0.3635157294	0.0970350532
H	-1.5834369932	0.2712370696	-1.1279024605
H	-2.0439637730	0.5816023843	0.5573965068
H	-0.0990620911	1.9376793627	0.8657343247
H	0.0149964741	1.9266931208	-0.8892393812
H	1.5660876786	0.3529234552	1.1291683654
H	2.0151720866	0.6587437682	-0.5600905344
H	1.2202299265	-1.6744482323	0.1440217767
H	-1.1521986438	-1.7259860503	-0.1153934505

1,2,3-triazolidine

Atom	x (Å)	y (Å)	z (Å)
N	-0.8076153928	-1.0016247605	0.1024582541
N	-1.1859830989	0.4344657193	0.1836299181
N	-0.0089128331	1.2310010884	-0.1501260594
C	1.1033328061	0.3752478663	0.2541420590
C	0.6342351813	-1.0230692099	-0.1779259551
H	1.2243065432	0.4281690391	1.3379711577
H	2.0232313678	0.7091399606	-0.2224054275
H	1.1085951048	-1.8426278835	0.3605146436
H	0.8142997868	-1.1680558585	-1.2467793156
H	-0.9395882799	-1.3251724750	1.0532472753
H	0.0439439806	1.3067106279	-1.1659102175
H	-1.8438231658	0.5909208858	-0.5725823328

1,2,4-triazolidine

Atom	x (Å)	y (Å)	z (Å)

Continued on Next Page...

Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
N	0.7642080664	-1.0166167744	0.0863504082
N	-0.6541552689	-1.0922037562	-0.1536007608
C	-1.1544035054	0.2292257486	0.2386380084
N	-0.1035653040	1.1969699368	-0.0885758667
C	1.1384046538	0.4329800296	0.0742817340
H	-2.0923567253	0.4698359345	-0.2596094614
H	-1.3175222261	0.2269289575	1.3191161926
H	1.6392925077	0.6832851774	1.0125173917
H	1.8188530709	0.6547765925	-0.7488102581
H	0.9050137865	-1.3852880889	1.0181034367
H	-0.7684389081	-1.2097327751	-1.1552716272
H	-0.1983701475	1.4670930177	-1.0597431973

perhydroquinoline

Atom	x (Å)	y (Å)	z (Å)
C	-1.2352476276	-1.4564978152	-0.2043378944
C	-2.5299171910	0.7198060032	-0.2314540641
C	0.0075801778	0.7446333891	-0.2614582214
C	-1.2631739520	1.4657805721	0.1982295930
C	0.0193731191	-0.7078502304	0.2421838110
C	-2.5115320158	-0.7374731989	0.2417000252
H	-2.6062848883	0.7419861651	-1.3233774700
H	-0.0037893646	0.6926739512	-1.3567556665
H	-1.2494643547	1.5614244271	1.2897254589
H	0.0141669944	-0.6652550574	1.3486073526
H	-2.5780333178	-0.7616272115	1.3343120071
H	-1.2141506138	-1.5451181649	-1.2943507919
H	-3.4171093092	1.2288949765	0.1518021931
N	1.2225820441	-1.3804325104	-0.2461907501
C	1.2911857178	1.4648402799	0.1638630458
C	2.5375778276	0.6800240780	-0.2549268201
C	2.4567819044	-0.7633739413	0.2355697006
H	2.5219427798	-0.7678551175	1.3377925666

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	3.3030383312	-1.3410201113	-0.1399655832
H	-3.3896486996	-1.2680179215	-0.1324149708
H	-1.2710472002	2.4841181569	-0.1989116434
H	1.2876965737	1.5863265645	1.2530963165
H	1.3135851325	2.4719704003	-0.2600078446
H	2.6197610527	0.6756453094	-1.3447025055
H	3.4396686313	1.1543383599	0.1378733504
H	-1.2180565191	-2.4757010670	0.1938642220
H	1.1969047676	-2.3599342858	0.0100055833

perhydroisoquinoline

Atom	x (Å)	y (Å)	z (Å)
C	-1.2442718316	-1.4722354362	-0.1794311250
C	-2.5382200163	0.7060652493	-0.2558210078
C	-0.0009492877	0.7321453422	-0.2547522686
C	-1.2773391354	1.4612099782	0.1756136267
C	0.0090194862	-0.7158760750	0.2705182642
C	-2.5252731463	-0.7439690458	0.2389868944
H	-2.6029394526	0.7119320159	-1.3490430790
H	-0.0045988714	0.6756926963	-1.3525557007
H	-1.2738034461	1.5719372659	1.2657045962
H	0.0078073415	-0.6695694497	1.3661180152
H	-2.6002207109	-0.7514791120	1.3313689974
H	-1.2287860367	-1.5815378220	-1.2696238496
H	-3.4301091064	1.2205713224	0.1089901386
C	1.3014187526	-1.4200603723	-0.1428313517
C	1.2779017880	1.4644258552	0.1649351691
C	2.5231933472	0.6762213389	-0.2356001849
N	2.4588966444	-0.6674104244	0.3339713310
H	-3.4019769504	-1.2777776789	-0.1347558100
H	-1.2840824364	2.4736045067	-0.2374914539
H	1.2802716682	1.6015101651	1.2500336231
H	1.3075864490	2.4587743333	-0.2883904246

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	2.5939793828	0.6599487879	-1.3375851179
H	3.4219808810	1.1695573564	0.1380771040
H	-1.2364233646	-2.4849341539	0.2330542542
H	3.3125026859	-1.1738478449	0.1393075539
H	1.3359996453	-2.4216688514	0.2911341513
H	1.3018757207	-1.5412209470	-1.2411253456

perhydro-4H-quinolizine

Atom	x (Å)	y (Å)	z (Å)
C	0.2974374738	-0.7044167880	0.0000000000
C	0.2085665210	-0.7042479524	-2.5419033996
N	-0.2184157534	0.6727829784	0.0000000000
C	-0.1570186505	-1.4481091781	-1.2592396482
H	1.2968920743	-0.6901742264	-2.6606687002
H	-1.2424483641	-1.5746107042	-1.2095104967
H	1.4060875159	-0.6788046231	0.0000000000
H	-0.1946726952	-1.2241290516	-3.4133834695
H	0.2832011214	-2.4479398309	-1.2547251690
C	-0.1570186505	-1.4481091781	1.2592396482
H	0.2832011214	-2.4479398309	1.2547251690
H	-1.2424483641	-1.5746107042	1.2095104967
C	0.2085665210	-0.7042479524	2.5419033996
H	1.2968920743	-0.6901742264	2.6606687002
H	-0.1946726952	-1.2241290516	3.4133834695
C	-0.3124906377	0.7299090391	2.4754336760
H	0.0181823484	1.3063833469	3.3421322911
H	-1.4055436204	0.7258360071	2.4851811041
C	0.1681480164	1.4117198089	1.2001893916
H	1.2668902656	1.5353920213	1.2487940097
H	-0.2563309976	2.4149794367	1.1271789372
C	0.1681480164	1.4117198089	-1.2001893916
H	-0.2563309976	2.4149794367	-1.1271789372
H	1.2668902656	1.5353920213	-1.2487940097

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-0.3124906377	0.7299090391	-2.4754336760
H	-1.4055436204	0.7258360071	-2.4851811041
H	0.0181823484	1.3063833469	-3.3421322911

perhydrocinnoline

Atom	x (Å)	y (Å)	z (Å)
C	0.0179955540	-0.7103259513	-0.2709516087
C	-2.5037875600	-0.7319219357	-0.2430692445
C	0.0122345161	0.7372360890	0.2618530474
C	-1.2276051741	-1.4668207681	0.1821559857
H	-2.5754938783	-0.7480505478	-1.3353437258
H	-0.0146386836	0.6647567543	1.3587208353
H	-1.2124228377	-1.5695040364	1.2734681723
H	0.0294326338	-0.6744736567	-1.3647812313
H	-3.3827442482	-1.2610246446	0.1309954639
H	-1.2064266698	-2.4774255397	-0.2288679612
N	1.2356695267	-1.4339620615	0.1112512285
N	2.3706166747	-0.7165793430	-0.3845330107
C	2.5286386460	0.5978747731	0.2335189820
C	1.3119382361	1.4523006021	-0.1238425105
H	1.3212024011	1.6380104326	-1.2013410986
H	1.3722906168	2.4231592231	0.3746412172
C	-1.2524076277	1.4746822257	-0.1862135028
H	-1.2588092607	2.4894533255	0.2208413264
H	-1.2381693709	1.5795744446	-1.2766384884
C	-2.5178907811	0.7230421097	0.2397510018
H	-2.5921155774	0.7388980524	1.3321450986
H	-3.4063156739	1.2343379406	-0.1374136287
H	1.2703871442	-1.4619370992	1.1349438809
H	3.1842974222	-1.3019407295	-0.2558082184
H	2.6229176248	0.5323109082	1.3316012059
H	3.4462793468	1.0489184326	-0.1494712165

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)

perhydrophthalazine

Atom	x (Å)	y (Å)	z (Å)
C	0.0186408545	-0.7263157287	-0.2578016483
C	-2.5090230482	-0.7561664832	-0.2202601046
C	0.0077908533	0.7275303693	0.2492130785
C	-1.2282457000	-1.4769198214	0.2148632550
H	-2.5846810872	-0.7939319911	-1.3118333437
H	-0.0091489158	0.6875952403	1.3481356958
H	-1.2100069431	-1.5617348752	1.3070800811
H	0.0025814886	-0.6925032878	-1.3535366937
H	-3.3863532847	-1.2778719615	0.1683434055
H	-1.2213955640	-2.4982906014	-0.1756455030
C	1.3315914744	-1.4060286952	0.1343298717
N	2.4418971982	-0.6014962699	-0.3708589898
N	2.5085539432	0.6978749869	0.2242244184
C	1.3055711426	1.4429577286	-0.1517796802
H	1.3383986943	1.5900512870	-1.2336288126
H	1.3608502055	2.4269944195	0.3198783046
C	-1.2591938898	1.4541861800	-0.2077709845
H	-1.2689012935	2.4749278070	0.1843442287
H	-1.2483995005	1.5414862394	-1.2996705464
C	-2.5230072704	0.7079217832	0.2339906809
H	-2.5946029668	0.7442108014	1.3260490546
H	-3.4129036729	1.2112531840	-0.1504061243
H	3.3369877728	-1.0496143238	-0.2324653515
H	1.3694372103	-1.5319955813	1.2310697181
H	1.3964532775	-2.4005985165	-0.3137501358
H	2.5097340216	0.6049991103	1.2438811255

perhydroquinazoline

Atom	x (Å)	y (Å)	z (Å)

Continued on Next Page...

Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	0.0280345117	-0.7180434165	-0.2606145031
C	-2.4988266351	-0.7515230536	-0.2454368129
C	0.0106352724	0.7310963849	0.2669206693
C	-1.2191909583	-1.4808369805	0.1772997774
H	-2.5712790918	-0.7634362729	-1.3378345344
H	0.0024428245	0.6745340753	1.3646445574
H	-1.2043441485	-1.5895734188	1.2683378429
H	0.0217835335	-0.6646940604	-1.3579894471
H	-3.3752159398	-1.2864348014	0.1264781439
H	-1.1897168751	-2.4894715823	-0.2387907789
N	1.2518102678	-1.4391102849	0.1019204244
C	2.4521350641	-0.6870856445	-0.2579030232
H	2.5140329459	-0.6783367853	-1.3499185253
H	3.3253358446	-1.2197688519	0.1178965176
N	2.5204003696	0.7014502820	0.1924193931
C	1.3051421884	1.4424468304	-0.1522741980
H	1.2987095322	1.5862580961	-1.2388219568
H	1.3609167731	2.4381459928	0.2928567893
C	-1.2581131578	1.4599790286	-0.1816543884
H	-1.2717126066	2.4755740185	0.2237626918
H	-1.2463956290	1.5643806285	-1.2724653864
C	-2.5198821776	0.7014380056	0.2434851403
H	-2.5920888685	0.7125001718	1.3360426914
H	-3.4113686831	1.2101325227	-0.1300833957
H	1.2505505833	-1.6288950746	1.0994337482
H	2.6624930602	0.7277231903	1.1960975635

perhydroquinoxaline

Atom	x (Å)	y (Å)	z (Å)
C	0.0223692713	-0.7307200522	-0.2629148687
C	-2.5042044873	-0.7173221735	-0.2223690811
C	0.0320816597	0.7224632551	0.2425990691
C	-1.2339104904	-1.4609904385	0.2030434807

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-2.5869015215	-0.7476859684	-1.3133974845
H	0.0217803590	0.6738355251	1.3490850039
H	-1.2126458116	-1.5523691249	1.2954118589
H	0.0130231446	-0.6822074436	-1.3581183384
H	-3.3866925872	-1.2280745448	0.1685072118
H	-1.2238745128	-2.4766212065	-0.1956233701
N	1.2328497313	-1.4677452955	0.1087401679
C	2.4492446473	-0.7416570273	-0.2603911267
H	2.5260334154	-0.7471716885	-1.3507639300
H	3.3131603851	-1.2795666061	0.1333703490
C	2.4591645501	0.7084473649	0.2255736701
H	3.3301447799	1.2338313609	-0.1719643240
H	2.5433142035	0.7114007612	1.3268734146
N	1.2465549046	1.3771521650	-0.2405175823
C	-1.2199039322	1.4676362900	-0.2132801072
H	-1.2056438643	2.4906918687	0.1747803904
H	-1.1988138533	1.5467000110	-1.3039908151
C	-2.4919078159	0.7444688735	0.2400068983
H	-2.5571333623	0.7773959525	1.3323767870
H	-3.3737950868	1.2660986414	-0.1374036694
H	1.2278590418	-1.6357733226	1.1101582622
H	1.2498632320	2.3521738232	0.0329271335

perhydro1,8-naphthyridine

Atom	x (Å)	y (Å)	z (Å)
C	0.0014322290	-0.7682175051	-0.2733443804
C	-2.5237886048	-0.6993596350	-0.2338435011
C	-0.0059978528	0.6876787064	0.2115782463
C	-1.2744258100	-1.4809507566	0.1824933335
H	-2.6205306457	-0.7135606091	-1.3220235171
H	-0.0052322871	0.6603855276	1.3266852884
H	-1.2589737992	-1.5883708890	1.2728526590
H	0.0007474861	-0.7125425947	-1.3660824735

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-3.4222698682	-1.1621236397	0.1801927345
H	-1.3014769667	-2.4933200032	-0.2274457299
C	1.2850864033	-1.4674420574	0.1816004525
C	2.5259162706	-0.6727996754	-0.2355753312
H	2.6221723627	-0.6861448889	-1.3238084764
H	3.4294297858	-1.1260816219	0.1780043623
C	2.4182205177	0.7774892292	0.2291905417
H	3.2592014786	1.3619084657	-0.1462365052
H	2.4698084977	0.8019221759	1.3315665371
N	1.1826227818	1.3709135390	-0.2822928606
N	-1.2021288036	1.3585153241	-0.2810378904
C	-2.4310458771	0.7518909361	0.2311087234
H	-2.4821670351	0.7755484396	1.3335216504
H	-3.2783893602	1.3274927874	-0.1436376644
H	1.1432902708	2.3533972341	-0.0366065921
H	1.2714792848	-1.5749984553	1.2719692371
H	1.3225341275	-2.4794797016	-0.2283434713
H	-1.1730245857	2.3411986680	-0.0347033724

perhydro1,5-naphthyridine

Atom	x (Å)	y (Å)	z (Å)
C	-0.0174747920	-0.7264307470	-0.2485925557
C	-2.4483498127	-0.7460621770	-0.2161826333
C	0.0174747920	0.7264307470	0.2485925557
N	-1.2204976494	-1.3728097127	0.2706279750
H	-2.5207992281	-0.7722660047	-1.3171021044
H	0.0271981419	0.6786017691	1.3513869929
H	-0.0271981419	-0.6786017691	-1.3513869929
H	-3.3016711234	-1.2999917246	0.1782247608
C	1.2437526607	-1.4666080465	0.1898459144
C	2.5020843168	-0.7091442252	-0.2458620279
H	2.5858790125	-0.7278937436	-1.3351385231
H	3.3942578932	-1.1926664741	0.1571294677

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	2.4483498127	0.7460621770	0.2161826333
H	3.3016711234	1.2999917246	-0.1782247608
H	2.5207992281	0.7722660047	1.3171021044
N	1.2204976494	1.3728097127	-0.2706279750
C	-1.2437526607	1.4666080465	-0.1898459144
C	-2.5020843168	0.7091442252	0.2458620279
H	-2.5858790125	0.7278937436	1.3351385231
H	-3.3942578932	1.1926664741	-0.1571294677
H	1.2105883686	2.3582548933	-0.0385919665
H	1.2229647029	-1.5675940468	1.2788909330
H	1.2470149546	-2.4798503789	-0.2222577366
H	-1.2470149546	2.4798503789	0.2222577366
H	-1.2229647029	1.5675940468	-1.2788909330
H	-1.2105883686	-2.3582548933	0.0385919665

perhydropteridine

Atom	x (Å)	y (Å)	z (Å)
C	0.0089650200	-0.7197824407	-0.2506627440
C	-2.4025023526	-0.7829374393	-0.2353675973
C	-0.0298123048	0.7302399061	0.2522420347
N	-1.1687701900	-1.4215931927	0.2291730193
H	-2.4901636768	-0.7931352083	-1.3321609684
H	-0.0142990505	0.6781287728	1.3558266717
H	0.0413154900	-0.6722646485	-1.3527834068
H	-3.2545716548	-1.3251963124	0.1764627043
N	1.2102740114	-1.4231417487	0.1750039064
C	2.4121404068	-0.6824116060	-0.2115198567
H	2.4901423630	-0.7326850013	-1.3005406477
H	3.2823759577	-1.1856129462	0.2073296941
N	2.4611727889	0.7297743505	0.1668859815
C	1.2421408767	1.4444756223	-0.2167214293
H	1.2161081736	1.5335168854	-1.3063968274
H	1.2857219582	2.4599597134	0.1834498157

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-1.1235877157	-2.3867626181	-0.0767136113
N	-1.2446637684	1.3632238486	-0.2435494805
C	-2.4398919190	0.6668274522	0.2352610331
H	-2.5167229651	0.6754879405	1.3334126217
H	-3.3243272090	1.1605470190	-0.1698524517
H	-1.2734740282	2.3409717468	0.0195535487
H	1.1748700450	-1.5432404702	1.1829644788
H	2.6047107437	0.8098493747	1.1670665111

perhydropyrazino[2,3-b]pyrazine

Atom	x (Å)	y (Å)	z (Å)
C	-0.0032913814	-0.7293174579	-0.2629945502
C	-2.4155757521	-0.7256141455	-0.2139692263
C	-0.0006323626	0.7294953995	0.2170672637
N	-1.1934489231	-1.3871275178	0.2464341291
H	-2.5182984366	-0.7494059303	-1.3089515701
H	0.0098728598	0.6918613643	1.3287978082
H	0.0254887276	-0.6866108874	-1.3623984214
H	-3.2760494458	-1.2377309273	0.2185321220
N	1.1768297491	-1.4587340882	0.1753894507
C	2.4038915048	-0.7564630884	-0.2095245495
H	2.5014002107	-0.8162816110	-1.2959262661
H	3.2567785797	-1.2765569152	0.2282324599
C	2.4100809662	0.7168650279	0.2083441079
H	3.2826475742	1.2227856050	-0.2087898881
H	2.4870688016	0.7712437417	1.3079389772
N	1.2016527759	1.3678506730	-0.3003128938
N	-1.1999635225	1.3861784744	-0.2767895429
C	-2.4047094435	0.7305260356	0.2366152393
H	-2.4639011875	0.7562763697	1.3355433293
H	-3.2791665571	1.2459942982	-0.1618037196
H	-1.1983380275	2.3677308305	-0.0242521344
H	1.2056550786	2.3531943974	-0.0652841684

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	1.1309311015	-1.5589534600	1.1852087368
H	-1.1761178899	-2.3598131885	-0.0360136933

perhydropyrimido[4,5-d]pyrimidine

Atom	x (Å)	y (Å)	z (Å)
C	0.0068979466	-0.7455843286	-0.2738883447
N	-2.4892863605	-0.7085411660	-0.1756136597
C	-0.0086880150	0.7091760822	0.2100675573
C	-1.2753002262	-1.4486024467	0.1849410883
H	0.0002926997	0.6828686406	1.3248215130
H	-1.2675996958	-1.5675930697	1.2735342477
H	0.0193083961	-0.7029962355	-1.3651518910
H	-1.3383764294	-2.4517794254	-0.2399509037
C	1.2959376482	-1.4194191655	0.1892336596
H	1.3677296131	-2.4266033650	-0.2252894652
H	1.2794007176	-1.5183215629	1.2887681994
N	2.4352665119	-0.6337087320	-0.2858206979
C	2.3924165601	0.7364839998	0.2038730994
H	3.2577106849	1.2757495258	-0.1816806055
H	2.4365191228	0.7683491543	1.3143950213
N	1.1817010511	1.3824487734	-0.2916463095
N	-1.2215798289	1.3547427936	-0.2727677646
C	-2.4141377978	0.6733215996	0.2516008666
H	-2.4350051826	0.6718887507	1.3529807883
H	-3.2960733542	1.2084504243	-0.0992648601
H	-1.2342740324	2.3323213901	0.0003420485
H	1.1803925285	2.3554903102	-0.0064075684
H	3.3074073915	-1.0668942811	-0.0113904932
H	-2.6043379494	-0.7298926662	-1.1827535258

perhydro-1H-indene

Atom	x (Å)	y (Å)	z (Å)

Continued on Next Page...

Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-0.2984068525	-2.4910291240	-0.9708188503
C	0.1447521165	-1.4918001132	-0.9608850109
C	0.2560952711	0.7242235571	-2.2308913655
C	0.2856916478	0.7121650700	0.2759750826
C	-0.1447521165	1.4918001132	-0.9608850109
C	-0.2856916478	-0.7121650700	0.2759750826
C	-0.2560952711	-0.7242235571	-2.2308913655
H	1.3484369231	0.7163150206	-2.3080296387
H	1.3804841266	0.6196871971	0.2499694878
H	-1.2313986590	1.6309163915	-0.9406159344
H	-1.3804841266	-0.6196871971	0.2499694878
H	-1.3484369231	-0.7163150206	-2.3080296387
H	1.2313986590	-1.6309163915	-0.9406159344
H	-0.1100912830	1.2458823502	-3.1180183497
H	0.2984068525	2.4910291240	-0.9708188503
H	0.1100912830	-1.2458823502	-3.1180183497
C	0.1108382392	-1.2382151483	1.6590074106
C	0.0000000000	0.0000000000	2.5941149561
H	0.8702325902	0.0737973508	3.2462220705
H	-0.8702325902	-0.0737973508	3.2462220705
C	-0.1108382392	1.2382151483	1.6590074106
H	0.5109353713	2.0701656233	1.9913257966
H	-1.1411739013	1.6020304517	1.6300023234
H	-0.5109353713	-2.0701656233	1.9913257966
H	1.1411739013	-1.6020304517	1.6300023234

perhydrobenzofuran

Atom	x (Å)	y (Å)	z (Å)
C	2.5029355226	-0.1308514160	-0.0547298669
C	1.6992463713	1.1881450107	0.0711263434
H	3.1016096691	-0.1666380134	-0.9660174670
H	1.7305293899	1.5650541511	1.0955274977
C	0.2828023928	0.7356043456	-0.2893296371

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-0.9020418561	-1.4845786561	-0.2097767296
C	-2.2051143623	0.7308888557	-0.2227143209
C	-2.1822380331	-0.7428784181	0.2197258295
C	-0.9398721209	1.5042687328	0.1923672170
C	0.2874874963	-0.6813630813	0.2705707203
H	-0.8567939873	-1.5787021145	-1.2982647225
H	-2.2976729861	0.7739210363	-1.3125458260
H	-2.2665362659	-0.7885652569	1.3101416871
H	-0.9058440470	1.6108036654	1.2817636861
H	0.2435701018	-0.6228087205	1.3717660668
H	0.2216034745	0.6415668640	-1.3799154334
H	-0.8873131797	-2.4944221265	0.2040991645
H	-3.0941534217	1.2199400429	0.1809535030
H	-3.0593264968	-1.2582676599	-0.1758167439
H	-0.9641709361	2.5150092032	-0.2212454640
O	1.5499304440	-1.2087136182	-0.1186637168
H	3.1709293966	-0.2809793577	0.7978122653
H	2.0847554343	1.9698325314	-0.5824460525

perhydrobenzothiophene

Atom	x (Å)	y (Å)	z (Å)
C	2.4294891494	0.6119827984	-0.1920389033
C	1.2676227924	1.5406762414	0.1869596568
H	2.7375088121	0.7633552804	-1.2251648108
H	1.2605998821	1.7114055561	1.2666396872
C	-0.0168688708	0.8285881523	-0.2277960468
C	-1.0228165900	-1.4864070220	-0.1718883865
C	-2.5159507777	0.5848811961	-0.2908618254
C	-2.3854181400	-0.8678379254	0.1867256508
C	-1.3464051881	1.4659766761	0.1755778489
C	0.0856565351	-0.5828289505	0.3513124645
H	-0.9250425547	-1.5889143397	-1.2560841468
H	-2.5522915977	0.5995307080	-1.3848113077

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-2.5154312762	-0.9029951493	1.2730725033
H	-1.3802318590	1.5854518596	1.2637800728
H	-0.0042227359	-0.5194503761	1.4394890344
H	-0.0069343779	0.7316740217	-1.3205319643
H	-0.9432566960	-2.4896410742	0.2508435017
H	-3.4631835030	1.0044207171	0.0542902558
H	-3.1888861521	-1.4726004941	-0.2386649656
H	-1.4369376211	2.4673308440	-0.2524004510
S	1.8079065580	-1.1288972589	-0.0215590515
H	3.2973766707	0.7458072792	0.4493153562
H	1.3754305404	2.5135932599	-0.2968391728

perhydro-1H-indole

Atom	x (Å)	y (Å)	z (Å)
H	-0.9349634604	-2.4948696380	0.2310084683
C	-0.9336118300	-1.4844713766	-0.1865959242
C	-2.2193074912	0.7313441817	-0.2235308250
C	0.2763870377	0.7209735724	-0.2859870674
C	-0.9474271599	1.4963326076	0.1821388434
C	0.2831351215	-0.6983913094	0.2772861290
C	-2.2069970264	-0.7344566626	0.2408139664
H	-2.3103206780	0.7580698239	-1.3141280266
H	0.2232179493	0.6221757064	-1.3762008488
H	-0.9153208680	1.6174084488	1.2703045036
H	0.2300924921	-0.6191481491	1.3793870942
H	-2.2854570039	-0.7629039326	1.3325576684
H	-0.8932627362	-1.5891073879	-1.2744005647
H	-3.1042620968	1.2349447379	0.1716677651
H	-0.9630277647	2.5022535719	-0.2445235226
H	-3.0902779966	-1.2493587707	-0.1424949217
N	1.5851728029	-1.1878995508	-0.1692044230
H	1.8798813742	-2.0173463458	0.3279325549
C	2.5487263729	-0.0733609136	-0.0007328158

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	3.2343112317	-0.0467629718	-0.8499404834
H	3.1581237055	-0.1803662464	0.9029566320
C	1.6811054760	1.2116482278	0.0796650181
H	2.0434930394	1.9983062949	-0.5813968565
H	1.6850515090	1.6124820819	1.0956896362

perhydro-2H-isoindole

Atom	x (Å)	y (Å)	z (Å)
H	-0.9578652761	-2.4937876953	0.2650828092
C	-0.9453630596	-1.4900148838	-0.1670387356
C	-2.2152437320	0.7321494458	-0.2482988058
C	0.2848265544	0.7123847187	-0.2912893034
C	-0.9423113722	1.4957887160	0.1549406591
C	0.2808311503	-0.7089823438	0.2839579658
C	-2.2162966512	-0.7253705054	0.2400195839
H	-2.2991417315	0.7419365910	-1.3400351333
H	0.2508386533	0.6190210644	-1.3849366951
H	-0.9151615164	1.6265583040	1.2420709846
H	0.2455834934	-0.6201206184	1.3773652669
H	-2.2972984364	-0.7358718073	1.3318484923
H	-0.9201141986	-1.6153381625	-1.2549798020
H	-3.0996775967	1.2479831225	0.1318809499
H	-0.9543198008	2.4979442730	-0.2812562530
H	-3.1022782429	-1.2395734974	-0.1386583189
C	1.6732518156	-1.2065793975	-0.0938450519
H	1.6737195052	-1.5632202311	-1.1327177547
H	2.0099162650	-2.0321851336	0.5374567019
C	1.6816083500	1.2002918880	0.0969426248
H	2.0718442722	1.9572472258	-0.5862646670
H	1.6642689897	1.6472519054	1.0977101255
N	2.5302684071	-0.0157693228	0.0987705527
H	3.2531631580	0.0371693444	-0.6020431961

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)

perhydroindolizine

Atom	x (Å)	y (Å)	z (Å)
H	-0.9927804481	-2.4575515734	0.3137961973
C	-0.9669830337	-1.4650450950	-0.1421502528
C	-2.1590320338	0.7592323850	-0.3160701631
N	0.2785511030	0.6458613143	-0.2330345594
C	-0.8711684801	1.4465598859	0.1410846131
C	0.2620291409	-0.7023206849	0.3327461962
C	-2.2393730126	-0.6810499953	0.2019667624
H	-2.1818569128	0.7557731187	-1.4088099842
H	-0.9048113198	1.6075631607	1.2360217837
H	0.2202130363	-0.6414154987	1.4397261643
H	-2.3679185005	-0.6663903940	1.2892577405
H	-0.8956807878	-1.6035054054	-1.2247267471
H	-3.0223329224	1.3351853079	0.0239744299
H	-0.7827800790	2.4318328900	-0.3217448311
H	-3.1188077695	-1.1818170302	-0.2078302077
C	1.5847783633	1.1917057291	0.1034369505
H	1.8181267857	2.0546577404	-0.5219849539
H	1.6205373564	1.5266716917	1.1553809348
C	1.6336290019	-1.2495079762	-0.0731629751
H	1.5692384952	-1.7068961347	-1.0611230323
H	1.9905706124	-2.0101672339	0.6204922615
C	2.5465400268	0.0050620753	-0.1114157779
H	3.0547999511	0.0842713714	-1.0711146690
H	3.3146964270	-0.0217586487	0.6602171194

perhydrobenzimidazole

Atom	x (Å)	y (Å)	z (Å)
H	-0.9169654628	-2.5216486056	0.2055655051
C	-0.8988592580	-1.5066068289	-0.1977812309

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-2.1826297174	0.7198245907	-0.2444767469
C	0.2946274826	0.7020313682	-0.2397568592
C	-0.9236075729	1.4849875204	0.2068900915
C	0.2896641802	-0.7169432982	0.3320492804
C	-2.1865515964	-0.7568025089	0.1908255852
H	-2.2448143777	0.7689423964	-1.3359004254
H	0.2640137638	0.6144351028	-1.3331155207
H	-0.9190930916	1.5919224305	1.2972664561
H	0.1661006751	-0.6264251556	1.4245865959
H	-2.3072445895	-0.8063418258	1.2779596231
H	-0.8136011146	-1.5984953327	-1.2840195556
H	-3.0770467783	1.2168255981	0.1362557127
H	-0.9168994434	2.4918579955	-0.2143761445
H	-3.0568082927	-1.2595990548	-0.2355794214
N	1.6368003425	-1.1837764444	-0.0143137145
H	2.0084256897	-1.7994701548	0.6949380371
C	2.4800490194	0.0451412390	-0.1547293274
N	1.6270248282	1.2159882685	0.0957281092
H	3.3379295745	0.0404348397	0.5194892801
H	2.8563435676	0.0982530863	-1.1785274638
H	1.6459251718	1.4361907735	1.0871191341

perhydro-1H-indazole

Atom	x (Å)	y (Å)	z (Å)
H	-0.8975354969	-2.5105690787	0.1146330238
C	-0.9019655125	-1.4832329853	-0.2585185881
C	-2.1863076604	0.7440914093	-0.1327295942
C	0.2912873242	0.7236159492	-0.3114833275
C	-0.8954029056	1.4908044773	0.2549617322
C	0.3141898824	-0.7102162602	0.2186453059
C	-2.1616843238	-0.7489783452	0.2413358057
H	-2.3260595636	0.8365828417	-1.2142882860
H	0.1508384017	0.6472072750	-1.3937837766

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-0.8128360668	1.5634038910	1.3445509364
H	0.2820427365	-0.6696666253	1.3245832056
H	-2.2117402428	-0.8436158833	1.3306707294
H	-0.8923652992	-1.5363882141	-1.3502976491
H	-3.0525187153	1.2207508603	0.3310799806
H	-0.9292492922	2.5135749360	-0.1276979771
H	-3.0564771103	-1.2376883327	-0.1490294704
N	1.6405829199	-1.1247408855	-0.2369056362
H	1.9663671179	-1.9908211268	0.1758000095
N	2.5205379858	-0.0562214785	0.2296692924
C	1.7469340775	1.1822888108	-0.0660618328
H	2.1591576529	1.6702526034	-0.9492224268
H	1.8390456931	1.8726389976	0.7737192120
H	2.5568943975	-0.1220998361	1.2485923315

octahydro-1H-pyrrolo[2,3-b]pyridine

Atom	x (Å)	y (Å)	z (Å)
H	-1.0167798184	-2.5087405923	0.2602719608
C	-0.9681109546	-1.5053934002	-0.1684906754
C	-2.1236861049	0.7690973404	-0.2277865988
C	0.2643834097	0.6779829353	-0.2604787441
N	-0.8813837136	1.4125490374	0.2279249326
C	0.2677750540	-0.7475237092	0.2942892150
C	-2.2062719030	-0.6877342127	0.2416274204
H	-2.2081158701	0.7875457219	-1.3270684914
H	0.2618969529	0.6103439479	-1.3657390068
H	0.2110735155	-0.6395344642	1.3834410235
H	-2.2974945445	-0.7011770120	1.3307415190
H	-0.9433337694	-1.6276782308	-1.2566632446
H	-2.9676324757	1.3347048434	0.1688123554
H	-3.1154890200	-1.1379536719	-0.1620931512
C	1.6805372224	-1.2073758792	-0.0768021089
H	1.6981406146	-1.6392733717	-1.0797200349

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	2.0726392013	-1.9596670090	0.6070782047
C	2.5067711963	0.1227896814	-0.0392704095
H	3.0618123807	0.2528479192	-0.9693509320
H	3.2331362683	0.1364667023	0.7720898610
N	1.5502903919	1.2481603212	0.1282774035
H	1.4810537768	1.4837384631	1.1135417060
H	-0.8457058105	2.3689156397	-0.1063002043

perhydroimidazo[1,2-a]pyrazine

Atom	x (Å)	y (Å)	z (Å)
H	-0.7826988146	2.4438241201	-0.3570300426
C	-0.8404044164	1.4748969111	0.1427999066
N	-2.1370778483	-0.5910464831	0.3057005749
C	0.2613167004	-0.6880995537	0.3303971500
C	-0.9977942847	-1.4058821559	-0.1145385285
N	0.2906992397	0.6574993421	-0.2514739824
C	-2.1205708652	0.7528151849	-0.2725399227
H	0.2499689451	-0.6298129321	1.4328379308
H	-0.9483327272	-1.5506359807	-1.2067672793
H	-2.1660648039	0.7405101774	-1.3726711905
H	-0.8566837425	1.6576217382	1.2310141360
H	-1.0620799948	-2.3846757317	0.3609169126
H	-2.9897981545	1.2993610089	0.0958727269
C	1.6310126006	1.1446914838	0.0393642411
H	1.6956472449	1.6018771301	1.0395741477
H	1.9443010289	1.8931573072	-0.6901407133
C	2.4842236508	-0.1562801932	-0.0116221201
H	3.0990138509	-0.2454091012	0.8844183450
H	3.1497588100	-0.1822776152	-0.8726818831
N	1.5214149664	-1.2832564281	-0.0793811153
H	1.4265604274	-1.5569059041	-1.0512325987
H	-3.0074868130	-1.0593513250	0.0949303051

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)

octahydro-1H-purine

Atom	x (Å)	y (Å)	z (Å)
C	-0.2467321443	-0.7075114838	-0.3279445765
C	-2.4533336757	-0.0181550636	0.1147972071
C	-0.2927457499	0.7071445720	0.2509342846
N	-1.5584301973	-1.2152654483	0.0380471908
H	-3.2702792759	-0.0635007117	-0.6068590967
H	-0.2710514509	0.6149058099	1.3441926460
H	-0.1243580231	-0.6128159032	-1.4209632527
H	-2.8874164636	0.0359805552	1.1149874032
N	0.8966457784	-1.4816057255	0.1233824856
C	2.1117752266	-0.7121632812	-0.1894866349
H	2.2388564407	-0.7474915280	-1.2746172036
H	2.9678395264	-1.2131262303	0.2589569646
N	2.1487270325	0.6995252460	0.2082848136
C	0.9533561631	1.4660686117	-0.1781277153
H	0.9616081883	1.5997855672	-1.2653807993
H	1.0067743920	2.4591891605	0.2682121514
N	-1.6283994003	1.1851090014	-0.1123561787
H	-1.8992337488	-1.9008886882	-0.6207863495
H	0.8145162951	-1.6453029554	1.1224736943
H	2.2829307649	0.7703229901	1.2098095816
H	-1.6383796781	1.4148195052	-1.1012666159

perhydropentalene

Atom	x (Å)	y (Å)	z (Å)
H	0.5726933028	2.0624944308	1.7089818716
C	-0.0710799888	1.2543028264	1.3617942812
C	0.3231300865	0.6916401211	0.0000000000
C	-0.3231300865	-0.6916401211	0.0000000000
C	0.0710799888	-1.2543028264	1.3617942812

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	0.0000000000	0.0000000000	2.2955834504
H	-1.0906837897	1.6457826104	1.3251075042
H	1.4107268019	0.5350468372	0.0000000000
H	-1.4107268019	-0.5350468372	0.0000000000
H	1.0906837897	-1.6457826104	1.3251075042
H	-0.5726933028	-2.0624944308	1.7089818716
H	0.8720361109	0.0448127385	2.9480216934
H	-0.8720361109	-0.0448127385	2.9480216934
C	-0.0710799888	1.2543028264	-1.3617942812
H	0.5726933028	2.0624944308	-1.7089818716
H	-1.0906837897	1.6457826104	-1.3251075042
C	0.0000000000	0.0000000000	-2.2955834504
H	-0.8720361109	-0.0448127385	-2.9480216934
H	0.8720361109	0.0448127385	-2.9480216934
C	0.0710799888	-1.2543028264	-1.3617942812
H	1.0906837897	-1.6457826104	-1.3251075042
H	-0.5726933028	-2.0624944308	-1.7089818716

perhydropyrrolizine

Atom	x (Å)	y (Å)	z (Å)
H	0.6064452069	2.0131912739	1.7294088868
C	-0.0655627989	1.2440155843	1.3505287403
C	0.3671942159	0.6844512362	0.0000000000
N	-0.2597394717	-0.6276104882	0.0000000000
C	0.0539120940	-1.2277293649	1.2779177633
C	-0.0882674636	-0.0273521445	2.2552048541
H	-1.0635457349	1.6764391245	1.2715675302
H	1.4726142784	0.5808628562	0.0000000000
H	1.0843950236	-1.6239462994	1.3038049199
H	-0.6219023336	-2.0505954527	1.5140806628
H	0.7237821160	-0.0214457144	2.9813859841
H	-1.0200216209	-0.0864263090	2.8154598007
C	-0.0655627989	1.2440155843	-1.3505287403

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	0.6064452069	2.0131912739	-1.7294088868
H	-1.0635457349	1.6764391245	-1.2715675302
C	-0.0882674636	-0.0273521445	-2.2552048541
H	-1.0200216209	-0.0864263090	-2.8154598007
H	0.7237821160	-0.0214457144	-2.9813859841
C	0.0539120940	-1.2277293649	-1.2779177633
H	1.0843950236	-1.6239462994	-1.3038049199
H	-0.6219023336	-2.0505954527	-1.5140806628

perhydro-1,4-dihydropyrrolo[3,2-b]pyrrole

Atom	x (Å)	y (Å)	z (Å)
N	1.2756439462	-1.2154058855	0.1442525157
C	2.2272519489	-0.0606974520	0.0523285843
C	1.3507692374	1.2287716175	-0.0799234722
C	-0.0157152957	0.6857816071	0.2984993448
C	0.0060184084	-0.6943703457	-0.3342384430
H	2.9041637791	-0.1519743917	-0.8018940690
H	2.8438290575	-0.0274853819	0.9518281525
H	-0.0300551283	0.5347867102	1.3841445722
H	0.0027822812	-0.5507753429	-1.4299616421
C	-1.3614040050	-1.2282545282	0.0707185428
C	-2.2276526286	0.0895851020	0.0377117554
H	-2.8107699966	0.1765590807	0.9549880894
H	-2.9320853185	0.0992973497	-0.7933401906
N	-1.3023409033	1.2629992322	-0.0726244944
H	1.6109899421	-2.0057043892	-0.3885229967
H	-1.2642892838	1.5594831082	-1.0419075170
H	-1.7573500618	-1.9962429829	-0.5930497106
H	-1.3190728910	-1.6402394156	1.0797665579
H	1.7074495477	2.0349671455	0.5585500199
H	1.3496013641	1.5913971626	-1.1105145992

Continued on Next Page...

Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)

perhydro-1,4-dihydroimidazo[4,5-d]imidazole

Atom	x (Å)	y (Å)	z (Å)
N	1.2637701088	-1.1668487473	0.2992298979
C	2.1617507258	-0.0125088036	-0.0116653016
N	1.2786351738	1.1949101772	-0.0961220353
C	-0.0246250223	0.6912548982	0.2714143633
C	0.0124777035	-0.7078629434	-0.2923564548
H	2.6783895431	-0.1434618202	-0.9703135855
H	2.9179705939	0.0941783094	0.7688795161
H	-0.1419634487	0.5961005994	1.3586649051
H	0.1186352042	-0.6356255297	-1.3912127302
N	-1.3037226340	-1.1940889022	0.0724047291
C	-2.1572855143	0.0644584466	0.0794546675
H	-2.5784068814	0.1841756304	1.0775212135
H	-2.9776276965	0.0064766021	-0.6354553118
N	-1.2905362307	1.2325028655	-0.2126673670
H	1.6221099340	-2.0085238375	-0.1344767863
H	-1.2216281001	1.3662839294	-1.2179681740
H	-1.6588263983	-1.8517206126	-0.6069532703
H	1.6002899392	1.9124507384	0.5378967241

perhydro-N-ethylindole

Atom	x (Å)	y (Å)	z (Å)
H	-0.2693751625	-2.4293424419	0.1584552846
C	-0.7666889133	-1.5419334245	-0.2383971415
C	-2.9976529557	-0.2778584372	-0.2463057247
C	-0.8347875116	0.9680568996	-0.2906353903
C	-2.2823179102	1.0146459693	0.1801578521
C	-0.1058646475	-0.2600113462	0.2503871708
C	-2.2436062215	-1.5421207653	0.1940012253
H	-3.0946628462	-0.2818086265	-1.3367006324

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-0.8341175819	0.8698365577	-1.3817662814
H	-2.3140602309	1.1170976653	1.2702233083
H	-0.1806892022	-0.2443846316	1.3574480432
H	-2.2919979339	-1.6245954879	1.2846425987
H	-0.6864532677	-1.5888483203	-1.3283324708
H	-4.0139672738	-0.2970803525	0.1532718412
H	-2.8004184768	1.8844048735	-0.2314382790
H	-2.7451943993	-2.4275452144	-0.2018448565
N	1.2699924728	-0.0097499360	-0.1724741244
C	1.5161363610	1.4246122841	0.0801322688
H	2.1743983185	1.8376528872	-0.6848790050
H	2.0161457819	1.5711444158	1.0496123173
C	0.1225549750	2.1031048703	0.0858138450
H	0.0675177984	2.9457943505	-0.6025574301
H	-0.1118478226	2.4822610872	1.0822854497
C	2.2752342868	-0.8940786363	0.3921118877
H	1.9273099642	-1.9209993005	0.2729249365
H	2.3899071179	-0.7217177014	1.4789148521
C	3.6337010722	-0.7544460707	-0.2874061587
H	4.0572651153	0.2400331537	-0.1438531493
H	3.5425077632	-0.9316529171	-1.3595873207
H	4.3405733303	-1.4763004041	0.1243260836

perhydro-N-ethylindazole

Atom	x (Å)	y (Å)	z (Å)
H	-0.2932168895	-2.4541139294	0.1388959565
C	-0.7847038070	-1.5574776035	-0.2445549079
C	-2.9916202614	-0.2332793381	-0.1480136398
C	-0.8106065244	0.9454757269	-0.3147513807
C	-2.2255197002	1.0458693419	0.2380458312
C	-0.0950270932	-0.2890489541	0.2291352009
C	-2.2473481691	-1.5221760723	0.2416804744
H	-3.1506746424	-0.2272698467	-1.2308995352

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-0.8860910145	0.8050362748	-1.3971580710
H	-2.1974186066	1.1554175223	1.3272120792
H	-0.1413671707	-0.2654320737	1.3378556395
H	-2.2543307500	-1.6214245457	1.3317060751
H	-0.7429344237	-1.6066496059	-1.3360511566
H	-3.9836096555	-0.2331645034	0.3085845624
H	-2.7446199025	1.9234876529	-0.1544495580
H	-2.7869685099	-2.3879616578	-0.1471072267
N	1.2777080090	-0.0182505206	-0.1976978421
N	1.5056839578	1.3545553805	0.2306774808
C	0.2294900753	2.0567452066	-0.0627824352
H	0.3498898222	2.6928250376	-0.9397609003
H	-0.0318393215	2.6954917252	0.7821388072
H	1.5954263811	1.3216723481	1.2526970966
C	2.3039102250	-0.8864443536	0.3474796075
H	1.9966371547	-1.9140159738	0.1487612103
H	2.3595823987	-0.7788382913	1.4485136433
C	3.6734325222	-0.6300380629	-0.2689646400
H	3.9966439111	0.3928602123	-0.0856002714
H	3.6367134091	-0.7839534490	-1.3474768130
H	4.4140785761	-1.3102786473	0.1542617130

octahydro-1Methylpurine

Atom	x (Å)	y (Å)	z (Å)
C	-0.2639090023	-0.6540931032	-0.3640054474
C	-2.4666356388	0.0301516562	-0.0261886824
C	-0.2834284862	0.7179361498	0.3006410846
N	-1.5741290312	-1.1579816783	-0.0211910669
H	-3.1273521686	0.0367050074	-0.9013203519
H	-0.2526673610	0.5594926578	1.3853212417
H	-0.1582366509	-0.5007765221	-1.4573303945
H	-3.0928081665	0.0150724156	0.8688457423
N	0.8676930748	-1.4752321765	0.0272257547

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	2.0921101007	-0.7094424403	-0.2656042633
H	2.1985673785	-0.6849991870	-1.3528347354
H	2.9465395177	-1.2497447683	0.1380144247
N	2.1589959312	0.6743885433	0.2152111316
C	0.9700759126	1.4841813487	-0.0974616623
H	0.9625382752	1.6915916351	-1.1731899432
H	1.0492554097	2.4435338809	0.4141865833
N	-1.6104287512	1.2378601965	-0.0372147972
H	0.8013582237	-1.6738517251	1.0216483993
H	2.3186416260	0.6838224649	1.2153530059
H	-1.5862928573	1.6126053554	-0.9788280580
C	-2.0466240086	-2.2832368254	-0.8023574595
H	-1.3109746789	-3.0850836316	-0.7591404343
H	-2.2167681542	-2.0273175761	-1.8622570156
H	-2.9835714943	-2.6604226777	-0.3905010562

N-ethylperhydropurine

Atom	x (Å)	y (Å)	z (Å)
H	-0.1723337111	-2.3807394498	-0.3327856595
C	-0.7161163535	-1.4541369527	-0.5238626209
C	-2.7943996832	-0.2932421979	0.1001585252
C	-0.8474666091	0.9924251157	-0.2166367296
N	-2.0447241934	0.8612694443	0.6056447026
C	0.0188162075	-0.2362207477	0.0129926653
N	-1.9812757369	-1.5012875289	0.2210150148
H	-3.1113265043	-0.1255316115	-0.9515702992
H	-1.1258024598	1.0121449877	-1.2867921436
H	0.1121300585	-0.3644679050	1.1006925688
H	-0.8432952461	-1.3541984091	-1.6130805790
H	-3.6915072069	-0.4228721522	0.7051541582
N	1.2623227473	0.1990791130	-0.6032111212
C	1.4279646465	1.5573566411	-0.0643748332
H	2.0298631930	2.1684609856	-0.7417102461

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	1.9239667148	1.5538445338	0.9165029800
N	0.0580523660	2.0945589347	0.0902848289
H	-0.0868742434	2.8620014526	-0.5492963211
H	-2.5269432760	-2.3092364539	-0.0452015802
H	-2.6200557000	1.6930911283	0.5408684246
C	2.4243052103	-0.6773307860	-0.5090346679
H	3.2466047398	-0.1779005989	-1.0281199364
H	2.2044773248	-1.5749396887	-1.0918753314
C	2.8917963096	-1.0974777345	0.8927745363
H	3.7658574502	-1.7452028917	0.8064534920
H	2.1214946778	-1.6536448865	1.4276999824
H	3.1756952775	-0.2434763414	1.5073271901

perhydrofluorene

Atom	x (Å)	y (Å)	z (Å)
H	-1.3882967323	0.0877092503	2.5378638137
C	-1.6902188525	-0.2744143853	1.5519293923
C	-3.5779495847	-0.1762666149	-0.1815902196
C	-1.1918181852	-0.2935312003	-0.9190002437
C	-2.5758019911	0.2374783523	-1.2727048030
C	-0.7359746746	0.2069810470	0.4656651398
C	-3.1162081890	0.2096359371	1.2324859455
H	-3.7136696977	-1.2619327425	-0.2274270642
H	-1.2821244327	-1.3833213420	-0.8326425790
H	-2.5405324562	1.3294092037	-1.3541506095
H	-0.7682912794	1.3058819601	0.4584642434
H	-3.1440981525	1.2998691701	1.3316357132
H	-1.6711640073	-1.3690477942	1.5982847123
H	-4.5576793979	0.2638099646	-0.3809601369
H	-2.9071281092	-0.1383904339	-2.2444539967
H	-3.8212431933	-0.1827042898	1.9689040448
C	0.7359746746	-0.2069810470	0.4656651398
C	2.5758019911	-0.2374783523	-1.2727048030

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	3.1162081890	-0.2096359371	1.2324859455
C	3.5779495847	0.1762666149	-0.1815902196
C	1.6902188525	0.2744143853	1.5519293923
C	1.1918181852	0.2935312003	-0.9190002437
H	2.5405324562	-1.3294092037	-1.3541506095
H	3.1440981525	-1.2998691701	1.3316357132
H	3.7136696977	1.2619327425	-0.2274270642
H	1.6711640073	1.3690477942	1.5982847123
H	1.2821244327	1.3833213420	-0.8326425790
H	0.7682912794	-1.3058819601	0.4584642434
H	2.9071281092	0.1383904339	-2.2444539967
H	3.8212431933	0.1827042898	1.9689040448
H	4.5576793979	-0.2638099646	-0.3809601369
H	1.3882967323	-0.0877092503	2.5378638137
C	0.0000000000	0.0000000000	-1.8647573368
H	-0.2026360626	0.8523361084	-2.5165486841
H	0.2026360626	-0.8523361084	-2.5165486841

perhydro-9-ethylfluorene

Atom	x (Å)	y (Å)	z (Å)
H	-1.8690857033	-2.8098025308	-0.1821944004
C	-2.0260057333	-1.7536301905	-0.4151606839
C	-3.6609535666	0.1956321905	-0.1140968946
C	-1.1909699057	0.6023643629	-0.1014288245
C	-2.5316217511	1.0736880342	0.4509571057
C	-0.9449119792	-0.8806608133	0.2111059745
C	-3.4073235129	-1.3060876323	0.0923810311
H	-3.7561653267	0.3958156476	-1.1864031519
H	-1.2516633825	0.6761393360	-1.1961963931
H	-2.5198239604	1.0076632336	1.5444062036
H	-0.9961591922	-1.0156949200	1.3010198112
H	-3.4782290681	-1.5362486058	1.1606685339
H	-1.9836826445	-1.6619244968	-1.5063597588

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-4.6168645572	0.4729466971	0.3360699265
H	-2.7173313439	2.1223417831	0.2028752470
H	-4.1948324782	-1.8828941329	-0.3979949784
C	0.5155438234	-1.0341446947	-0.2042308765
C	2.6029614336	0.3785321081	-0.0197454895
C	2.7433619507	-2.1682503835	-0.3029549441
C	3.4058891959	-0.9043402807	0.2613738837
C	1.2786197469	-2.3081101836	0.1385558843
C	1.1628430151	0.1999196917	0.4599485793
H	2.6224018539	0.5973575737	-1.0917491114
H	2.7787871279	-2.1342382046	-1.3969654665
H	3.5145823061	-1.0150729825	1.3454935566
H	1.2321469884	-2.4824526352	1.2194859579
H	1.2253430661	-0.0364879354	1.5289625666
H	0.5647991502	-0.9015176875	-1.2945240208
H	3.0896523037	1.2172198481	0.4809363964
H	3.3156452608	-3.0497165344	-0.0046837227
H	4.4173818242	-0.8060372156	-0.1395521961
H	0.8258849990	-3.1803304010	-0.3398812462
C	0.0994815459	1.3497779864	0.3283260667
C	0.4213176003	2.5124936200	-0.6248576078
H	0.8478994819	2.1221681597	-1.5534024778
H	-0.5245445914	2.9815979950	-0.9124441737
C	1.3309376712	3.5980803252	-0.0478174607
H	1.4850607244	4.4034397260	-0.7681970456
H	2.3117434091	3.2126529706	0.2274702573
H	0.8875653729	4.0379611953	0.8482751134
H	-0.0596251545	1.7815709762	1.3215208293

perhydro-9H-carbazole

Atom	x (Å)	y (Å)	z (Å)
H	-1.4467566739	-2.5482999030	0.0348839776
C	-1.7194701128	-1.5481532903	-0.3107508923

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-3.5488160056	0.2465824161	-0.1686197350
C	-1.1498982738	0.9000642107	-0.2847983177
C	-2.5108346783	1.2934723482	0.2726249932
C	-0.7383657759	-0.5006937295	0.1996133493
C	-3.1363181515	-1.1932056590	0.1781627201
H	-3.6876229276	0.3247551452	-1.2520575224
H	-1.2551736769	0.8398653085	-1.3792757640
H	-2.4512971636	1.3465072521	1.3633486705
H	-0.7882058881	-0.5018654439	1.2966486822
H	-3.1701129339	-1.3216348320	1.2648903500
H	-1.6969537315	-1.5753213836	-1.4056290000
H	-4.5197188239	0.4679077867	0.2795442482
H	-2.8051052063	2.2862114205	-0.0765525319
H	-3.8641369834	-1.8943297296	-0.2363610486
C	0.7363595657	-0.5069017076	-0.1965093371
C	2.5010480291	1.2941244195	-0.2458104011
C	3.1280373050	-1.1989415044	-0.2008365445
C	3.5444268199	0.2370799016	0.1613572603
C	1.7150117034	-1.5652881200	0.2934719817
C	1.1522381726	0.8801922258	0.3171278281
H	2.4404761115	1.3664306486	-1.3374793914
H	3.1540092502	-1.3136391211	-1.2894079186
H	3.6984746125	0.3011900529	1.2428580950
H	1.6997966094	-1.6063025816	1.3879066799
H	1.2770135527	0.7949101889	1.4057566406
H	0.7844156871	-0.4880961394	-1.2943769745
H	2.7996837675	2.2775097794	0.1261723350
H	3.8619385275	-1.9022922902	0.1986162842
H	4.5078355657	0.4657160184	-0.2989594233
H	1.4430348092	-2.5614892538	-0.0634441588
N	-0.0058217758	1.7673446019	0.0706782283
H	0.1933716939	2.4272479641	-0.6689343636

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)

perhydro-N-ethylcarbazole

Atom	x (Å)	y (Å)	z (Å)
H	-1.7430180821	-2.9029095523	0.0860098770
C	-1.9279264785	-1.8881329315	-0.2744040110
C	-3.6016275647	0.0502949458	-0.1905138798
C	-1.1509169770	0.5048958967	-0.2497729829
C	-2.4912546938	1.0086016875	0.2751040036
C	-0.8762825653	-0.9190691332	0.2489583024
C	-3.3208709119	-1.4164306229	0.1764124147
H	-3.7050352895	0.1319239587	-1.2774750296
H	-1.2346201951	0.4554761736	-1.3524375917
H	-2.4516358414	1.0532342493	1.3671840843
H	-0.9398270631	-0.9054804243	1.3448794484
H	-3.3933987771	-1.5316872253	1.2626632713
H	-1.8824584287	-1.9283554148	-1.3680391248
H	-4.5610672094	0.3573686229	0.2308523851
H	-2.7030144603	2.0208802926	-0.0773884703
H	-4.0941242149	-2.0575883550	-0.2526320356
C	0.5885214438	-1.0644952370	-0.1400741953
C	2.5150194855	0.5168763295	-0.3456845961
C	2.8779242213	-2.0298573844	-0.1866519300
C	3.4526475027	-0.6286737403	0.0837153753
C	1.4527376066	-2.2109170630	0.3640274528
C	1.1593425032	0.2875401861	0.3220966814
H	2.4110621048	0.5259923840	-1.4343755342
H	2.8563382831	-2.2031832663	-1.2673509050
H	3.6532194107	-0.5268837205	1.1549802496
H	1.4689491970	-2.2112161477	1.4588855920
H	1.3638062412	0.2105626875	1.3999561227
H	0.6287646484	-1.0803582076	-1.2380713915
H	2.9567784261	1.4727537234	-0.0587049172
H	3.5467200958	-2.7852485064	0.2317056769

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	4.4167542064	-0.5255949867	-0.4185902271
H	1.0525494403	-3.1788026956	0.0528235750
N	0.0448887940	1.2545124678	0.1434832350
C	0.2838963064	2.5176369342	-0.5347738652
H	0.9396083233	2.4033024631	-1.4100719901
H	-0.6742941334	2.8658683166	-0.9246214858
C	0.8498755194	3.5970927636	0.3879795261
H	1.0043618471	4.5311615873	-0.1568276853
H	1.8082373418	3.2977916790	0.8134326380
H	0.1648029375	3.7846912657	1.2151569370

perhydro-1,8-diazacarbazole

Atom	x (Å)	y (Å)	z (Å)
H	-1.5218801736	-2.5635808704	0.0531227605
C	-1.7536425518	-1.5567350200	-0.3012994634
C	-3.4565318920	0.3482713883	-0.1019648100
C	-1.1447655917	0.8622945334	-0.3056889608
N	-2.3839118061	1.2392475326	0.3600754942
C	-0.7303926922	-0.5375856706	0.1796814585
C	-3.1371128735	-1.1190795947	0.2199372124
H	-3.6213486320	0.4377534216	-1.1900341958
H	-1.3147501311	0.8003008483	-1.3977202873
H	-0.7773753589	-0.5119201771	1.2737219371
H	-3.1616790274	-1.2504701778	1.3045399255
H	-1.7577865513	-1.5970744524	-1.3955840711
H	-4.3860809044	0.6386006633	0.3889657841
H	-3.9215709472	-1.7534109423	-0.1981787155
C	0.7379702321	-0.5452841414	-0.2307144560
N	2.4101278879	1.2523232475	-0.2565842690
C	3.1361449302	-1.1304947463	-0.2158795481
C	3.4553416275	0.3138362269	0.1910794870
C	1.7403268967	-1.5809515786	0.2542399087
C	1.1310845576	0.8425847040	0.2920783627

Continued on Next Page...

Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	3.1857641587	-1.2086756753	-1.3050327725
H	3.5808738297	0.3472462363	1.2855445275
H	1.7144470824	-1.6457079399	1.3471208687
H	1.1856815130	0.7793220277	1.3932401421
H	0.7976391111	-0.5003640279	-1.3247677643
H	3.9095855847	-1.7871178302	0.1877252246
H	4.4031143023	0.6221758671	-0.2516578913
H	1.5164377944	-2.5787880091	-0.1288250653
N	0.0105437497	1.7392659451	-0.0488987519
H	2.6412483730	2.1825789014	0.0762524427
H	-2.6134354983	2.2051979010	0.1586409391
H	0.2567550007	2.2348644097	-0.8972404528

perhydro-N-methyl-1,8-diazacarbazole

Atom	x (Å)	y (Å)	z (Å)
H	-1.5595591693	-2.7656484751	-0.1448494101
C	-1.7745376215	-1.7270714658	-0.4057729593
C	-3.4701187479	0.1599314707	-0.0953865430
C	-1.1436449585	0.6723020395	-0.1283380864
N	-2.4172321391	0.9874257251	0.5089124897
C	-0.7581421918	-0.7733259833	0.2072719870
C	-3.1750891547	-1.3328016342	0.1007533255
H	-3.5767911812	0.3559231515	-1.1762708758
H	-1.2565111442	0.7397720999	-1.2336066896
H	-0.8150389737	-0.8700275048	1.2966811312
H	-3.2454980926	-1.5646991867	1.1663834077
H	-1.7380676799	-1.6593156661	-1.4980185131
H	-4.4214234004	0.4137089006	0.3737219211
H	-3.9439342120	-1.9186516843	-0.4074403405
C	0.7065502628	-0.7534282916	-0.2066114706
N	2.4151841406	0.9903319871	-0.1127657478
C	3.0852524327	-1.4011346936	-0.3134952425
C	3.4449444744	-0.0100672397	0.2212562775

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	1.6895750213	-1.8583804978	0.1459312946
C	1.1413640545	0.5638673613	0.4499735487
H	3.1088049847	-1.3751140289	-1.4058861381
H	3.5916929217	-0.0846087224	1.3115002764
H	1.6876880786	-2.0332624645	1.2267073799
H	1.2583457605	0.3751737827	1.5334481566
H	0.7546311089	-0.5962143378	-1.2904960121
H	3.8505631495	-2.1106423065	0.0076833480
H	4.3906602492	0.3203819048	-0.2098579079
H	1.4252604100	-2.8047785964	-0.3305712067
N	-0.0067151861	1.4872932663	0.2865934842
C	0.1899202740	2.6879019173	-0.5052419640
H	0.4475986657	2.4938028844	-1.5561473288
H	-0.7265759348	3.2798397131	-0.4838320939
H	0.9720631376	3.3128027852	-0.0738658854
H	2.6936062127	1.8796987094	0.2859948770
H	-2.6407435519	1.9691350807	0.3965935105

perhydro-N-ethyl-1,8-diazacarbazole

Atom	x (Å)	y (Å)	z (Å)
H	-1.7064971685	-2.9045617345	-0.3936100367
C	-1.8679716941	-1.8371636438	-0.5590027037
C	-3.4833759834	0.0898347722	-0.1097164231
C	-1.1359616988	0.4956296421	-0.0322589934
N	-2.4155019794	0.8081484971	0.6014239208
C	-0.8303951743	-0.9945098767	0.1686282337
C	-3.2628442989	-1.4269268249	-0.0501935070
H	-3.5459163999	0.3925854599	-1.1690678498
H	-1.2196718920	0.6794052748	-1.1251681600
H	-0.9259955379	-1.1855679103	1.2426258417
H	-3.3732282008	-1.7542624565	0.9866184798
H	-1.7978382694	-1.6676809799	-1.6384117775
H	-4.4370859121	0.3439204595	0.3543665539

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-4.0434759162	-1.9241050062	-0.6298637663
C	0.6445175420	-1.0083868202	-0.2053827209
N	2.4255154520	0.6376132366	0.0084868733
C	2.9871627560	-1.7603675605	-0.3789568297
C	3.4130165515	-0.4299066628	0.2546029360
C	1.5700962081	-2.1882568965	0.0459976813
C	1.1414521553	0.2175998798	0.5728006790
H	3.0132409798	-1.6558776844	-1.4665566333
H	3.5643116764	-0.5922727926	1.3345058534
H	1.5585120068	-2.4587296466	1.1066308217
H	1.3009857745	-0.0819722216	1.6278820608
H	0.7234170615	-0.7469421577	-1.2668719334
H	3.7185383419	-2.5263098263	-0.1128960255
H	4.3693469408	-0.1106613994	-0.1610533655
H	1.2606457698	-3.0737042909	-0.5132463453
N	0.0232117069	1.1651309292	0.5224748197
C	0.2249779967	2.5807772698	0.2920502696
H	-0.6378587786	3.1180321764	0.6991042982
H	1.0684600434	2.9054416369	0.9071315239
H	2.7502305852	1.4806054137	0.4686746443
H	-2.5979796611	1.8041604861	0.5626647138
C	0.4540028601	3.0268158751	-1.1604889893
H	1.3279739931	2.5338497972	-1.5829842555
H	0.6061644321	4.1078610237	-1.2013521044
H	-0.4057612684	2.7943275623	-1.7905917845

perhydrodibenzoborole

Atom	x (Å)	y (Å)	z (Å)
H	-1.3361796412	0.0601550030	2.4703716072
C	-1.6656814442	-0.2744047153	1.4832045929
C	-3.6102457572	-0.1686335300	-0.1767322950
C	-1.2396584615	-0.1742418873	-1.0202943329
C	-2.6652660423	0.2992289317	-1.2946649047

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-0.7312661723	0.2299872866	0.3872684912
C	-3.1016838524	0.2090702712	1.2217743968
H	-3.7117609167	-1.2577627356	-0.2362277976
H	-1.2635611719	-1.2883851080	-1.0099176540
H	-2.6799355837	1.3929691950	-1.3479307032
H	-0.7304830257	1.3289383809	0.4312830677
H	-3.1316130514	1.2985687163	1.3308785957
H	-1.6447076440	-1.3702027169	1.4990620575
H	-4.6108197772	0.2431747268	-0.3290140145
H	-3.0185081100	-0.0613772267	-2.2634167372
H	-3.7765171600	-0.1927295786	1.9810629270
C	0.7312661723	-0.2299872866	0.3872684912
C	2.6652660423	-0.2992289317	-1.2946649047
C	3.1016838524	-0.2090702712	1.2217743968
C	3.6102457572	0.1686335300	-0.1767322950
C	1.6656814442	0.2744047153	1.4832045929
C	1.2396584615	0.1742418873	-1.0202943329
H	2.6799355837	-1.3929691950	-1.3479307032
H	3.1316130514	-1.2985687163	1.3308785957
H	3.7117609167	1.2577627356	-0.2362277976
H	1.6447076440	1.3702027169	1.4990620575
H	1.2635611719	1.2883851080	-1.0099176540
H	0.7304830257	-1.3289383809	0.4312830677
H	3.0185081100	0.0613772267	-2.2634167372
H	3.7765171600	0.1927295786	1.9810629270
H	4.6108197772	-0.2431747268	-0.3290140145
H	1.3361796412	-0.0601550030	2.4703716072
B	0.0000000000	0.0000000000	-1.9585902867
H	0.0000000000	0.0000000000	-3.1521403069

perhydro-5Me-dibenzoborole

Atom	x (Å)	y (Å)	z (Å)
H	-1.3303513766	-2.7569108491	0.0803187104

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-1.6599703472	-1.7745739060	-0.2684269271
C	-3.6068187743	-0.1158037404	-0.1887714873
C	-1.2352654303	0.7290431158	-0.2053196845
C	-2.6616584464	1.0081082313	0.2653090247
C	-0.7304170765	-0.6697476736	0.2254216389
C	-3.0981189838	-1.5096266857	0.2061118291
H	-3.7070020475	-0.0695305689	-1.2786295751
H	-1.2634512291	0.6963555398	-1.3167288405
H	-2.6775712574	1.0752288767	1.3586288853
H	-0.7371866876	-0.6982703030	1.3251465773
H	-3.1321917547	-1.6066637042	1.2967013010
H	-1.6342279565	-1.8046885242	-1.3638927836
H	-4.6079688924	0.0411632471	0.2203333082
H	-3.0199949211	1.9710413806	-0.1071886257
H	-3.7710883776	-2.2738256666	-0.1897074604
C	0.7341504064	-0.6740723800	-0.2243140579
C	2.6672597439	0.9990429666	-0.2990111331
C	3.0995812709	-1.5187177851	-0.1999860636
C	3.6126263589	-0.1192543618	0.1685183587
C	1.6629329736	-1.7723767191	0.2849485254
C	1.2426796857	0.7310108799	0.1838125406
H	2.6781045264	1.0489297307	-1.3933360467
H	3.1287478496	-1.6347213614	-1.2888498959
H	3.7187302764	-0.0549337221	1.2569230373
H	1.6414617279	-1.7838468000	1.3808530201
H	1.2766977446	0.7130066558	1.2945918780
H	0.7398612794	-0.7197061087	-1.3234552957
H	3.0297232097	1.9666724635	0.0567637397
H	3.7727578735	-2.2772690906	0.2062188843
H	4.6119024757	0.0289540346	-0.2483621698
H	1.3297740185	-2.7597216848	-0.0458587565
B	0.0036527667	1.6860756335	-0.0213525074
C	-0.0091627472	3.2516685535	-0.0004728531

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	0.9195261413	3.7135410940	-0.3403751857
H	-0.1431918068	3.5654285223	1.0438332860
H	-0.8445302159	3.6900167098	-0.5503961955

perhydro[b,d]dibenzofuran

Atom	x (Å)	y (Å)	z (Å)
H	-1.4918670784	0.0160089986	2.5645199496
C	-1.7386453377	-0.3228202697	1.5557820812
C	-3.5177591159	-0.1516417954	-0.2947809879
C	-1.1230274097	-0.2916626246	-0.8673348552
C	-2.4486693720	0.2900337171	-1.3138582651
C	-0.7370372658	0.1962047683	0.5328323814
C	-3.1435766151	0.1740142078	1.1624761464
H	-3.6654643880	-1.2319597767	-0.3909123308
H	-1.2360906970	-1.3855591967	-0.8281069858
H	-2.3776549958	1.3804395965	-1.3539162138
H	-0.7921821445	1.2927034535	0.5343546830
H	-3.1792963309	1.2587187444	1.3051178903
H	-1.7185045931	-1.4174689833	1.5753635615
H	-4.4766557810	0.3098388386	-0.5376705710
H	-2.7117392613	-0.0555063999	-2.3153445024
H	-3.8936841832	-0.2483641048	1.8344704960
C	0.7370372658	-0.1962047683	0.5328323814
C	2.4486693720	-0.2900337171	-1.3138582651
C	3.1435766151	-0.1740142078	1.1624761464
C	3.5177591159	0.1516417954	-0.2947809879
C	1.7386453377	0.3228202697	1.5557820812
C	1.1230274097	0.2916626246	-0.8673348552
H	2.3776549958	-1.3804395965	-1.3539162138
H	3.1792963309	-1.2587187444	1.3051178903
H	3.6654643880	1.2319597767	-0.3909123308
H	1.7185045931	1.4174689833	1.5753635615
H	1.2360906970	1.3855591967	-0.8281069858

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	0.7921821445	-1.2927034535	0.5343546830
H	2.7117392613	0.0555063999	-2.3153445024
H	3.8936841832	0.2483641048	1.8344704960
H	4.4766557810	-0.3098388386	-0.5376705710
H	1.4918670784	-0.0160089986	2.5645199496
O	0.0000000000	0.0000000000	-1.7149889547

perhydrodibenzothiophene

Atom	x (Å)	y (Å)	z (Å)
H	-1.2566224215	0.1433242108	2.6437577195
C	-1.6297596653	-0.2454073214	1.6935010173
C	-3.6225809227	-0.1773616670	0.0893377605
C	-1.2978349384	-0.3389631486	-0.7829321711
C	-2.6879490264	0.2112456924	-1.0699549119
C	-0.7361517552	0.2032682793	0.5372216814
C	-3.0698762311	0.2403550873	1.4595784830
H	-3.7675831900	-1.2622444894	0.0767512856
H	-1.3731206226	-1.4264106013	-0.7005937701
H	-2.6364121598	1.2985510096	-1.1718464412
H	-0.7771677709	1.2992681257	0.4918837597
H	-3.0861946413	1.3324738446	1.5334720455
H	-1.6114100169	-1.3377951160	1.7709047634
H	-4.6084562688	0.2664509823	-0.0639042208
H	-3.0780693473	-0.1783386619	-2.0121197026
H	-3.7245210580	-0.1307705320	2.2509806169
C	0.7361517552	-0.2032682793	0.5372216814
C	2.6879490264	-0.2112456924	-1.0699549119
C	3.0698762311	-0.2403550873	1.4595784830
C	3.6225809227	0.1773616670	0.0893377605
C	1.6297596653	0.2454073214	1.6935010173
C	1.2978349384	0.3389631486	-0.7829321711
H	2.6364121598	-1.2985510096	-1.1718464412
H	3.0861946413	-1.3324738446	1.5334720455

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	3.7675831900	1.2622444894	0.0767512856
H	1.6114100169	1.3377951160	1.7709047634
H	1.3731206226	1.4264106013	-0.7005937701
H	0.7771677709	-1.2992681257	0.4918837597
H	3.0780693473	0.1783386619	-2.0121197026
H	3.7245210580	0.1307705320	2.2509806169
H	4.6084562688	-0.2664509823	-0.0639042208
H	1.2566224215	-0.1433242108	2.6437577195
S	0.0000000000	0.0000000000	-2.0623008302

perhydro-3,6-diazacarbazole

Atom	x (Å)	y (Å)	z (Å)
H	-1.5022416312	-2.5211367908	0.0875725522
C	-1.7415448124	-1.5202767815	-0.2771100270
C	-3.5099204530	0.1920861157	-0.1456044494
C	-1.1492930383	0.9040369579	-0.2778733552
C	-2.5129577746	1.2776639102	0.2841377335
C	-0.7317866449	-0.4933985733	0.2127076754
N	-3.0504433020	-1.1371279211	0.2647245867
H	-3.6516496581	0.2656825642	-1.2378896711
H	-1.2628375908	0.8348398901	-1.3706882834
H	-0.7766585108	-0.4986221169	1.3069327005
H	-1.7242616268	-1.5575747800	-1.3800864026
H	-4.4827611013	0.3694458102	0.3149765252
C	0.7300190933	-0.5001931078	-0.2186249769
C	2.5091906836	1.2766268796	-0.2462848592
N	3.0442061519	-1.1408514335	-0.2805350366
C	3.5047175953	0.1787716366	0.1590064614
C	1.7347863112	-1.5384901151	0.2541369581
C	1.1493332835	0.8839541852	0.3025315562
H	3.6451224758	0.2313725173	1.2517636560
H	1.7180734013	-1.5941645960	1.3559322060
H	1.2652295883	0.7920866686	1.3913629950

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	0.7751257116	-0.4854323611	-1.3135118450
H	4.4771112862	0.3657712415	-0.2985930434
H	1.4996542749	-2.5336531374	-0.1278792648
N	-0.0031627643	1.7781224986	0.0563130433
H	-2.8450632961	2.2493042324	-0.0889169384
H	-2.4619990804	1.3388516905	1.3729029349
H	2.8410363638	2.2376177436	0.1540773286
H	2.4711838600	1.3586229452	-1.3362854236
H	3.7419971116	-1.8401326846	-0.0654428656
H	-3.7467096976	-1.8329196129	0.0338591356
H	0.1930347899	2.4173885246	-0.7023296065

perhydro-4,5-diazacarbazole

Atom	x (Å)	y (Å)	z (Å)
N	1.6277119589	-1.5361686030	0.2324156159
C	3.5051662787	0.1826656231	0.1753758121
C	1.1425360318	0.9210024729	0.2903382972
C	2.5169790644	1.2841278578	-0.2528540045
C	0.7337136392	-0.4816008998	-0.2082483175
C	3.0051578018	-1.2306003899	-0.1827457592
H	3.6568840242	0.2421431472	1.2582197238
H	1.2348313302	0.8464992453	1.3852957695
H	0.7801633445	-0.4751971146	-1.3053408855
H	4.4829638669	0.3476221783	-0.2840626941
C	-0.7320274075	-0.4863728158	0.1987389925
C	-2.5061245962	1.2825837897	0.2327236524
C	-2.9966773906	-1.2386250556	0.2019504654
C	-3.5011871574	0.1734078811	-0.1627059594
N	-1.6227548559	-1.5530747954	-0.2185080801
C	-1.1473630532	0.9008648886	-0.3270415855
H	-3.6716748508	0.2239267217	-1.2423608975
H	-1.2689350538	0.8007857494	-1.4153821467
H	-0.7755001126	-0.4600779427	1.2966372214

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-4.4695702785	0.3438233001	0.3140686153
N	0.0068919574	1.7904236080	-0.0801655918
H	-2.8432193124	2.2495055382	-0.1488915996
H	-2.4473540802	1.3679543404	1.3236709478
H	3.6673659067	-1.9838332684	0.2464222356
H	3.0493141150	-1.3586557840	-1.2692719215
H	-1.5792622987	-1.6753155831	-1.2245968184
H	1.5782607647	-1.6403349005	1.2402614521
H	-3.6653079695	-1.9921120735	-0.2163243247
H	-3.0345380034	-1.3579395157	1.2898363786
H	2.8481122195	2.2585016598	0.1142627385
H	2.4648421216	1.3566509394	-1.3429470034
H	-0.1916340046	2.4704668012	0.6408306711

pyrimidine

Atom	x (Å)	y (Å)	z (Å)
H	-2.1454664073	0.0000000000	-1.1148667707
C	-1.1802887238	0.0000000000	-0.6205300403
N	1.1922501213	0.0000000000	0.7126859807
N	-1.1922501213	0.0000000000	0.7126859807
C	0.0000000000	0.0000000000	-1.3492461795
C	1.1802887238	0.0000000000	-0.6205300403
C	0.0000000000	0.0000000000	1.3069149793
H	0.0000000000	0.0000000000	-2.4298204865
H	2.1454664073	0.0000000000	-1.1148667707
H	0.0000000000	0.0000000000	2.3909583473

pyridazine

Atom	x (Å)	y (Å)	z (Å)
N	0.6644048378	0.0000000000	1.2216081575
C	-0.6888506265	0.0000000000	-1.1782054603
C	1.3187268964	0.0000000000	0.0634272412

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
N	-0.6644048378	0.0000000000	1.2216081575
C	-1.3187268964	0.0000000000	0.0634272412
C	0.6888506265	0.0000000000	-1.1782054603
H	2.3984050729	0.0000000000	0.1469585800
H	-2.3984050729	0.0000000000	0.1469585800
H	1.2655869501	0.0000000000	-2.0929065183
H	-1.2655869501	0.0000000000	-2.0929065183

1,3,5-triazine

Atom	x (Å)	y (Å)	z (Å)
N	-1.3685449311	0.0000001370	0.0000000000
C	1.2904826641	-0.0000001292	0.0000000000
C	-0.6452416940	-1.1175908500	0.0000000000
C	-0.6452414702	1.1175909792	0.0000000000
N	0.6842723342	1.1851944637	0.0000000000
N	0.6842720969	-1.1851946007	0.0000000000
H	-1.1872440190	2.0563671487	0.0000000000
H	2.3744879498	-0.0000002377	0.0000000000
H	-1.1872444308	-2.0563669110	0.0000000000

1H-pyrrole

Atom	x (Å)	y (Å)	z (Å)
C	0.0132883425	-0.9915809482	-0.7104772925
C	0.0681608957	0.3175787023	-1.1216279882
N	0.1011499627	1.1049863059	0.0000000000
C	0.0681608957	0.3175787023	1.1216279882
C	0.0132883425	-0.9915809482	0.7104772925
H	-0.0227713694	-1.8524247157	-1.3558469069
H	0.0861149436	0.7485018162	-2.1069480507
H	0.0861149436	0.7485018162	2.1069480507
H	-0.0227713694	-1.8524247157	1.3558469069
H	0.1434484118	2.1072869851	0.0000000000

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)

1H-imidazole

Atom	x (Å)	y (Å)	z (Å)
C	1.1319211674	-0.2999923147	-0.0033713092
C	0.6344726584	0.9714943427	0.0545130224
N	-0.7330505023	0.8212319463	0.0819688363
C	-0.9928292443	-0.5157939962	0.0402985349
N	0.1104080202	-1.2196917943	-0.0117054069
H	2.1633405243	-0.6059321023	-0.0392453587
H	1.1063622485	1.9367270773	0.0779893331
H	-1.9954460669	-0.9094300361	0.0504001026
H	-1.4114178053	1.5609938773	0.1245162456

1H-pyrazole

Atom	x (Å)	y (Å)	z (Å)
N	0.9720421886	-0.4423875768	-0.0915163176
N	0.7804929765	0.8884959646	-0.0745307601
C	-0.5383190225	1.0288593543	-0.0219190884
C	-1.1979732517	-0.2167042701	-0.0051607622
C	-0.1839176765	-1.1457720806	-0.0517021535
H	-0.9687627174	2.0162242877	0.0020808145
H	-2.2549767242	-0.4089187334	0.0349371649
H	-0.1962549872	-2.2216073327	-0.0591956138
H	1.9094362145	-0.8002136130	-0.1308272837

1H-1,2,3-triazole

Atom	x (Å)	y (Å)	z (Å)
N	-0.4661458256	-0.9483510151	-0.1065185320
N	-1.1411470969	0.2148995632	-0.0720027228
N	-0.2593201369	1.1637087203	-0.0053834337
C	0.9879382682	0.6174671912	0.0044817961
C	0.8695686305	-0.7458984118	-0.0610706270

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	1.8724168604	1.2261303804	0.0564384182
H	1.5861532741	-1.5460799879	-0.0778309294
H	-0.9754379737	-1.8141974403	-0.1601199694

1H-1,2,4-triazole

Atom	x (Å)	y (Å)	z (Å)
N	0.8261624896	0.6775149833	-0.0732536584
N	-0.4628462888	1.0865255047	-0.0623883989
C	-1.1132641224	-0.0596570680	-0.0029016971
N	-0.3255433551	-1.1692209397	0.0239405919
C	0.8895846363	-0.6661045734	-0.0216427401
H	-2.1890167491	-0.0988334622	0.0214004457
H	1.8145411911	-1.2178645847	-0.0195547808
H	1.5691451983	1.3532561400	-0.1152787623

naphthalene

Atom	x (Å)	y (Å)	z (Å)
H	3.3645215766	-1.2402275820	0.0000000000
C	2.4238428070	-0.7058025573	0.0000000000
H	1.2392614266	-2.4798275384	0.0000000000
C	1.2406174149	-1.3969645822	0.0000000000
C	1.2406174149	1.3969645822	0.0000000000
C	0.0000000000	-0.7139541915	0.0000000000
C	2.4238428070	0.7058025573	0.0000000000
C	0.0000000000	0.7139541915	0.0000000000
C	-1.2406174149	-1.3969645822	0.0000000000
H	3.3645215766	1.2402275820	0.0000000000
H	-1.2392614266	2.4798275384	0.0000000000
H	1.2392614266	2.4798275384	0.0000000000
C	-2.4238428070	-0.7058025573	0.0000000000
H	-1.2392614266	-2.4798275384	0.0000000000
H	-3.3645215766	-1.2402275820	0.0000000000

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-2.4238428070	0.7058025573	0.0000000000
H	-3.3645215766	1.2402275820	0.0000000000
C	-1.2406174149	1.3969645822	0.0000000000

isoquinoline

Atom	x (Å)	y (Å)	z (Å)
H	3.3876425423	-1.0801058078	0.0000000000
C	2.4121289659	-0.6093096780	0.0000000000
H	1.3315996086	-2.4473962005	0.0000000000
C	1.2716538431	-1.3667605000	0.0000000000
C	1.2572813257	1.3586618004	0.0000000000
C	0.0110103063	-0.7267898023	0.0000000000
N	2.4172155366	0.7488879542	0.0000000000
C	0.0043139980	0.6954655646	0.0000000000
C	-1.2252796880	-1.4154964161	0.0000000000
H	-1.2232458667	2.4705572066	0.0000000000
C	-2.4055964573	-0.7182729520	0.0000000000
H	-1.2255805462	-2.4979384934	0.0000000000
H	-3.3470671454	-1.2514424459	0.0000000000
C	-2.4101528771	0.6943355266	0.0000000000
H	-3.3529339432	1.2244455172	0.0000000000
C	-1.2281926598	1.3878279578	0.0000000000
H	1.2745100570	2.4452887685	0.0000000000

4H-quinolizine

Atom	x (Å)	y (Å)	z (Å)
C	-0.0176704482	-0.7447053420	0.0000000000
C	-2.4683030064	-0.7111287829	0.0000000000
N	-0.0703971522	0.6765097068	0.0000000000
C	-1.3100597806	-1.4009003457	0.0000000000
H	-1.3043318954	-2.4819104318	0.0000000000
H	-3.4133321360	-1.2373577677	0.0000000000

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	1.1641710358	-1.3940674291	0.0000000000
H	1.1341814620	-2.4750917125	0.0000000000
C	2.5076576638	-0.7177027927	0.0000000000
H	3.1073316309	-1.0259677999	-0.8687911667
H	3.1073316309	-1.0259677999	0.8687911667
C	2.3326961249	0.7757343058	0.0000000000
H	3.2133134493	1.4040683607	0.0000000000
C	1.1435737845	1.3729066966	0.0000000000
H	1.0399672559	2.4485773967	0.0000000000
C	-1.2649661700	1.3563015281	0.0000000000
H	-1.1724167127	2.4327319433	0.0000000000
C	-2.4573585347	0.7265462035	0.0000000000
H	-3.3708802017	1.2993180628	0.0000000000

cinnoline

Atom	x (Å)	y (Å)	z (Å)
N	2.3307466872	0.8087174542	0.0000000000
N	1.1801993017	1.4067709809	0.0000000000
C	1.2864309387	-1.3579570700	0.0000000000
C	0.0285854778	0.6769603455	0.0000000000
C	2.3907135884	-0.5485966618	0.0000000000
C	0.0234383490	-0.7442089592	0.0000000000
C	-1.1996087951	1.3810506721	0.0000000000
H	-1.2184227099	-2.5134636510	0.0000000000
H	1.3822086163	-2.4362738090	0.0000000000
C	-2.3807965541	0.6909332319	0.0000000000
H	-1.1631515296	2.4612992978	0.0000000000
H	-3.3214896106	1.2247051349	0.0000000000
C	-2.3873791499	-0.7249024598	0.0000000000
H	-3.3333495489	-1.2496958046	0.0000000000
C	-1.2145427820	-1.4309579092	0.0000000000
H	3.3943627212	-0.9516887927	0.0000000000

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)

phtalazine

Atom	x (Å)	y (Å)	z (Å)
N	0.6817551513	0.0000000000	2.4235653419
C	1.3246894847	0.0000000000	1.2860513522
C	-1.3246894847	0.0000000000	1.2860513522
C	0.7055726916	0.0000000000	0.0092410962
N	-0.6817551513	0.0000000000	2.4235653419
C	-0.7055726916	0.0000000000	0.0092410962
C	1.4051103650	0.0000000000	-1.2149314263
H	-2.4874012170	0.0000000000	-1.2112953380
H	-2.4075068439	0.0000000000	1.3610116213
C	0.7054859403	0.0000000000	-2.3965485988
H	2.4874012170	0.0000000000	-1.2112953380
H	1.2354931426	0.0000000000	-3.3394410485
C	-0.7054859403	0.0000000000	-2.3965485988
H	-1.2354931426	0.0000000000	-3.3394410485
C	-1.4051103650	0.0000000000	-1.2149314263
H	2.4075068439	0.0000000000	1.3610116213

quinazoline

Atom	x (Å)	y (Å)	z (Å)
H	3.2633700662	-1.1843531666	0.0000000000
C	2.3173348222	-0.6550314139	0.0000000000
N	1.2285588925	-1.3809452058	0.0000000000
C	1.2702322663	1.3544820095	0.0000000000
C	0.0444754765	-0.7095853528	0.0000000000
N	2.4066481217	0.7011073970	0.0000000000
C	0.0126792500	0.7101104314	0.0000000000
C	-1.1752002545	-1.4232576611	0.0000000000
H	-1.2383026126	2.4710477416	0.0000000000
H	1.3199527725	2.4403299338	0.0000000000

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-2.3646097248	-0.7408736063	0.0000000000
H	-1.1352785699	-2.5033119355	0.0000000000
H	-3.2980255312	-1.2879802326	0.0000000000
C	-2.3948129583	0.6721869536	0.0000000000
H	-3.3474197470	1.1841153427	0.0000000000
C	-1.2264992696	1.3883007651	0.0000000000

quinoxaline

Atom	x (Å)	y (Å)	z (Å)
H	-1.2498780597	0.0000000000	3.2496342653
C	-0.7080837417	0.0000000000	2.3096023603
N	-1.4118479372	0.0000000000	1.2053159093
N	1.4118479372	0.0000000000	1.2053159093
C	-0.7125313270	0.0000000000	0.0387859696
C	0.7080837417	0.0000000000	2.3096023603
C	0.7125313270	0.0000000000	0.0387859696
C	-1.4055890716	0.0000000000	-1.1930331485
H	1.2498780597	0.0000000000	3.2496342653
H	2.4863800865	0.0000000000	-1.1673412333
C	-0.7068126939	0.0000000000	-2.3716404121
H	-2.4863800865	0.0000000000	-1.1673412333
H	-1.2371734702	0.0000000000	-3.3144217107
C	0.7068126939	0.0000000000	-2.3716404121
H	1.2371734702	0.0000000000	-3.3144217107
C	1.4055890716	0.0000000000	-1.1930331485

1,8-naphthyridine

Atom	x (Å)	y (Å)	z (Å)
H	3.1910518200	0.0000000000	1.3601492408
C	2.2867909084	0.0000000000	0.7593983376
N	1.1530680933	0.0000000000	1.4181250504
C	1.2450311429	0.0000000000	-1.3913347422

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	0.0000000000	0.0000000000	0.7019829947
C	2.3935563252	0.0000000000	-0.6499524461
C	0.0000000000	0.0000000000	-0.7251986279
N	-1.1530680933	0.0000000000	1.4181250504
H	3.3688858196	0.0000000000	-1.1161799355
H	-1.2723558940	0.0000000000	-2.4741411884
H	1.2723558940	0.0000000000	-2.4741411884
C	-2.2867909084	0.0000000000	0.7593983376
H	-3.1910518200	0.0000000000	1.3601492408
C	-2.3935563252	0.0000000000	-0.6499524461
H	-3.3688858196	0.0000000000	-1.1161799355
C	-1.2450311429	0.0000000000	-1.3913347422

1,5-naphthyridine

Atom	x (Å)	y (Å)	z (Å)
H	3.3372529386	-1.1700260431	0.0000000000
C	2.3697110102	-0.6871559397	0.0000000000
C	1.2111812533	-1.4147266106	0.0000000000
N	1.1700868987	1.4014288820	0.0000000000
C	-0.0247107895	-0.7302983520	0.0000000000
C	2.2940313979	0.7243762317	0.0000000000
C	0.0095177028	0.6926671475	0.0000000000
N	-1.1853042637	-1.4390563286	0.0000000000
H	3.2087960222	1.3081633781	0.0000000000
H	-1.2174065255	2.4584215301	0.0000000000
C	-2.3092228412	-0.7620168626	0.0000000000
H	-3.2240211771	-1.3457562653	0.0000000000
C	-2.3849087789	0.6495468124	0.0000000000
H	-3.3524593910	1.1324068140	0.0000000000
C	-1.2263989927	1.3771102563	0.0000000000
H	1.2022165358	-2.4960386504	0.0000000000

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)

pteridine

Atom	x (Å)	y (Å)	z (Å)
H	3.2385741234	-1.1797714310	0.0000000000
C	2.2863891417	-0.6612056534	0.0000000000
N	1.1969761676	-1.3864078004	0.0000000000
N	1.1383722764	1.4487546698	0.0000000000
C	0.0315948860	-0.6924465120	0.0000000000
C	2.2508068853	0.7590827936	0.0000000000
C	-0.0090305695	0.7223875644	0.0000000000
C	-1.2131710130	-1.3635183805	0.0000000000
H	3.1816918858	1.3168590030	0.0000000000
N	-2.3505138297	-0.7141961626	0.0000000000
H	-1.2296498965	-2.4485896654	0.0000000000
C	-2.2704914531	0.6439424459	0.0000000000
H	-3.2211190626	1.1641146354	0.0000000000
N	-1.1895575417	1.3839684931	0.0000000000

pyrazino[2,3-b]pyrazine

Atom	x (Å)	y (Å)	z (Å)
H	3.2012844298	-1.2497311225	0.0000000000
C	2.2606246492	-0.7093131736	0.0000000000
N	1.1585760849	-1.4147377019	0.0000000000
N	1.1585760849	1.4147377019	0.0000000000
C	0.0000000000	-0.7118184453	0.0000000000
C	2.2606246492	0.7093131736	0.0000000000
C	0.0000000000	0.7118184453	0.0000000000
N	-1.1585760849	-1.4147377019	0.0000000000
H	3.2012844298	1.2497311225	0.0000000000
C	-2.2606246492	-0.7093131736	0.0000000000
H	-3.2012844298	-1.2497311225	0.0000000000
C	-2.2606246492	0.7093131736	0.0000000000

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-3.2012844298	1.2497311225	0.0000000000
N	-1.1585760849	1.4147377019	0.0000000000

pyrimido[4,5-d]pyrimidine

Atom	x (Å)	y (Å)	z (Å)
N	2.3796244254	0.0000000000	-0.6651881256
H	1.3184987749	0.0000000000	-2.4237383816
C	1.2559943011	0.0000000000	-1.3388759730
N	1.1653170155	0.0000000000	1.4071173355
C	0.0000000000	0.0000000000	-0.6973918763
C	2.2628304129	0.0000000000	0.6910432253
C	0.0000000000	0.0000000000	0.7169297334
C	-1.2559943011	0.0000000000	-1.3388759730
H	3.2008905369	0.0000000000	1.2340569909
N	-2.3796244254	0.0000000000	-0.6651881256
H	-1.3184987749	0.0000000000	-2.4237383816
C	-2.2628304129	0.0000000000	0.6910432253
N	-1.1653170155	0.0000000000	1.4071173355
H	-3.2008905369	0.0000000000	1.2340569909

benzo[b]thiophene

Atom	x (Å)	y (Å)	z (Å)
H	-1.5438440000	-2.4455990000	0.0000000000
C	-1.4000230000	-1.3728900000	0.0000000000
C	-1.0357600000	1.4218570000	0.0000000000
C	-0.1014710000	-0.8430330000	0.0000000000
C	-2.4861450000	-0.5190080000	0.0000000000
C	-2.3055940000	0.8714770000	0.0000000000
C	0.0595710000	0.5602660000	0.0000000000
H	-3.4889200000	-0.9246940000	0.0000000000
H	-3.1690780000	1.5229840000	0.0000000000
H	-0.8986890000	2.4945680000	0.0000000000

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	1.1608140000	-1.5268440000	0.0000000000
H	1.2579360000	-2.6027980000	0.0000000000
C	2.2178340000	-0.6832230000	0.0000000000
H	3.2644960000	-0.9384930000	0.0000000000
S	1.7536390000	0.9961850000	0.0000000000

1H-indole

Atom	x (Å)	y (Å)	z (Å)
H	-0.9024286322	-2.4903481074	0.0746878951
C	-0.9247166399	-1.4084980280	0.0502771237
C	-0.9915634242	1.4270185347	-0.0139005601
C	0.2491484546	-0.6571751919	0.0544577883
C	-2.1249408594	-0.7201587312	0.0136045958
C	-2.1578667300	0.6843260175	-0.0181593173
C	0.2403813531	0.7607655673	0.0227658836
H	-3.0546415673	-1.2730935693	0.0093152862
H	-3.1144474547	1.1886868775	-0.0463496643
H	-1.0286405368	2.5083973482	-0.0385222928
N	1.5666622226	-1.0546325592	0.0869699011
H	1.8881271543	-2.0043986749	0.1118295222
C	2.3789723751	0.0595822975	0.0765083630
H	3.4501618770	-0.0454653244	0.0979756389
C	1.6092321512	1.1856421195	0.0377907478
H	1.9745222567	2.1981044242	0.0219690887

2H-isoindole

Atom	x (Å)	y (Å)	z (Å)
C	-0.9914748910	-0.0135805163	1.4257552931
C	-2.1575094484	0.0128473986	-0.7127782809
C	0.2393129339	-0.0414850109	-0.7232451851
C	-0.9914748910	-0.0135805163	-1.4257552931
C	0.2393129339	-0.0414850109	0.7232451851

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-2.1575094484	0.0128473986	0.7127782809
H	-1.0045528692	-0.0132661157	-2.5081295101
H	-3.1055715248	0.0343167868	1.2338852951
H	-1.0045528692	-0.0132661157	2.5081295101
H	-3.1055715248	0.0343167868	-1.2338852951
C	1.5676518063	-0.0717943954	1.1311461261
H	2.0128405251	-0.0817688414	2.1096504881
C	1.5676518063	-0.0717943954	-1.1311461261
H	2.0128405251	-0.0817688414	-2.1096504881
N	2.3314253554	-0.0891999610	0.0000000000
H	3.3359865808	-0.1122866540	0.0000000000

indolizine(delta-coniceine)

Atom	x (Å)	y (Å)	z (Å)
H	-1.0267672828	-2.4659343540	-0.2051772982
C	-0.9998338090	-1.4042575283	-0.0031918401
C	-2.0793579855	0.7078783073	0.4455413142
N	0.2812702692	0.6198642062	0.3310036087
C	-0.8772613188	1.3330619545	0.5153879936
C	0.2584691036	-0.7669531355	0.0666473181
C	-2.1481576208	-0.6892109218	0.1811237595
H	-0.7593717189	2.3879246444	0.7123054524
H	-3.1113351864	-1.1762031053	0.1278250247
H	-2.9795569210	1.2854633915	0.5932910772
C	1.5841319705	1.0463364791	0.3586661295
H	1.8240171862	2.0778038415	0.5460589384
C	1.5790734937	-1.1777044854	-0.0665864621
H	1.9013701983	-2.1836676140	-0.2723675797
C	2.3932464638	-0.0454028584	0.1163277415
H	3.4693451571	-0.0188108182	0.0768778031

1H-benzo[d]imidazole

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
Atom	x (Å)	y (Å)	z (Å)
H	-0.9025316802	-2.5151119053	-0.0600900391
C	-0.9119446537	-1.4335860789	-0.0397744206
C	-0.9534036488	1.4169468367	0.0140095443
C	0.2605009258	-0.6846183162	-0.0446433339
C	-2.1039893379	-0.7264125374	-0.0074183861
C	-2.1243408853	0.6776814833	0.0190701611
C	0.2582302893	0.7258744859	-0.0183183051
H	-3.0400676491	-1.2682627558	-0.0024481490
H	-3.0777264473	1.1878577997	0.0439004438
H	-0.9635980955	2.4977201224	0.0342662322
N	1.5977406929	-1.0282183241	-0.0726980885
H	1.9819922140	-1.9557187738	-0.0947133607
N	1.5586725914	1.2081776974	-0.0302393140
C	2.3098498829	0.1452358241	-0.0622566367
H	3.3884358017	0.1460044420	-0.0796483477

1H-indazole

Atom	x (Å)	y (Å)	z (Å)
H	-0.9111178462	-2.5020392698	0.0000000000
C	-0.9231542159	-1.4205911744	0.0000000000
C	-0.9706825583	1.4277666172	0.0000000000
C	0.2582215774	-0.6716347451	0.0000000000
C	-2.1108999623	-0.7173548036	0.0000000000
C	-2.1377326372	0.6923406626	0.0000000000
C	0.2522226609	0.7418530145	0.0000000000
H	-3.0466783322	-1.2601195194	0.0000000000
H	-3.0930600682	1.1990537551	0.0000000000
H	-0.9979964558	2.5092636656	0.0000000000
N	1.5727051124	-1.0339175756	0.0000000000
H	1.9667022179	-1.9566807979	0.0000000000
N	2.4054160736	0.0351392536	0.0000000000
C	1.6321209302	1.0993587274	0.0000000000

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	2.0734935036	2.0825591897	0.0000000000

1H-pyrrolo[2,3-b]pyridine

Atom	x (Å)	y (Å)	z (Å)
N	-0.8583051272	-1.4313290106	0.0000000000
C	-1.0130511981	1.4107814947	0.0000000000
C	0.2103721389	-0.6464909373	0.0000000000
C	-2.0225010822	-0.7843114724	0.0000000000
C	-2.1456550210	0.6121193122	0.0000000000
C	0.2285155431	0.7740685273	0.0000000000
H	-2.9115119949	-1.4040691564	0.0000000000
H	-3.1322497797	1.0539192736	0.0000000000
H	-1.0926345851	2.4902053883	0.0000000000
N	1.5142424503	-1.0736174016	0.0000000000
H	1.7948279914	-2.0377904821	0.0000000000
C	2.3469830786	0.0250284359	0.0000000000
H	3.4160383394	-0.1001956126	0.0000000000
C	1.6036292238	1.1713103073	0.0000000000
H	1.9941070229	2.1743783336	0.0000000000

imidazo[1,2-a]pyrazine

Atom	x (Å)	y (Å)	z (Å)
H	-0.8370601997	-2.4523862407	0.0000000000
C	-0.8883920952	-1.3746696910	0.0000000000
N	-2.1036628392	0.6996248981	0.0000000000
C	0.2864808516	0.7208975255	0.0000000000
C	-0.9724488222	1.3578781583	0.0000000000
N	0.2930191576	-0.6795338255	0.0000000000
C	-2.0471284010	-0.6640973717	0.0000000000
H	-1.0012776729	2.4410324656	0.0000000000
H	-2.9936504169	-1.1863263049	0.0000000000
C	1.6061858762	-1.0619634985	0.0000000000

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	1.9053500623	-2.0941429731	0.0000000000
C	2.3278397500	0.1153328233	0.0000000000
H	3.4013879225	0.2114898396	0.0000000000
N	1.5219268269	1.2045651950	0.0000000000

7H-purine

Atom	x (Å)	y (Å)	z (Å)
C	-0.9629672313	-1.3777152392	0.0495530332
C	-2.0232306194	0.6527452556	-0.0218647796
C	0.2075749356	0.7221933077	0.0233223042
N	-0.9316697034	1.4094901984	-0.0172994089
C	0.2372934568	-0.6887672490	0.0582706944
N	-2.0995890221	-0.6890188698	0.0089208405
H	-2.9715048845	1.1751115469	-0.0546094117
H	-1.0297636568	-2.4602115892	0.0743171778
N	1.5754368361	-1.0150408992	0.0942892549
C	2.2581991875	0.1745189268	0.0797652040
H	3.3364580951	0.1970605829	0.1018902801
N	1.4909448417	1.2286006024	0.0379511943
H	1.9811237783	-1.9338735900	0.1243209741

1,4-dihydropentalene

Atom	x (Å)	y (Å)	z (Å)
C	1.3413203522	1.1981084792	0.0000000000
C	-0.0144542616	0.6778925260	0.0000000000
C	0.0144542616	-0.6778925260	0.0000000000
C	1.4349455295	-1.1496864188	0.0000000000
C	2.1996011074	0.1563879165	0.0000000000
H	1.6196262955	2.2419402954	0.0000000000
H	1.6794587667	-1.7597232287	-0.8759428567
H	1.6794587667	-1.7597232287	0.8759428567
H	3.2770833178	0.2155079701	0.0000000000

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-1.4349455295	1.1496864188	0.0000000000
H	-1.6794587667	1.7597232287	-0.8759428567
H	-1.6794587667	1.7597232287	0.8759428567
C	-2.1996011074	-0.1563879165	0.0000000000
H	-3.2770833178	-0.2155079701	0.0000000000
C	-1.3413203522	-1.1981084792	0.0000000000
H	-1.6196262955	-2.2419402954	0.0000000000

1H-pyrrolizine

Atom	x (Å)	y (Å)	z (Å)
C	1.3346637841	1.1758317122	0.0000000000
C	0.0392819489	0.7250451906	0.0000000000
N	0.0746765506	-0.6539144556	0.0000000000
C	1.3715417484	-1.0995381325	0.0000000000
C	2.1727063139	0.0195988051	0.0000000000
H	1.6610073014	2.2015878165	0.0000000000
H	1.6149890193	-2.1467383430	0.0000000000
H	3.2495441456	0.0141471366	0.0000000000
C	-1.4017700992	1.1495904515	0.0000000000
H	-1.6658278125	1.7475247150	-0.8771496022
H	-1.6658278125	1.7475247150	0.8771496022
C	-2.1175255808	-0.1890371121	0.0000000000
H	-3.1877146107	-0.3085475082	0.0000000000
C	-1.2249082787	-1.1824417767	0.0000000000
H	-1.3804396177	-2.2485132142	0.0000000000

1,4-dihydropyrrolo[3,2-b]pyrrole

Atom	x (Å)	y (Å)	z (Å)
C	1.3265372456	-1.1774090454	0.0000000000
C	2.1187425754	-0.0495657617	0.0000000000
N	1.3286179922	1.0841305460	0.0000000000
C	0.0089046330	0.6960191860	0.0000000000

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-0.0089046330	-0.6960191860	0.0000000000
H	3.1915930085	0.0308911366	0.0000000000
N	-1.3286179922	-1.0841305460	0.0000000000
C	-2.1187425754	0.0495657617	0.0000000000
H	-3.1915930085	-0.0308911366	0.0000000000
C	-1.3265372456	1.1774090454	0.0000000000
H	-1.6746523311	-2.0244708162	0.0000000000
H	1.6746523311	2.0244708162	0.0000000000
H	1.6832035007	-2.1925755403	0.0000000000
H	-1.6832035007	2.1925755403	0.0000000000

1,4-dihydroimidazo[4,5-d]imidazole

Atom	x (Å)	y (Å)	z (Å)
N	1.2767527909	-1.1954378525	-0.0632665450
C	2.0270698628	-0.1117693450	0.0358058686
N	1.3057735600	1.0616207589	0.1101007772
C	-0.0164284943	0.6837798128	0.0517785684
C	0.0164284943	-0.6837798128	-0.0517785684
H	3.1035565448	-0.1113469775	0.0594536343
N	-1.3057735600	-1.0616207589	-0.1101007772
C	-2.0270698628	0.1117693450	-0.0358058686
H	-3.1035565448	0.1113469775	-0.0594536343
N	-1.2767527909	1.1954378525	0.0632665450
H	-1.6844137819	-1.9885487074	-0.1855782455
H	1.6844137819	1.9885487074	0.1855782455

N-ethylindole

Atom	x (Å)	y (Å)	z (Å)
C	-0.5735549293	-1.4188884306	0.0738327103
C	-2.6979824894	-0.3389398097	-0.4050164390
C	-0.7689216745	1.0328746960	-0.0076841183
C	-2.1334703130	0.9192205116	-0.3017507787

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-0.0046553948	-0.1490624395	0.1798155749
C	-1.9248274254	-1.4967875912	-0.2183946677
H	-2.3932861629	-2.4679422040	-0.3058988770
H	0.0128207423	-2.3171888424	0.2126545718
H	-3.7507255739	-0.4378464005	-0.6335300667
H	-2.7373527671	1.8057656839	-0.4467370493
N	1.2903641463	0.2284724805	0.4701503482
C	1.3518298977	1.6072071314	0.4562421170
H	2.2852852244	2.1045973827	0.6613769008
C	0.1253612258	2.1351761331	0.1739084930
H	-0.1128810143	3.1832092726	0.1128792486
C	2.4190627136	-0.6629847518	0.6716903394
H	2.0788949312	-1.5158586531	1.2613812076
H	3.1506991303	-0.1326644761	1.2819630409
C	3.0627937452	-1.1404868353	-0.6293839071
H	3.4416275932	-0.2973569944	-1.2072649858
H	2.3449232681	-1.6786913661	-1.2475314718
H	3.8971118863	-1.8098092172	-0.4137512813

N-ethylindazole

Atom	x (Å)	y (Å)	z (Å)
H	-0.4504549234	-2.4513853371	0.0000000000
C	-0.9520197157	-1.4938253370	0.0000000000
C	-2.2953833601	1.0181236644	0.0000000000
C	-0.2406941771	-0.2875986233	0.0000000000
C	-2.3302317152	-1.4108720744	0.0000000000
C	-2.9980672055	-0.1691723031	0.0000000000
C	-0.8945121264	0.9661962584	0.0000000000
H	-2.9148124724	-2.3212045448	0.0000000000
H	-4.0794483240	-0.1545464908	0.0000000000
H	-2.8138305329	1.9677700745	0.0000000000
N	1.0989117857	-0.0264607874	0.0000000000
N	1.3413215895	1.3068834835	0.0000000000

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	0.1700082935	1.9089775483	0.0000000000
H	0.1212716911	2.9855902762	0.0000000000
C	2.1754838372	-1.0108158197	0.0000000000
H	2.0529607850	-1.6492036988	-0.8791688155
H	2.0529607850	-1.6492036988	0.8791688155
C	3.5597346886	-0.3843983443	0.0000000000
H	4.3046114736	-1.1804987462	0.0000000000
H	3.7133858116	0.2377432503	0.8790478616
H	3.7133858116	0.2377432503	-0.8790478616

N-methylpurine

Atom	x (Å)	y (Å)	z (Å)
C	-0.7304145824	-1.4568204739	0.0000000000
C	-2.4671391934	0.0382389076	0.0000000000
C	-0.4194529271	0.9283323766	0.0000000000
N	-1.7327200943	1.1454794442	0.0000000000
C	0.1307548472	-0.3730566438	0.0000000000
N	-2.0426524418	-1.2372038009	0.0000000000
H	-3.5418629588	0.1736221794	0.0000000000
H	-0.3935097936	-2.4879257365	0.0000000000
N	1.4973368810	-0.1958397244	0.0000000000
C	1.6857980687	1.1624658601	0.0000000000
H	2.6832843876	1.5756677298	0.0000000000
N	0.5866800575	1.8686347033	0.0000000000
C	2.5191349247	-1.2235815867	0.0000000000
H	3.4967009793	-0.7473810478	0.0000000000
H	2.4362489227	-1.8512570935	-0.8875876660
H	2.4362489227	-1.8512570935	0.8875876660

N-ethylpurine

Atom	x (Å)	y (Å)	z (Å)
C	-0.6833361031	-1.4606173815	0.1863080771

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-2.7128200232	-0.4708386368	-0.2022463888
C	-0.9684927483	0.9150613157	-0.0531512730
N	-2.2800276596	0.7843321252	-0.2399693874
C	-0.1209955983	-0.1951624642	0.1645594336
N	-1.9941561017	-1.5885295130	0.0001267454
H	-3.7756377697	-0.6184200807	-0.3509780762
H	-0.1098667211	-2.3670466759	0.3487854836
N	1.1441790127	0.3315980234	0.3241074478
C	0.9876999240	1.6875412548	0.1915885083
H	1.8387174834	2.3467046357	0.2774079238
N	-0.2381692168	2.0820585669	-0.0300090803
C	2.3942892766	-0.3874773575	0.5342635912
H	3.1088030542	0.3277653201	0.9414329666
H	2.2271919527	-1.1420339540	1.3044631660
C	2.9456416423	-1.0282134439	-0.7364359771
H	3.8784065282	-1.5479121724	-0.5154688016
H	3.1459091602	-0.2742785274	-1.4975146849
H	2.2459059074	-1.7525970344	-1.1520606740

9H-fluorene

Atom	x (Å)	y (Å)	z (Å)
H	-1.3119043545	0.0000000000	2.5289475456
C	-1.6473136605	0.0000000000	1.4999514642
C	-2.5358034799	0.0000000000	-1.1664785171
C	-0.7329294847	0.0000000000	0.4508786283
C	-3.0067449394	0.0000000000	1.2073433752
C	-3.4493241280	0.0000000000	-0.1140519417
C	-1.1806546438	0.0000000000	-0.8808435344
H	-3.7289922349	0.0000000000	2.0129430716
H	-4.5106822126	0.0000000000	-0.3236440980
H	-2.8867213462	0.0000000000	-2.1909737510
C	0.7329294847	0.0000000000	0.4508786283
C	3.4493241280	0.0000000000	-0.1140519417

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	1.6473136605	0.0000000000	1.4999514642
C	1.1806546438	0.0000000000	-0.8808435344
C	2.5358034799	0.0000000000	-1.1664785171
C	3.0067449394	0.0000000000	1.2073433752
H	1.3119043545	0.0000000000	2.5289475456
H	2.8867213462	0.0000000000	-2.1909737510
H	3.7289922349	0.0000000000	2.0129430716
H	4.5106822126	0.0000000000	-0.3236440980
C	0.0000000000	0.0000000000	-1.8238126941
H	0.0000000000	0.8767215555	-2.4778838957
H	0.0000000000	-0.8767215555	-2.4778838957

9-ethylfluorene

Atom	x (Å)	y (Å)	z (Å)
H	0.6598050624	-2.8744522927	-1.3087103370
C	0.3276450839	-1.9009703102	-1.6453919621
C	-0.5389383913	0.6187668669	-2.5346674817
C	-0.0059894195	-0.9050731511	-0.7328262079
C	0.2274696859	-1.6280769039	-3.0053623158
C	-0.2023116885	-0.3789148363	-3.4482312453
C	-0.4385382777	0.3542501307	-1.1786911375
H	0.4845399598	-2.3922141498	-3.7269239903
H	-0.2761209418	-0.1828314205	-4.5096544003
H	-0.8745563331	1.5855064320	-2.8890668872
C	-0.0059894195	-0.9050731511	0.7328262079
C	-0.2023116885	-0.3789148363	3.4482312453
C	0.3276450839	-1.9009703102	1.6453919621
C	-0.4385382777	0.3542501307	1.1786911375
C	-0.5389383913	0.6187668669	2.5346674817
C	0.2274696859	-1.6280769039	3.0053623158
H	0.6598050624	-2.8744522927	1.3087103370
H	-0.8745563331	1.5855064320	2.8890668872
H	0.4845399598	-2.3922141498	3.7269239903

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-0.2761209418	-0.1828314205	4.5096544003
C	-0.7504784984	1.2578266969	0.0000000000
C	-0.0093019080	2.6124176316	0.0000000000
H	-0.3398310664	3.1819502128	0.8723024648
H	-0.3398310664	3.1819502128	-0.8723024648
C	1.5154385081	2.5143362154	0.0000000000
H	1.8805688274	1.9859318869	0.8809937604
H	1.9623085772	3.5093258276	0.0000000000
H	1.8805688274	1.9859318869	-0.8809937604
H	-1.8238716692	1.4809747094	0.0000000000

N-ethylcarbazole

Atom	x (Å)	y (Å)	z (Å)
H	0.3066840104	-3.0812115012	-1.3970709307
C	0.1631292934	-2.0489630262	-1.6886859644
C	-0.2079771966	0.6434829905	-2.4728586817
C	0.0251256893	-1.0541821644	-0.7218849342
C	0.1156278709	-1.7007093241	-3.0300943797
C	-0.0676828942	-0.3671061829	-3.4137369184
C	-0.1642505067	0.2899750727	-1.1256762182
H	0.2228067282	-2.4635088361	-3.7890632683
H	-0.0984305666	-0.1162929025	-4.4657014049
H	-0.3418389940	1.6694683350	-2.7864335741
C	0.0251256893	-1.0541821644	0.7218849342
C	-0.0676828942	-0.3671061829	3.4137369184
C	0.1631292934	-2.0489630262	1.6886859644
C	-0.1642505067	0.2899750727	1.1256762182
C	-0.2079771966	0.6434829905	2.4728586817
C	0.1156278709	-1.7007093241	3.0300943797
H	0.3066840104	-3.0812115012	1.3970709307
H	-0.3418389940	1.6694683350	2.7864335741
H	0.2228067282	-2.4635088361	3.7890632683
H	-0.0984305666	-0.1162929025	4.4657014049

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
N	-0.2884112359	1.0896532163	0.0000000000
C	-0.4690995985	2.5292212469	0.0000000000
H	-1.0674625069	2.7916952809	0.8731281817
H	-1.0674625069	2.7916952809	-0.8731281817
C	0.8427162490	3.3138790667	0.0000000000
H	1.4381822231	3.0790655718	0.8820620055
H	0.6410962787	4.3862248406	0.0000000000
H	1.4381822231	3.0790655718	-0.8820620055

N-methyl-1,8-diazacarbazole

Atom	x (Å)	y (Å)	z (Å)
H	0.0157532838	-2.8552735197	-1.5017356694
C	0.0069101152	-1.7968209961	-1.7272670357
N	-0.0152199578	0.9687530129	-2.3645277625
C	0.0000636117	-0.8423576405	-0.7198666849
C	0.0019814616	-1.3489403980	-3.0435843777
C	-0.0098707317	0.0221034005	-3.3067000256
C	-0.0114399174	0.5223284596	-1.1182206226
H	0.0075919525	-2.0490907816	-3.8666761652
H	-0.0143180080	0.3752341043	-4.3312751351
C	0.0000636117	-0.8423576405	0.7198666849
C	-0.0098707317	0.0221034005	3.3067000256
C	0.0069101152	-1.7968209961	1.7272670357
C	-0.0114399174	0.5223284596	1.1182206226
N	-0.0152199578	0.9687530129	2.3645277625
C	0.0019814616	-1.3489403980	3.0435843777
H	0.0157532838	-2.8552735197	1.5017356694
H	0.0075919525	-2.0490907816	3.8666761652
H	-0.0143180080	0.3752341043	4.3312751351
N	-0.0243774976	1.3315532121	0.0000000000
C	-0.0061253106	2.7804612789	0.0000000000
H	-0.5129485436	3.1368486254	0.8927468848
H	-0.5129485436	3.1368486254	-0.8927468848

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	1.0163732630	3.1628839752	0.0000000000

N-ethyl-1,8-diazacarbazole

Atom	x (Å)	y (Å)	z (Å)
H	-0.3274169681	-3.0999060970	-1.5012123974
C	-0.1747993187	-2.0525236584	-1.7270372538
N	0.2238943489	0.6840448419	-2.3648356009
C	-0.0388133711	-1.1074156014	-0.7198400085
C	-0.1080129716	-1.6099186003	-3.0434379119
C	0.0902492816	-0.2532570390	-3.3067167591
C	0.1587887885	0.2431281238	-1.1178245095
H	-0.2082600532	-2.3029064805	-3.8664937113
H	0.1428948859	0.0957101837	-4.3313823423
C	-0.0388133711	-1.1074156014	0.7198400085
C	0.0902492816	-0.2532570390	3.3067167591
C	-0.1747993187	-2.0525236584	1.7270372538
C	0.1587887885	0.2431281238	1.1178245095
N	0.2238943489	0.6840448419	2.3648356009
C	-0.1080129716	-1.6099186003	3.0434379119
H	-0.3274169681	-3.0999060970	1.5012123974
H	-0.2082600532	-2.3029064805	3.8664937113
H	0.1428948859	0.0957101837	4.3313823423
N	0.2809678554	1.0444040706	0.0000000000
C	0.4799577722	2.4875175481	0.0000000000
H	1.0668511777	2.7275531491	0.8848347016
H	1.0668511777	2.7275531491	-0.8848347016
C	-0.8303574603	3.2701612627	0.0000000000
H	-1.4203169542	3.0380854489	-0.8862385309
H	-0.6229718587	4.3412255753	0.0000000000
H	-1.4203169542	3.0380854489	0.8862385309

5H-dibenzoborole

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
Atom	x (Å)	y (Å)	z (Å)
H	-1.2528245953	0.0000000000	2.4415044785
C	-1.6148371411	0.0000000000	1.4213125443
C	-2.6005108970	0.0000000000	-1.2065078972
C	-0.7433186452	0.0000000000	0.3484413226
C	-2.9926038769	0.0000000000	1.1731741860
C	-3.4853743564	0.0000000000	-0.1245374249
C	-1.2299050651	0.0000000000	-0.9833631301
H	-3.6826415817	0.0000000000	2.0070828858
H	-4.5537337566	0.0000000000	-0.2943948635
H	-2.9876955764	0.0000000000	-2.2180020788
C	0.7433186452	0.0000000000	0.3484413226
C	3.4853743564	0.0000000000	-0.1245374249
C	1.6148371411	0.0000000000	1.4213125443
C	1.2299050651	0.0000000000	-0.9833631301
C	2.6005108970	0.0000000000	-1.2065078972
C	2.9926038769	0.0000000000	1.1731741860
H	1.2528245953	0.0000000000	2.4415044785
H	2.9876955764	0.0000000000	-2.2180020788
H	3.6826415817	0.0000000000	2.0070828858
H	4.5537337566	0.0000000000	-0.2943948635
B	0.0000000000	0.0000000000	-1.9384213280
H	0.0000000000	0.0000000000	-3.1275767173

dibenzo-5Me-borole

Atom	x (Å)	y (Å)	z (Å)
H	-1.2450673200	-2.7690330196	0.0000000000
C	-1.6100371570	-1.7498959274	0.0000000000
C	-2.5941601735	0.8752458787	0.0000000000
C	-0.7388398623	-0.6747549416	0.0000000000
C	-2.9866800298	-1.5049292720	0.0000000000
C	-3.4788848326	-0.2064736146	0.0000000000
C	-1.2232370822	0.6554314304	0.0000000000

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-3.6764457657	-2.3390461687	0.0000000000
H	-4.5473251210	-0.0361524343	0.0000000000
H	-2.9865202120	1.8852982896	0.0000000000
C	0.7465028652	-0.6796239823	0.0000000000
C	3.4903094216	-0.2236624526	0.0000000000
C	1.6128276499	-1.7583694048	0.0000000000
C	1.2389257255	0.6476813620	0.0000000000
C	2.6105810127	0.8619649832	0.0000000000
C	2.9909221420	-1.5193771608	0.0000000000
H	1.2442686900	-2.7762574526	0.0000000000
H	3.0062879061	1.8706555465	0.0000000000
H	3.6764216235	-2.3570438568	0.0000000000
H	4.5595688647	-0.0588676377	0.0000000000
B	0.0133158045	1.6241498046	0.0000000000
C	0.0012794081	3.1861042561	0.0000000000
H	0.9888539892	3.6480233080	0.0000000000
H	-0.5464332735	3.5639932334	0.8700601184
H	-0.5464332735	3.5639932334	-0.8700601184

dibenzo[b,d]furan

Atom	x (Å)	y (Å)	z (Å)
H	-1.4654793533	0.0000000000	2.5592977280
C	-1.7199672914	0.0000000000	1.5079276099
C	-2.4133576566	0.0000000000	-1.2435397730
C	-0.7243127255	0.0000000000	0.5318341814
C	-3.0479247250	0.0000000000	1.1040286278
C	-3.3890953599	0.0000000000	-0.2528541787
C	-1.0975807341	0.0000000000	-0.8199047933
H	-3.8332470464	0.0000000000	1.8474310879
H	-4.4322091639	0.0000000000	-0.5385207803
H	-2.6638473781	0.0000000000	-2.2944972619
C	0.7243127255	0.0000000000	0.5318341814
C	3.3890953599	0.0000000000	-0.2528541787

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	1.7199672914	0.0000000000	1.5079276099
C	1.0975807341	0.0000000000	-0.8199047933
C	2.4133576566	0.0000000000	-1.2435397730
C	3.0479247250	0.0000000000	1.1040286278
H	1.4654793533	0.0000000000	2.5592977280
H	2.6638473781	0.0000000000	-2.2944972619
H	3.8332470464	0.0000000000	1.8474310879
H	4.4322091639	0.0000000000	-0.5385207803
O	0.0000000000	0.0000000000	-1.6467788956

dibenzo[b,d]thiophene

Atom	x (Å)	y (Å)	z (Å)
H	-1.2232811117	0.0000000000	2.6610785609
C	-1.6073944566	0.0000000000	1.6496089655
C	-2.6286478462	0.0000000000	-0.9677089589
C	-0.7250928805	0.0000000000	0.5649036063
C	-2.9737729295	0.0000000000	1.4270595651
C	-3.4822623862	0.0000000000	0.1244362948
C	-1.2560692636	0.0000000000	-0.7389065161
H	-3.6548264806	0.0000000000	2.2671302721
H	-4.5520899030	0.0000000000	-0.0347091328
H	-3.0221586679	0.0000000000	-1.9749056836
C	0.7250928805	0.0000000000	0.5649036063
C	3.4822623862	0.0000000000	0.1244362948
C	1.6073944566	0.0000000000	1.6496089655
C	1.2560692636	0.0000000000	-0.7389065161
C	2.6286478462	0.0000000000	-0.9677089589
C	2.9737729295	0.0000000000	1.4270595651
H	1.2232811117	0.0000000000	2.6610785609
H	3.0221586679	0.0000000000	-1.9749056836
H	3.6548264806	0.0000000000	2.2671302721
H	4.5520899030	0.0000000000	-0.0347091328
S	0.0000000000	0.0000000000	-1.9715079466

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)

9H-carbazole

Atom	x (Å)	y (Å)	z (Å)
H	-1.4061314923	0.0000000000	2.5492435215
C	-1.6938772423	0.0000000000	1.5060536445
C	-2.4730852356	0.0000000000	-1.2147670047
C	-0.7232565693	0.0000000000	0.5041667303
C	-3.0338216209	0.0000000000	1.1498833597
C	-3.4162402075	0.0000000000	-0.1974707336
C	-1.1297745141	0.0000000000	-0.8517098930
H	-3.7946388546	0.0000000000	1.9183288391
H	-4.4678386606	0.0000000000	-0.4513240184
H	-2.7758026739	0.0000000000	-2.2536887426
C	0.7232565693	0.0000000000	0.5041667303
C	3.4162402075	0.0000000000	-0.1974707336
C	1.6938772423	0.0000000000	1.5060536445
C	1.1297745141	0.0000000000	-0.8517098930
C	2.4730852356	0.0000000000	-1.2147670047
C	3.0338216209	0.0000000000	1.1498833597
H	1.4061314923	0.0000000000	2.5492435215
H	2.7758026739	0.0000000000	-2.2536887426
H	3.7946388546	0.0000000000	1.9183288391
H	4.4678386606	0.0000000000	-0.4513240184
N	0.0000000000	0.0000000000	-1.6486825309
H	0.0000000000	0.0000000000	-2.6518148745

1,8-diazacarbazole

Atom	x (Å)	y (Å)	z (Å)
H	-1.5035184768	0.0000000000	2.5720371984
C	-1.7288427574	0.0000000000	1.5136152156
N	-2.3677840238	0.0000000000	-1.2534217702
C	-0.7211455610	0.0000000000	0.5581367909

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-3.0444739040	0.0000000000	1.0654484320
C	-3.3091369107	0.0000000000	-0.3057317588
C	-1.1235266813	0.0000000000	-0.8043813493
H	-3.8674215836	0.0000000000	1.7657191677
H	-4.3338628078	0.0000000000	-0.6579823186
C	0.7211455610	0.0000000000	0.5581367909
C	3.3091369107	0.0000000000	-0.3057317588
C	1.7288427574	0.0000000000	1.5136152156
C	1.1235266813	0.0000000000	-0.8043813493
N	2.3677840238	0.0000000000	-1.2534217702
C	3.0444739040	0.0000000000	1.0654484320
H	1.5035184768	0.0000000000	2.5720371984
H	3.8674215836	0.0000000000	1.7657191677
H	4.3338628078	0.0000000000	-0.6579823186
N	0.0000000000	0.0000000000	-1.6019833281
H	0.0000000000	0.0000000000	-2.6072818873

3,6-diazacarbazole

Atom	x (Å)	y (Å)	z (Å)
H	-1.4673749250	0.0000000000	2.5299545116
C	-1.7193177481	0.0000000000	1.4751869057
C	-2.4753429270	0.0000000000	-1.1833918164
C	-0.7237671925	0.0000000000	0.5013347598
N	-3.0147986894	0.0000000000	1.1747592587
C	-3.3665008406	0.0000000000	-0.1200260570
C	-1.1265280144	0.0000000000	-0.8524953534
H	-4.4321296677	0.0000000000	-0.3174326644
C	0.7237671925	0.0000000000	0.5013347598
C	3.3665008406	0.0000000000	-0.1200260570
C	1.7193177481	0.0000000000	1.4751869057
C	1.1265280144	0.0000000000	-0.8524953534
C	2.4753429270	0.0000000000	-1.1833918164
N	3.0147986894	0.0000000000	1.1747592587

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Table S9 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	1.4673749250	0.0000000000	2.5299545116
H	4.4321296677	0.0000000000	-0.3174326644
N	0.0000000000	0.0000000000	-1.6498483325
H	2.8269916622	0.0000000000	-2.2058728774
H	-2.8269916622	0.0000000000	-2.2058728774
H	0.0000000000	0.0000000000	-2.6538050023

4,5-diazacarbazole

Atom	x (Å)	y (Å)	z (Å)
N	1.5844915471	0.0000000000	1.5110683072
C	2.4748732380	0.0000000000	-1.1904560334
C	0.7250698918	0.0000000000	0.4923090659
C	2.8742229381	0.0000000000	1.1924977772
C	3.3588033849	0.0000000000	-0.1226639464
C	1.1250864089	0.0000000000	-0.8678166354
H	4.4259082881	0.0000000000	-0.2962698864
C	-0.7250698918	0.0000000000	0.4923090659
C	-3.3588033849	0.0000000000	-0.1226639464
N	-1.5844915471	0.0000000000	1.5110683072
C	-1.1250864089	0.0000000000	-0.8678166354
C	-2.4748732380	0.0000000000	-1.1904560334
C	-2.8742229381	0.0000000000	1.1924977772
H	-4.4259082881	0.0000000000	-0.2962698864
N	0.0000000000	0.0000000000	-1.6690759059
H	2.8234437666	0.0000000000	-2.2149715632
H	-3.5730451164	0.0000000000	2.0210086577
H	3.5730451164	0.0000000000	2.0210086577
H	-2.8234437666	0.0000000000	-2.2149715632
H	0.0000000000	0.0000000000	-2.6728725803