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Supporting Information:

Theoretical study on conformational energies of transition metal complexes

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1 General remarks

The systems evaluated in this study were generally chosen to cover most transition metals as well as various ligand types and coordination motifs and elements involved in the ligand sphere. The structures of the TMCONF5 subset were chosen to represent the X-ray structure conformation, energetically low lying conformers at the B97-3c and GFN2-xTB levels, an energetically high lying conformer at the B97-3c level and a structure in between the high and low lying conformers at the GFN2-xTB level. By this selection process, a sufficiently large conformational energy range was covered for the TMCONF5 subset. The varying number of evaluated conformers for the TMCONF40 set results from subsequent removal of enantiomers and identical structures originating from the B97-3c reoptimization.

In some cases (**SIGSUX**, **MOGWIP**, **EGOZUV**, **BOBXAS**) GFN1-xTB consistently produced highly erroneous results based on the underlying optimization method. This issue was observed mainly for early transition metals, and can be addressed to an erroneous charge estimate. The corresponding compounds were considered as unreasonable outliers and were excluded from the evaluation. In the case of UFF **UWUBEV** and **NOXPAR** were excluded accordingly.

As all geometry inputs were initially generated by the `crest` program in conjunction with the GFN2-xTB method, in some cases chemical transformations differing from the X-ray input structure are observed (**FEGGII**, **DUGVEH**, **DEFVIT**, **CAFKOJ**, **GOZYAX**). Nevertheless, the resulting structures were re-optimized with B97-3c to obtain the reference geometries and thus, were still used to evaluate energy differences of their conformers.

Based on qualitative fractional occupation density (FOD) analysis, some structures of the original benchmark set of Minenkov *et al.* were discarded. The respective FOD plots are depicted in Figure S1.

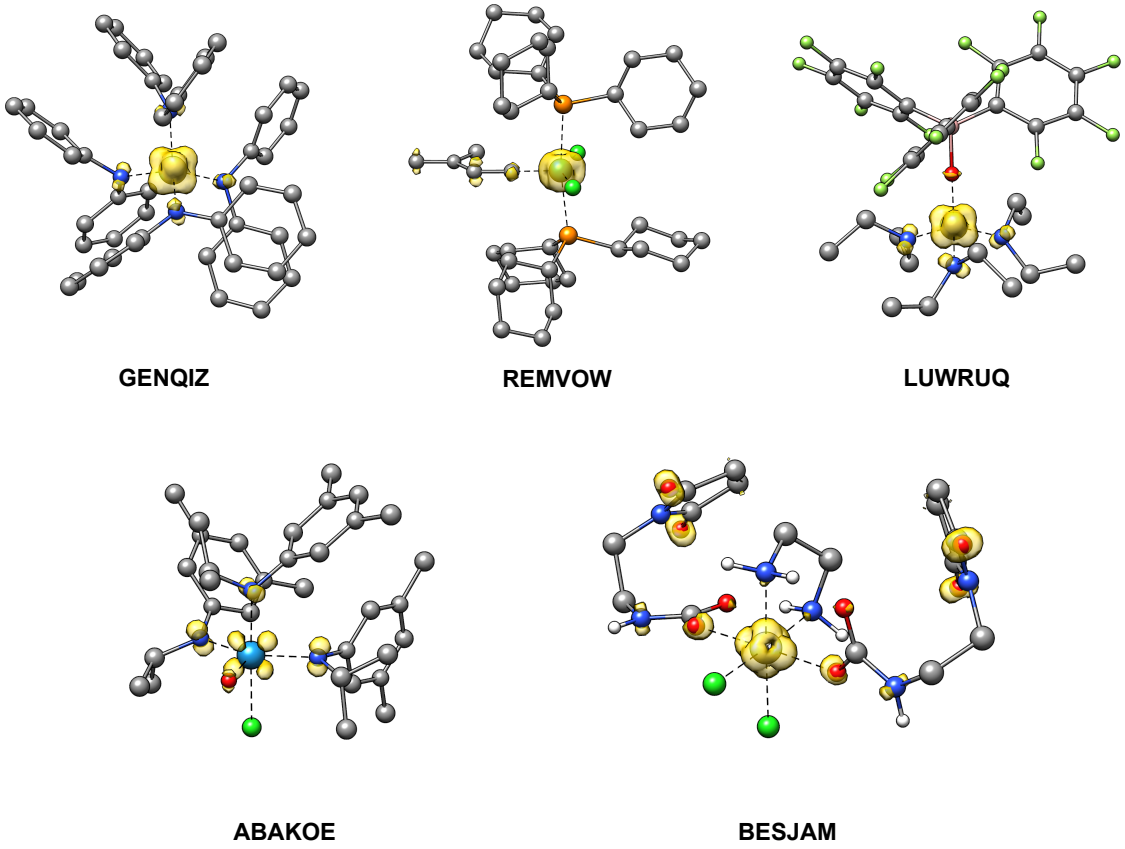

Figure S1: Qualitative FOD analysis of discarded structures. The isosurface value is set to σ = 0.005 e·bohr^{-}3.

2 Statistical measures

Mean deviation (MD):

$$MD = \frac{1}{n}\sum_{i}^{n}(E_{x_i} - E_{r_i}) \tag{S1}$$

Mean absolute deviation (MAD):

$$MAD = \frac{1}{n}\sum_{i}^{n}(|E_{x_i} - E_{r_i}|) \tag{S2}$$

Pearson correlation coefficient (r_p):

$$r_p = \frac{\sum_{i=1}^{n}(E_{x_i} - \overline{E}_x)(E_{r_i} - \overline{E}_r)}{\sqrt{\sum_{i=1}^{n}(E_{x_i} - \overline{E}_x)^2 \sum_{i=1}^{n}((E_{r_i} - \overline{E}_r)^2}} \tag{S3}$$

Spearman correlation coefficient (r_s):

$$r_s = \frac{\sum_{i=1}^{n}(R_{x_i} - \overline{R}_x)(R_{r_i} - \overline{R}_r)}{\sqrt{\sum_{i=1}^{n}(R_{x_i} - \overline{R}_x)^2 \sum_{i=1}^{n}((R_{r_i} - \overline{R}_r)^2}} \tag{S4}$$

With E_i being the relative energy of the i^{th} of n conformers, and $\overline{E}$ the average relative conformer energy over all n conformers for the tested method x and the reference r. For the Spearman correlation coefficient ρ_s the same notation is applied for conformer rankings R instead of their relative conformer energies.

3 Tabulated Data

Table S1: DLPNO-CCSD(T1)/def2-TZVPP/*VeryTightPNO* energy contributions and conformational energies.

Compound	#	E_0 / a.u.	E_{corr} / a.u.	E_{CC} / a.u.	ΔE_{conf} / kcal·mol^{-1}
AXURER	1-CC	-2335.647616806	-3.532125154	-2339.179741960	0.000
	2-CC	-2335.646642303	-3.531931297	-2339.178573600	0.733
	3-CC	-2335.644220411	-3.530611584	-2339.174831995	3.081
	4-CC	-2335.644343349	-3.529247757	-2339.173591106	3.860
	5-CC	-2335.640072244	-3.531497151	-2339.171569395	5.128
AYISEG	1-CC	-2511.716755331	-8.388613477	-2520.105368808	0.000
	2-CC	-2511.706591515	-8.394192042	-2520.100783557	2.877
	3-CC	-2511.706037280	-8.393212928	-2520.099250208	3.839
	4-CC	-2511.702944282	-8.394666688	-2520.097610970	4.868
	5-CC	-2511.698406556	-8.395560162	-2520.093966718	7.155
HAYGUJ	1-CC	-1416.825151316	-4.651155123	-1421.476306439	0.000
	2-CC	-1416.819625969	-4.656926132	-1421.476552101	-0.154
	3-CC	-1416.814470405	-4.655496558	-1421.469966963	3.978
	4-CC	-1416.812359084	-4.656875551	-1421.469234635	4.438
	5-CC	-1416.809034407	-4.657366401	-1421.466400808	6.216
WECSEC	1-CC	-2865.408256915	-4.946961607	-2870.355218522	0.000
	2-CC	-2865.407930474	-4.945817054	-2870.353747528	0.923
	3-CC	-2865.403138532	-4.948201252	-2870.351339784	2.434
	4-CC	-2865.399586700	-4.950021705	-2870.349608405	3.520
	5-CC	-2865.397191621	-4.947869676	-2870.345061297	6.374
YIDHAX	1-CC	-1522.468113235	-6.058651789	-1528.526765024	0.000
	2-CC	-1522.468048132	-6.057446548	-1528.525494680	0.797
	3-CC	-1522.468499339	-6.055961892	-1528.524461231	1.446
	4-CC	-1522.463615449	-6.060817551	-1528.524433000	1.463
	5-CC	-1522.464771468	-6.058000726	-1528.522772194	2.506

Table S2: DLPNO-CCSD(T1)/def2-QZVPP/*VeryTightPNO* energy contributions.

Compound	#	E_0 / a.u.	E_{corr} / a.u.	E_{CC} / a.u.
AXURER	1-CC	-2335.719068440	-3.805072151	-2339.524140591
	2-CC	-2335.718223292	-3.804641757	-2339.522865049
	3-CC	-2335.715775226	-3.803462524	-2339.51923775
	4-CC	-2335.716076171	-3.802054487	-2339.518130658
	5-CC	-2335.711670464	-3.804147578	-2339.515818042
AYISEG	1-CC	–	–	–
	2-CC	–	–	–
	3-CC	–	–	–
	4-CC	–	–	–
	5-CC	–	–	–
HAYGUJ	1-CC	-1416.880183611	-4.934282186	-1421.814465797
	2-CC	-1416.874522600	-4.939708095	-1421.814230695
	3-CC	-1416.869365218	-4.938458014	-1421.807823232
	4-CC	-1416,867204151	-4,939873591	-1421.807077742
	5-CC	-1416.863893700	-4.940218761	-1421.804112461
WECSEC	1-CC	-2865.491449875	-5.391680591	-2870.883130466
	2-CC	-2865.491126846	-5.390810085	-2870.881936931
	3-CC	-2865.486298686	-5.392774565	-2870.879073251
	4-CC	-2865.482633868	-5.394556251	-2870.877190119
	5-CC	-2865.480178747	-5.391915482	-2870.872094229
YIDHAX	1-CC	-1522.528014804	-6.463180505	-1528.991195309
	2-CC	-1522.527965761	-6.461740210	-1528.989705971
	3-CC	-1522.528598606	-6.460551098	-1528.989149704
	4-CC	-1522.523451940	-6.465010759	-1528.988462699
	5-CC	-1522.524723625	-6.462258199	-1528.986981824

Table S3: DLPNO-CCSD(T1)/CBS(def2-TZVPP/def2-QZVPP)/*VeryTightPNO* energy contributions and conformational energies.

Compound	#	E_0 / a.u.	E_{corr} / a.u.	E_{CC} / a.u.	ΔE_{conf} / kcal·mol^{-1}
AXURER	1-CC	-2335.728910094	-4.007254961	-2339.736165056	0.000
	2-CC	-2335.728082764	-4.006649355	-2339.734732119	0.899
	3-CC	-2335.725631092	-4.005574181	-2339.731205274	3.112
	4-CC	-2335.725956556	-4.004133396	-2339.730089952	3.812
	5-CC	-2335.721532309	-4.006110707	-2339.727643016	5.348
AYISEG	1-CC	–	–	–	–
	2-CC	–	–	–	–
	3-CC	–	–	–	–
	4-CC	–	–	–	–
	5-CC	–	–	–	–
HAYGUJ	1-CC	-1416.887763687	-5.144005780	-1422.031769468	0.000
	2-CC	-1416.882083990	-5.149176060	-1422.031260050	0.320
	3-CC	-1416.876926358	-5.148058937	-1422.024985294	4.257
	4-CC	-1416.874758439	-5.149501613	-1422.024260052	4.712
	5-CC	-1416.871449947	-5.149738872	-1422.021188819	6.639
WECSEC	1-CC	-2865.502908764	-5.721101816	-2871.224010580	0.000
	2-CC	-2865.502586205	-5.720434307	-2871.223020513	0.621
	3-CC	-2865.497753057	-5.722087885	-2871.219840942	2.616
	4-CC	-2865.494072676	-5.723840855	-2871.217913531	3.826
	5-CC	-2865.491609285	-5.720838057	-2871.212447342	7.256
YIDHAX	1-CC	-1522.536265568	-6.762831183	-1529.299096751	0.000
	2-CC	-1522.536218737	-6.761216774	-1529.297435511	1.042
	3-CC	-1522.536876600	-6.760246583	-1529.297123184	1.238
	4-CC	-1522.531693740	-6.764412913	-1529.296106653	1.876
	5-CC	-1522.532981356	-6.761707956	-1529.294689313	2.766

Table S4: Subset DFT/def2-QZVP conformational energies in kcal·mol^{-1}.

Compound	#	B97-3c	PBEh-3c	PBE0-D4	MN15	ωB97X-V	ωB97M-V	PWPB95-D4	B2PLYP-D4
AXURER	1-CC	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	2-CC	0.333	-0.169	-0.043	1.489	0.818	1.045	0.738	0.289
	3-CC	3.045	1.819	2.765	2.755	2.767	2.844	2.759	2.912
	4-CC	3.415	2.720	2.893	4.166	3.559	3.911	3.739	3.198
	5-CC	4.983	3.572	4.830	5.165	5.068	5.241	5.040	4.867
AYISEG	1-CC	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	2-CC	1.304	2.879	1.535	1.899	2.092	2.220	1.390	1.495
	3-CC	2.150	3.729	2.469	2.775	2.860	2.990	2.465	2.338
	4-CC	3.969	5.766	3.659	3.454	3.853	3.943	3.087	3.616
	5-CC	5.732	7.242	5.299	4.971	5.407	5.369	4.573	5.184
HAYGUJ	1-CC	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	2-CC	-0.033	-0.113	0.356	-0.406	0.237	0.065	0.122	0.297
	3-CC	4.034	3.438	4.514	2.996	3.861	3.722	3.696	4.354
	4-CC	4.547	3.746	4.942	3.226	4.347	4.230	4.229	4.766
	5-CC	6.358	5.756	6.766	5.064	6.153	6.000	6.021	6.604
WECSEC	1-CC	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	2-CC	0.265	0.662	0.457	0.722	0.776	0.768	0.679	0.689
	3-CC	1.634	1.455	2.054	2.427	1.919	1.709	2.684	2.558
	4-CC	2.772	2.809	3.363	3.490	2.991	2.736	3.906	3.762
	5-CC	6.088	5.336	6.561	5.958	5.340	5.015	6.965	7.095
YIDHAX	1-CC	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	2-CC	1.506	-0.531	0.898	1.148	0.825	0.945	1.000	0.980
	3-CC	1.217	1.160	1.234	1.648	1.306	1.459	1.376	1.378
	4-CC	2.347	-0.024	1.619	1.692	1.464	1.576	1.749	1.735
	5-CC	3.115	0.629	2.765	2.434	2.550	2.633	2.566	3.051

Table S5: **ADUHOY**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.116	-0.079	0.508	0.619	0.837	0.620	2.460	6.514
3	0.532	0.256	0.215	0.223	0.398	-0.067	-0.007	-0.183
4	1.225	1.034	0.904	0.807	0.211	0.623	5.914	-4.040
5	1.523	1.310	1.649	1.678	0.969	1.489	8.326	0.974
6	1.632	1.623	2.128	2.065	0.991	0.820	1.044	0.791
7	1.977	1.976	2.411	2.329	1.494	0.864	1.441	2.711
8	2.579	2.640	2.612	2.098	1.811	2.665	5.330	-262.760
9	3.852	3.865	4.340	4.141	3.514	4.077	8.702	-251.754
10	4.154	4.456	3.831	4.036	2.883	2.502	5.633	3.143
11	4.399	4.318	4.553	4.095	2.796	3.612	7.284	-257.878

Table S6: **ADUHOY**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	4.985	4.878	-2.103	1.954	1.132	1.041	3.880
3	-0.031	-0.748	-13.289	0.551	0.065	-6.379	0.584
4	1.022	2.304	-9.740	0.079	-0.181	-8.312	7.706
5	2.763	3.248	-15.320	0.349	0.488	-11.367	9.754
6	2.137	1.921	-7.240	0.902	0.552	-3.405	1.293
7	2.647	1.843	-10.759	1.313	0.648	-4.650	1.722
8	3.929	6.477	-16.731	2.051	1.782	-11.524	9.185
9	6.384	9.144	-12.042	2.599	2.547	-10.647	10.906
10	4.236	4.094	-10.573	2.663	1.854	-5.045	6.266
11	7.070	8.807	9.107	2.103	1.999	4.531	4.993

Table S7: **ADUHOY**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	1.644	1.680	0.806
3	0.526	0.737	0.127
4	-2.357	-2.295	0.448
5	-1.695	-1.828	0.973
6	1.646	1.387	0.704
7	1.372	1.288	0.669
8	0.909	1.170	1.657
9	2.888	2.987	3.565
10	1.564	2.024	3.343
11	1.180	1.331	1.859

Table S8: **AKECIC**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.162	0.173	0.669	0.233	1.454	0.549	-0.063	3.600
3	0.264	0.290	0.690	0.367	1.466	0.681	0.015	2.634
4	0.627	0.534	1.278	0.513	2.352	0.914	0.612	8.162
5	0.682	0.528	1.253	0.501	2.320	0.930	0.558	7.711
6	0.769	0.708	1.250	0.569	2.386	1.056	0.640	6.982
7	1.272	1.535	1.515	1.540	1.256	0.899	2.225	-3.382
8	1.427	1.699	1.785	1.588	1.590	1.417	2.224	-5.142
9	1.474	1.589	1.885	1.572	1.906	1.302	2.111	-4.999
10	1.597	1.233	2.308	1.115	3.293	0.236	0.884	16.068
11	1.693	1.721	1.920	1.700	2.021	1.375	2.087	-5.557
12	1.876	1.943	2.150	1.641	2.475	1.579	2.547	-3.031
13	1.940	1.583	2.668	1.948	1.291	0.580	1.652	25.934
14	2.012	2.079	2.612	1.974	3.093	1.946	2.386	0.095
15	4.255	4.276	4.693	4.393	2.141	0.772	0.901	26.738
16	4.506	4.559	4.739	4.624	2.436	0.939	0.881	24.030
17	5.205	5.053	5.725	5.145	4.274	1.664	1.076	27.280
18	5.304	5.073	5.589	5.188	4.024	1.678	1.043	26.609
19	5.620	5.149	6.002	5.300	3.772	1.529	1.753	30.468
20	6.409	6.747	6.617	7.616	4.101	3.255	5.931	12.636
21	7.311	7.594	8.153	8.373	5.924	4.117	6.929	35.133

Table S9: **AKECIC**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	9.909	5.643	1.577	2.961	2.347	-4.832	-1.136
3	4.064	1.875	-2.341	1.891	1.260	-6.229	0.880
4	8.072	4.996	-0.388	3.743	2.354	-7.512	-1.390
5	3.454	1.699	-2.719	1.469	1.035	-8.407	-0.480
6	9.014	5.090	-1.950	2.651	1.951	-6.508	0.462
7	2.652	1.468	-1.230	1.391	1.609	-6.355	3.012
8	2.308	1.636	0.955	1.961	1.922	-2.737	3.232
9	2.964	2.099	-0.611	2.539	2.074	-4.820	3.145
10	2.689	1.950	-3.746	3.097	0.335	-4.939	-0.411
11	3.392	2.491	-0.668	2.421	2.208	-5.060	3.251
12	2.665	2.037	-3.582	3.032	2.105	-4.006	3.515
13	3.464	2.239	-1.882	-0.560	0.878	-10.063	0.580
14	4.579	2.416	-2.472	3.766	2.397	-4.725	1.891
15	15.811	3.574	-1.789	3.829	1.314	-6.268	0.415
16	6.412	4.813	-0.076	1.297	1.670	-8.414	0.041
17	7.708	5.454	-0.587	3.769	2.364	-7.337	-1.310
18	6.097	4.936	-3.132	3.932	2.180	-6.283	0.244
19	6.230	5.084	-2.410	3.893	2.243	-6.280	0.217
20	8.182	6.311	2.487	3.812	3.888	-4.584	6.507
21	9.034	7.826	4.128	4.196	4.657	-4.758	5.811

Table S10: **AKECIC**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	0.470	0.323	-1.058
3	0.809	0.720	-0.513
4	0.473	0.613	-1.582
5	0.467	0.605	-1.735
6	0.726	0.883	-1.295
7	0.692	1.321	0.693
8	0.225	1.141	0.334
9	0.041	0.978	-0.106
10	0.605	0.803	-1.715
11	0.072	0.991	0.052
12	0.467	1.664	0.018
13	-1.654	-1.374	-5.149
14	0.596	1.454	-0.815
15	1.896	1.662	2.061
16	2.334	2.265	3.191
17	2.899	2.877	2.213
18	3.005	2.966	2.584
19	2.641	2.603	0.779
20	3.154	3.201	3.823
21	2.555	2.446	1.499

Table S11: **AMOZEH**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.600	0.550	0.824	1.279	1.179	1.973	1.896	2.099
3	0.729	0.643	0.990	2.160	0.402	0.980	0.848	-0.728
4	0.767	0.588	1.230	1.376	1.921	1.644	1.072	6.908
5	0.878	0.265	0.160	1.034	-1.043	0.094	-0.346	-3.495
6	1.074	0.313	0.524	1.437	0.678	0.809	0.529	2.460
7	1.194	0.742	1.249	1.515	1.799	1.371	0.951	7.269
8	1.335	0.338	0.526	1.556	1.316	0.083	-0.860	-0.049
9	1.494	0.556	0.438	1.382	-1.100	-0.094	-0.539	-2.824
10	1.673	0.776	0.796	1.310	0.594	0.295	-0.501	2.688
11	3.002	2.453	2.155	3.679	1.179	1.259	-0.295	-6.493
12	3.235	3.109	2.479	3.638	1.913	1.830	-3.579	-9.144
13	3.387	1.994	2.129	3.493	1.761	1.880	-0.895	-4.608
14	3.534	2.723	2.836	2.574	0.690	0.014	-0.493	3.198
15	3.620	2.978	3.023	2.862	0.891	0.624	0.265	0.863
16	3.645	3.123	3.108	4.451	1.428	2.271	0.374	-5.412
17	3.713	2.383	2.390	3.568	2.021	2.127	-0.425	-2.993
18	4.204	3.632	2.928	4.627	3.110	1.517	-2.337	-9.790
19	4.238	3.860	3.469	3.742	1.733	1.551	1.369	3.782
20	4.407	3.925	3.849	5.327	3.036	1.009	-1.444	-4.463
21	4.576	5.031	4.128	6.283	4.461	3.971	-0.637	-3.397
22	4.634	3.685	3.329	5.415	1.823	1.300	-3.635	-7.362
23	4.740	4.063	4.746	5.293	0.481	0.618	-80.884	1.352
24	4.820	4.578	3.638	5.842	2.331	1.745	-1.986	-9.734
25	4.840	4.334	3.738	6.198	2.140	2.484	-3.710	-10.817
26	5.138	4.499	4.082	6.018	2.426	2.693	-2.153	-8.438
27	5.273	4.508	4.119	5.286	1.516	1.371	-1.290	-1.470
28	5.376	4.613	4.138	5.520	1.447	1.239	-1.441	-4.076
29	7.343	6.549	6.668	6.836	1.546	2.449	-80.711	23.944

Table S12: **AMOZEH**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	1.402	2.002	1.497	1.151	1.517	-0.312	1.000
3	0.262	-0.100	0.054	1.281	1.528	-0.136	1.372
4	2.289	1.217	1.532	0.360	0.944	-0.591	-0.843
5	-0.026	0.112	-0.049	-0.448	0.529	-1.378	0.746
6	1.783	0.983	0.523	0.464	0.848	0.796	1.394
7	2.407	0.897	1.299	0.290	0.954	-0.787	-0.865
8	1.272	0.231	0.880	0.552	0.273	0.454	0.389
9	-0.038	-0.023	1.155	-0.337	0.289	-0.632	0.327
10	0.437	0.554	0.479	1.056	0.401	0.258	0.612
11	2.371	1.744	3.077	1.235	1.431	0.201	2.056
12	3.017	2.923	2.288	1.637	1.498	4.175	79.381
13	1.986	1.544	2.539	1.291	1.638	0.685	1.011
14	2.664	2.594	3.531	1.245	0.033	1.440	-0.374
15	2.759	2.009	3.346	1.548	1.193	1.507	1.544
16	2.607	2.001	2.420	2.025	1.976	0.576	2.306
17	2.160	1.885	2.416	1.713	1.991	0.713	1.099
18	4.453	3.619	2.733	0.868	0.412	-1.435	-0.638
19	3.322	2.734	4.794	2.162	1.946	1.847	2.209
20	4.975	4.268	6.355	1.507	0.350	1.870	-0.278
21	4.839	4.584	4.573	2.390	2.990	1.517	1.252
22	3.127	3.033	3.110	2.178	1.362	5.201	80.060
23	5.166	4.064	2.680	0.713	1.120	-0.665	1.844
24	4.662	3.905	3.433	1.309	1.166	0.135	0.439
25	3.827	3.975	3.149	1.853	1.464	4.549	80.315
26	4.416	4.401	4.642	1.780	1.702	0.434	1.168
27	4.329	3.880	4.033	1.315	1.096	-0.583	0.183
28	5.130	3.894	3.308	1.260	1.179	-0.960	0.257
29	7.211	6.534	6.751	1.828	2.318	1.648	1.232

Table S13: **AMOZEH**: Conformational heats of formation in kcal·mol^{-1}.

SPE	PM6	PM6-D3H4X	PM7
GEO	B97-3c	B97-3c	B97-3c
1	0.000	0.000	0.000
2	2.871	3.265	2.718
3	2.653	2.656	1.497
4	4.079	3.896	2.121
5	-1.775	-2.325	-1.200
6	2.501	2.650	1.442
7	4.593	4.214	2.661
8	1.335	1.180	0.510
9	-1.787	-2.413	-1.154
10	-0.804	-1.201	-1.071
11	-0.614	-1.131	2.174
12	-1.520	-1.215	2.363
13	-2.093	-1.618	0.289
14	-4.019	-2.992	-1.733
15	-3.797	-2.797	-0.498
16	-0.458	-0.740	2.187
17	-1.274	-0.804	1.046
18	1.034	1.757	3.806
19	-3.238	-2.056	-0.503
20	2.492	2.393	3.145
21	5.850	6.278	6.706
22	-1.860	-1.890	1.648
23	1.425	1.522	-0.819
24	3.690	4.701	4.179
25	-1.183	-0.567	4.522
26	-1.006	-0.081	4.910
27	-2.612	-2.063	-0.079
28	-2.554	-2.078	-0.024
29	1.009	0.731	1.503

Table S14: **AXURER**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.342	0.286	0.369	0.317	0.506	0.566	0.621	1.991
3	0.682	1.301	0.149	-1.635	1.860	5.736	7.364	20.474
4	0.703	0.764	0.290	-0.148	-0.451	3.731	-1.631	22.084
5	1.526	1.133	1.090	0.716	0.691	2.605	-5.504	33.141
6	1.740	1.942	1.861	0.885	0.240	4.651	3.726	6.892
7	1.969	2.035	1.392	0.430	1.739	6.519	-0.250	41.265
8	2.004	2.161	2.304	1.180	1.326	4.171	3.585	0.473
9	2.045	2.076	2.260	1.604	1.211	3.108	2.749	-3.225
10	2.072	2.159	2.309	1.248	1.358	4.176	3.445	1.821
11	2.393	2.296	2.537	1.491	1.437	5.226	2.195	16.099
12	2.474	2.381	2.539	1.572	1.356	3.764	3.136	0.753
13	2.757	2.511	2.777	2.111	1.655	3.300	2.105	1.984
14	2.826	2.781	2.980	1.885	1.838	4.337	2.687	9.280
15	3.612	3.427	3.234	2.797	1.387	5.499	-1.302	27.638
16	4.745	4.636	4.979	3.634	2.407	6.805	5.801	2.524
17	5.210	5.103	4.908	3.710	2.705	8.803	3.525	12.177

Table S15: **AXURER**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.241	0.385	3.187	-0.079	0.021	3.787	-0.020
3	2.325	4.862	19.768	3.085	3.551	14.824	2.957
4	-1.698	2.240	2.760	0.314	0.292	4.164	0.027
5	-0.975	0.161	1.707	1.676	0.223	0.849	-1.096
6	2.469	2.950	14.832	3.468	4.282	13.273	3.009
7	-3.295	2.620	14.143	3.231	5.258	15.505	-3.462
8	1.924	0.586	-0.199	2.052	0.049	-0.083	0.014
9	0.767	1.233	11.863	1.737	0.035	8.524	3.096
10	0.887	0.631	14.458	1.755	0.053	12.684	3.066
11	0.729	4.958	10.312	1.684	3.974	7.711	-0.942
12	0.408	1.236	11.533	2.102	0.040	8.649	3.115
13	1.280	2.992	12.256	1.908	2.807	8.353	3.160
14	1.529	4.365	13.282	2.041	3.619	9.570	3.266
15	0.471	0.118	1.753	2.768	0.221	0.828	-1.101
16	2.038	1.269	23.539	3.663	0.058	17.200	6.587
17	2.401	4.661	14.796	3.424	3.803	13.138	3.019

Table S16: **AXURER**: Conformational heats of formation in kcal·mol^{-1}.

SPE	PM6	PM6-D3H4X	PM7
GEO	B97-3c	B97-3c	B97-3c
1	0.000	0.000	0.000
2	0.212	0.145	0.633
3	-2.620	-4.003	6.917
4	-2.478	-2.061	4.494
5	-3.958	-3.235	5.120
6	-1.406	-1.538	1.853
7	-3.593	-3.987	7.847
8	-3.285	-3.365	0.535
9	-4.267	-4.193	-0.581
10	-3.542	-3.581	0.523
11	-0.393	-0.818	4.097
12	-3.853	-3.724	-0.343
13	-3.641	-3.535	0.549
14	-2.509	-2.662	2.483
15	-7.018	-6.242	4.655
16	-7.302	-7.202	0.808
17	-2.185	-2.207	6.737

Table S17: **AYISEG**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.260	0.091	-0.008	0.033	-1.048	-0.619	-2.480	-14.151
3	0.315	0.110	-0.023	0.046	-1.102	-0.670	-2.367	-14.295
4	0.840	0.758	1.256	1.385	0.287	0.834	-2.009	-13.156
5	1.020	0.841	1.332	1.531	0.658	1.057	-2.718	-14.493
6	5.592	4.655	5.446	4.618	4.961	4.247	8.769	-19.077
7	5.759	4.619	5.116	3.822	1.713	1.727	4.285	-9.068
8	5.927	4.825	5.156	4.443	4.040	2.608	9.529	-14.503
9	5.934	5.102	5.754	5.426	3.305	1.752	6.117	-15.418
10	6.147	4.994	5.982	4.739	2.524	2.616	5.079	-7.653
11	6.151	5.391	6.677	6.060	5.644	3.481	13.489	-23.861
12	6.222	5.732	6.833	4.037	3.797	2.321	-3.283	-4.331
13	6.735	7.503	8.607	6.059	2.123	-0.289	-10.554	16.188
14	6.955	7.233	8.089	5.525	2.706	2.717	-4.728	2.637
15	7.062	7.163	7.855	4.168	-0.223	-0.943	-12.334	3.005
16	7.377	7.134	6.967	7.784	2.883	2.792	-5.025	-17.736
17	7.533	7.610	8.599	6.051	2.314	1.034	-0.228	-1.249
18	7.832	7.463	7.045	7.516	3.659	2.059	-3.146	-20.662
19	7.848	7.465	7.270	7.999	5.456	4.480	10.014	-11.255
20	8.027	7.578	6.820	7.238	2.505	0.083	-0.444	-3.701
21	8.156	7.508	8.496	7.864	4.225	3.278	-6.877	1.273
22	8.295	8.112	7.193	8.072	2.813	1.633	-1.809	-0.875
23	8.860	8.924	9.685	9.676	3.168	1.532	2.197	-9.870
24	8.911	8.852	8.135	8.930	3.826	0.416	2.199	-11.223
25	10.124	10.376	10.659	11.318	3.503	1.092	1.097	4.095
26	12.515	12.161	13.019	10.496	4.196	0.045	-6.904	12.392
27	12.693	12.229	13.370	10.948	5.160	0.827	-6.529	14.705
28	15.650	15.540	15.791	13.376	4.136	0.735	-5.716	16.258

Table S18: **AYISEG**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.121	1.417	4.376	-0.580	-0.772	1.237	-3.759
3	-0.252	0.298	-3.139	-0.589	-0.718	-1.367	1.271
4	3.061	0.783	1.989	-0.574	0.010	1.843	-12.990
5	1.536	1.246	-31.219	0.091	0.691	-18.645	-1.939
6	16.017	8.821	7.690	0.491	1.896	-3.594	-51.753
7	7.084	7.453	15.125	2.009	0.565	11.123	-55.964
8	4.535	7.382	26.783	2.071	0.686	22.231	-54.630
9	11.077	7.961	4.363	2.444	0.986	-0.828	-50.756
10	15.382	7.644	41.509	1.142	0.951	18.361	-67.203
11	8.479	8.804	14.272	2.534	2.024	12.231	-56.191
12	18.502	12.102	30.498	1.980	0.677	10.966	-68.425
13	9.100	5.221	-6.563	3.099	0.669	-11.875	-46.556
14	15.952	8.482	7.579	0.974	2.289	-3.917	-53.892
15	6.114	4.740	-27.481	0.942	0.108	-12.554	2.843
16	11.882	10.218	17.026	-1.470	-4.375	-1.749	-101.468
17	12.250	8.252	0.610	1.628	0.700	-11.294	-49.093
18	10.791	10.806	0.061	-0.300	-5.517	-6.149	-97.445
19	10.397	9.966	-6.651	0.536	-4.982	-5.924	-97.781
20	6.954	8.960	-7.113	0.007	-6.551	-6.541	-30.725
21	9.751	10.364	12.459	1.134	-2.626	7.953	-32.783
22	10.074	8.668	6.328	-1.504	-5.493	-6.159	-97.258
23	10.351	9.987	10.641	1.894	-4.034	-3.291	-101.526
24	9.155	9.707	-9.359	-0.347	-6.678	-9.805	-91.926
25	11.997	12.834	-10.710	-0.938	-6.334	-10.193	-89.914
26	13.194	13.655	-3.876	-0.697	-8.435	-6.595	-106.792
27	12.920	13.344	-4.317	0.453	-7.383	-8.412	-106.954
28	15.426	16.031	-4.495	1.782	-6.386	-8.088	-105.608

Table S19: **AYISEG**: Conformational heats of formation in kcal·mol^{-1}.

SPE	PM6	PM6-D3H4X	PM7
GEO	B97-3c	B97-3c	B97-3c
1	0.000	0.000	0.000
2	-1.106	-1.166	0.070
3	-1.066	-1.102	0.069
4	-0.610	-0.806	0.578
5	-0.095	-0.428	0.692
6	-9.333	-9.693	-2.709
7	-14.218	-14.202	-3.021
8	-10.436	-10.176	-3.097
9	-15.271	-14.683	-3.436
10	-14.831	-14.937	-3.080
11	-12.468	-12.319	-4.750
12	-14.374	-13.045	0.084
13	-33.344	-32.329	-6.527
14	-18.960	-18.122	-1.008
15	-30.227	-29.234	-3.824
16	-24.351	-24.403	-7.326
17	-20.581	-19.122	-0.319
18	-24.357	-23.775	-7.315
19	-14.260	-14.241	-6.334
20	-23.442	-22.412	-7.341
21	-25.950	-25.065	-7.475
22	-23.571	-22.796	-7.005
23	-6.906	-5.379	-1.249
24	-24.345	-23.052	-7.804
25	-23.673	-23.259	-8.067
26	-30.119	-27.750	-10.844
27	-27.803	-25.423	-9.534
28	-29.727	-27.179	-8.076

Table S20: **BIDHON**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.387	0.134	0.070	0.308	0.493	0.385	-0.445	1.608
3	0.397	0.585	0.687	-0.562	2.389	-0.574	1.306	11.955
4	0.431	0.492	0.901	0.372	0.814	-0.367	-0.779	2.923
5	0.437	0.505	0.649	-0.759	2.121	-0.777	1.420	8.193
6	0.589	0.497	0.721	-0.553	3.199	-0.152	1.210	1.270
7	0.680	0.382	0.339	0.327	1.531	0.890	-0.584	-5.831
8	0.836	1.092	0.808	-0.221	1.791	-0.707	2.224	4.626
9	0.907	1.026	0.789	-0.271	2.122	-0.667	2.190	4.913
10	1.068	0.594	0.633	0.359	0.770	-0.116	-0.550	3.000
11	1.140	1.287	1.354	0.095	2.624	-0.225	1.553	8.281
12	1.432	1.465	1.729	0.470	3.803	0.221	0.999	0.306
13	1.478	1.341	1.559	0.270	3.681	0.273	1.525	0.960
14	1.706	1.955	2.837	0.611	1.090	-1.300	0.039	34.233
15	1.855	2.148	1.873	0.592	1.752	-0.185	1.043	18.174
16	1.975	2.350	2.738	0.249	2.914	-0.718	1.041	15.201
17	2.027	2.154	1.856	0.549	2.227	0.029	1.103	14.861
18	2.085	2.393	2.801	0.134	2.671	-0.841	0.857	22.133
19	2.139	2.254	2.552	0.410	3.136	-1.098	0.058	7.345
20	2.688	2.931	2.575	1.208	2.434	0.366	1.398	15.353
21	2.805	2.910	2.616	1.305	2.701	0.450	1.375	14.020
22	2.989	3.261	2.967	0.541	3.537	0.064	0.020	11.327
23	3.042	3.345	3.176	0.536	3.755	0.033	1.098	15.777
24	3.151	3.466	3.779	1.135	3.085	-0.492	1.240	24.431
25	3.162	3.202	2.893	0.516	3.547	0.131	0.299	8.232
26	3.386	3.129	2.770	1.929	4.620	1.946	0.263	-0.496

Table S21: **BIDHON**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	-2.106	1.378	-1.205	0.412	0.302	0.117	-0.717
3	6.419	4.506	2.701	-2.093	-0.781	7.496	-0.387
4	-0.736	-0.580	-1.950	-0.451	-0.944	-1.346	-0.857
5	6.869	5.054	2.422	-2.017	-1.860	7.310	-0.177
6	8.744	5.052	3.288	-2.586	-0.900	8.382	-0.466
7	3.362	2.495	0.888	-0.523	0.611	2.398	-1.356
8	-3.306	-14.225	3.499	-0.439	1.864	10.022	-1.611
9	-2.977	-14.304	1.225	-0.626	1.934	6.651	-0.425
10	5.171	3.068	0.123	-0.705	-0.734	1.136	-0.672
11	6.935	5.947	3.504	-1.891	0.143	7.961	-0.356
12	8.026	4.972	2.423	-2.148	-0.748	7.795	-0.232
13	8.845	5.172	3.009	-2.323	-0.778	7.774	-0.596
14	3.769	3.299	-0.113	-1.464	-0.278	4.325	-0.434
15	3.498	1.807	2.708	-1.431	-3.065	7.394	-0.254
16	1.072	-13.234	-0.844	0.900	3.150	11.145	-2.699
17	4.062	2.747	1.174	-1.507	-2.839	6.381	-0.324
18	-0.128	-14.402	-1.836	0.618	3.021	8.264	-1.243
19	2.477	-15.444	-1.092	0.962	3.096	10.445	-0.717
20	4.004	1.813	3.310	-1.253	-3.011	7.554	-0.183
21	4.377	3.010	3.043	-1.331	-2.734	7.528	-0.268
22	-0.680	3.528	-2.753	0.888	-0.480	6.311	-0.687
23	-0.887	3.538	-1.905	1.880	-0.022	7.154	-0.868
24	1.465	-13.435	-1.097	1.049	3.395	8.715	-1.263
25	-0.423	3.982	-2.718	1.077	-0.334	6.637	-0.997
26	5.879	3.802	0.581	0.871	-2.681	7.399	0.170

Table S22: **BIDHON**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	0.268	0.687	0.089
3	-0.602	0.442	-3.468
4	1.313	1.014	0.528
5	-0.765	0.276	-3.472
6	-0.397	0.671	-2.904
7	1.335	2.008	1.845
8	-1.387	0.303	-5.054
9	-0.946	0.570	-4.740
10	1.311	1.460	0.753
11	-0.351	0.566	-3.180
12	0.237	1.302	-1.392
13	0.164	1.359	-2.194
14	0.093	0.502	-2.887
15	-0.536	1.276	-4.941
16	-1.926	1.395	-2.061
17	-0.631	1.262	-5.165
18	-1.797	1.424	-2.001
19	-2.661	0.306	-2.430
20	0.112	1.972	-4.447
21	0.066	1.975	-4.348
22	-1.089	1.639	-2.001
23	-1.236	1.867	-1.788
24	-1.328	1.883	-1.294
25	-1.451	1.469	-2.269
26	1.369	3.513	-2.461

Table S23: **CNETPA**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.673	0.605	0.817	0.128	1.073	0.813	2.404	-7.336
3	1.388	0.999	0.907	0.815	0.664	0.364	2.534	-1.563
4	1.755	1.854	2.151	1.528	1.919	1.717	3.273	-1.403
5	2.332	2.153	1.994	2.404	-0.333	0.283	5.386	-1.102
6	3.370	3.020	2.962	3.103	2.213	1.378	3.867	1.056
7	3.582	3.457	3.371	3.658	1.015	1.787	5.092	-2.578
8	3.739	4.093	4.869	3.980	1.125	2.545	10.853	-6.310
9	3.788	4.260	4.747	4.735	1.132	1.596	9.343	-0.530
10	3.854	3.910	4.147	3.774	1.358	1.905	8.990	-2.113
11	3.988	4.152	4.555	4.681	0.411	1.668	10.238	3.677
12	4.014	4.060	3.931	3.773	1.614	1.721	6.377	-4.411
13	4.054	4.176	4.774	4.346	0.962	1.968	10.119	-3.713
14	4.630	4.918	5.534	5.296	1.754	2.451	10.039	-2.302
15	4.664	4.701	5.104	4.795	1.642	2.509	10.718	-2.351
16	4.844	5.259	5.697	5.381	1.833	2.856	11.070	3.265
17	4.983	5.269	5.277	5.791	1.740	2.256	7.373	-1.957
18	5.409	5.326	5.635	5.207	2.014	2.371	12.817	0.561
19	5.511	5.626	6.080	5.348	2.605	3.071	10.310	-4.926
20	5.517	5.398	5.689	5.307	1.971	2.431	10.100	-4.038
21	5.547	5.674	6.176	5.373	2.471	3.444	12.264	-2.358
22	6.117	6.168	6.915	7.299	1.397	2.688	15.708	2.726
23	6.137	6.020	6.564	6.445	2.573	3.355	11.635	0.801
24	6.327	5.963	6.351	6.265	2.283	3.395	12.742	3.662
25	6.675	6.942	8.089	6.921	2.725	4.349	17.700	-2.495

Table S24: **CNETPA**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.511	0.572	-4.609	1.282	0.833	-1.298	2.878
3	2.479	0.151	-3.863	0.360	0.478	-0.827	1.195
4	4.197	2.737	2.619	1.011	1.579	2.253	3.069
5	5.406	1.076	-2.728	-1.681	0.428	-0.613	2.012
6	4.800	2.902	-0.973	1.204	1.630	1.160	1.506
7	6.009	3.481	-1.145	0.273	2.956	0.482	4.603
8	5.861	5.782	-3.099	0.450	2.281	-3.453	11.202
9	6.364	4.469	-1.885	0.068	1.585	-1.749	7.736
10	6.387	5.021	-3.855	0.211	1.520	-0.704	1.192
11	7.005	5.520	0.060	-0.908	1.443	-0.436	6.740
12	6.920	3.319	-1.202	0.330	1.810	0.490	4.216
13	6.099	5.667	0.992	0.097	1.549	1.199	9.591
14	6.899	5.501	-2.580	0.855	2.431	-2.798	9.081
15	6.485	6.957	0.206	0.774	2.054	0.227	9.290
16	6.826	5.502	-0.729	1.047	2.890	-1.975	9.504
17	7.104	4.401	0.281	0.879	2.707	1.336	5.313
18	7.696	7.589	0.105	0.672	1.909	0.454	9.098
19	8.346	6.601	6.224	1.489	2.464	5.419	5.647
20	7.931	7.015	0.257	1.027	1.911	0.699	9.101
21	7.992	7.281	6.437	1.550	3.051	3.041	7.126
22	8.648	7.340	-1.118	0.276	2.589	0.507	4.610
23	9.155	5.012	2.002	0.985	1.581	3.489	10.501
24	8.588	7.943	0.049	0.948	2.685	0.151	9.287
25	9.825	9.901	-3.014	1.446	3.902	-3.349	11.195

Table S25: **CNETPA**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	-0.371	0.161	1.041
3	-0.849	-0.187	-0.070
4	-1.420	-1.299	0.313
5	-0.746	-0.291	0.860
6	0.638	0.991	0.456
7	1.634	1.939	2.751
8	0.469	0.984	3.266
9	0.008	0.447	1.376
10	-1.107	-0.819	1.277
11	1.561	1.805	3.745
12	0.087	0.871	3.166
13	0.665	0.736	2.178
14	0.641	1.224	2.920
15	0.557	0.853	2.953
16	2.500	3.028	5.452
17	2.183	2.239	4.089
18	-0.065	0.593	2.967
19	-0.478	0.214	2.952
20	-0.292	0.042	2.585
21	0.988	1.597	4.453
22	1.541	2.398	6.352
23	2.037	2.400	3.083
24	2.766	3.052	3.060
25	1.771	2.107	4.992

Table S26: **EFOYEG**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.257	0.337	0.410	0.318	0.240	0.193	-0.068	-6.146
3	0.891	0.811	0.384	1.376	-0.084	0.081	-0.097	3.733
4	1.004	0.914	0.746	1.445	0.649	0.161	-0.214	-3.030
5	1.291	1.432	1.335	1.270	0.771	0.233	16.113	-9.507
6	1.628	1.789	1.873	2.169	0.767	0.865	0.486	-8.719
7	1.915	1.732	1.756	2.788	0.920	-0.431	0.950	-1.603
8	2.184	1.634	1.747	2.250	1.105	-0.809	-0.805	-13.003
9	2.335	2.187	2.261	3.012	1.249	-0.235	1.365	-0.501
10	2.402	2.031	2.240	2.391	1.471	-0.532	-0.220	-12.829
11	2.440	2.414	1.998	2.917	0.860	-0.438	0.471	4.710
12	2.468	1.889	2.012	1.962	1.808	-1.097	15.938	-11.113
13	2.768	2.391	2.463	3.031	1.564	0.050	-3.073	-4.813
14	3.081	2.771	3.200	2.703	4.923	0.430	15.337	-21.950
15	3.160	2.625	2.868	2.412	2.793	-0.024	17.041	-4.038
16	4.738	3.974	3.982	3.807	3.053	1.453	1.403	-6.211
17	4.930	4.066	4.007	3.875	3.772	0.238	16.073	-10.642
18	6.205	6.394	6.084	7.299	0.237	3.038	-1.127	159.601
19	7.443	7.451	7.304	7.823	1.386	4.470	0.310	158.739
20	8.401	7.883	7.392	8.678	4.256	4.415	0.050	149.169
21	8.407	8.440	8.014	9.064	5.106	5.446	-19.971	159.470
22	8.443	8.469	8.009	8.379	5.882	5.490	-20.110	147.026
23	8.816	8.443	7.650	8.471	3.968	4.027	0.253	146.880
24	9.425	9.853	9.301	11.104	1.370	4.729	-2.891	182.844
25	12.214	12.673	11.865	14.169	0.943	5.639	3.641	4.453
26	12.431	13.086	12.250	14.223	1.529	6.020	4.303	4.799
27	12.942	13.252	12.795	15.082	1.769	6.526	4.366	7.619
28	14.308	14.485	13.527	15.827	0.631	6.216	5.044	13.285

Table S27: **EFOYEG**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.336	1.187	0.165	0.384	0.229	0.243	0.270
3	0.628	0.781	-0.195	-0.433	-0.107	0.203	0.426
4	1.395	1.186	4.301	0.351	-0.094	2.781	-0.508
5	1.555	2.019	1.961	0.643	0.119	0.584	0.056
6	1.885	2.079	2.294	0.831	0.877	1.180	0.854
7	2.552	1.862	2.883	0.317	-0.340	2.825	0.740
8	1.613	1.796	5.751	1.448	-0.833	4.364	-1.817
9	3.030	2.351	3.142	0.682	-0.231	3.004	1.036
10	2.113	2.889	6.078	1.739	-0.845	4.611	-0.925
11	3.047	2.718	2.403	0.019	-0.731	2.555	-26.217
12	2.724	2.554	1.888	1.480	-1.345	4.311	-0.508
13	3.654	3.139	0.645	0.320	-0.244	2.685	0.162
14	5.575	4.061	9.471	1.792	-0.071	7.795	-1.566
15	4.109	5.073	4.298	2.446	-1.442	4.111	-1.280
16	4.536	4.856	4.332	2.394	0.623	3.561	-0.607
17	5.892	5.486	4.036	1.146	-0.830	3.193	0.434
18	7.559	5.893	15.811	-0.683	3.608	9.142	-33.902
19	9.684	7.766	18.878	0.169	4.897	9.033	-33.228
20	10.617	7.332	12.881	-0.367	4.341	11.522	-32.755
21	11.974	9.852	13.602	0.214	6.786	11.071	-32.443
22	11.270	9.324	21.000	-0.274	3.316	10.215	-31.867
23	10.687	8.110	15.831	-0.442	3.868	10.880	-32.475
24	11.933	10.239	21.256	0.735	4.450	8.959	-34.248
25	12.711	11.736	22.561	0.827	5.511	10.069	-32.879
26	13.014	12.227	22.631	1.360	6.237	10.613	-32.308
27	14.602	14.153	23.961	1.623	6.268	11.550	-32.054
28	13.865	10.691	24.508	0.492	5.424	11.381	-31.563

Table S28: **EFOYEG**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	1.051	0.903	1.012
3	1.974	1.198	0.312
4	0.850	0.084	-0.182
5	3.062	2.536	3.278
6	2.104	1.698	2.343
7	0.140	-1.166	-2.318
8	1.006	-0.773	-2.787
9	0.632	-0.589	-2.007
10	1.496	-0.105	-1.987
11	2.889	1.271	-0.695
12	0.891	-0.788	-2.548
13	2.692	1.494	0.053
14	2.445	1.065	0.461
15	1.759	0.683	-2.362
16	2.344	1.776	-0.407
17	4.667	3.275	2.090
18	15.165	12.988	23.821
19	15.303	13.816	24.309
20	12.518	10.807	19.953
21	11.521	10.375	18.749
22	12.837	11.848	19.860
23	14.620	12.754	21.962
24	12.597	10.731	19.443
25	15.873	14.585	23.398
26	16.526	15.453	24.061
27	15.624	14.644	22.844
28	16.272	14.612	22.829

Table S29: **ESOGEA**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.079	0.126	0.554	0.241	0.687	0.150	0.506	3.529
3	0.493	0.054	0.445	0.395	1.599	1.689	-19.719	-6.041
4	0.542	-0.317	-0.492	0.010	0.566	0.289	-19.975	-4.274
5	0.553	0.707	0.355	0.832	0.845	0.361	0.278	2.769
6	0.578	-0.268	-0.018	-0.032	0.331	1.148	0.232	-7.558
7	0.599	-0.091	-0.340	-0.180	0.448	0.666	-20.309	-5.107
8	0.805	0.509	0.177	0.871	0.715	0.665	-18.189	-2.610
9	0.814	-0.199	-0.524	0.114	0.545	0.255	-20.094	-5.380
10	0.881	1.172	0.738	1.326	0.691	0.320	0.386	3.793
11	0.893	0.969	0.696	1.041	0.899	0.579	0.610	4.940
12	0.922	-0.142	-0.452	0.066	0.644	2.251	-21.047	-13.422
13	1.077	1.525	1.596	1.884	1.043	0.096	1.264	8.038
14	1.104	0.054	-0.355	0.391	0.551	2.228	-0.475	-14.435
15	1.245	1.452	1.180	1.439	0.732	0.433	0.799	6.642
16	1.488	0.681	0.217	0.982	0.446	-0.036	-19.774	-3.931
17	1.590	0.946	0.277	1.092	0.832	0.784	-19.096	-3.313
18	1.608	1.079	0.519	1.172	1.087	1.197	-18.368	-3.319
19	1.625	0.556	-0.233	0.621	1.090	1.037	-20.185	-6.221
20	1.652	0.902	0.542	1.395	1.255	2.277	-0.221	-14.314
21	1.665	0.749	0.072	0.676	0.395	-0.069	-19.560	-2.955
22	1.813	0.489	0.394	0.608	0.454	0.689	-0.305	-10.552
23	1.868	1.434	2.331	1.580	1.631	0.598	0.837	0.759
24	1.972	1.192	0.276	1.333	1.156	1.385	-21.024	-9.032
25	2.081	1.503	1.399	1.429	1.588	1.483	-0.337	-5.524
26	2.189	0.994	0.076	1.107	0.736	0.968	-20.424	-8.031

Table S30: **ESOGEA**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	-0.109	-0.060	1.073	0.809	0.036	0.754	22.670
3	0.401	1.158	-1.992	1.476	0.483	-1.779	23.123
4	-0.618	-0.468	63.979	0.316	-0.955	57.324	-37.267
5	0.676	0.011	-1.426	0.889	0.115	-1.722	23.175
6	-0.140	0.640	1.715	0.072	-0.344	-1.091	-1.995
7	-0.433	-0.073	5.596	0.173	-0.624	1.392	-2.346
8	-0.344	-0.223	3.386	0.751	0.138	1.065	0.582
9	-0.575	-0.486	4.338	0.079	-0.971	1.888	-2.357
10	0.207	0.190	1.541	0.786	0.277	0.383	22.910
11	1.294	0.309	1.264	0.819	0.293	1.131	23.182
12	-0.658	0.318	-0.916	0.272	-0.124	-0.936	-3.134
13	1.048	0.630	4.100	1.047	0.123	1.435	23.497
14	-0.800	0.295	-0.522	0.142	-0.143	-1.004	-3.295
15	1.976	0.533	2.149	0.583	0.440	1.182	23.180
16	0.093	-0.446	4.658	0.022	-0.676	2.468	-1.993
17	0.155	0.414	3.444	0.604	0.431	1.467	-2.365
18	0.308	0.448	6.447	0.693	0.380	2.975	0.567
19	0.765	-0.322	-0.674	2.113	-0.339	0.583	-2.206
20	0.923	0.846	6.094	0.603	0.604	3.010	-0.166
21	-0.369	-0.349	6.759	0.298	-0.682	3.393	-2.590
22	-0.242	0.446	1.600	0.307	-0.473	0.306	-2.917
23	1.590	1.846	4.155	1.953	0.570	1.559	22.615
24	0.762	0.471	-0.278	0.404	0.490	0.728	-1.289
25	1.575	0.892	0.227	1.574	0.589	-0.662	22.621
26	-0.247	-0.224	58.871	0.540	-0.331	54.775	-38.100

Table S31: **ESOGEA**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	-0.303	-0.360	0.500
3	0.526	0.793	1.007
4	1.391	1.469	2.464
5	1.420	1.417	2.293
6	-1.511	-1.712	-2.530
7	-0.322	-0.520	-0.664
8	1.863	1.857	2.698
9	1.381	1.382	2.758
10	2.003	2.137	2.052
11	1.164	1.384	1.946
12	0.182	-0.158	0.733
13	2.571	2.936	3.525
14	0.529	0.176	0.605
15	1.114	1.454	1.018
16	1.240	1.693	1.335
17	0.859	1.214	0.828
18	1.163	1.403	2.094
19	0.534	0.553	0.794
20	1.171	1.446	1.643
21	1.094	1.228	0.383
22	-0.034	-0.091	0.783
23	-1.815	-1.435	-2.688
24	1.335	1.564	1.230
25	0.365	0.408	1.292
26	1.604	1.637	1.769

Table S32: **GOZYAX**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.261	0.393	0.429	0.541	0.275	0.345	1.496	-4.355
3	0.424	0.200	0.391	0.786	-0.007	0.692	1.079	-3.756
4	0.696	0.578	0.644	0.647	0.420	0.987	1.285	-3.364
5	0.776	0.968	0.925	0.527	0.922	0.738	1.125	-0.782
6	0.862	0.606	0.478	0.790	0.061	1.242	0.832	-6.169
7	0.963	1.084	0.886	1.150	0.759	1.110	1.259	-0.027
8	1.292	1.171	1.522	1.373	0.734	1.308	2.490	-2.092
9	1.332	1.393	1.511	1.619	0.432	2.068	3.450	-6.615
10	1.775	1.866	1.931	1.913	0.807	2.132	3.621	-6.806
11	1.800	1.781	1.527	1.516	1.563	2.941	2.941	-12.380
12	1.895	2.055	2.179	2.087	0.965	2.186	3.870	-6.436
13	1.949	1.520	1.976	2.007	0.715	2.155	0.641	-14.733
14	2.024	1.848	2.401	2.311	1.096	1.765	3.762	-1.386
15	2.057	1.404	1.703	1.552	0.195	0.984	0.681	-7.995
16	2.061	2.308	2.431	2.133	1.332	2.380	3.933	-8.755
17	2.086	2.085	2.354	2.008	1.220	2.243	3.824	-10.356
18	2.253	1.986	1.850	1.782	0.906	2.554	3.448	-6.974
19	2.452	2.271	2.517	2.638	1.273	1.705	4.130	-5.933
20	2.468	2.347	2.260	1.992	1.176	2.406	3.797	-6.583
21	2.539	2.913	2.533	3.292	1.688	3.037	-0.339	-4.660
22	2.598	2.535	3.025	3.147	1.622	1.430	4.981	-5.772
23	2.613	2.592	2.395	2.154	1.292	2.698	4.121	-6.119
24	2.644	2.538	2.703	2.579	1.594	2.165	4.138	-4.364
25	2.678	2.614	2.467	2.167	1.424	2.619	4.053	-6.018
26	2.773	2.878	2.742	2.233	1.752	2.814	4.399	-7.934
27	2.894	3.130	3.130	3.291	1.964	2.693	1.976	0.392
28	2.907	2.825	2.912	2.424	1.786	2.650	4.150	-8.607
29	3.238	3.220	3.272	2.813	2.405	2.750	4.679	-7.174
30	3.746	4.459	3.930	4.680	2.573	2.275	2.011	15.916

Table S33: **GOZYAX**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.079	0.900	5.860	0.338	0.272	3.675	-1.133
3	-0.015	0.634	3.965	-0.019	0.716	1.605	-91.327
4	0.308	0.731	-0.736	0.521	0.872	-1.816	2.771
5	0.797	0.794	1.784	0.990	0.858	1.291	0.994
6	0.220	1.125	5.153	0.148	0.815	2.977	-1.982
7	0.614	0.972	2.398	0.897	1.085	1.036	1.266
8	0.927	1.657	3.148	0.846	1.574	1.611	1.267
9	1.554	1.583	-1.689	0.438	2.079	0.150	3.018
10	2.078	1.972	-0.795	0.759	2.226	0.801	3.249
11	0.708	2.446	1.405	1.851	2.865	2.598	1.634
12	2.166	2.113	0.862	0.919	2.369	0.114	2.151
13	1.795	4.089	-5.508	0.420	1.562	-4.737	2.463
14	2.693	2.742	2.688	0.933	1.667	1.036	0.078
15	1.321	2.771	4.636	0.118	0.912	0.856	-90.731
16	2.364	2.142	0.932	1.341	2.626	1.379	1.651
17	2.391	2.409	0.943	1.137	2.316	1.590	3.450
18	2.263	1.552	1.273	0.708	2.258	1.185	3.492
19	4.117	2.291	4.441	0.337	1.051	2.978	-0.990
20	2.783	2.021	1.238	0.972	2.301	1.961	3.689
21	3.067	4.549	-0.369	1.285	2.070	1.016	0.491
22	3.962	2.483	4.372	1.186	1.166	2.985	-0.003
23	2.811	2.040	4.711	1.066	2.663	3.684	0.915
24	3.530	2.416	5.251	1.327	1.903	4.076	-0.361
25	2.911	2.236	1.378	1.165	2.442	1.639	3.779
26	3.260	2.367	1.463	1.528	2.831	2.005	3.121
27	4.401	3.257	2.257	1.272	2.271	1.775	2.663
28	3.371	2.532	1.198	1.521	2.497	1.923	3.703
29	3.984	3.135	5.125	2.049	2.284	5.274	0.060
30	7.544	2.760	4.034	0.842	1.889	2.208	2.431

Table S34: **GOZYAX**: Conformational heats of formation in kcal·mol^{-1}.

SPE	PM6	PM6-D3H4X	PM7
GEO	B97-3c	B97-3c	B97-3c
1	0.000	0.000	0.000
2	-0.027	0.256	0.614
3	0.359	-0.173	0.300
4	-0.639	0.060	0.125
5	0.276	1.079	1.048
6	-0.020	0.634	0.374
7	-0.516	0.095	0.544
8	0.547	0.525	0.660
9	-0.717	1.157	-0.938
10	0.026	1.859	-0.518
11	1.144	2.832	1.592
12	-0.549	1.420	-0.476
13	4.846	4.558	0.507
14	-0.221	1.183	-0.245
15	1.961	1.804	1.022
16	0.412	2.454	0.084
17	0.944	2.780	-0.228
18	0.021	2.092	-0.720
19	1.106	2.467	-0.260
20	0.006	2.030	-0.348
21	3.924	4.763	-0.917
22	1.662	2.461	0.460
23	0.203	2.255	-0.232
24	1.305	2.970	0.390
25	0.325	2.486	-0.379
26	0.828	3.009	0.099
27	1.878	3.397	-0.299
28	0.863	3.000	-0.172
29	2.639	4.663	1.466
30	1.958	3.406	1.758

Table S35: **HAYGUJ**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
19 1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
12 2	0.022	-0.097	-0.039	-0.035	-0.044	-0.343	0.066	-1.160
26 3	0.410	0.043	0.041	-0.120	0.331	0.351	0.337	-4.188
29 4	0.823	0.607	0.543	0.324	0.676	0.456	0.657	-5.259
17 5	1.090	0.968	0.647	0.850	-0.539	0.068	0.078	-6.420
21 6	1.144	0.691	0.413	1.182	0.125	0.651	0.374	-0.115
22 7	1.151	1.213	0.728	1.716	0.350	1.432	2.201	3.964
9 8	1.396	0.897	0.436	0.940	-0.920	-0.054	-0.231	-5.569
14 9	1.566	1.262	0.844	1.205	0.698	0.865	1.024	-7.318
11 10	1.636	0.968	0.657	0.709	-0.459	0.311	-0.172	-5.617
18 11	1.688	1.158	0.906	1.233	0.345	0.736	0.130	-6.189
24 12	1.701	1.472	1.024	1.836	-0.114	0.621	1.100	1.780
20 13	1.737	1.310	1.021	1.749	-0.516	-0.102	1.024	-0.613
23 14	2.302	2.241	1.711	2.149	0.089	0.789	2.027	2.001
28 15	2.673	2.521	2.408	2.338	-0.111	1.234	0.909	2.781
13 16	2.691	2.457	2.450	2.440	-0.412	0.908	0.680	2.274
16 17	2.719	2.323	1.902	2.825	-0.567	0.433	1.221	-0.689
27 18	3.248	2.938	2.953	2.822	0.520	1.897	0.877	-3.218
8 19	3.360	2.444	1.887	1.027	-0.618	2.839	2.176	5.634
30 20	3.478	3.163	3.049	3.798	1.937	1.629	2.134	2.182
7 21	3.524	2.528	1.986	1.069	-0.830	3.004	2.195	6.596
2 22	4.705	4.274	4.175	4.204	-0.483	1.202	1.492	9.597
25 23	4.924	4.749	4.539	4.275	-0.767	1.023	1.657	9.887
3 24	4.940	4.534	4.515	4.399	-0.378	1.158	1.541	8.853
10 25	5.003	4.948	4.151	2.774	-0.704	4.016	3.721	19.716
6 26	5.102	4.687	4.632	4.533	-0.129	1.252	1.751	9.659
15 27	5.113	4.924	5.111	4.569	-0.019	0.856	1.449	7.018
5 28	5.203	4.949	4.922	4.749	-0.233	1.217	1.582	8.000
1 29	5.411	5.035	5.025	4.673	-0.251	0.871	1.714	4.948
4 30	5.799	5.476	4.787	3.244	-1.408	3.741	4.090	17.536

Table S36: **HAYGUJ**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	-0.481	-0.341	-2.556	-0.439	-0.294	-0.321	0.661
3	0.045	6.310	4.836	0.664	-1.734	6.015	0.701
4	0.643	7.830	4.862	0.960	1.776	5.916	1.206
5	-4.873	5.669	0.265	-0.020	-1.579	0.042	1.302
6	-3.737	7.775	1.258	0.447	-1.574	0.127	0.021
7	-3.493	6.768	6.919	0.290	-0.921	2.762	1.125
8	-5.075	5.585	10.370	-0.480	-1.880	10.099	0.676
9	-1.915	7.309	6.439	-0.251	-0.940	0.865	0.861
10	-3.848	5.913	-3.202	-0.366	-1.447	-4.461	0.836
11	-4.076	6.941	-2.080	0.176	-1.538	-3.374	1.081
12	-4.245	7.001	11.881	0.489	-1.103	5.268	0.902
13	-3.426	7.437	19.054	0.133	-1.590	13.119	0.475
14	-2.079	6.454	11.385	0.385	-0.532	4.642	1.729
15	1.618	5.829	12.413	0.629	1.683	11.790	0.537
16	-1.934	7.941	-28.526	-0.163	-0.890	-15.121	-67.430
17	-3.414	7.191	14.346	-0.112	-1.209	6.815	2.152
18	2.191	7.030	5.954	0.748	1.980	3.942	1.121
19	3.872	4.198	-6.032	-0.670	3.111	-0.627	1.056
20	0.835	10.635	14.477	0.955	0.032	6.882	2.338
21	5.408	2.803	-5.903	-0.691	3.694	-0.393	1.074
22	0.556	9.103	10.347	-1.321	-1.088	2.954	0.962
23	-0.039	8.166	6.964	0.442	-0.069	3.752	1.537
24	1.062	9.420	10.425	-1.242	-1.072	2.398	0.875
25	4.475	4.548	-5.640	-0.278	3.271	-0.306	1.188
26	1.082	9.502	11.207	-0.978	-0.955	3.339	0.963
27	-0.425	9.169	9.959	-0.311	-1.384	3.026	1.172
28	1.443	9.458	8.445	-1.020	-0.976	1.559	1.420
29	1.134	8.951	9.425	-1.447	-1.390	1.846	0.999
30	5.856	3.980	-10.507	-1.282	2.910	-6.677	2.609

Table S37: **HAYGUJ**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	0.806	0.560	-0.255
3	-0.784	0.119	-0.179
4	-0.193	0.682	-0.175
5	1.945	2.273	0.122
6	-0.258	0.123	-0.722
7	1.025	1.624	-2.277
8	1.099	1.461	-0.762
9	0.425	1.200	-1.468
10	0.372	1.229	-0.080
11	-0.470	0.396	-0.575
12	0.329	1.003	-2.119
13	0.835	1.045	-1.939
14	1.418	2.217	-1.415
15	1.959	2.581	1.814
16	2.081	2.578	1.683
17	1.379	1.522	-0.353
18	0.433	1.434	1.839
19	3.934	4.944	3.057
20	1.739	2.080	0.838
21	4.541	5.556	3.503
22	4.035	4.413	2.520
23	4.596	5.061	2.673
24	4.674	4.808	2.361
25	8.347	9.691	6.383
26	4.577	4.887	2.745
27	4.620	4.752	2.826
28	4.276	4.668	2.251
29	4.398	4.698	2.602
30	8.548	9.642	5.917

Table S38: **MECYUR**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	2.007	2.927	1.313	3.903	-1.471	-0.148	1.537	-31.406
3	2.071	2.821	1.457	3.993	0.186	-0.736	-0.114	7.992
4	2.075	2.809	1.279	3.818	-1.723	-0.329	1.277	-34.918
5	2.209	2.254	0.944	2.025	-1.212	-1.016	-0.400	19.872
6	2.229	2.987	1.462	4.044	0.241	-0.732	-0.297	8.356
7	2.263	2.272	0.941	1.990	-1.165	-0.990	-0.584	20.570
8	2.820	2.976	1.622	3.019	-0.301	-0.922	3.201	20.490
9	3.269	1.942	0.727	1.424	0.584	-0.012	3.974	13.420
10	3.293	2.331	1.242	2.204	0.104	-0.020	3.441	11.356
11	3.338	1.984	0.724	1.447	0.521	-0.200	4.341	12.502
12	3.731	2.296	0.948	1.578	0.770	1.225	6.953	-37.323
13	3.795	2.398	0.957	2.394	1.410	0.636	3.113	18.493
14	3.872	2.829	1.630	2.196	-0.078	-1.607	3.023	23.209
15	4.104	4.712	3.471	5.939	-0.341	0.067	1.430	-30.868
16	4.970	4.677	3.032	5.240	-0.034	-0.859	4.880	15.703
17	5.124	4.720	3.608	4.945	0.652	-0.361	1.390	27.843
18	5.178	4.131	3.224	4.296	1.411	0.568	4.729	-39.365
19	5.726	5.840	3.800	6.469	0.640	0.226	6.614	-23.768
20	7.748	5.901	4.893	6.519	1.428	-0.017	3.430	13.345

Table S39: **MECYUR**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	3.453	0.391	11.573	-0.688	-0.524	8.886	-5.859
3	2.357	-1.094	0.723	0.191	0.597	0.704	0.099
4	1.595	-0.909	10.378	-1.696	-0.440	8.039	-5.363
5	1.101	0.685	-0.039	-0.403	-0.329	1.924	-1.905
6	2.410	-1.228	0.734	0.188	0.601	0.577	0.101
7	1.431	0.726	-0.015	-0.434	-0.279	1.926	-1.901
8	0.807	-0.445	7.721	0.603	-0.124	5.694	-1.413
9	0.737	-0.724	8.762	0.126	-0.167	6.662	-1.729
10	0.814	-0.384	9.372	0.261	-0.466	6.663	-1.773
11	1.145	-0.809	8.161	0.195	-0.167	7.426	-1.406
12	5.510	2.983	10.538	0.423	0.755	2.836	0.614
13	1.830	0.507	6.031	0.242	-0.540	7.061	-4.046
14	2.071	0.383	0.490	-0.295	-0.196	2.318	-1.891
15	3.107	1.082	8.694	-0.168	0.420	7.364	-3.429
16	1.361	1.616	9.960	0.625	-0.187	11.260	2.532
17	2.966	3.257	2.771	1.497	0.034	4.039	-1.445
18	3.938	2.963	11.707	1.555	-0.253	8.780	-1.640
19	5.370	2.849	12.294	0.853	1.525	10.488	-3.173
20	3.696	2.901	3.274	1.113	0.337	4.879	-1.628

Table S40: **MECYUR**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	2.404	0.966	3.645
3	8.423	8.990	7.745
4	0.961	-1.186	2.839
5	6.685	7.553	5.646
6	8.328	8.885	7.766
7	6.773	7.668	5.694
8	11.195	12.887	8.645
9	8.611	9.890	5.296
10	6.240	6.357	6.263
11	8.310	9.623	5.230
12	11.898	13.285	7.586
13	9.172	9.827	6.176
14	8.734	11.015	5.384
15	0.821	-1.236	3.821
16	9.144	9.515	6.973
17	9.829	11.047	8.219
18	6.829	7.098	6.806
19	4.739	4.641	4.029
20	4.925	5.168	6.099

Table S41: **NOXPAR**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.626	0.474	0.342	0.360	-1.178	-0.224	2.369	16.639
3	0.816	0.805	0.787	0.607	-0.404	0.185	2.696	14.741
4	1.115	0.896	0.958	1.140	-0.241	-0.008	2.751	14.641
5	1.285	1.244	1.143	1.150	0.445	-0.292	1.387	14.493
6	1.321	1.406	1.272	1.093	1.653	0.976	0.116	-2.250
7	1.447	1.461	1.340	1.193	1.688	0.953	0.021	-2.535
8	1.572	1.169	1.125	1.145	0.314	0.405	-0.509	3.396
9	2.201	1.715	1.722	1.887	1.794	1.170	-0.853	4.501
10	2.408	1.842	1.712	1.962	1.729	0.580	0.516	9.125
11	2.474	2.475	2.738	2.823	1.954	0.770	1.146	14.179
12	2.685	2.855	2.719	3.265	2.211	0.589	1.857	18.707
13	2.747	2.662	2.707	2.968	-1.611	-0.042	18.276	30.990
14	6.430	6.825	6.257	8.243	5.123	5.336	7.721	263.315
15	8.412	7.938	7.218	7.899	3.114	2.771	4.840	250.878
16	8.521	8.562	7.924	9.154	2.674	3.250	6.955	254.474
17	8.546	8.713	8.117	8.924	0.879	2.505	4.465	247.836
18	8.608	8.485	7.536	8.619	-1.107	1.101	86.078	138.319
19	8.725	8.579	7.565	8.673	-1.137	1.120	85.562	139.029
20	9.116	8.867	7.753	9.191	-2.621	0.369	-1.538	133.743
21	9.387	9.225	8.223	9.465	-1.752	0.425	89.770	133.745
22	10.159	9.815	9.389	10.365	1.589	1.245	4.738	250.629
23	10.850	10.325	9.353	10.378	1.231	2.409	4.884	553.780
24	11.218	10.531	9.733	11.055	2.637	2.044	6.331	553.330
25	11.513	11.132	10.289	11.604	-0.183	1.266	2.557	553.077

Table S42: **NOXPAR**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	-1.510	-0.749	-21.329	-0.021	-0.075	-13.912	16.958
3	-4.208	-10.878	-17.764	-0.907	1.814	-12.285	15.159
4	-4.238	-11.161	-17.990	-0.751	1.735	-12.369	15.130
5	-1.453	-1.272	-15.605	-1.046	-0.084	-10.372	14.305
6	-1.597	1.089	-18.099	-0.278	0.893	-14.768	13.296
7	-1.509	1.518	-18.212	-0.282	0.884	-14.762	13.309
8	-1.766	1.000	-19.826	-1.522	-0.082	-15.002	13.988
9	-0.590	-6.962	-20.543	-0.611	2.179	-14.811	13.474
10	-0.212	1.358	-19.948	-0.249	0.085	-14.749	13.395
11	1.389	1.846	-18.739	-0.767	-0.171	-12.269	14.081
12	1.757	0.574	-17.209	0.054	0.284	-11.396	13.526
13	-2.470	-7.581	-18.831	-2.045	1.222	-14.605	15.225
14	2.254	-5.746	-17.301	0.104	3.141	-11.848	15.005
15	4.789	-5.206	-17.849	1.514	2.927	-11.549	15.000
16	3.501	-5.057	-17.168	-0.278	2.085	-12.439	15.192
17	2.608	-3.111	-16.919	0.740	3.059	-10.266	15.586
18	1.950	1.725	-17.310	-0.424	1.781	-12.517	15.408
19	1.994	2.007	-17.271	-0.427	1.792	-12.514	15.414
20	0.896	-3.880	-19.683	-1.004	2.046	-14.242	15.303
21	1.248	-4.857	-18.903	-0.034	2.342	-13.333	15.262
22	5.444	-4.130	-17.656	-0.452	1.974	-12.444	15.388
23	3.956	-3.858	-20.382	-0.204	2.884	-14.070	15.202
24	4.492	-4.046	-16.869	-0.310	2.387	-12.350	15.216
25	4.391	-3.466	-16.895	-0.383	2.490	-12.411	15.346

Table S43: **NOXPAR**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	2.054	2.379	-0.178
3	3.530	3.691	0.604
4	1.739	1.746	1.199
5	-0.690	-0.308	1.456
6	-1.937	-1.261	2.846
7	-2.132	-1.441	2.479
8	-0.157	-0.337	1.575
9	-1.601	-1.521	2.403
10	-1.826	-1.441	3.661
11	1.114	1.379	5.247
12	4.765	5.093	7.106
13	6.641	6.329	3.506
14	13.355	13.289	9.759
15	3.070	3.752	10.646
16	9.747	9.162	12.575
17	11.139	11.206	10.948
18	8.433	8.976	9.816
19	7.830	8.310	9.614
20	8.970	8.817	7.510
21	9.462	9.136	8.532
22	7.040	6.876	11.877
23	10.158	10.293	10.685
24	8.146	8.365	14.758
25	11.387	11.663	10.452

Table S44: **RIFVAF**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.116	0.194	0.145	0.111	-0.706	-0.056	0.665	0.600
3	0.144	0.251	0.157	0.436	0.622	0.767	0.261	-3.181
4	0.232	0.270	0.199	0.578	0.567	0.728	0.268	-5.265
5	0.432	0.436	0.179	0.773	0.405	1.001	0.025	-8.783
6	0.715	0.640	1.320	-0.317	1.448	0.389	0.739	1.512
7	1.113	0.800	1.320	0.994	1.532	1.337	1.429	-20.283
8	1.232	1.430	2.527	1.462	-0.900	0.375	0.800	-10.690
9	1.254	1.620	2.771	1.592	0.216	0.594	0.959	-7.352
10	1.332	1.114	1.183	1.158	-1.089	0.595	-0.379	-2.215
11	1.586	1.088	1.658	0.706	-1.574	0.220	0.004	-13.397
12	1.631	1.365	1.388	1.226	-1.437	0.341	-0.469	-8.094
13	1.896	1.605	1.930	1.763	0.919	0.269	-0.488	-4.419
14	2.029	1.482	2.240	1.620	-0.995	1.444	1.354	-27.963
15	2.150	2.155	3.088	1.569	0.113	1.469	1.177	-5.107
16	2.276	2.059	3.136	1.790	-2.023	-0.455	0.179	-8.112
17	2.448	1.741	2.389	1.882	-0.541	2.199	1.059	-33.389
18	2.477	2.435	3.267	1.801	0.589	1.824	0.825	-10.892
19	2.535	2.055	2.174	1.633	0.875	1.592	-0.022	-5.180
20	2.563	2.266	3.082	2.688	1.843	1.924	1.722	-4.880
21	2.709	2.868	4.267	2.525	2.386	2.661	2.901	-13.600
22	2.741	2.237	2.931	1.396	-0.862	0.554	-1.630	-1.550
23	2.918	2.408	3.061	1.961	-1.108	0.840	-1.145	-6.936
24	2.919	2.462	3.898	2.553	0.963	1.647	0.923	-6.932
25	3.011	2.087	2.485	2.197	-0.721	2.140	-0.104	-37.966

Table S45: **RIFVAF**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	-2.185	0.825	-0.091	-0.515	0.631	0.729	0.889
3	-1.401	1.505	1.813	-0.364	0.109	-0.821	0.095
4	0.449	1.102	2.069	-1.017	0.140	-0.837	-0.015
5	-0.102	1.216	0.636	-0.401	0.442	-1.126	-0.232
6	1.094	0.917	2.869	0.137	0.659	0.013	-0.832
7	1.697	3.961	3.158	0.669	1.233	-0.702	0.500
8	0.714	2.032	4.472	-1.569	-0.928	1.035	-0.204
9	1.226	2.116	5.224	-0.164	-0.438	2.459	0.027
10	-1.567	-0.458	-0.718	-0.303	0.499	0.163	0.255
11	-1.761	0.096	1.910	-0.948	0.013	-0.693	-0.315
12	-1.026	0.680	-0.894	-0.789	0.223	-1.488	0.567
13	-1.411	0.331	0.398	0.546	0.154	0.397	0.299
14	-2.090	1.950	0.050	-0.027	0.313	-1.795	0.832
15	1.521	3.642	4.482	-0.259	0.061	-0.514	0.114
16	0.379	2.126	3.842	-1.578	-0.791	0.030	-0.690
17	0.557	1.610	3.179	-0.035	0.954	-1.506	1.477
18	1.635	3.631	3.820	-0.151	0.319	-1.297	-0.136
19	0.512	2.187	1.420	-0.529	0.534	-1.043	0.039
20	2.126	2.545	4.809	0.534	1.407	1.740	-0.328
21	2.750	4.927	8.061	0.211	0.218	4.005	1.074
22	0.082	1.929	0.939	-0.078	0.223	-1.275	0.188
23	0.442	2.358	2.218	-1.236	0.211	-2.039	0.492
24	1.303	3.961	3.430	0.719	1.514	-0.610	0.435
25	0.757	2.608	1.454	-0.807	0.329	-2.851	0.216

Table S46: **RIFVAF**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	-0.176	-0.115	1.043
3	0.675	1.005	1.416
4	0.866	1.103	1.632
5	0.629	0.972	1.973
6	-1.302	-1.223	-0.929
7	1.077	0.867	1.676
8	0.031	-0.140	1.606
9	-0.147	-0.145	1.246
10	0.117	-0.193	2.708
11	1.442	0.997	2.715
12	-0.087	-0.203	2.171
13	1.628	1.559	1.382
14	2.079	1.757	3.516
15	0.715	0.659	1.121
16	0.026	-0.774	1.509
17	1.998	2.010	2.936
18	0.658	0.583	1.645
19	1.456	2.048	1.121
20	0.518	0.220	1.781
21	1.339	1.953	4.183
22	0.083	-0.018	-0.560
23	0.832	0.834	1.131
24	0.682	0.487	0.273
25	2.353	2.213	4.003

Table S47: **UWUBEV**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	1.027	0.830	0.483	0.512	-0.999	-0.621	-1.328	-349.720
3	1.527	1.373	1.291	1.320	1.524	1.348	1.573	-256.551
4	1.826	1.022	0.987	0.926	-0.021	-0.439	0.634	-260.618
5	1.954	1.875	1.417	1.768	2.782	1.954	0.789	-268.647
6	2.036	1.864	1.468	1.846	2.839	2.080	1.047	-268.128
7	2.390	1.921	1.260	1.237	3.900	2.128	0.352	-353.118
8	2.639	2.179	1.718	2.073	2.508	1.549	0.725	-268.956
9	4.492	5.407	5.247	5.202	2.090	2.474	2.556	-585.922
10	5.267	4.938	3.738	4.055	4.924	3.828	3.611	-638.638

Table S48: **UWUBEV**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	-0.837	-0.113	4.641	-1.418	-0.451	13.921	52.182
3	0.833	2.172	8.770	0.411	2.018	18.769	51.983
4	-0.616	0.171	8.071	-1.450	-0.202	17.856	52.129
5	-0.758	2.213	9.759	-0.072	1.007	19.808	51.549
6	-0.705	1.954	9.749	-0.247	1.061	19.726	51.518
7	4.655	3.037	8.052	3.332	2.183	19.884	50.891
8	-0.750	2.063	9.408	-0.223	1.077	19.385	51.512
9	3.688	-0.186	4.816	2.748	0.036	14.849	52.160
10	1.770	4.063	9.642	0.683	2.290	20.264	51.843

Table S49: **UWUBEV**: Conformational heats of formation in kcal·mol^{-1}.

SPE	PM6	PM6-D3H4X	PM7
GEO	B97-3c	B97-3c	B97-3c
1	0.000	0.000	0.000
2	-0.176	-0.485	-0.883
3	0.123	0.850	0.611
4	-0.136	0.048	-0.365
5	0.379	0.444	0.872
6	0.592	0.702	1.186
7	-3.106	-2.267	-1.248
8	0.311	0.404	0.867
9	1.803	1.560	0.439
10	0.246	2.110	1.628

Table S50: **WECSEC**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.003	-0.217	0.177	-0.060	0.328	0.066	-0.628	-2.864
3	0.056	0.006	0.019	0.031	-0.022	-0.022	0.000	0.388
4	0.765	0.604	0.610	0.503	-0.186	0.233	-0.266	-0.850
5	0.931	0.783	0.733	0.333	0.232	0.312	-0.065	-3.720
6	1.914	1.294	2.070	1.038	2.012	1.730	-21.974	-0.547
7	2.030	1.608	1.540	1.666	0.215	0.088	-1.198	4.475
8	2.091	1.336	2.065	1.103	2.002	1.541	-21.902	1.791
9	2.611	1.720	2.001	1.253	0.829	1.419	-23.063	-1.557
10	2.633	1.585	1.909	1.224	0.572	1.582	0.148	-2.533
11	2.641	2.038	2.821	1.494	2.616	2.149	-21.237	1.114
12	2.645	2.027	2.148	1.190	1.200	1.762	-21.990	0.345
13	2.723	1.845	2.118	1.398	0.925	1.423	-22.911	-0.680
14	2.791	2.193	2.242	1.397	1.032	1.652	1.332	1.133
15	2.836	1.634	1.968	1.307	0.730	1.390	0.182	0.818
16	2.951	1.929	2.044	1.176	0.965	1.403	0.189	0.131
17	2.967	2.439	2.521	2.703	0.967	1.079	1.657	10.239
18	3.100	2.036	2.133	1.321	1.030	1.436	0.289	0.868
19	3.355	2.477	2.803	2.234	1.837	2.021	-20.169	7.368
20	3.638	2.892	3.303	2.346	2.006	2.748	-19.532	6.339
21	3.897	2.788	2.988	2.049	2.347	2.558	1.188	8.196
22	3.994	3.326	3.102	2.931	2.437	3.094	-19.034	13.208
23	4.022	2.901	3.184	2.705	2.499	3.121	3.569	14.617
24	4.064	2.655	3.113	2.246	1.490	2.093	2.391	7.488

Table S51: **WECSEC**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	-1.068	-0.560	-4.320	0.368	0.431	-0.803	0.401
3	-3.279	-0.231	-3.639	0.299	0.002	-0.655	0.493
4	0.290	0.604	-2.038	-0.679	0.123	-0.669	0.332
5	0.392	0.377	1.206	0.174	0.438	1.431	0.452
6	5.563	3.548	1.984	-0.725	0.861	-2.252	0.730
7	-0.795	1.593	-3.567	0.123	-0.010	-0.286	0.515
8	2.588	3.664	-8.295	0.802	0.880	-2.820	-17.181
9	3.624	3.140	1.203	-1.675	0.766	-2.640	0.131
10	2.406	2.955	-9.133	-0.756	0.767	-4.234	-18.314
11	6.279	4.121	2.138	0.345	1.611	-1.198	1.974
12	1.866	3.421	-7.451	-0.152	1.484	-2.928	-17.934
13	3.604	3.350	1.078	-1.526	0.794	-2.664	0.090
14	1.916	3.511	-7.754	-0.110	1.538	-3.477	-17.837
15	2.482	3.043	-9.049	-0.730	0.825	-4.580	-18.253
16	1.735	2.860	-3.829	-0.729	0.740	-2.728	1.324
17	1.637	2.386	0.120	0.815	0.475	2.249	0.640
18	1.693	2.973	-3.983	-0.593	0.774	-2.689	1.303
19	6.088	4.492	-8.811	-1.476	1.210	-4.681	-18.661
20	4.070	4.704	-7.057	0.507	1.373	-2.761	-17.913
21	3.200	5.210	-1.135	0.521	1.311	0.387	1.387
22	5.248	5.305	3.497	-0.690	1.898	-0.224	0.132
23	2.755	5.738	0.897	0.431	1.143	0.017	1.251
24	5.391	3.908	-9.472	-0.140	1.273	-4.610	-18.656

Table S52: **WECSEC**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	-0.763	-0.976	-0.820
3	0.012	0.048	0.065
4	0.031	-0.074	-0.464
5	0.708	0.750	0.203
6	7.337	7.066	-5.438
7	1.773	0.945	2.194
8	7.319	6.852	-5.228
9	8.236	7.526	-4.352
10	8.176	7.161	-4.040
11	8.062	7.984	-4.021
12	9.163	8.725	-3.092
13	8.580	7.844	-3.863
14	9.071	8.433	-2.416
15	8.122	7.046	-3.427
16	8.390	7.338	-3.773
17	2.485	1.572	2.090
18	8.724	7.659	-3.519
19	7.948	7.752	-4.656
20	9.904	9.523	-3.102
21	9.964	8.619	-0.622
22	10.513	9.705	-1.298
23	9.497	8.471	-0.903
24	8.881	7.456	-3.452

Table S53: **YIDHAX**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.403	-0.308	0.200	-1.545	-2.852	-3.334	-3.743	1.658
3	0.430	0.525	0.901	-1.492	-1.235	-3.768	-2.861	3.450
4	0.539	0.164	0.546	-1.424	-2.382	-2.898	-0.728	-0.628
5	0.567	0.121	0.471	-0.801	-2.348	-2.381	-2.487	0.251
6	0.568	0.330	0.687	-1.956	-1.989	-3.190	0.426	0.846
7	0.666	0.622	1.595	-0.655	-0.319	0.799	6.336	-11.988
8	0.721	0.687	0.986	0.154	-0.323	-0.006	-1.644	20.469
9	0.732	0.790	1.428	0.451	-0.854	-0.450	-3.512	20.211
10	0.909	0.652	1.091	-1.252	-1.982	-2.773	0.221	0.560
11	1.192	1.039	1.202	-1.953	-0.834	-2.269	1.570	1.010
12	1.279	1.078	1.412	-0.853	-1.084	-4.061	-3.045	1.887
13	1.364	1.611	2.995	-0.185	0.057	0.434	3.129	24.251
14	1.428	1.445	1.938	-0.974	-0.794	-2.508	2.797	-4.408
15	1.514	1.267	0.811	-0.296	-0.174	-0.743	1.138	14.221
16	1.539	1.337	1.985	-0.127	0.069	0.038	3.466	10.850
17	1.671	1.583	1.764	2.858	-0.885	-1.149	-2.586	12.362
18	1.736	1.437	2.085	-0.950	-0.717	-2.024	0.886	11.624
19	1.881	1.673	2.809	-0.244	0.557	0.922	6.431	-2.811
20	2.027	1.805	2.231	-0.348	-0.847	-2.475	2.255	4.125
21	2.051	2.023	2.509	-1.001	-1.672	-2.891	1.633	-7.011
22	2.250	1.998	2.363	-0.828	0.708	0.169	6.028	-15.574
23	2.409	2.248	2.536	-0.153	0.117	-1.943	2.177	6.768
24	2.620	2.627	2.947	-0.594	-0.961	-2.332	1.973	-4.945
25	3.985	3.587	4.682	0.338	-0.215	-3.003	1.848	-3.418

Table S54: **YIDHAX**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	-1.658	-0.051	3.195	-1.459	-3.300	-1.247	-5.174
3	2.728	3.258	13.261	-0.632	-4.748	7.289	-3.049
4	1.850	2.334	5.269	-2.032	-4.541	0.008	-3.753
5	-1.072	0.463	29.879	-1.125	-2.234	12.517	8.279
6	1.929	2.284	1.410	-2.043	-4.983	-1.969	1.208
7	0.787	1.448	29.567	0.277	0.552	13.657	17.461
8	-0.213	0.823	31.835	0.448	-0.487	15.365	9.189
9	0.670	1.674	6.172	-0.075	-0.815	1.809	-5.997
10	2.259	2.751	1.098	-1.604	-4.318	-1.072	-1.002
11	2.250	2.604	6.128	-1.143	-4.446	3.585	1.628
12	3.678	4.928	8.464	-0.448	-4.870	4.374	-3.437
13	4.511	2.849	25.684	-0.296	0.241	10.762	17.123
14	3.248	3.273	-0.918	-1.397	-4.775	-1.375	3.833
15	-0.694	0.347	28.379	0.830	-1.121	14.331	14.212
16	5.066	5.297	31.898	0.103	-3.045	15.194	2.040
17	0.669	1.301	5.560	0.445	-1.128	0.728	-3.931
18	3.625	3.227	30.843	-1.647	-4.356	15.912	1.230
19	5.698	5.693	35.842	-0.613	-2.778	18.499	1.189
20	3.311	3.529	2.529	-0.849	-3.978	-1.205	2.912
21	3.083	5.533	6.228	0.871	-2.682	2.044	2.468
22	3.723	4.102	22.170	-0.200	-2.778	9.979	8.685
23	4.334	4.536	4.671	0.211	-3.179	0.404	2.529
24	3.446	3.990	1.282	-0.953	-3.863	-0.750	3.079
25	4.564	5.838	34.986	-0.275	-4.536	17.487	0.068

Table S55: **YIDHAX**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	-2.572	-2.391	-4.047
3	-0.922	-0.266	0.026
4	-2.463	-1.418	-2.696
5	-2.637	-2.168	-3.372
6	-1.649	-0.472	-1.928
7	0.933	1.559	1.035
8	0.634	1.873	0.622
9	1.409	2.123	0.539
10	-1.894	-0.795	-2.143
11	-1.385	0.277	-1.018
12	0.016	0.442	0.999
13	3.325	4.219	4.051
14	-1.297	-0.811	1.102
15	-1.819	-0.259	0.292
16	1.977	2.875	4.987
17	-4.862	-4.845	-2.057
18	-1.917	0.211	0.132
19	2.009	3.268	2.402
20	-0.708	0.572	-0.976
21	-4.314	-3.242	-2.001
22	0.644	2.395	1.819
23	0.442	1.586	-0.094
24	-3.554	-2.014	-0.734
25	1.287	2.380	0.188

Table S56: **YILDAA**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.859	1.165	1.302	0.521	0.753	1.181	-1.171	6.865
3	1.021	1.269	1.417	1.434	0.082	1.454	0.252	-6.200
4	1.122	1.232	1.424	1.417	0.121	1.549	0.088	-6.361
5	1.716	1.748	1.819	1.250	1.306	1.730	-1.007	10.464
6	1.777	1.765	1.949	1.204	1.392	1.357	-0.702	8.057
7	1.804	1.777	1.888	1.980	0.719	2.172	0.448	-3.754
8	1.860	1.823	1.993	2.033	0.769	1.747	0.659	-5.108
9	1.924	1.946	2.166	2.213	0.936	2.022	0.361	-6.142
10	2.089	2.033	2.144	1.348	1.928	2.023	-1.324	6.136
11	2.102	1.952	2.168	1.435	1.606	1.785	-0.880	8.424
12	2.310	2.456	2.742	2.212	1.356	1.851	-0.926	-6.447
13	2.604	3.060	3.122	3.067	1.859	3.530	1.447	-1.849
14	2.802	2.690	3.119	2.716	1.476	3.314	0.233	-7.706
15	3.004	3.310	3.197	3.533	1.598	2.039	1.508	-2.062
16	3.188	3.510	3.783	3.357	2.424	2.884	0.517	-2.951
17	3.372	3.427	3.411	3.411	2.327	3.411	2.140	0.319
18	3.527	3.621	3.546	3.741	2.282	3.541	2.230	1.015
19	3.678	3.620	3.687	3.916	2.254	3.508	2.141	0.819
20	4.242	4.176	3.855	3.081	2.944	2.325	-1.854	1.778
21	4.250	4.097	3.948	2.961	3.008	1.926	-1.500	-0.377
22	4.367	4.408	3.953	3.595	3.819	1.435	-1.409	2.753
23	5.060	5.064	5.057	4.454	2.919	3.434	-0.483	-12.293
24	5.141	5.027	5.086	4.482	2.948	3.482	-0.479	-12.124
25	5.824	5.936	5.008	7.432	3.808	3.387	3.183	8.843
26	6.769	7.067	5.759	7.022	4.454	3.910	0.493	14.031

Table S57: **YILDAA**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	1.207	1.659	-0.294	0.798	1.551	-0.980	-0.278
3	1.261	1.094	0.307	0.218	1.543	-0.602	-0.243
4	1.868	-0.836	-3.567	0.521	4.739	-3.873	2.452
5	1.689	1.676	5.948	1.388	2.255	2.979	-1.484
6	1.807	1.674	14.140	1.499	2.027	8.152	-2.005
7	2.150	-0.735	4.920	1.144	5.533	1.107	1.186
8	1.839	1.394	11.456	0.922	2.067	6.469	-1.713
9	2.498	-0.692	3.267	1.346	5.329	-0.053	2.270
10	2.122	0.663	15.366	2.026	3.675	9.619	-4.288
11	2.046	1.976	3.049	1.675	2.102	1.306	-0.306
12	2.738	-0.421	0.131	1.332	4.204	-0.690	1.351
13	3.703	1.059	-1.616	2.041	6.447	-1.762	3.865
14	3.184	-0.201	-2.408	1.461	5.810	-2.928	3.200
15	3.032	3.039	2.417	1.718	2.140	1.186	0.885
16	3.903	1.004	1.216	2.277	5.087	0.212	2.609
17	3.882	1.414	-0.320	2.552	6.526	-0.705	4.213
18	4.187	1.170	7.494	2.349	6.730	3.618	2.869
19	4.229	1.417	2.252	2.434	6.622	0.368	4.202
20	4.221	3.107	15.200	2.569	3.009	7.709	-5.532
21	4.370	2.883	18.244	2.651	2.817	11.127	-9.640
22	4.404	5.785	3.353	3.386	1.464	1.920	0.051
23	5.534	3.468	0.088	2.503	4.967	-2.103	2.524
24	5.539	2.988	0.237	2.518	5.026	-1.962	2.518
25	5.686	4.751	12.398	3.384	2.879	7.520	0.489
26	7.080	5.667	9.725	3.366	4.310	4.365	-1.083

Table S58: **YILDAA**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	1.938	2.031	2.853
3	-0.576	-0.513	-0.047
4	-0.721	-0.641	-0.267
5	0.784	0.754	3.181
6	-0.067	0.258	3.270
7	-1.496	-1.422	0.268
8	-2.588	-2.288	0.234
9	-1.632	-1.303	-0.243
10	0.958	1.141	3.440
11	1.636	2.134	2.775
12	0.189	0.189	0.779
13	0.755	1.483	0.977
14	-0.465	0.297	-0.256
15	-1.414	-0.705	-0.024
16	-0.208	0.280	1.702
17	0.137	1.221	0.832
18	0.135	1.319	1.034
19	-0.850	0.221	0.479
20	1.714	1.256	4.406
21	0.583	0.494	4.365
22	2.415	2.670	4.648
23	1.268	1.206	2.232
24	1.421	1.368	2.161
25	-1.751	-0.948	0.399
26	0.883	0.972	6.635

Table S59: **AKUGOD**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.252	0.384	0.449	0.035	0.480	0.362	1.308	2.599
3	0.416	0.224	0.304	0.206	0.153	0.163	0.827	1.859
4	1.487	2.194	1.407	2.219	-0.213	-0.159	1.906	-1.228
5	2.054	2.310	1.469	2.509	0.076	-0.075	2.672	-0.977
6	2.126	2.506	1.617	2.753	-0.324	0.143	2.660	-2.225
7	2.628	2.547	2.519	2.527	1.949	1.387	2.055	7.502
8	2.637	2.992	2.846	2.681	1.908	1.697	2.207	2.304
9	2.697	2.827	2.788	2.968	1.455	1.461	2.654	10.095
10	2.798	3.698	2.708	3.966	-0.643	0.229	3.314	3.597
11	2.833	3.067	3.008	2.902	1.486	2.003	2.940	5.091
12	2.934	2.628	2.589	2.651	1.880	1.447	1.937	5.746
13	3.490	3.767	3.883	3.476	2.529	2.335	3.186	-1.766
14	3.562	3.508	3.284	3.169	3.320	1.518	2.186	4.448
15	3.977	4.109	4.148	3.876	3.369	2.314	3.884	5.572
16	4.094	4.046	4.176	3.934	2.993	2.284	4.320	9.727
17	4.147	4.357	4.483	4.586	2.886	1.005	3.008	15.310
18	4.183	4.069	4.387	4.281	2.766	1.245	4.344	18.110
19	4.657	5.338	5.198	5.316	2.473	2.753	3.812	9.734
20	4.774	4.768	5.031	4.438	4.068	2.692	4.590	2.625
21	4.876	5.111	4.865	5.236	2.790	2.965	3.387	8.306
22	5.109	4.922	4.767	4.988	3.537	2.725	2.844	9.784
23	5.186	6.206	5.346	6.115	2.655	2.088	3.762	13.662
24	5.364	6.200	4.880	6.426	1.360	1.580	4.755	7.453
25	5.495	5.926	4.823	6.436	1.155	1.171	5.176	18.239
26	6.783	7.433	7.175	8.492	4.115	3.480	7.358	14.031

Table S60: **AKUGOD**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	1.072	1.646	2.190	0.032	-0.044	1.783	0.862
3	0.943	1.050	0.723	0.011	-0.084	0.397	0.063
4	1.683	1.653	2.976	-0.665	-0.346	-0.045	1.266
5	1.573	2.485	3.924	-0.301	-0.638	0.929	1.451
6	2.077	2.042	4.681	-0.912	-0.328	1.050	1.147
7	3.000	3.151	3.959	1.573	1.469	2.487	1.881
8	3.348	2.921	4.990	1.820	1.391	2.783	1.532
9	3.138	3.146	4.143	1.159	1.226	2.531	1.920
10	2.797	3.204	5.344	-0.857	-0.253	0.612	2.183
11	3.401	4.149	6.936	1.181	1.409	4.478	2.106
12	2.963	3.261	4.073	1.660	1.463	2.322	2.101
13	4.355	4.081	7.953	2.295	1.854	4.530	1.797
14	3.925	4.002	8.516	2.892	1.286	6.445	0.478
15	4.442	4.249	7.381	3.311	2.250	5.328	2.989
16	4.664	5.680	8.887	2.704	1.485	6.619	3.540
17	4.331	4.473	6.402	2.985	0.910	4.047	2.613
18	4.685	4.544	6.967	2.696	1.245	4.435	3.828
19	5.175	5.357	7.563	2.283	2.364	4.110	2.862
20	5.528	4.951	9.550	3.791	1.510	5.746	2.859
21	5.186	5.269	6.395	2.475	2.813	3.436	3.094
22	5.287	5.272	4.388	3.177	2.944	1.650	3.382
23	6.358	6.155	8.365	1.336	0.936	3.532	3.450
24	4.911	5.240	11.336	1.071	1.061	5.770	2.836
25	5.133	4.967	7.724	0.542	1.185	2.312	4.255
26	7.355	7.682	9.209	3.838	3.116	5.875	6.554

Table S61: **AKUGOD**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	0.158	0.945	-0.794
3	-0.077	0.588	-0.284
4	-1.693	-2.396	-3.059
5	-0.565	-1.197	-3.576
6	-0.891	-1.431	-2.984
7	0.017	1.225	0.747
8	0.798	1.085	-1.528
9	1.139	1.663	-0.875
10	-0.902	-2.043	-3.440
11	0.661	1.376	-1.307
12	-0.119	1.058	0.733
13	-0.031	0.511	-2.478
14	-0.353	0.187	-0.502
15	2.190	3.130	-1.662
16	2.094	3.289	-1.494
17	1.964	2.597	-1.044
18	2.031	3.447	-1.616
19	1.592	1.457	-2.049
20	1.256	2.273	-2.770
21	0.357	1.256	0.457
22	-0.202	1.406	1.730
23	0.460	0.485	-2.417
24	-0.964	-1.114	-3.024
25	0.920	1.362	-2.464
26	3.251	3.014	1.159

Table S62: **BOBXAS**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.101	0.091	0.148	0.065	0.033	38.589	0.684	0.316
3	0.202	-0.012	0.005	0.018	-0.028	16.571	0.021	-0.007
4	0.760	0.783	1.072	1.404	0.362	137.350	2.513	7.904
5	0.861	2.036	2.282	2.118	0.438	-8.411	-3.693	2.491
6	1.138	2.318	2.673	1.949	0.600	135.212	-3.162	4.787
7	1.227	2.534	2.748	2.789	1.027	-43.784	-0.101	3.481
8	1.314	2.920	3.298	2.970	1.259	22.500	-2.234	1.150
9	1.658	3.136	4.017	3.881	1.424	340.003	-4.772	3.429
10	1.720	2.946	3.322	2.797	1.521	186.170	-3.928	15.548
11	1.758	3.229	4.089	3.408	1.634	465.986	-2.117	11.896
12	2.061	4.558	6.127	5.896	3.613	222.207	8.079	-1.108
13	2.067	3.381	4.219	3.722	1.350	435.558	-5.602	3.764
14	2.387	4.021	5.469	4.871	2.488	-19.173	-0.677	-13.797
15	2.863	4.160	5.572	4.890	1.698	-643.350	-0.245	-25.857
16	2.866	3.550	3.941	3.289	0.895	286.346	-1.374	10.683
17	2.945	4.247	6.049	5.532	2.639	-193.693	5.267	-8.860
18	2.957	4.152	5.642	4.871	1.731	-584.253	0.086	-24.348
19	3.033	4.122	5.626	4.761	2.531	-701.055	-0.015	-27.793
20	3.060	4.071	5.730	4.915	1.941	-716.299	-0.323	-25.829
21	3.276	4.409	5.447	5.098	2.872	-521.752	-0.398	-23.410
22	3.417	4.554	5.542	5.287	3.389	-583.779	0.200	-21.281
23	3.541	4.419	4.682	4.327	2.193	675.223	-4.495	13.959
24	3.756	5.725	7.149	6.840	3.692	558.669	24.103	-0.087
25	3.925	4.546	4.668	4.312	1.860	632.733	-4.386	9.632
26	3.950	5.387	7.320	6.363	4.083	-360.394	1.949	-11.357
27	4.677	5.000	5.555	4.769	1.102	168.499	-4.044	-11.033
28	4.740	4.956	5.164	4.581	0.857	36.810	-2.201	-12.617
29	4.746	5.393	6.308	6.369	2.265	-67.620	0.803	-7.097

Table S63: **BOBXAS**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	-0.021	0.269	-1.377	0.172	0.247	-0.775	0.004
3	-0.004	0.114	-0.047	-0.001	-0.002	-0.042	-0.001
4	0.953	1.337	-1.756	0.367	0.847	-1.099	-0.027
5	6.222	8.450	3.083	-1.493	1.413	-0.349	0.399
6	6.658	9.011	0.615	-1.210	1.529	-0.903	-0.090
7	6.931	9.163	5.735	-1.001	1.720	3.763	-0.107
8	7.097	9.261	2.227	-0.983	1.996	0.871	0.036
9	9.232	10.865	0.024	-1.168	2.087	-3.778	0.905
10	7.720	9.315	6.113	-0.687	1.589	3.497	0.455
11	7.977	10.402	3.441	-0.419	2.154	-0.470	0.655
12	10.997	12.060	0.465	0.680	3.271	-3.243	1.488
13	8.187	9.377	0.076	-0.966	2.713	-3.673	0.905
14	10.229	12.032	4.025	-0.566	2.367	1.840	2.260
15	10.023	12.036	6.328	-0.801	3.312	5.524	2.226
16	7.773	10.290	1.673	-0.870	1.915	-0.151	-0.030
17	11.376	14.281	8.960	0.076	3.220	7.459	3.491
18	9.923	11.926	6.189	-0.801	3.328	5.385	2.246
19	10.390	11.751	6.958	-0.307	3.569	6.087	2.579
20	10.232	11.320	7.392	-0.722	3.482	6.320	2.324
21	10.312	12.012	6.088	-0.510	3.076	4.469	2.015
22	10.236	11.098	6.711	-0.454	3.280	5.019	1.998
23	10.248	11.038	7.123	-0.662	2.010	1.919	1.738
24	10.980	11.974	3.690	1.254	4.549	-5.697	8.281
25	9.159	10.517	5.776	-0.699	2.140	0.597	1.756
26	12.708	14.116	6.478	0.372	3.899	5.938	2.701
27	9.388	10.659	6.259	-0.863	1.797	1.221	1.419
28	8.938	10.601	8.057	-1.048	2.012	4.461	1.438
29	10.535	12.841	6.706	-0.007	2.835	5.005	2.648

Table S64: **BOBXAS**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	-0.032	0.204	-0.749
3	0.002	0.010	-0.056
4	-0.950	-0.610	-1.169
5	9.389	9.835	-6.030
6	9.484	10.053	-4.699
7	9.373	9.755	-5.899
8	10.767	11.394	-4.463
9	11.324	11.069	-4.021
10	9.633	10.577	-4.780
11	9.447	10.713	-4.948
12	13.195	15.036	-0.146
13	11.647	11.426	-4.575
14	12.313	13.091	-0.197
15	12.717	13.122	1.192
16	10.353	11.515	-3.802
17	12.388	13.819	1.601
18	12.948	13.438	1.367
19	12.920	13.587	1.913
20	12.493	13.015	0.918
21	12.660	12.892	1.511
22	12.512	13.072	1.826
23	12.074	12.629	-4.175
24	14.817	15.987	-1.482
25	11.766	12.316	-3.844
26	12.457	14.696	0.749
27	12.141	12.237	-2.662
28	11.959	12.093	-1.947
29	12.600	13.367	-0.345

Table S65: **CAFKOJ**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1 1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
7 2	0.092	-0.137	-1.156	-0.081	3.549	-1.730	-1.123	44.631
3 3	0.533	0.330	-0.803	0.558	2.077	-1.353	-2.300	19.545
8 4	0.544	-0.075	-0.120	-1.044	1.830	-1.191	-0.740	21.475
6 5	0.605	0.558	-1.751	1.000	2.758	-4.056	0.668	38.876
10 6	0.612	0.319	-1.641	0.854	2.495	-3.790	0.733	36.032
24 7	0.964	0.489	-0.888	0.074	3.033	1.313	1.170	42.236
11 8	1.011	0.123	-0.134	-0.687	2.266	-0.854	0.876	21.783
2 9	1.045	0.550	-0.276	1.416	0.943	-2.824	-1.791	4.355
30 10	1.142	0.633	-0.368	-0.544	4.410	-0.177	0.298	25.016
19 11	1.219	0.998	0.308	1.479	1.830	-0.022	-0.025	-4.596
15 12	1.382	1.199	0.015	0.752	3.403	-4.061	1.394	37.573
27 13	1.462	1.247	1.481	0.910	3.406	-0.016	-2.416	-6.459
25 14	1.945	2.327	0.171	2.492	2.415	1.687	-2.160	25.414
13 15	2.230	1.517	-0.149	2.067	4.374	-3.435	-2.038	29.380
14 16	2.376	1.676	-0.108	2.244	4.031	-2.832	-1.893	33.444
20 17	2.410	2.213	0.476	2.524	3.208	-2.045	-0.244	25.887
17 18	2.445	1.508	3.349	0.208	2.178	-2.069	-3.625	-14.400
29 19	2.569	3.159	0.536	2.909	2.982	1.532	0.129	36.314
21 20	2.739	2.520	2.547	2.258	3.237	-2.195	6.955	27.339
26 21	3.055	2.548	3.336	1.394	2.991	-1.179	5.156	5.494
16 22	3.509	2.531	0.943	2.803	3.826	0.816	1.275	46.597
23 23	3.550	3.981	3.276	4.550	2.990	0.561	3.542	-3.566
18 24	4.209	3.979	1.804	3.880	4.918	3.082	-0.671	29.827
28 25	4.265	4.531	3.600	5.066	3.469	0.039	-1.819	-14.731

Table S66: **CAFKOJ**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	-3.743	0.307	6.666	4.978	-3.526	6.129	-3.515
3	-1.228	-10.218	-1.326	0.402	-0.181	-1.592	-3.364
4	-3.812	5.865	6.739	4.179	-3.220	8.716	1.581
5	-3.676	-1.569	46.578	4.906	-4.904	40.931	33.718
6	-3.548	-1.473	52.505	4.862	-4.880	44.493	-100.301
7	-3.142	3.892	9.142	5.719	-3.874	8.155	-1.388
8	-3.813	5.491	6.772	4.104	-3.233	8.604	1.534
9	-2.622	-13.088	3.054	1.900	-0.689	8.099	-0.131
10	-0.710	3.743	-18.630	4.193	-4.540	-9.785	3.740
11	-2.394	-9.461	4.538	2.951	1.276	7.250	0.230
12	-2.738	-2.135	-3.012	4.680	-4.877	2.959	2.727
13	1.318	-6.984	-27.949	2.719	-0.889	-15.841	5.701
14	-0.229	-7.935	6.912	2.763	1.895	12.752	-2.710
15	-1.033	0.738	5.281	1.915	-4.460	9.746	-0.097
16	-1.584	1.062	5.275	1.939	-4.381	9.815	-0.183
17	-1.089	-8.615	53.942	5.451	-1.140	44.862	-95.899
18	0.254	1.053	-32.160	3.474	-4.498	-16.278	5.475
19	-1.367	-8.624	16.793	3.516	0.832	20.643	-2.518
20	-2.045	4.036	20.280	5.826	-4.479	25.514	-1.193
21	0.294	1.676	-29.130	3.958	-4.676	-16.536	10.100
22	-0.262	-7.656	27.317	3.614	-1.407	28.987	-0.953
23	2.139	-6.797	5.918	4.243	0.702	7.708	4.311
24	0.766	6.310	33.258	3.531	-3.228	6.052	0.242
25	1.906	-7.068	5.612	4.306	0.642	7.182	4.294

Table S67: **CAFKOJ**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	10.622	11.397	2.077
3	4.175	4.610	-6.852
4	0.019	0.721	-2.719
5	12.740	13.392	5.818
6	9.794	10.675	2.381
7	14.098	14.426	10.797
8	1.292	1.978	-2.710
9	-1.755	-1.567	-3.233
10	6.413	7.231	1.224
11	0.213	0.177	-1.085
12	9.081	10.198	2.365
13	-4.438	-3.841	-11.675
14	11.131	11.470	7.479
15	8.461	9.231	0.640
16	8.216	9.076	2.121
17	6.673	7.396	2.216
18	-10.389	-8.981	-10.536
19	13.136	13.706	8.505
20	7.708	8.088	5.676
21	-1.653	-0.997	3.763
22	9.770	10.194	5.764
23	4.095	4.086	3.890
24	12.418	13.043	4.468
25	3.995	3.864	3.400

Table S68: **CESHIS**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.201	-0.424	0.097	1.243	0.050	0.679	-3.610	-4.102
3	0.736	0.698	1.202	1.139	2.119	0.756	1.749	2.768
4	1.503	-0.025	1.635	2.995	0.580	-2.370	-3.528	-0.359
5	1.648	0.859	1.135	2.374	1.041	-0.059	0.423	-15.310
6	1.734	1.851	2.094	2.674	-0.702	-0.037	1.735	10.455
7	2.230	2.073	2.378	3.098	-0.700	-0.758	-0.711	11.970
8	2.258	0.984	2.257	3.457	0.998	-1.696	-3.854	0.367
9	2.312	1.062	1.875	1.652	1.112	0.148	-1.156	5.303
10	2.435	0.955	1.280	1.724	2.263	0.403	0.228	0.824
11	2.540	2.530	2.700	3.636	-0.236	1.085	1.729	15.694
12	2.976	2.396	2.763	2.938	3.946	2.673	1.688	3.090
13	3.478	2.615	3.003	4.387	1.060	0.748	1.454	3.515
14	3.484	3.691	4.127	4.696	0.349	1.353	1.300	23.319
15	3.651	3.381	3.482	4.025	0.841	0.792	1.458	3.732
16	4.158	3.423	4.244	4.093	2.184	1.370	1.837	19.521
17	4.870	5.236	4.381	7.973	6.210	5.719	-11.464	-12.717
18	4.985	4.451	4.560	7.851	2.726	0.045	-2.751	5.608
19	6.876	7.277	6.674	9.011	6.772	5.404	-15.635	-7.871
20	8.163	8.450	6.839	9.677	9.329	7.051	-12.523	-0.786
21	8.782	8.825	6.759	10.424	8.156	5.618	-13.325	-8.016
22	12.767	11.271	9.854	11.480	9.454	7.240	-9.995	6.527

Table S69: **CESHIS**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	-1.144	0.296	1.203	1.226	0.589	2.149	-6.622
3	1.325	3.246	8.091	2.116	-0.169	7.198	-0.555
4	1.242	1.031	5.355	1.277	-1.728	3.356	-6.690
5	2.887	0.526	8.324	-0.145	-0.678	3.273	-3.322
6	1.615	1.641	-1.532	-0.570	0.321	-5.618	1.528
7	2.260	2.829	4.168	-0.099	-0.623	1.665	-4.500
8	2.036	2.149	5.678	1.389	-0.911	3.419	-6.705
9	2.676	2.081	4.814	1.619	0.003	-0.393	-4.706
10	2.871	1.215	10.967	1.332	0.574	6.136	-3.476
11	2.202	2.805	4.946	-0.010	1.263	1.592	-0.672
12	3.618	3.715	3.775	3.674	2.529	3.387	-1.395
13	2.849	3.089	6.356	1.117	0.465	3.870	-4.479
14	3.338	4.082	4.643	1.629	1.914	-1.317	0.098
15	3.677	4.094	5.938	0.695	0.507	3.419	-2.516
16	3.937	5.009	8.978	2.347	1.005	2.332	-0.710
17	33.547	38.590	48.241	0.735	-4.785	13.221	73.950
18	5.301	5.987	3.735	2.517	-0.793	1.142	-4.729
19	37.336	38.999	41.798	0.624	-5.105	6.537	93.745
20	36.496	38.249	39.378	0.464	-5.524	4.802	94.196
21	34.088	35.516	34.371	-0.061	-7.689	3.605	73.261
22	36.178	37.898	39.608	0.731	-4.628	3.873	75.849

Table S70: **CESHIS**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	2.379	1.164	-2.732
3	1.815	3.047	0.177
4	7.709	5.111	-2.833
5	2.807	3.012	-4.415
6	1.833	1.966	1.807
7	-0.258	0.087	-3.030
8	6.122	4.633	-2.075
9	-0.472	-0.051	-6.789
10	4.056	4.949	-3.043
11	2.714	2.852	0.485
12	4.111	4.934	1.624
13	1.220	2.670	-3.146
14	3.815	3.899	-0.929
15	0.537	1.457	0.169
16	2.864	3.771	-2.697
17	6.527	6.379	4.850
18	5.748	3.585	5.896
19	8.324	7.139	0.910
20	5.840	6.009	1.479
21	6.452	5.658	2.100
22	9.748	9.488	2.989

Table S71: **CODDIJ**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.652	0.607	0.925	-0.178	2.008	-0.814	-1.250	9.863
3	1.108	0.467	0.694	1.273	2.879	2.280	0.558	-4.128
4	1.212	1.301	1.725	0.416	3.317	0.556	-0.303	7.611
5	1.262	1.103	1.317	0.461	1.782	0.090	1.244	10.401
6	1.369	1.508	2.073	1.370	0.899	0.357	-0.512	-2.041
7	1.404	1.497	1.773	0.332	2.516	-0.548	-1.047	10.282
8	1.902	1.973	2.197	1.628	-0.141	-0.697	-1.309	-0.924
9	2.083	1.849	2.033	1.564	2.437	1.085	0.264	8.366
10	3.287	3.609	3.462	3.016	2.860	1.091	0.502	7.144
11	3.352	3.679	3.581	3.350	3.851	2.361	1.832	6.407
12	4.541	4.174	4.183	4.151	4.637	3.390	2.377	-0.721
13	4.632	4.279	4.074	3.976	3.344	2.022	1.000	0.745
14	4.676	4.619	4.470	4.466	3.757	1.694	0.596	1.525

Table S72: **CODDIJ**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	3.502	2.771	-3.473	-1.427	-2.068	-2.558	-1.985
3	-0.154	0.858	-1.137	3.274	2.183	-2.106	-0.587
4	4.113	2.941	-3.358	-0.548	-2.064	-1.126	0.368
5	1.194	1.064	0.033	0.972	0.629	0.057	-0.079
6	4.420	4.435	-3.723	-2.044	-2.105	-2.568	-2.043
7	4.516	3.584	-3.388	-1.549	-2.563	-2.717	-0.802
8	4.374	4.302	2.337	-2.668	-2.676	3.125	-0.518
9	2.243	1.679	3.397	1.451	1.550	1.692	-1.236
10	5.802	5.674	2.307	-0.140	-0.710	2.877	-0.292
11	6.454	2.887	2.108	0.890	-2.058	4.245	0.858
12	6.565	6.422	-3.597	1.745	0.261	-2.873	-1.894
13	5.773	5.788	2.080	0.874	-0.335	2.834	-0.466
14	6.049	6.643	1.645	1.682	0.259	2.047	-3.382

Table S73: **CODDIJ**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	-2.146	-0.665	4.676
3	2.393	2.565	1.940
4	-0.261	1.958	6.910
5	0.317	1.039	3.539
6	-0.192	1.603	2.319
7	-1.540	0.574	6.161
8	-1.390	0.521	1.198
9	-0.441	0.248	2.051
10	-1.622	1.262	5.932
11	-0.596	2.310	6.928
12	1.765	4.251	6.382
13	0.329	2.857	5.364
14	-0.069	2.414	5.200

Table S74: **DEFVIT**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	1.025	0.484	0.659	-0.251	2.181	1.719	2.456	5.041
3	1.382	1.544	1.783	0.522	1.203	2.669	1.646	2.226
4	1.400	2.454	2.075	2.324	0.728	-0.661	1.856	7.553
5	1.465	1.815	1.588	1.087	1.116	3.198	2.713	4.823
6	1.495	2.217	1.921	2.419	-0.165	-1.872	2.490	9.225
7	1.658	3.623	2.509	2.481	0.110	-0.695	1.860	-5.202
8	1.726	3.988	3.307	2.637	0.705	0.769	4.873	-4.043
9	2.375	4.261	3.489	2.859	-1.558	-1.780	2.043	-8.639
10	2.707	3.161	3.175	1.827	3.488	4.573	2.396	9.473
11	2.795	6.182	5.085	5.215	-0.589	-2.196	9.401	-8.515
12	2.839	2.760	3.000	1.574	3.579	2.206	2.515	10.363
13	2.858	3.412	3.752	2.709	1.002	-1.167	4.352	-2.634
14	3.223	4.447	3.779	1.670	2.607	4.245	2.080	-10.718
15	3.350	4.194	3.928	3.477	2.897	2.675	17.267	14.249
16	3.456	6.825	6.578	4.653	3.196	4.844	1.628	-34.904
17	3.528	5.206	4.586	4.413	-0.431	-3.213	4.777	-7.068
18	3.545	4.546	4.648	3.926	2.535	0.792	4.407	-8.633
19	4.016	6.174	5.815	3.755	2.180	-0.224	7.710	-9.847
20	4.132	4.961	5.236	4.087	3.471	0.919	4.480	6.355
21	4.287	4.794	4.420	4.239	5.288	4.949	18.227	27.112
22	4.795	5.548	4.925	5.365	2.671	2.745	6.170	5.118
23	5.359	6.380	5.954	6.010	-0.614	-3.346	7.188	1.833
24	5.631	6.346	6.078	6.650	1.665	-0.512	9.436	22.031
25	6.825	7.413	7.069	6.248	4.998	6.010	19.779	15.713
26	7.893	7.850	9.111	5.347	1.960	1.862	12.572	-4.719

Table S75: **DEFVIT**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	3.528	-1.958	-0.856	1.841	-2.265	1.656	-2.255
3	1.581	-3.015	-2.340	-0.270	0.425	-0.035	-2.138
4	2.676	3.950	16.734	1.157	-0.949	6.603	1.102
5	0.776	-3.138	21.268	0.481	-1.044	2.940	69.324
6	2.365	-1.635	11.984	0.915	-2.080	9.322	0.991
7	6.152	-1.772	-0.392	0.047	-2.121	-6.751	2.470
8	4.751	-1.947	-0.912	0.211	-2.134	-20.054	182.132
9	1.398	-0.403	6.267	-0.658	-0.934	0.973	-0.282
10	4.483	2.693	15.863	2.890	1.356	3.510	69.464
11	3.247	-1.500	13.470	0.015	-2.157	-11.546	180.907
12	6.210	4.461	8.482	2.798	-0.275	5.454	-2.105
13	2.977	-2.714	-2.837	-0.729	-2.168	-1.160	-2.076
14	5.068	2.590	-3.542	0.893	-1.406	-7.021	3.078
15	3.430	3.551	20.813	2.951	1.407	2.164	68.342
16	0.847	2.272	8.847	3.687	0.972	-15.046	187.296
17	4.742	-3.541	9.749	-0.732	-1.718	2.170	-0.462
18	0.799	-3.890	3.133	0.769	-0.525	-4.074	-1.373
19	6.534	1.894	-18.222	1.898	-1.361	-23.498	1.867
20	6.247	3.080	0.799	2.073	-0.236	2.312	-2.236
21	4.160	-3.037	7.791	1.720	-1.018	-16.010	183.222
22	4.857	-0.335	11.791	0.085	-0.819	1.560	67.946
23	4.942	-3.795	8.682	-0.798	-1.704	1.292	-0.491
24	6.223	1.342	21.192	1.896	0.835	2.645	68.366
25	5.503	5.732	10.294	2.687	1.030	4.193	68.026
26	5.634	2.358	6.535	2.820	-1.873	-10.319	182.814

Table S76: **DEFVIT**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	0.607	0.517	2.385
3	3.059	3.166	-0.263
4	-1.399	-1.531	-4.638
5	2.814	3.002	2.116
6	-2.100	-2.192	-4.545
7	2.477	2.746	-7.986
8	5.792	6.087	-5.986
9	3.238	3.335	-8.974
10	0.885	1.109	-3.457
11	12.528	11.986	3.261
12	-2.295	-2.144	-2.786
13	6.779	6.374	3.705
14	4.648	4.588	-4.081
15	2.516	2.672	-0.046
16	3.978	4.319	-7.959
17	7.825	7.413	-0.223
18	6.598	6.090	5.224
19	11.966	11.557	3.479
20	4.416	4.227	0.354
21	3.956	3.970	4.311
22	10.728	10.630	10.639
23	10.684	10.598	3.612
24	9.402	9.323	10.434
25	10.042	9.967	9.074
26	13.840	13.802	6.524

Table S77: **DILQAQ**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	3.461	4.288	4.700	2.943	0.399	2.856	8.293	38.165
3	3.625	3.261	3.536	2.968	-1.475	-0.107	5.215	21.054
4	4.154	2.979	6.316	3.197	2.444	4.791	14.179	31.027
5	4.595	4.399	7.224	5.280	1.168	2.786	13.124	17.193
6	5.187	5.040	4.802	4.724	0.111	0.993	-0.280	10.614
7	5.584	3.849	5.055	2.904	-1.256	1.313	11.770	48.618
8	5.709	6.147	8.011	5.536	-1.780	-0.167	5.628	11.359
9	6.442	6.166	6.217	5.516	0.120	2.374	4.409	24.198
10	6.511	6.502	7.477	5.536	1.920	3.860	9.618	32.116
11	6.633	6.683	8.409	6.033	-1.599	1.626	9.497	23.555
12	7.030	6.476	6.274	5.493	0.671	1.600	3.944	27.920
13	7.288	7.335	8.953	6.815	-0.694	0.875	3.566	9.309
14	8.788	7.833	9.269	7.522	3.753	3.891	3.887	35.011
15	12.312	12.361	12.445	11.398	3.390	5.014	4.739	35.825
16	13.559	13.459	12.951	12.732	5.116	5.533	1.809	24.671
17	14.340	14.712	16.567	14.129	0.174	-0.986	7.835	39.183

Table S78: **DILQAQ**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	-13.959	-16.848	5.652	2.144	5.526	11.924	12.958
3	-11.566	-10.640	2.930	-0.031	2.383	5.592	6.296
4	-7.322	-10.345	36.583	2.282	1.903	18.951	4.088
5	-4.744	-7.524	17.203	-0.322	-1.250	10.099	7.242
6	-0.357	-1.377	6.389	-2.153	-1.361	-0.312	-0.775
7	-8.141	-10.681	11.913	-0.974	3.961	2.078	9.145
8	-3.823	-9.208	5.797	0.246	2.795	-3.214	3.848
9	-9.847	-7.154	8.836	1.369	3.962	7.025	6.270
10	-5.202	-8.834	22.438	0.501	4.898	7.926	7.404
11	-6.922	-10.460	7.392	1.660	5.066	4.149	9.650
12	-7.314	-10.733	7.612	-0.841	1.053	4.324	5.436
13	-1.704	-7.673	7.868	0.011	4.044	-3.039	2.615
14	3.071	2.112	22.005	0.347	-1.712	6.290	4.960
15	-2.937	-4.098	13.389	1.716	2.775	5.532	5.667
16	1.899	-0.458	13.048	-2.448	-1.077	2.165	0.731
17	1.463	0.362	13.616	-1.293	-5.384	-3.038	5.391

Table S79: **DILQAQ**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	3.891	4.089	4.528
3	5.088	5.172	6.511
4	4.186	4.646	1.922
5	6.212	7.166	8.903
6	4.176	4.542	7.340
7	6.936	6.472	8.655
8	6.759	7.220	3.874
9	5.863	6.112	9.611
10	6.130	6.697	8.576
11	6.412	6.849	6.643
12	5.738	5.767	7.374
13	2.165	2.176	1.539
14	9.285	9.720	13.652
15	9.537	10.365	13.803
16	10.154	11.679	15.549
17	6.952	8.279	7.447

Table S80: **DUGVEH**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	2.413	2.600	2.156	3.431	-1.305	-1.264	2.359	14.724
3	2.491	2.587	2.168	3.472	-1.391	-1.237	2.385	15.434
4	7.737	12.639	3.676	19.330	-10.022	9.331	24.224	2.072
5	7.766	13.116	4.209	19.871	-9.538	10.082	98.216	-6.451
6	7.968	13.445	4.765	19.997	-9.506	10.609	97.963	3.966
7	8.226	13.295	4.174	19.653	-7.835	10.291	96.292	-4.611
8	8.265	14.087	5.131	20.800	-9.169	11.750	98.650	4.459
9	8.351	13.490	4.715	20.787	-10.157	10.016	24.104	4.430
10	8.371	13.789	4.417	19.665	-9.080	10.632	98.378	4.077
11	8.630	13.756	5.102	20.098	-10.075	10.211	98.324	6.751
12	10.082	15.802	6.862	21.394	-8.771	11.907	24.322	14.693
13	10.569	16.662	8.050	24.686	-5.404	13.147	28.076	10.836
14	11.474	16.443	7.452	23.764	-6.390	12.090	100.047	18.744
15	12.564	16.937	8.879	23.401	-3.181	13.626	101.875	28.580
16	12.593	18.515	8.964	24.023	-6.882	11.430	24.593	16.301
17	13.346	18.159	9.278	26.284	-4.625	14.446	27.827	17.055
18	14.481	19.444	9.409	26.624	-5.700	12.818	100.632	-1.280
19	14.499	20.277	10.741	28.762	-3.309	15.413	104.081	12.636
20	14.579	19.328	9.468	24.891	-3.664	13.794	27.878	30.345
21	14.649	19.542	10.792	26.918	-3.598	14.015	26.117	30.317
22	14.797	20.899	10.848	27.964	-5.128	11.729	25.427	-6.225
23	15.023	20.084	11.074	27.836	-3.646	14.879	26.406	29.650
24	15.301	19.952	9.559	26.120	-6.893	12.418	26.252	-0.407
25	17.570	23.840	14.484	29.472	-2.027	12.758	25.836	28.811
26	17.607	23.762	13.236	27.539	-4.128	16.150	21.469	32.493

Table S81: **DUGVEH**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.354	-38.871	34.119	-0.069	8.305	22.035	19.288
3	0.303	-38.843	33.579	-0.067	8.301	21.667	19.323
4	17.581	-12.219	33.701	-16.388	10.910	13.734	38.875
5	14.607	-8.382	29.426	-17.345	9.364	6.116	40.229
6	13.878	-14.163	-2.264	-16.246	12.512	-0.760	22.626
7	25.071	-15.473	70.880	-11.152	16.535	51.827	5.624
8	12.194	-13.002	-2.125	-16.412	10.968	1.128	22.589
9	19.562	-10.954	27.985	-15.492	10.613	8.312	38.301
10	11.498	-22.584	-1.837	-16.853	13.224	-1.645	21.847
11	12.970	-7.666	37.267	-17.782	10.645	15.646	38.333
12	12.511	-11.487	-3.953	-13.887	11.599	-2.279	21.901
13	22.398	-16.056	37.513	-11.758	15.893	17.038	38.740
14	24.801	-21.389	33.037	-16.539	14.347	5.712	36.227
15	21.834	-4.751	16.699	-12.285	13.346	14.033	22.780
16	16.751	-7.314	-3.646	-12.068	12.689	-2.204	22.733
17	26.088	-17.458	5.214	-12.002	16.843	4.662	24.456
18	26.251	-4.802	34.744	-11.838	13.056	29.734	-8.028
19	38.608	6.400	147.449	-12.706	13.778	116.746	26.091
20	24.351	-3.499	64.284	-10.575	14.078	50.409	9.228
21	30.946	-13.178	33.046	-13.069	14.500	13.330	37.136
22	31.525	-15.340	138.880	-9.462	14.752	111.590	26.679
23	30.479	-14.278	33.362	-13.823	15.549	11.955	36.919
24	21.281	-17.200	32.013	-13.577	15.052	29.722	-7.171
25	35.688	2.490	141.701	-10.444	13.974	113.924	25.101
26	28.592	-7.373	36.388	-14.238	14.385	9.181	37.950

Table S82: **DUGVEH**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	-5.236	-4.762	2.916
3	-5.286	-4.862	3.039
4	42.608	41.408	9.780
5	40.807	39.534	14.268
6	41.987	41.197	10.189
7	41.480	41.150	7.062
8	44.402	43.838	12.017
9	46.870	45.770	11.601
10	48.542	47.936	10.090
11	46.143	45.148	9.590
12	48.879	48.953	8.299
13	52.123	51.612	14.022
14	50.864	49.619	15.205
15	31.344	30.730	12.837
16	49.494	50.441	7.298
17	54.637	53.930	14.353
18	47.131	45.473	15.136
19	54.152	53.002	20.041
20	36.995	37.302	19.195
21	54.329	53.056	16.623
22	39.303	38.177	15.398
23	58.235	57.125	17.683
24	47.439	45.648	12.057
25	45.302	45.115	15.942
26	61.883	60.950	11.632

Table S83: **EGOZUV**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.473	0.092	-0.191	0.018	-0.161	-65.199	-0.812	-1.034
3	0.685	0.703	-0.004	0.395	1.742	-668.326	-3.289	-9.587
4	0.786	0.320	-0.034	0.327	-0.579	-50.076	-0.179	1.135
5	0.997	0.674	0.678	1.069	-0.667	-341.566	2.175	3.679
6	1.056	0.717	0.549	1.045	1.151	255.148	-0.978	-3.672
7	1.118	0.492	0.145	0.081	0.905	-264.783	-0.746	-2.016
8	1.123	0.871	0.557	1.066	1.112	304.356	-0.830	-2.999
9	1.144	0.773	0.650	1.148	-0.368	-197.614	2.403	3.684
10	1.184	0.829	0.047	0.521	2.215	-981.269	-3.223	-10.870
11	1.275	0.679	0.282	0.550	-0.850	186.548	0.066	1.819
12	1.397	0.966	0.134	0.434	0.786	-309.384	-1.382	-3.308
13	1.419	0.604	0.004	0.379	-0.555	9.791	-0.074	1.698
14	1.487	1.161	0.718	1.181	1.463	246.709	-1.135	-4.603
15	1.849	0.942	0.169	0.449	0.154	-91.796	-0.824	0.515
16	1.867	1.066	0.264	0.471	-0.453	139.521	-0.635	0.125
17	2.022	1.776	0.845	1.007	1.350	-620.360	-2.509	-12.207
18	2.086	1.524	0.687	1.334	1.793	-578.390	-0.089	-4.554
19	2.095	1.576	0.715	1.153	1.713	-426.574	-0.328	-3.269
20	2.160	1.501	0.817	1.405	1.292	-710.335	-1.081	-7.902
21	2.387	2.347	2.011	3.044	1.125	390.489	2.103	9.263
22	2.409	2.106	1.702	1.972	1.130	-545.554	0.470	-5.655
23	2.653	1.681	1.200	2.022	0.102	-60.177	2.566	5.541
24	2.677	2.670	2.448	3.056	0.825	-283.731	0.803	-18.480
25	2.795	1.700	0.737	1.012	0.067	478.768	0.419	4.208
26	3.455	4.579	4.060	4.682	2.563	1047.116	3.935	14.219
27	4.464	5.048	4.254	5.260	2.420	1135.996	4.206	14.635
28	5.133	5.550	4.462	5.361	2.521	1063.072	4.014	16.484

Table S84: **EGOZUV**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	-1.654	-1.422	2.309	-0.541	-0.633	1.674	-2.965
3	-0.526	-0.480	-2.566	0.427	-1.559	-0.738	-1.654
4	-0.648	-0.617	-0.322	-0.668	-0.595	-0.392	-0.205
5	-1.677	-0.631	4.303	-0.373	-0.163	2.744	-2.731
6	0.682	0.393	-0.930	0.490	0.213	-1.431	-0.427
7	0.141	0.150	-1.649	0.032	-0.509	0.222	-0.012
8	0.331	0.544	-1.583	0.640	0.222	-1.277	-0.064
9	-1.406	-0.778	-0.123	-0.469	-0.253	-1.015	-0.620
10	-0.167	-0.791	-1.482	0.233	-1.588	-0.384	-2.125
11	-1.582	-1.243	-0.946	-0.871	-0.715	-0.440	-0.118
12	4.767	2.556	1.819	-0.139	1.827	1.575	-1.767
13	-0.672	-0.507	3.490	-0.770	-0.651	2.649	-2.352
14	1.708	1.564	-2.305	0.916	1.798	-1.153	0.153
15	-0.496	-0.234	-1.260	-0.775	-0.782	-0.635	0.436
16	-1.194	-1.079	4.148	-0.944	-0.851	3.605	-2.402
17	-0.074	-0.292	-2.421	0.974	-0.319	-1.725	-0.306
18	0.255	-0.283	-1.522	-0.042	-1.486	-0.440	-2.245
19	-0.237	-0.094	-2.098	-0.185	-1.585	-0.246	-1.753
20	-0.167	-0.760	-1.644	0.276	-1.546	-0.541	-2.121
21	0.737	1.179	1.274	0.545	-0.120	0.934	-1.043
22	0.066	0.849	-2.793	1.046	-0.363	-2.284	-0.204
23	-0.976	0.667	-1.959	0.148	-0.563	-0.036	-1.736
24	0.286	1.130	-0.901	1.174	0.669	-0.743	-0.903
25	-0.454	-0.275	-1.697	-0.755	-0.818	-1.090	0.503
26	4.266	2.884	-1.195	0.068	2.283	-0.032	2.067
27	4.076	3.535	-1.353	0.011	2.762	-0.297	1.762
28	4.360	2.773	1.650	0.067	2.499	3.194	1.712

Table S85: **EGOZUV**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	-0.386	-0.817	0.136
3	-1.764	-2.051	-2.759
4	-0.529	-0.903	0.352
5	-0.502	-0.404	0.163
6	0.244	0.000	3.079
7	-1.482	-1.384	-2.986
8	0.461	0.278	3.062
9	-0.436	-0.158	0.110
10	-1.606	-2.104	-3.350
11	-0.538	-0.579	0.552
12	-0.946	-0.981	-1.133
13	-0.784	-1.016	-0.097
14	0.358	0.122	2.063
15	-0.854	-0.835	-1.136
16	-0.898	-0.857	-0.436
17	-1.911	-2.155	-0.250
18	-1.421	-1.677	-3.181
19	-2.133	-2.031	-4.268
20	-1.178	-1.652	-3.920
21	2.738	2.571	6.381
22	-1.732	-1.539	-1.326
23	0.714	0.683	-0.075
24	-0.382	-0.507	-0.577
25	0.194	0.682	-0.476
26	5.472	6.381	8.719
27	5.912	6.453	8.361
28	5.597	6.414	5.457

Table S86: **FEGGII**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.514	-0.751	-0.370	-0.918	1.304	1.101	-1.064	3.905
3	0.514	-1.017	-1.035	-1.488	0.841	0.304	-1.586	3.408
4	0.601	0.358	1.055	0.139	0.949	0.660	1.220	4.923
5	0.746	-0.146	0.216	-0.943	1.999	2.790	0.320	3.332
6	1.362	1.719	1.860	1.526	1.502	2.802	2.538	1.749
7	1.556	0.437	0.576	-0.908	2.383	2.853	0.145	4.092
8	1.800	1.098	0.603	0.557	0.277	0.826	-0.558	2.930
9	2.297	1.624	1.371	1.246	0.249	0.130	-1.741	6.226
10	2.456	1.593	2.034	0.971	2.860	3.091	3.786	13.087
11	2.699	1.880	2.246	1.242	2.999	3.815	2.373	14.119
12	2.873	0.627	0.583	0.029	0.005	0.937	0.450	9.294
13	2.923	2.153	3.162	2.327	2.488	1.343	5.544	18.567
14	3.021	2.322	2.361	2.438	0.655	0.858	-1.329	8.083
15	3.624	2.957	3.921	3.016	1.249	3.172	5.396	5.771
16	3.711	2.549	3.189	3.035	0.729	1.034	3.602	7.209
17	3.802	3.067	3.828	3.765	1.259	2.156	4.276	9.155
18	4.135	2.325	2.049	2.293	-0.037	1.050	0.476	6.039
19	4.544	2.735	1.931	2.113	1.982	1.760	-1.453	6.489
20	4.614	3.901	3.856	3.555	3.443	4.864	5.308	11.668
21	4.964	3.649	4.003	2.857	2.322	4.371	4.753	13.499
22	5.263	5.038	4.840	4.345	3.259	4.873	3.919	6.577
23	5.524	4.622	4.426	4.315	3.862	4.193	2.821	5.553
24	5.560	5.206	6.033	5.552	2.432	4.259	6.422	9.423
25	5.683	3.527	3.165	1.856	4.945	5.725	4.277	10.630
26	5.979	4.772	5.076	4.557	3.963	3.783	3.797	16.948
27	6.530	4.979	4.827	4.236	3.131	5.177	4.143	24.316
28	7.919	6.474	5.725	4.870	3.982	6.490	4.619	16.611

Table S87: **FEGGII**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.191	-1.636	1.976	2.011	2.190	1.650	-1.761
3	-1.376	-1.887	0.986	0.695	0.372	1.092	-2.959
4	0.455	-0.649	3.880	1.211	1.497	3.434	-0.622
5	0.848	-0.731	2.394	1.885	4.392	2.533	1.580
6	1.627	1.505	2.583	1.631	3.212	2.600	2.844
7	1.314	-0.902	1.059	2.501	3.597	2.320	0.262
8	0.519	-0.554	1.908	-0.247	0.473	1.269	-0.917
9	1.329	-0.286	2.337	0.212	0.148	0.344	-2.797
10	2.174	-0.193	7.041	2.520	3.752	6.170	2.031
11	1.932	0.613	6.763	2.799	3.847	4.932	1.793
12	-0.446	-1.335	1.900	0.462	1.454	1.143	-1.207
13	2.356	-0.218	6.645	2.706	2.822	6.886	2.657
14	2.270	-0.038	3.237	0.666	1.407	0.390	-2.177
15	3.499	1.444	8.624	1.374	4.220	5.625	3.770
16	2.949	0.707	9.772	0.660	1.735	5.964	1.326
17	3.397	1.271	9.993	1.339	3.015	5.838	1.088
18	1.972	0.012	2.390	0.310	1.964	0.570	0.068
19	7.456	0.313	11.811	3.748	1.999	4.967	-0.182
20	3.291	0.244	5.124	3.695	0.007	5.496	5.059
21	4.567	1.741	7.864	1.571	4.252	5.375	3.816
22	4.653	3.275	5.937	2.935	5.283	4.628	4.290
23	4.461	3.076	7.285	3.607	4.809	5.626	1.523
24	5.778	3.415	12.914	2.341	5.252	7.631	5.100
25	3.833	1.681	5.993	3.707	5.785	5.654	4.331
26	3.134	2.584	13.700	0.671	2.773	8.196	1.868
27	4.737	2.954	5.809	3.127	5.717	4.931	2.626
28	6.282	0.836	8.547	3.594	1.766	8.064	3.184

Table S88: **FEGGII**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	1.877	3.203	-7.695
3	-0.978	-0.561	-8.965
4	4.707	6.620	-1.513
5	-2.194	1.290	-6.756
6	-0.863	2.189	2.352
7	-1.070	2.704	-4.941
8	3.825	4.320	-0.940
9	0.682	1.186	-2.260
10	4.019	6.642	-3.511
11	3.422	6.208	-2.324
12	1.736	1.487	-4.096
13	0.610	2.888	-5.284
14	3.557	4.843	-0.673
15	1.178	5.270	-2.519
16	3.503	4.851	-4.338
17	6.927	9.118	-1.436
18	6.143	6.202	-0.916
19	0.832	1.559	-0.191
20	3.785	6.295	-3.377
21	0.805	5.110	-2.119
22	3.435	6.970	2.547
23	6.918	8.853	1.493
24	2.607	6.546	0.330
25	2.078	6.993	3.229
26	4.173	6.192	-2.408
27	4.236	6.009	-0.394
28	4.232	7.580	-2.558

Table S89: **FODBOP**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	1.327	1.653	1.427	1.785	0.477	0.617	-0.165	-0.764
3	1.598	1.595	0.946	1.055	0.686	0.174	0.027	7.125
4	1.833	2.146	1.572	1.700	-0.168	0.012	-0.753	-8.025
5	1.885	2.112	1.586	2.156	0.770	0.630	-0.168	-1.746
6	2.052	2.518	2.702	2.608	1.394	1.643	7.530	9.960
7	2.131	2.697	1.873	2.571	0.351	-0.409	-0.740	-10.082
8	2.744	3.028	3.012	3.033	2.700	2.607	6.440	4.353
9	2.805	2.596	2.289	2.666	1.332	1.112	5.807	0.372
10	2.976	2.926	2.158	2.345	0.586	0.115	-0.454	-11.981
11	3.045	3.325	2.576	3.125	1.065	0.550	-0.165	-2.345
12	3.307	3.317	3.041	3.318	2.003	1.729	5.810	4.877
13	3.378	3.386	3.074	3.127	1.740	1.541	-0.466	-10.424
14	3.429	2.701	2.272	2.372	1.990	1.077	1.351	3.627
15	3.814	3.604	2.691	3.162	1.474	1.203	-1.696	-10.499
16	3.844	3.846	3.174	3.384	2.343	1.460	0.585	-1.278
17	3.852	3.915	3.174	3.553	1.787	0.897	0.016	-3.485
18	3.914	4.076	3.227	3.606	1.432	0.569	0.033	-2.081
19	3.975	4.708	3.730	4.519	1.239	0.513	1.016	-5.315
20	3.984	4.676	4.906	4.939	2.776	3.170	3.906	12.290
21	4.083	3.718	3.466	3.540	3.068	2.252	1.387	2.687
22	4.187	3.383	2.472	2.745	1.771	0.662	0.670	-4.070
23	4.246	5.163	5.072	5.159	2.289	2.443	1.185	0.343
24	4.298	3.536	2.946	3.075	3.164	1.930	2.606	7.180
25	4.491	5.174	4.523	5.105	1.371	1.882	-1.249	-22.009
26	4.558	4.624	3.446	4.198	1.279	0.946	-1.317	-15.174
27	4.963	5.402	4.912	5.550	2.055	1.489	0.348	-1.027
28	5.145	5.642	4.888	5.899	2.592	2.175	1.261	-4.646
29	5.148	5.265	4.456	5.066	2.612	1.900	1.307	3.128
30	7.247	7.123	5.941	6.614	2.949	2.259	2.083	1.872

Table S90: **FODBOP**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	1.561	1.650	-1.397	0.248	0.422	-0.629	0.184
3	0.812	0.609	-2.063	0.641	0.328	-0.482	-0.063
4	0.976	1.023	-1.093	0.198	0.317	-0.795	-4.277
5	1.708	1.595	-0.793	0.542	0.530	-0.153	0.200
6	2.484	2.777	7.720	1.240	1.276	5.212	1.557
7	1.586	1.142	3.110	0.493	0.198	2.904	-5.573
8	3.512	3.413	10.119	2.487	2.431	9.095	-0.266
9	1.972	1.997	0.086	1.323	1.143	0.323	0.642
10	1.774	1.455	1.399	0.862	0.717	1.722	-4.548
11	2.474	2.075	0.137	1.031	0.590	0.453	-0.163
12	2.695	2.922	-0.676	2.045	1.639	-0.216	0.678
13	2.221	2.458	2.157	2.267	1.983	3.603	-0.540
14	2.391	1.992	2.625	1.980	1.404	2.282	-2.540
15	2.184	2.402	0.974	1.971	1.510	2.468	-5.913
16	3.109	2.882	3.631	2.312	1.603	3.220	0.027
17	3.141	2.517	1.075	1.742	1.249	1.487	-4.135
18	2.872	2.449	1.739	1.594	1.043	1.536	-4.201
19	3.627	3.031	6.101	1.157	0.974	4.228	-3.952
20	4.820	4.651	6.324	2.587	3.177	4.671	3.406
21	3.451	3.375	7.483	2.997	2.287	7.212	0.445
22	1.977	1.791	6.542	2.004	1.116	4.942	-4.112
23	4.726	4.702	2.782	2.409	2.615	1.087	1.585
24	3.300	2.774	5.310	2.651	1.890	4.640	1.083
25	3.535	3.802	4.587	1.924	2.315	4.483	-5.798
26	2.814	2.795	9.563	1.483	1.357	7.841	-2.646
27	4.377	3.999	4.550	2.327	2.111	3.212	-3.830
28	5.167	4.614	6.490	2.412	2.490	5.563	-3.759
29	4.677	3.915	6.378	2.400	2.148	4.361	0.473
30	5.655	5.261	8.994	3.116	2.511	6.614	-3.698

Table S91: **FODBOP**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	0.928	0.696	1.284
3	0.314	1.371	0.958
4	-1.095	-0.764	2.495
5	2.832	2.530	2.292
6	-0.318	0.534	2.121
7	-0.812	-0.882	2.454
8	3.616	3.856	2.322
9	-0.446	-1.013	2.587
10	0.353	0.694	3.568
11	1.791	1.887	3.852
12	1.285	2.010	2.078
13	3.755	3.944	3.269
14	-1.654	-1.075	-0.118
15	2.511	2.928	2.971
16	2.101	3.107	2.329
17	-1.600	-1.289	4.479
18	-3.352	-3.031	2.085
19	-1.181	-1.472	3.437
20	1.111	1.992	0.203
21	0.521	1.499	0.272
22	-0.471	0.270	1.598
23	1.830	2.489	2.398
24	-0.085	1.244	-0.151
25	2.701	2.528	6.312
26	-0.285	-0.057	3.658
27	-0.885	-1.648	2.851
28	-0.160	-0.216	3.278
29	-1.700	-1.469	2.806
30	2.700	4.045	5.459

Table S92: **FONLID**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.169	0.207	0.496	0.309	2.053	1.086	2.175	-4.252
3	0.325	0.364	0.453	0.459	1.806	1.307	2.187	-1.693
4	0.394	0.453	0.179	0.602	1.476	1.668	3.466	-2.464
5	0.412	0.400	0.849	0.519	2.782	2.130	3.275	-4.978
6	0.496	0.999	0.749	0.532	2.188	1.584	4.356	-1.742
7	0.512	0.872	0.080	0.619	1.051	1.709	4.452	2.679
8	0.519	0.582	0.742	0.688	2.656	2.716	3.402	-2.410
9	0.567	0.680	0.834	0.717	2.939	2.910	4.461	-1.221
10	0.571	0.665	0.898	0.788	3.238	2.707	4.132	-4.281
11	0.742	0.931	0.748	1.126	3.447	3.166	5.680	-4.096
12	0.765	1.338	0.782	0.976	2.263	1.936	5.299	2.164
13	0.767	1.317	0.908	0.871	2.351	1.897	5.127	0.800
14	0.781	0.971	0.744	1.226	3.773	3.379	5.746	-4.965
15	0.790	1.341	0.784	0.983	2.259	1.925	5.290	2.163
16	0.803	0.897	0.461	0.999	2.639	2.166	4.784	-3.008
17	0.831	1.095	0.836	0.633	2.147	2.314	5.842	0.045
18	0.840	1.064	0.787	1.079	2.342	2.204	2.463	0.139
19	0.925	0.905	1.152	0.368	1.920	1.272	3.703	1.880
20	1.010	1.253	0.863	1.154	2.938	2.566	4.592	-1.164
21	1.032	1.266	1.426	1.341	3.668	3.014	4.211	-3.123
22	1.082	1.527	0.931	1.564	2.846	1.715	4.767	2.084
23	1.093	1.388	0.970	0.893	2.334	2.712	6.694	2.886
24	1.105	1.404	1.304	1.385	3.522	3.522	4.654	0.121
25	1.186	1.636	0.800	1.423	1.742	0.667	3.191	4.083
26	1.199	1.717	0.936	1.538	2.550	1.011	3.614	3.806
27	1.253	1.427	0.814	1.666	0.800	0.120	-1.014	0.821
28	1.306	1.677	1.504	1.604	3.288	2.545	3.817	1.998
29	1.552	1.931	1.308	1.476	2.939	1.853	5.121	4.098
30	1.565	1.942	0.990	2.331	3.253	2.857	5.147	-1.257

Table S93: **FONLID**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	-0.465	2.343	-4.945	-0.826	-1.202	-4.912	4.395
3	-0.752	1.528	0.827	-1.128	-0.329	-2.646	1.980
4	-0.032	1.975	-7.335	0.521	2.959	-5.233	5.953
5	-0.112	2.310	-9.258	0.198	0.200	-7.607	5.882
6	4.416	5.150	10.241	0.502	2.908	-2.108	-29.431
7	-0.665	1.554	2.934	0.481	0.221	1.079	0.414
8	-0.396	1.621	1.350	-0.156	1.137	-1.128	3.087
9	0.939	1.589	2.691	-0.439	-0.322	-2.640	4.185
10	1.378	3.457	4.647	-0.117	-1.218	-1.613	5.484
11	1.895	4.996	-8.624	0.403	2.112	-4.655	6.390
12	2.255	1.892	2.644	0.455	1.095	-5.946	7.153
13	4.434	5.329	9.023	0.590	2.169	-1.797	4.548
14	1.506	5.434	5.555	-0.280	0.328	0.661	1.911
15	2.128	1.912	2.181	0.456	1.093	-6.169	7.169
16	1.232	4.105	-7.429	0.469	2.279	-4.193	4.254
17	3.475	4.436	-8.887	0.258	2.074	-4.921	3.202
18	-0.385	2.071	1.898	-0.565	0.189	-2.538	-30.777
19	0.829	3.595	-0.930	0.129	1.106	-2.110	3.083
20	1.404	5.611	12.256	-0.064	0.540	4.889	-36.469
21	1.471	3.465	4.946	0.294	-0.763	-1.820	3.367
22	2.419	4.554	8.181	0.170	1.857	1.804	-36.843
23	3.539	3.016	-7.152	0.354	0.692	-4.034	3.575
24	0.666	2.188	2.856	-0.044	0.184	-0.898	2.395
25	-0.539	0.430	5.696	0.156	1.758	1.719	-32.256
26	2.666	3.279	5.609	0.482	3.310	-1.305	4.102
27	-2.785	2.314	3.842	0.572	-1.205	3.394	1.071
28	1.490	3.263	6.790	0.385	1.116	0.346	4.211
29	2.765	0.067	-3.675	0.376	2.192	-4.628	5.026
30	1.329	3.680	-2.912	-0.036	1.533	0.263	4.740

Table S94: **FONLID**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	1.631	2.667	0.915
3	1.564	2.534	1.046
4	3.715	4.079	1.147
5	2.618	4.131	1.475
6	2.340	3.830	2.479
7	1.834	2.603	1.863
8	2.488	4.036	1.767
9	3.010	4.465	1.940
10	3.272	4.863	2.009
11	5.233	6.636	2.725
12	2.618	3.971	2.566
13	2.288	3.801	2.715
14	5.620	7.088	3.056
15	2.629	3.990	2.584
16	4.371	5.166	2.160
17	2.913	4.193	2.698
18	1.748	2.984	1.817
19	1.421	2.309	1.011
20	4.080	5.442	2.820
21	3.588	5.474	2.672
22	3.621	4.527	2.193
23	2.741	4.023	2.897
24	3.206	5.034	2.789
25	1.614	2.298	1.524
26	2.599	3.394	1.934
27	1.634	1.618	0.850
28	2.289	3.960	2.253
29	3.128	4.527	2.701
30	5.687	6.496	3.378

Table S95: **HIGTIA**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.489	0.822	0.552	-0.895	1.467	1.160	-4.212	2.613
3	0.685	0.796	0.614	-0.760	1.652	1.048	-4.125	2.205
4	1.100	1.082	1.341	0.896	0.971	1.055	-0.047	2.284
5	1.192	1.167	1.300	0.837	1.052	1.062	0.043	3.121
6	1.204	1.118	1.365	0.913	0.967	1.099	-0.040	2.663
7	1.258	1.149	1.399	0.919	1.060	1.115	0.044	2.512
8	1.271	1.185	1.404	0.918	1.138	1.162	0.071	2.303
9	1.412	1.246	1.393	0.969	1.065	1.052	-0.028	1.238
10	3.109	2.467	2.074	1.000	4.225	2.658	-2.272	2.596
11	3.146	2.427	2.089	1.007	4.390	2.730	-2.136	2.742
12	3.203	2.144	2.138	0.581	5.206	3.021	-1.958	2.089
13	4.312	3.631	3.594	3.325	2.013	1.352	-4.150	0.863
14	8.155	5.929	4.738	4.082	6.468	2.805	0.127	2.462

Table S96: **HIGTIA**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	7.403	1.431	-3.952	4.656	3.227	5.625	-1.710
3	15.409	5.205	-4.042	4.471	3.381	5.622	-1.712
4	0.748	0.957	0.181	2.251	1.569	2.666	0.142
5	0.913	1.151	0.781	2.259	1.610	3.350	0.098
6	0.800	1.176	-0.017	2.249	1.569	2.413	0.140
7	0.607	1.218	0.094	2.248	1.462	2.588	0.140
8	0.858	1.053	0.770	2.249	1.587	3.228	0.111
9	0.754	1.077	0.399	2.257	1.538	2.873	0.122
10	9.433	3.105	0.938	4.517	2.950	8.101	-2.265
11	8.741	2.852	1.173	4.541	2.956	8.241	-2.267
12	4.536	2.266	-1.489	4.422	1.782	4.678	-1.383
13	4.693	2.292	-1.526	4.424	1.783	4.686	-1.373
14	15.460	5.431	-3.005	4.456	3.360	6.303	-1.750

Table S97: **HIGTIA**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	2.927	2.289	-2.607
3	2.783	2.289	-2.641
4	2.420	2.132	0.663
5	1.959	1.739	0.619
6	2.474	2.172	0.741
7	2.201	1.881	0.671
8	2.224	1.882	0.634
9	2.327	1.990	0.562
10	0.989	1.254	-0.896
11	0.685	1.006	-0.885
12	-1.431	-1.744	-2.350
13	5.246	4.852	-1.908
14	1.211	1.291	-0.713

Table S98: **LARJIZ**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.463	0.034	0.079	-0.286	0.466	-0.329	-0.125	-2.625
3	0.561	0.358	0.268	0.386	0.419	0.278	0.171	0.998
4	0.566	0.212	0.105	-0.278	0.583	-0.280	-0.085	-2.894
5	0.599	-0.464	0.528	-1.144	2.040	-1.479	1.423	11.350
6	0.732	0.760	0.315	0.584	0.201	1.271	1.318	2.534
7	0.776	-0.537	0.991	-1.676	0.668	-0.642	1.922	20.543
8	0.784	0.510	0.134	0.354	-0.138	1.011	0.864	0.007
9	0.865	0.202	0.993	-0.297	1.190	-1.118	0.425	9.397
10	0.992	0.953	1.024	0.788	1.132	1.133	0.027	-0.085
11	1.432	1.465	0.949	1.330	0.521	2.376	0.406	3.051
12	1.811	1.993	1.244	2.622	0.150	-0.447	1.319	2.725
13	1.987	0.797	1.921	0.287	2.351	0.972	3.443	25.189
14	2.069	1.149	1.300	1.821	3.585	-0.413	1.771	-0.388
15	2.396	1.692	2.336	2.008	2.717	1.495	2.823	23.794
16	2.531	2.562	2.058	2.884	1.439	-0.644	1.571	4.503
17	2.624	2.513	1.775	2.817	0.892	-1.138	1.447	3.541
18	2.657	2.344	1.502	2.682	3.551	1.895	0.488	-8.202
19	3.442	2.690	2.848	2.485	3.160	1.563	3.767	22.723
20	4.115	4.210	2.875	4.556	2.191	1.909	0.869	-0.171
21	4.454	4.390	3.498	5.223	3.921	2.066	1.086	1.269
22	5.056	4.689	4.128	5.212	4.007	3.124	2.790	22.440
23	5.188	5.261	4.789	5.320	4.228	2.571	2.295	10.190
24	5.245	5.142	4.460	5.616	4.437	2.744	0.892	4.015
25	5.442	5.277	4.071	5.741	3.969	1.734	1.273	9.785
26	5.962	5.654	4.990	4.975	3.157	0.896	6.332	29.267
27	6.034	5.811	5.326	6.097	4.401	5.608	3.212	11.972
28	7.189	6.436	6.140	6.511	4.630	4.593	3.654	14.140
29	7.226	7.601	6.367	8.580	5.501	2.931	2.642	6.311

Table S99: **LARJIZ**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.357	0.356	0.932	0.372	-0.684	1.240	0.395
3	2.813	2.250	0.163	1.743	0.248	0.455	0.120
4	0.626	0.192	2.162	1.086	-0.688	3.130	0.674
5	-0.097	1.267	1.833	2.292	-1.831	4.073	1.269
6	-0.040	-0.077	2.410	0.413	0.794	2.588	0.799
7	-0.222	1.637	3.456	1.662	-1.089	3.916	1.234
8	-0.289	0.036	2.585	0.096	0.355	2.390	0.587
9	0.652	1.423	4.329	1.270	-1.184	4.253	-0.618
10	0.399	0.856	6.189	1.689	1.309	5.717	0.065
11	0.556	0.966	5.619	0.514	2.452	4.060	0.178
12	1.501	1.681	2.005	-0.111	-0.721	2.317	1.351
13	1.300	2.920	8.478	2.897	0.259	9.524	1.249
14	1.362	2.053	4.315	3.612	-0.920	5.945	2.298
15	1.612	3.221	8.129	3.258	1.003	9.052	1.442
16	2.965	2.542	2.080	0.864	-1.000	3.820	2.112
17	2.085	1.948	1.911	0.504	-1.299	3.934	1.428
18	0.701	1.945	25.114	4.179	1.461	21.087	-2.691
19	4.154	3.649	5.824	2.268	0.976	6.911	2.676
20	2.329	3.120	3.955	2.417	1.639	3.088	0.610
21	3.413	3.566	4.474	3.949	1.859	3.920	0.696
22	4.676	4.657	8.104	2.988	2.910	10.011	1.895
23	4.543	4.287	6.378	3.842	3.064	6.554	2.208
24	3.912	4.106	11.947	4.536	3.086	10.753	-0.305
25	4.215	4.217	7.076	4.320	1.625	7.226	0.637
26	5.957	5.821	9.178	2.412	0.077	8.323	4.385
27	6.905	6.701	8.080	3.951	4.525	7.785	2.965
28	7.479	7.292	9.654	3.348	3.240	7.194	2.869
29	6.829	6.476	45.368	4.638	2.759	38.764	-5.415

Table S100: **LARJIZ**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	5.667	6.009	1.785
3	-1.046	-0.829	-0.097
4	5.053	5.465	1.981
5	1.074	2.884	-1.060
6	3.347	3.579	0.699
7	-0.816	1.188	-3.414
8	0.963	1.254	-0.472
9	9.394	10.108	2.372
10	5.493	5.873	2.235
11	3.838	4.188	1.740
12	-3.114	-3.186	0.635
13	-2.071	0.150	-3.500
14	-5.497	-5.033	-4.484
15	2.891	4.139	0.379
16	0.851	0.990	1.776
17	1.740	1.724	3.109
18	-4.618	-4.514	-2.751
19	1.259	3.101	-0.386
20	-8.126	-7.776	-1.664
21	-10.641	-10.065	-1.304
22	10.974	11.269	5.364
23	-9.262	-8.075	-1.385
24	-9.610	-8.545	-2.186
25	-2.249	-1.521	3.760
26	3.048	4.101	1.303
27	2.689	4.055	4.051
28	9.752	10.843	6.380
29	-16.704	-15.718	-1.233

Table S101: **LEHJAL**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	1.701	0.251	0.529	-0.776	2.720	-0.650	1.583	5.000
3	1.999	0.395	0.848	-0.968	3.060	-1.011	1.616	11.748
4	3.082	1.284	1.471	0.977	0.415	-1.516	-2.039	0.048
5	3.959	1.741	2.233	1.674	2.215	-0.211	-3.133	-2.471
6	3.968	1.586	1.806	0.270	2.343	-2.031	-0.350	4.924
7	4.030	2.380	2.683	0.893	3.702	1.009	3.820	8.304
8	4.120	1.648	2.572	-0.085	5.250	0.342	-0.160	0.100
9	4.124	1.588	2.009	0.274	2.645	-2.014	-0.112	5.251
10	4.153	1.796	2.289	1.769	2.329	-0.553	-3.235	-0.355
11	4.154	2.403	2.387	0.929	2.954	1.755	-0.528	10.278
12	4.246	1.675	2.248	1.805	2.246	-0.433	-3.146	0.655
13	4.444	1.572	2.612	0.206	5.276	0.001	-0.503	-1.142
14	4.879	3.247	2.996	1.462	3.632	1.640	4.068	5.514
15	4.890	3.926	3.425	3.976	2.198	2.394	2.319	-3.744
16	5.197	3.499	3.660	2.709	2.956	-0.027	1.672	6.074
17	5.912	2.990	3.827	1.560	3.895	0.150	-3.133	-2.125
18	6.142	3.611	4.297	2.593	3.981	-1.073	0.631	21.569
19	6.335	3.729	4.149	1.962	5.167	-0.367	3.575	10.899
20	7.541	5.134	6.016	3.235	6.892	2.041	0.628	3.781
21	7.718	6.976	6.943	7.000	2.682	1.844	2.934	24.277
22	7.763	4.863	5.065	4.398	3.359	1.180	-0.672	-1.173
23	8.968	5.158	6.337	4.109	4.868	0.803	0.421	12.416
24	10.758	9.651	10.255	8.396	9.601	7.560	5.295	14.378
25	13.650	10.032	11.186	9.795	9.378	3.439	2.116	49.976

Table S102: **LEHJAL**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.327	-0.061	-0.074	2.476	-0.137	1.645	1.747
3	1.733	0.478	-1.012	2.888	-0.718	1.253	3.166
4	18.698	20.652	14.612	2.517	-1.738	7.741	5.841
5	4.033	3.418	0.094	1.808	-0.781	0.990	-1.079
6	3.100	2.155	-3.205	0.933	-1.980	-0.123	1.440
7	3.181	1.766	3.000	3.226	1.687	2.584	4.090
8	5.483	3.921	1.688	2.918	-0.522	3.401	0.183
9	3.416	2.394	-3.124	1.164	-1.950	0.187	1.503
10	2.962	3.617	-0.492	1.597	-0.714	0.730	-1.092
11	2.358	1.106	1.134	2.965	-1.247	2.844	-1.683
12	2.724	3.705	1.926	1.621	-0.779	2.451	-1.519
13	5.214	3.099	0.716	3.084	-1.006	3.424	0.003
14	3.497	2.142	3.031	3.274	1.797	2.465	4.091
15	4.389	2.312	3.630	1.346	3.042	-0.853	2.440
16	4.570	3.584	0.434	1.589	0.307	0.298	3.321
17	4.155	5.771	1.491	3.591	-0.614	5.205	-1.117
18	6.901	6.161	-0.138	1.363	-1.921	2.132	4.337
19	5.813	3.999	0.083	3.070	-0.239	0.125	3.350
20	20.199	21.228	2.410	3.676	-1.210	5.040	3.808
21	8.089	7.586	4.451	1.457	1.677	3.784	4.530
22	5.811	5.099	1.859	2.467	1.272	0.608	1.376
23	12.531	6.678	3.865	3.464	0.567	4.895	0.735
24	17.897	20.603	12.618	1.980	0.328	7.645	7.381
25	16.626	19.601	7.312	2.846	0.824	4.832	4.696

Table S103: **LEHJAL**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	3.011	3.556	4.444
3	6.163	5.679	1.577
4	2.338	1.003	-1.436
5	0.903	0.196	-1.105
6	5.201	3.947	0.010
7	3.854	5.879	8.493
8	4.655	5.104	4.430
9	5.386	4.465	-0.227
10	1.309	0.401	-1.027
11	3.081	3.649	3.620
12	1.262	0.378	-1.824
13	3.985	4.404	3.985
14	1.103	4.971	8.989
15	1.227	3.271	-2.987
16	2.685	4.776	5.496
17	5.418	3.711	-1.184
18	6.071	7.540	9.059
19	5.069	8.129	9.903
20	5.361	7.290	6.186
21	5.844	5.846	2.745
22	1.426	2.303	5.615
23	9.178	6.513	3.902
24	7.428	10.517	13.855
25	8.850	9.050	7.252

Table S104: **MIYBAZ**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.038	-0.349	-0.127	-0.942	0.515	0.757	0.188	-2.742
3	0.610	0.768	0.615	0.862	-0.401	0.350	0.227	0.108
4	0.619	0.393	0.629	0.179	0.235	0.817	0.200	-2.501
5	0.640	0.661	0.888	0.048	0.621	1.127	1.066	-1.876
6	0.962	1.485	1.257	1.364	0.762	0.492	0.978	0.938
7	1.097	1.036	1.226	0.432	1.191	1.621	1.080	-1.883
8	1.152	1.583	1.397	1.591	-0.127	0.695	1.014	1.060
9	1.315	1.828	1.673	1.764	1.078	0.612	0.182	0.115
10	1.324	1.668	1.301	2.270	-0.758	0.158	0.207	2.610
11	1.379	2.204	1.895	2.204	0.824	0.742	1.195	2.547
12	1.389	1.708	1.799	0.937	0.989	1.499	1.904	-0.919
13	1.460	1.937	1.454	2.552	-0.102	0.106	0.328	3.793
14	1.533	1.339	1.219	0.823	0.977	0.706	1.532	0.047
15	1.535	1.647	1.626	1.680	1.136	1.049	0.327	0.626
16	1.585	2.049	2.151	1.425	1.269	1.974	1.974	-1.070
17	1.660	1.829	1.702	1.805	0.795	0.291	1.121	1.617
18	1.711	2.307	2.068	2.113	0.770	1.394	1.945	1.591
19	2.013	2.138	2.073	1.811	1.179	1.285	1.353	0.039
20	2.073	1.398	1.311	0.705	1.740	1.464	1.635	-3.293
21	2.189	2.217	1.746	2.424	0.872	0.805	1.309	2.406
22	2.292	2.670	2.497	2.613	1.107	1.841	1.632	-0.308
23	2.368	2.237	2.779	1.394	2.479	2.624	1.867	-0.590
24	2.415	3.228	2.917	3.088	1.775	0.969	1.880	-0.696
25	2.576	2.400	2.200	2.180	1.712	1.656	1.755	0.319
26	2.772	2.354	2.089	1.855	1.735	0.616	1.876	-3.135
27	2.839	3.383	3.193	2.939	1.652	2.242	2.360	0.399
28	2.984	2.899	2.721	2.539	2.069	1.891	2.328	1.357
29	4.100	4.278	3.748	4.175	1.713	1.232	2.127	-0.721

Table S105: **MIYBAZ**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.094	0.008	-0.062	0.160	1.080	0.487	0.375
3	0.526	0.396	1.054	-0.209	0.646	-0.216	0.017
4	0.920	0.000	0.615	0.497	1.052	0.129	0.311
5	0.849	1.041	0.902	0.601	1.433	0.780	1.145
6	0.977	0.994	1.353	1.465	0.593	0.271	0.700
7	1.438	0.069	1.510	0.920	2.573	1.454	1.161
8	1.311	1.304	1.712	0.217	0.908	-0.546	0.751
9	2.902	-0.466	1.891	0.852	1.711	-0.182	0.083
10	1.227	0.833	1.592	-0.261	0.518	-1.371	-0.283
11	2.236	1.280	2.011	0.879	1.291	-0.078	0.979
12	1.682	1.879	1.751	1.047	1.804	0.543	1.936
13	1.225	0.694	1.785	0.424	0.484	-0.860	-0.143
14	1.098	1.520	1.293	1.330	0.342	1.809	1.362
15	2.189	0.086	1.961	1.094	1.920	0.396	0.130
16	2.206	1.128	2.310	1.366	2.951	1.400	1.952
17	1.856	2.103	2.333	1.009	-0.256	1.107	0.858
18	1.926	1.786	2.239	1.160	1.610	0.529	1.536
19	2.434	1.629	1.876	1.166	1.388	0.025	1.320
20	1.992	0.469	1.793	1.739	1.373	2.792	1.789
21	1.828	1.934	2.213	1.188	0.705	1.841	1.053
22	3.006	0.874	2.669	1.426	2.525	0.551	1.292
23	4.216	2.048	2.631	1.830	2.980	2.173	1.883
24	3.058	1.781	4.339	2.107	1.375	1.776	0.873
25	2.941	1.123	2.624	1.468	1.803	1.665	1.706
26	2.304	1.598	3.657	1.957	0.069	3.831	1.103
27	3.674	1.723	3.575	1.839	2.731	1.238	2.030
28	4.025	1.746	3.203	2.213	2.056	2.456	2.190
29	3.890	1.888	5.331	1.635	1.866	2.522	1.168

Table S106: **MIYBAZ**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	-0.149	-0.103	0.856
3	0.300	0.288	-0.798
4	-0.571	-0.419	-0.207
5	0.144	0.591	0.588
6	0.462	0.783	0.143
7	-0.020	0.726	0.652
8	0.604	0.951	-0.774
9	-0.458	0.695	1.921
10	0.626	0.640	-2.414
11	0.551	1.665	0.453
12	0.454	1.336	0.711
13	0.669	0.902	-1.416
14	0.219	0.492	0.779
15	0.120	0.735	0.673
16	0.397	1.579	0.188
17	0.742	1.151	0.482
18	0.658	1.610	-0.716
19	-0.019	1.168	0.464
20	-0.206	0.669	1.290
21	0.660	1.417	0.008
22	-0.079	1.323	-0.863
23	0.599	1.708	1.590
24	1.387	2.106	1.752
25	0.375	1.553	0.971
26	0.598	0.829	1.678
27	0.237	1.842	-0.307
28	0.737	1.847	1.018
29	1.032	1.971	0.740

Table S107: **MOGWIP**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	1.490	0.920	-0.355	0.861	2.032	-1049.099	13.689	0.202
3	1.722	1.640	-0.218	1.883	-3.115	140.648	24.575	17.086
4	1.775	-0.381	-1.490	-0.855	-6.945	277.588	2.334	6.336
5	2.048	1.098	-0.020	1.237	-3.798	97.702	13.346	11.167
6	2.400	-0.287	-1.474	-0.626	-6.984	231.769	1.531	5.416
7	2.417	-0.325	-1.426	-0.600	-7.097	253.329	1.540	4.987
8	2.566	-0.241	-1.394	-0.396	-7.295	427.076	1.033	6.040
9	2.733	1.266	0.244	1.496	-4.576	276.115	3.776	8.003
10	2.825	1.751	0.507	2.039	-4.138	159.971	15.906	18.224
11	2.876	-0.086	-1.430	-0.393	-7.321	505.489	1.070	6.580
12	2.893	1.652	0.437	1.922	-4.584	375.868	7.444	17.898
13	3.459	3.344	2.086	2.543	1.817	512.039	-0.450	31.323
14	3.764	1.962	1.138	2.472	-4.551	375.720	6.569	18.562
15	3.814	0.969	-0.561	0.741	-6.169	384.935	2.699	10.997
16	3.959	2.497	1.823	3.560	-3.892	749.532	8.727	22.246
17	4.023	3.406	2.516	4.442	-0.743	-563.628	18.593	32.321
18	4.289	2.536	1.714	2.686	-3.733	566.194	4.496	13.260
19	4.397	2.500	1.014	2.937	-4.249	-945.974	14.030	9.368
20	4.755	3.580	2.815	3.287	1.300	317.879	15.074	13.755
21	4.915	2.484	1.206	2.582	-4.002	833.970	13.616	18.702
22	5.220	3.129	1.825	3.949	-2.904	654.373	17.552	28.590
23	5.344	3.986	2.657	4.415	-3.634	-442.210	16.357	9.490
24	5.630	3.328	1.820	3.562	-4.327	-470.389	14.731	14.046

Table S108: **MOGWIP**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	-0.375	-0.303	5.916	0.800	1.199	8.723	3.559
3	-8.379	-4.154	8.242	2.693	0.057	12.967	26.224
4	-9.229	-5.479	8.355	-0.197	-2.463	6.964	0.166
5	-7.171	-5.036	12.176	2.334	-1.538	12.122	2.602
6	-7.739	-4.523	7.812	0.473	-2.126	6.570	-0.025
7	-7.156	-3.502	7.980	0.635	-1.649	6.728	-0.016
8	-8.864	-6.695	9.117	-0.140	-3.527	7.141	-0.246
9	-8.106	-4.655	5.453	1.657	-1.547	5.655	1.021
10	-7.689	-4.559	10.480	2.193	-1.150	10.708	3.099
11	-10.066	-6.746	9.724	-0.710	-3.522	7.631	-0.246
12	-8.487	-4.599	10.150	1.812	-1.160	10.259	1.557
13	1.682	0.960	4.566	1.526	2.783	7.810	1.132
14	-7.427	-3.781	5.059	1.749	-0.480	5.685	0.864
15	-8.911	-5.588	4.823	-0.098	-2.722	4.498	0.101
16	-6.428	-3.559	5.489	2.140	-0.651	6.116	1.066
17	-5.312	-6.596	9.498	2.244	-3.108	8.316	1.740
18	-6.016	-3.242	9.518	2.569	-0.806	9.356	1.515
19	-5.343	-2.552	5.211	2.221	1.191	5.454	2.800
20	3.091	1.986	0.054	0.490	0.551	0.115	-0.017
21	-6.766	-3.744	4.876	2.250	-0.375	5.904	1.839
22	-6.962	-4.561	8.756	2.743	-1.479	9.947	2.384
23	-5.794	-2.874	5.329	2.544	1.892	7.173	5.374
24	-6.358	-3.405	11.761	1.633	0.583	10.221	12.733

Table S109: **MOGWIP**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	0.642	1.221	2.818
3	-5.044	-4.702	16.822
4	-7.058	-7.181	10.649
5	-6.459	-6.500	16.308
6	-7.724	-7.937	11.631
7	-8.011	-8.262	11.389
8	-8.500	-8.875	12.386
9	-6.436	-6.539	13.490
10	-7.103	-7.023	14.685
11	-8.520	-8.923	12.184
12	-7.579	-7.451	14.207
13	2.487	3.683	2.884
14	-7.200	-6.913	14.019
15	-7.392	-7.312	12.532
16	-6.777	-6.398	14.870
17	-3.740	-2.253	15.218
18	-6.102	-5.652	15.719
19	-3.732	-3.551	11.004
20	1.626	2.764	1.093
21	-6.908	-6.355	14.461
22	-8.037	-6.813	15.180
23	-4.123	-3.556	14.120
24	-4.789	-4.353	11.187

Table S110: **REPFID**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	1.394	1.818	1.963	1.429	2.491	3.808	0.827	-2.542
3	2.622	3.667	2.269	1.590	1.313	1.973	14.777	58.766
4	2.696	2.848	2.738	2.735	2.507	1.483	3.753	2.328
5	2.937	2.571	2.014	2.825	0.914	0.987	2.904	1.760
6	3.461	4.606	3.157	2.462	1.129	0.937	15.471	54.271
7	3.691	3.497	3.386	3.114	2.191	2.651	3.344	-3.098
8	3.713	4.157	2.800	3.306	-0.450	-0.516	10.756	49.659
9	3.769	4.039	4.454	4.574	3.031	2.450	2.952	1.172
10	3.790	4.024	3.623	3.294	3.938	4.464	3.270	-0.168
11	4.080	3.849	3.563	3.731	1.942	1.253	4.195	-4.160
12	4.112	4.315	3.574	2.382	4.041	6.370	4.373	3.820
13	4.215	4.650	4.204	3.104	3.559	7.561	4.005	-0.013
14	4.391	4.387	4.186	3.395	3.932	6.245	1.086	6.712
15	4.511	4.450	4.199	4.184	4.361	2.910	4.110	-0.311
16	4.548	5.008	4.296	3.295	4.165	8.905	6.189	0.381
17	4.595	5.006	4.577	3.051	4.257	6.158	2.777	-2.041
18	4.708	5.245	4.805	3.535	5.335	8.707	7.763	3.231
19	4.769	4.824	4.111	4.194	1.397	-0.594	13.932	39.734
20	4.891	5.395	5.089	4.360	4.605	7.498	3.277	-4.742
21	5.194	5.905	5.205	3.778	5.293	8.847	5.976	1.322
22	5.255	6.234	4.912	5.097	1.311	1.815	21.408	60.415
23	5.589	6.448	4.866	4.739	2.848	2.265	16.315	50.396
24	5.800	6.949	5.299	5.248	1.792	2.524	22.229	60.377
25	7.117	7.477	5.633	6.931	0.152	1.741	15.558	55.115
26	7.642	8.318	7.366	7.434	1.427	2.731	9.554	70.583
27	9.218	9.242	8.049	7.869	6.561	9.992	12.128	1.096
28	9.602	9.691	8.304	7.857	5.338	9.687	15.153	29.450
29	10.621	11.229	9.448	9.931	5.669	12.436	11.462	24.176

Table S111: **REPFID**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	-0.322	0.415	2.390	1.028	0.884	1.726	0.019
3	-2.393	-4.788	-2.162	2.316	0.788	4.433	-16.353
4	-0.578	-2.933	-8.812	1.528	-0.865	0.736	-12.275
5	-2.072	-2.629	-11.651	0.323	-2.191	-3.206	-12.394
6	-2.167	-3.591	-0.731	2.469	-0.244	3.658	-16.912
7	-0.246	-1.042	-6.210	1.316	-0.702	2.185	-12.289
8	-1.587	-5.673	-2.809	0.312	-1.141	2.556	-17.862
9	0.183	-0.373	-6.200	3.152	0.746	1.139	-12.092
10	2.165	-0.389	-9.785	1.830	1.050	0.171	-9.178
11	-0.138	-0.538	-8.478	1.533	-1.327	-0.593	-11.645
12	4.167	3.069	1.749	0.984	4.427	2.378	4.720
13	3.496	3.920	1.188	0.423	4.509	0.791	4.295
14	1.070	2.535	1.255	2.552	2.026	-0.362	0.195
15	1.484	-1.059	-10.082	2.510	-0.090	0.663	-9.616
16	3.745	4.765	2.092	0.506	5.132	2.692	4.756
17	4.395	5.678	-0.055	1.901	3.851	-0.181	4.149
18	5.139	4.240	1.535	1.111	5.565	2.909	6.610
19	-1.014	-3.648	-0.439	2.551	-1.272	1.613	-14.624
20	4.714	5.093	2.099	-0.369	5.114	3.437	2.728
21	4.986	5.773	2.821	1.432	6.108	2.744	5.621
22	0.378	-2.802	-0.184	2.276	1.896	2.379	-14.321
23	1.587	-2.437	0.913	1.564	-0.664	3.771	-12.139
24	0.601	-2.833	-1.178	3.025	2.715	1.881	-12.102
25	0.760	-2.367	-1.047	1.317	1.304	2.124	-16.616
26	1.134	-1.683	1.539	2.320	0.599	4.099	-15.035
27	6.161	6.776	4.882	2.763	5.333	4.944	5.197
28	5.123	5.247	3.211	2.482	4.537	4.267	6.127
29	5.848	2.534	-1.620	3.009	1.153	1.571	-11.507

Table S112: **REPFID**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	0.997	2.035	2.666
3	4.724	4.849	2.717
4	2.377	3.495	3.165
5	0.832	2.273	1.877
6	3.238	3.462	2.711
7	0.940	2.858	2.705
8	1.943	0.110	2.391
9	2.110	2.437	2.713
10	1.071	3.928	3.615
11	1.205	2.570	2.167
12	0.625	4.421	3.471
13	0.735	3.900	3.867
14	2.173	3.908	3.153
15	1.217	2.802	2.995
16	3.285	5.972	5.777
17	0.661	3.945	3.666
18	4.746	7.704	5.332
19	4.943	2.668	0.935
20	1.903	4.376	4.988
21	1.975	5.878	5.217
22	5.584	3.771	4.163
23	4.731	5.466	4.436
24	4.455	3.658	4.080
25	3.158	0.999	3.691
26	3.375	4.111	4.930
27	3.203	5.733	6.307
28	5.623	9.022	8.894
29	3.947	8.334	10.137

Table S113: **RESCUN**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.755	0.950	0.771	1.331	-1.268	0.039	2.709	11.160
3	1.372	1.010	1.110	0.456	1.757	1.713	1.332	20.021
4	1.857	1.824	1.546	1.381	1.350	1.831	-0.088	48.964
5	2.174	1.689	1.960	2.752	0.114	1.564	4.583	32.158
6	2.184	1.794	2.184	2.953	0.380	1.527	4.926	34.060
7	2.254	1.808	1.849	1.613	1.285	1.861	4.155	24.163
8	2.276	1.737	1.987	2.764	0.171	1.576	4.627	30.243
9	2.327	2.018	2.021	1.905	0.651	1.818	3.969	20.579
10	2.359	1.981	2.263	3.072	-0.381	1.552	4.565	40.146
11	2.827	2.367	2.378	2.747	0.442	2.468	4.248	76.718
12	2.829	2.252	2.226	2.695	0.905	2.703	4.428	76.219
13	3.007	2.321	2.372	2.692	0.619	2.506	4.110	72.554
14	3.736	3.115	3.361	1.238	5.242	4.223	8.936	-6.934
15	3.915	2.855	3.118	3.612	1.815	2.663	1.976	28.372
16	3.968	3.314	3.473	1.887	4.297	3.785	11.736	-5.067
17	5.031	4.306	3.802	3.611	2.356	2.861	3.944	59.946
18	5.385	4.530	3.832	3.782	2.988	2.990	3.702	62.700
19	5.612	5.070	4.527	4.792	1.667	3.018	6.707	54.324
20	5.847	4.993	4.468	4.710	2.223	2.945	6.963	55.666
21	6.031	5.115	4.434	4.744	1.624	3.045	6.579	54.514
22	6.305	5.987	6.262	6.063	1.884	3.245	1.962	3.159
23	7.542	6.734	5.251	5.704	5.007	4.264	6.925	13.796
24	7.675	7.060	6.515	6.824	3.138	4.586	8.576	11.490
25	7.882	7.192	5.540	6.331	5.306	4.643	6.924	12.250
26	7.892	7.039	6.354	6.715	2.316	4.541	8.121	14.195
27	8.576	7.759	8.481	8.414	2.929	4.638	6.300	28.879
28	9.106	8.057	6.669	6.471	5.488	6.078	8.377	4.404

Table S114: **RESCUN**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.385	0.631	-0.371	-1.641	0.252	0.609	0.218
3	-0.894	1.435	0.681	2.732	1.605	2.664	0.600
4	2.095	2.276	4.109	1.867	1.333	4.382	-0.403
5	2.635	2.082	6.076	-0.601	1.670	3.976	1.451
6	1.968	2.405	7.759	-0.240	1.595	5.089	1.402
7	4.709	1.832	8.454	3.099	1.964	5.808	-0.512
8	2.683	2.092	5.810	-0.603	1.663	3.781	1.464
9	1.660	2.135	3.391	0.342	1.844	3.867	0.544
10	2.922	2.447	5.998	-1.350	1.603	4.027	1.542
11	2.979	2.881	4.331	-0.515	1.524	3.880	-0.464
12	2.378	2.300	4.517	0.202	1.698	3.785	-0.433
13	2.907	2.850	4.259	-0.519	1.522	3.858	-0.440
14	6.363	5.124	11.248	2.470	3.773	6.927	4.492
15	3.180	2.069	6.101	1.104	1.246	5.537	1.668
16	6.684	4.803	9.441	1.346	3.461	7.253	4.630
17	5.216	5.284	6.856	1.785	2.268	7.242	0.307
18	4.929	5.533	6.771	1.958	2.272	8.168	0.437
19	5.649	5.529	3.642	0.350	2.612	7.076	0.588
20	5.043	5.889	6.575	1.244	2.501	7.345	0.332
21	5.970	5.507	5.976	0.477	2.656	6.462	0.329
22	7.703	6.370	6.784	-0.784	3.261	1.486	0.632
23	8.021	6.158	12.769	1.947	3.819	15.153	0.882
24	6.604	8.310	12.147	1.781	3.133	10.770	3.976
25	7.728	6.728	8.730	2.323	4.100	10.392	2.178
26	6.845	8.460	10.635	0.880	3.010	8.458	3.999
27	11.089	8.413	11.068	0.301	4.369	4.413	2.759
28	8.006	7.672	4.004	2.452	4.788	7.653	29.794

Table S115: **RESCUN**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	0.668	0.454	-0.746
3	1.713	1.910	1.912
4	3.952	3.460	2.892
5	3.104	2.096	0.633
6	2.766	1.706	0.020
7	2.176	1.975	1.073
8	2.978	1.983	0.521
9	2.423	2.413	1.545
10	3.380	2.372	0.743
11	4.643	3.605	2.177
12	4.800	3.687	2.438
13	4.621	3.598	2.362
14	7.246	8.990	10.058
15	3.147	2.400	1.788
16	6.653	8.291	8.651
17	5.993	4.480	3.157
18	6.551	5.260	4.186
19	6.378	4.649	2.345
20	6.000	4.206	1.703
21	6.754	5.053	3.162
22	1.997	2.524	9.392
23	8.385	6.996	9.418
24	7.056	5.442	2.275
25	9.107	7.674	9.560
26	7.459	5.872	3.659
27	3.946	4.501	10.473
28	10.602	10.292	13.200

Table S116: **SIGSUX**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.303	0.666	-0.200	-0.157	-6.337	-175.995	-1.752	2.617
3	1.161	1.621	1.105	0.014	-7.177	318.106	0.844	-3.998
4	1.243	1.415	1.052	1.266	-0.178	44.392	0.194	1.163
5	1.634	1.896	0.767	0.300	-8.361	-72.537	-1.832	-0.777
6	2.099	1.970	0.750	-0.166	-8.788	-196.923	-2.810	-3.990
7	2.338	2.297	1.025	0.739	-8.801	-141.917	-2.813	5.373
8	2.563	2.619	2.269	1.577	-7.576	338.730	-0.019	4.715
9	2.812	3.101	1.835	2.277	-4.119	155.660	0.664	5.484
10	3.007	2.630	2.441	1.531	-6.755	311.484	-3.024	-3.549
11	3.025	2.798	2.089	1.178	-7.895	109.273	-0.236	-4.847
12	3.039	3.377	1.943	1.551	-8.276	-211.338	-2.524	-2.035
13	3.409	3.153	1.688	1.141	-8.761	-338.272	-3.787	-5.750
14	3.726	3.627	2.088	1.561	-9.316	-225.262	-1.115	-4.470
15	3.985	3.955	1.950	2.697	-5.835	-129.479	0.185	9.777
16	4.022	4.850	3.145	2.936	-9.116	-72.352	2.291	0.057
17	4.101	4.287	3.672	3.131	-7.783	63.640	0.492	6.093
18	4.153	4.061	3.123	2.813	-6.880	-140.939	-2.428	6.814
19	4.159	4.235	3.712	3.069	-8.185	57.454	1.380	6.789
20	4.184	3.636	3.656	2.912	-5.395	253.833	-3.900	-2.311
21	4.213	4.026	3.476	2.484	-5.693	286.195	2.363	9.578
22	4.628	4.787	3.414	2.812	-8.405	332.009	0.166	-0.571
23	4.735	4.844	3.371	3.317	-8.408	-42.250	-0.188	13.081
24	5.190	4.881	3.141	1.891	-7.459	252.535	1.317	0.091
25	5.279	4.962	3.484	3.884	-7.176	-52.703	0.719	17.373
26	6.363	6.350	5.482	4.315	-3.025	646.448	0.969	-9.408
27	7.302	7.315	5.347	6.098	-5.933	138.408	2.199	20.212
28	8.972	8.689	6.868	6.999	-6.322	368.375	1.800	15.325

Table S117: **SIGSUX**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	-1.623	-0.592	2.552	-0.261	-1.853	5.458	-2.080
3	0.006	0.775	15.353	-0.146	0.492	12.460	6.528
4	1.097	2.163	-3.300	-0.132	0.224	-3.537	1.228
5	0.082	0.547	-12.033	-1.320	-1.920	-10.685	1.799
6	-1.128	-0.389	-11.761	-1.549	-1.746	-7.971	2.511
7	-0.574	1.299	-13.649	-0.752	-0.558	-17.414	1.455
8	0.921	1.060	-18.536	-0.186	-1.746	-14.086	8.702
9	-1.206	1.446	6.172	-1.028	-1.577	9.114	-3.412
10	1.161	3.190	-8.402	-0.089	-1.677	-11.951	0.926
11	2.841	2.512	-6.329	-0.312	1.426	-2.834	0.886
12	-0.600	0.205	-10.201	-1.202	-1.018	-10.778	-2.039
13	-1.217	-0.069	-12.499	-1.378	-2.227	-6.216	-1.019
14	-0.056	1.341	-16.522	-0.728	-1.572	-10.906	2.506
15	-0.169	1.118	10.486	0.027	-0.141	12.167	-3.648
16	2.305	3.645	-11.067	-0.660	-1.255	-3.546	2.585
17	0.867	2.255	-10.040	-0.944	-1.947	-7.099	6.412
18	-0.327	1.917	-7.798	-0.971	-1.788	-6.664	-3.707
19	4.955	6.679	-5.042	0.295	0.328	-8.581	5.391
20	2.247	3.529	0.948	-0.068	-1.360	-2.583	-3.994
21	5.359	4.840	-6.172	0.501	1.681	-5.275	-2.239
22	-0.282	1.897	-6.641	-1.460	-1.789	-1.611	3.289
23	0.757	3.458	5.751	0.258	-1.094	5.548	-0.829
24	1.305	2.076	0.053	-0.412	-0.798	2.035	-0.275
25	1.299	3.298	-0.374	-0.279	-1.389	2.112	0.090
26	9.293	8.116	-6.307	0.419	1.606	-7.068	8.502
27	1.478	3.387	-3.015	-0.669	-1.146	-3.249	0.652
28	1.941	4.281	-2.872	-0.391	-0.771	-0.856	-0.885

Table S118: **SIGSUX**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	-1.090	-1.477	-0.697
3	-0.652	0.017	0.263
4	0.156	0.239	1.207
5	0.984	0.526	2.968
6	0.002	-0.450	2.363
7	0.852	0.301	3.314
8	1.954	2.530	4.386
9	2.481	2.397	1.903
10	3.521	4.039	4.425
11	0.078	0.767	1.149
12	2.187	1.924	4.226
13	0.272	-0.165	3.655
14	2.504	2.061	5.118
15	2.082	2.258	4.561
16	5.914	5.091	4.260
17	2.749	3.058	6.111
18	2.178	2.487	5.826
19	2.521	2.688	5.940
20	4.741	4.992	6.109
21	3.607	5.002	7.076
22	3.934	4.348	4.783
23	4.671	4.427	4.768
24	3.015	3.533	4.891
25	4.350	4.399	5.178
26	1.412	2.214	2.045
27	5.577	6.141	6.042
28	7.480	8.322	7.660

Table S119: **TITVEX01**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.169	0.035	0.009	0.018	-0.235	-0.218	0.151	-0.217
3	0.173	0.109	0.043	0.002	-0.079	-0.089	-0.114	-0.078
4	1.205	0.700	0.822	0.803	0.452	0.154	1.044	4.162
5	1.603	1.927	2.166	2.146	0.927	0.670	3.279	7.580
6	1.714	1.589	1.581	1.655	1.218	0.214	0.826	7.517
7	2.559	2.376	2.227	2.451	0.608	0.514	3.761	8.985
8	2.965	4.034	4.548	4.125	1.361	1.225	8.074	14.604
9	3.049	3.173	3.743	3.895	0.912	0.636	4.691	11.628
10	3.233	3.527	3.453	3.894	1.395	1.053	3.798	4.537
11	3.758	3.969	3.862	4.475	1.869	1.555	3.917	4.387
12	3.911	4.027	3.866	4.429	1.803	1.450	3.541	4.162
13	4.541	4.609	4.556	3.876	2.519	1.239	3.830	12.244
14	5.108	5.849	7.195	4.761	2.522	1.444	6.854	17.648
15	5.180	6.020	7.124	4.771	2.591	1.453	6.943	17.820

Table S120: **TITVEX01**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	6.290	-9.587	-10.249	-7.767	-3.453	-4.633	1.793
3	5.998	-8.428	-9.182	-7.785	-2.143	-4.507	1.794
4	7.776	-8.742	1.490	-5.399	-2.994	3.939	0.260
5	6.560	-7.145	8.294	-4.242	-2.664	7.449	-2.993
6	4.495	-9.145	-5.510	4.035	-2.828	-1.860	2.448
7	10.088	-6.187	4.201	-1.582	-2.750	-3.293	9.720
8	-14.536	-3.903	-7.351	5.790	-2.739	1.365	1.443
9	-11.662	-5.169	-6.961	5.318	-2.815	-4.892	4.069
10	5.543	-6.237	5.517	-4.656	-2.396	5.564	-1.810
11	8.784	-6.179	5.074	-3.378	-2.418	5.249	-1.789
12	8.334	-6.316	5.276	-3.425	-2.434	5.388	-1.791
13	-10.568	-4.179	1.040	6.370	-1.817	2.830	-0.392
14	-11.038	-3.900	-2.701	7.326	-1.027	-5.434	8.278
15	-11.241	-3.921	-2.682	7.329	-1.026	-5.462	8.276

Table S121: **TITVEX01**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	0.355	0.177	-0.351
3	0.119	-0.024	-0.440
4	4.796	5.362	1.730
5	2.151	2.955	-1.817
6	7.221	7.432	2.284
7	0.641	1.821	-1.007
8	0.557	2.700	-2.456
9	5.079	6.354	-0.446
10	0.929	1.247	1.275
11	-1.880	-1.132	-0.647
12	-2.922	-2.234	-1.743
13	5.039	6.759	3.037
14	-0.176	0.583	-0.929
15	-0.387	0.372	-1.048

Table S122: **WOWSAC**: Conformational energies in kcal·mol^{-1}.

SPE GEO	PWPB95-D4 B97-3c	ωB97X-V B97-3c	B97-3c B97-3c	PBEh-3c B97-3c	GFN2-xTB B97-3c	GFN1-xTB B97-3c	GFN-FF B97-3c	UFF B97-3c
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.887	0.871	0.893	1.186	0.998	1.080	0.505	0.473
3	1.099	1.288	1.192	0.746	1.381	-0.007	1.194	6.663
4	1.271	1.326	1.145	1.022	1.027	-0.211	1.153	6.165
5	1.369	1.649	1.517	0.948	2.066	0.711	1.529	7.741
6	1.549	1.699	1.766	2.326	1.627	1.673	1.354	1.253
7	2.017	2.177	1.993	1.911	1.757	0.391	1.836	6.307
8	5.402	6.390	8.305	7.025	2.199	4.002	0.294	15.915
9	5.660	6.491	8.287	7.080	1.642	3.884	-0.024	16.398
10	5.734	6.610	8.506	7.242	2.685	4.306	0.287	15.633
11	5.973	6.923	8.437	7.643	1.085	3.581	0.303	15.633
12	6.165	7.067	8.625	7.508	1.741	3.926	0.285	16.124
13	8.509	7.998	11.763	9.666	3.839	6.758	-2.676	7.017
14	8.693	8.883	12.913	10.742	5.944	7.729	-2.723	6.609
15	9.893	9.759	13.588	11.144	5.683	8.648	-2.218	12.295
16	10.116	9.993	13.762	11.315	5.876	8.641	-2.108	12.786
17	10.251	10.123	14.022	11.509	5.560	8.901	-2.057	13.687
18	10.303	9.703	13.026	11.532	2.695	6.313	-2.565	13.466
19	14.483	13.765	17.385	14.780	1.433	5.992	-3.174	26.380
20	15.401	14.466	17.315	14.186	6.744	8.539	-0.885	26.803
21	15.435	14.328	17.173	13.986	5.896	8.079	-2.481	25.269

Table S123: **WOWSAC**: Conformational energies in kcal·mol^{-1}.

SPE GEO	B97-3c GFN2-xTB	B97-3c GFN1-xTB	B97-3c GFN-FF	GFN2-xTB GFN2-xTB	GFN1-xTB GFN1-xTB	GFN2-xTB GFN-FF	GFN-FF GFN-FF
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	1.081	0.612	1.977	1.022	0.811	3.794	-0.876
3	-0.168	1.053	0.315	3.473	-0.240	2.588	0.687
4	-1.309	0.955	-0.502	3.575	-0.275	0.484	0.891
5	-0.279	1.261	0.950	3.644	0.101	3.314	1.229
6	2.089	1.371	3.537	2.174	1.573	1.555	-0.544
7	-0.115	1.344	1.855	4.257	0.532	2.656	0.767
8	-2.122	7.123	8.164	5.810	4.923	-5.510	0.581
9	-2.095	7.473	8.686	5.783	5.287	-4.899	0.730
10	0.090	11.678	8.217	5.438	7.777	-7.363	-0.996
11	-4.075	6.849	7.163	5.978	4.901	-7.776	-0.937
12	-1.893	7.392	7.122	6.024	5.257	-8.108	-1.166
13	0.074	12.384	9.244	3.997	6.545	-6.869	-1.310
14	1.568	13.988	8.826	5.066	7.667	-2.232	-0.211
15	1.919	14.141	8.799	5.201	8.186	-2.335	-0.127
16	2.025	14.462	9.298	5.384	7.961	-1.795	-0.093
17	2.397	14.569	9.337	5.508	8.455	-1.715	0.059
18	0.392	12.033	11.088	5.901	7.266	-4.289	-1.437
19	1.398	16.460	15.264	5.760	6.594	-7.125	-0.517
20	8.267	17.671	14.704	5.637	8.059	-4.416	0.208
21	7.416	17.439	13.901	5.388	7.684	-5.372	0.430

Table S124: **WOWSAC**: Conformational heats of formation in kcal·mol^{-1}.

SPE GEO	PM6 B97-3c	PM6-D3H4X B97-3c	PM7 B97-3c
1	0.000	0.000	0.000
2	2.879	3.250	4.078
3	4.719	5.463	10.858
4	7.334	7.971	15.256
5	4.067	5.200	10.113
6	3.955	4.577	4.517
7	8.412	9.487	16.842
8	4.832	6.892	11.915
9	4.975	7.073	12.462
10	7.850	10.010	17.578
11	4.432	6.452	9.492
12	4.041	6.291	10.181
13	19.796	22.187	2.065
14	5.848	7.650	-18.381
15	11.453	13.638	-8.760
16	10.839	13.089	-9.589
17	13.386	15.657	-5.789
18	31.628	33.938	14.738
19	36.729	38.061	48.494
20	34.119	35.943	53.923
21	31.539	33.279	46.061