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Supporting information for:

A Look at the Density Functional Theory Zoo with the Advanced GMTKN55 Database for General Main Group Thermochemistry, Kinetics and Noncovalent Interactions

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SI.1 Details on the new MB16-43 set

SI.1.1 Creating the artificial molecules

The starting structures of the artificial molecules (AMs) were created by randomly placing 16 atoms inside a sphere with a radius of 4 a.u., whilst imposing a minimum interatomic distance of 1 a.u. The atoms were chosen based on a fixed element distribution (see Tab. S1). The distribution was based on the MB08-931 distribution from the original mindless benchmarking publication [S1] and adapted to promote the formation of single molecules. To achieve this, the occurence of hydrogen, alkaline and earth-alkaline metals was lowered. The probability of group 13-17 elements was increased, with the third-row elements being assigned half the probability of the second-row ones. Overall, this led to a much higher yield of systems containing a single molecule.

Table S1: Element distributions of the initial 3000, intermediate 255 and final 43 AMs.

	Set size		
Atom	3000	255	43
H	46.8750	39.78	40.59
Li	1.5625	1.23	1.91
Be	1.5625	0.07	0.15
B	6.2500	10.15	12.06
C	6.2500	7.16	6.76
N	6.2500	6.62	5.29
O	6.2500	6.20	6.18
F	6.2500	6.57	7.65
Na	1.5625	0.86	0.88
Mg	1.5625	2.50	2.35
Al	3.1250	5.00	5.29
Si	3.1250	4.31	4.56
P	3.1250	3.82	3.09
S	3.1250	3.21	3.24
Cl	3.1250	2.52	2.35

The resulting stuctures were then optimised at the PBE-D3/def2-SV(P) [S2–S5] level of theory; if the resulting structure was fragmented (e.g. more than one molecule was formed), it was eliminated from the set. In this procedure, two atoms were considered bonded when they were closer than 1.1 times the sum of their van-der-Waal radii. The remaining structures were then reoptimised with TPSS-D3/def2-TZVP. [S3–S6] Several diagnostics were then applied to verify a reasonable electronic structure: the gap between the highest occupied and lowest unoccupied molecular orbitals had to be greater than 0.5 eV and the D1/T1 diagnostics at the CCSD/cc-pVDZ level of theory had to be smaller than 0.1 and 0.03, respectively. Finally, the TURBOMOLE-based MP2/def2-TZVP energies were verified with ORCA in order to check if the electronic state of the wave-function guess was the same with both codes. This was done to ensure compatibility of the set with different QM codes. Of an original number of 3000 created AMs, 255 remained after applying this scheme.
The main differences between this set and the original MB08-165 [S1] are summarised in Tab. S2.

Table S2: Comparison of the MB08-165, and the intermediate 255, and the final 43 AMs

Property	MB08-165	255	43
number of atoms	8	16	16
average number of e^-	31.0	97.5	96.2
open shell systems	23.6 %	49.0 %	53.0 %
atom positions	corners of cube	random in sphere	random in sphere
reaction to	XH_n and Y_2	XH_n and Y_2	XH_n and Y_2
reaction energies (kcal/mol)	-400 to 400	-350 to 1250	-350 to 1250
allow fragments in AM?	yes	no	no

The main difference between the two sets is the system size, which is doubled. This also leads to a larger spread in the reaction energies. Note that the proportion of open-shell systems is about 50% of the set, opposed to 24% in MB08-165. The decomposition scheme of the AMs — i.e. the chemical reactions we built — is the same as in the previous study: group 1-2

and 13-15 (denoted here as X) are decomposed to the respective hydrides, and the rest react to their respective diatomics. No fractional numbers are allowed in the reaction schemes. For an example, see equation 1.

$$2\ H_6B_2N_2O_2FNaAlCl + 4\ H_2 \rightarrow\ 4\ BH_3 + 2\ N_2 + 2\ O_2 + F_2 + 2\ NaH + 2\ AlH_3 + Cl_2 \tag{1}$$

SI.1.2 Choosing a representative subset

In order to limit the number of calculations to make the set compatibale with others in GMTKN55, the original 255 structures were reduced to a represantative subset of 50 structures. This was done as follows: first, reference energies were calculated at an inexpensive composite level:

$$\begin{aligned} &\mathrm{E} = \mathrm{MP2(CBS)} + \Delta\mathrm{CCSD(T)} + \Delta\mathrm{MP2_{core}} \\ &\Delta\mathrm{CCSD(T)} = \mathrm{MP2/def2\text{-}TZVP} - \mathrm{CCSD(T)/def2\text{-}TZVP} \\ &\Delta\mathrm{MP2_{core}} = \mathrm{MP2_{full}/cc\text{-}pwCVTZ} - \mathrm{MP2_{fc}/cc\text{-}pVTZ}, \end{aligned} \tag{2}$$

where $\Delta MP2_{core}$ is the core-valence correction and "fc" refers to the frozen-core approximation.
Based on this reference, DFT calculations were carried out with a number of dispersion-corrected and dispersion-uncorrected functionals, including GGA-, hybrid- and double-hybrid methods with a large def2-QZVP basis set. For these methods, mean deviations, mean absolute deviations and standard deviations were calculated. Then, 50 AMs were chosen randomly, and the same statistical data were recalculated for this subset. This was repeated until the difference between the full-set and subset statistical data for all functionals was below 0.5 kcal/mol for all tested functionals. For this subset, accurate W1-F12 calculations were carried out. For 5 systems, W1-F12 energies could not be obtained for technical reasons, as they were either too large to obtain the fully core-correlated values necessary for W1-F12, or the explicitly-correlated calculations did not converge. Two additional systems had significant errors for all of the tested methods, and were further analysed by plotting their fractional occupation number weighted electron densities (FODs).[S7] The resulting plots indicated strong multi-reference character, which is why these two were also eliminated from the set.

SI.2 Parameters for the DFT-D3 dispersion correction

SI.2.1 Parameters for the DFT-D3 correcton with Becke-Johnson damping [DFT-D3(BJ)]

Tab. S3 shows all DFT-D3(BJ) parameters for all tested density functional approximations (DFAs); a description of DFT-D3(BJ) and its parameters is given in Ref. S4. For those parameters that were determined in this work, s_6 was fixed to unity, while a_1, a_2, and s_8 were fitted as described in the main text. The only exception is the double hybrid MW2PLYP, for which an s_6 of 0.66 had been determined according to instructions outlined in in Ref. S8 before the remaining parameters were fitted. Any work using DFT-D3(BJ) should cite Refs. S3 and S4 as well as the work that presented the respective functional parameters for the first time (see last column of Tab. S3).

Table S3: Parameters for the DFT-D3 correcton with Becke-Johnson damping [DFT-D3(BJ)]

Functional	s_6	a_1	s_8	a_2	cite Ref.
PBE	1.0	0.4289	0.7875	4.4407	S4
PBEhPBE	1.0	0.0000	1.1152	6.7184	this work
revPBE	1.0	0.5238	2.3550	3.5016	S4
RPBE	1.0	0.1820	0.8318	4.0094	this work
PW91	1.0	0.6319	1.9598	4.5718	S9
BLYP	1.0	0.4298	2.6996	4.2359	S4
BP86	1.0	0.3946	3.2822	4.8516	S4
BPBE	1.0	0.4567	4.0728	4.3908	S10
OPBE	1.0	0.5512	3.3816	2.9444	S10
OLYP	1.0	0.5299	2.6205	2.8065	S10
XLYP	1.0	0.0809	1.5669	5.3166	this work
mPWLYP	1.0	0.4831	2.0077	4.5323	S10
mPWPW91	1.0	0.3168	1.7974	4.7732	this work
rPW86PBE	1.0	0.4613	1.3845	4.5062	S4
B97-D3(BJ)	1.0	0.5545	2.2609	3.2297	S4
HCTH/407	1.0	0.0000	0.6490	4.8162	this work
TPSS	1.0	0.4535	1.9435	4.4752	S4
revTPSS	1.0	0.4426	1.4023	4.4723	this work
SCAN	1.0	0.538	0.000	5.420	S11
τHCTH	1.0	0.0000	1.2626	5.6162	this work
MN12L	1.0	0.0000	2.2674	9.1494	S12
B3LYP	1.0	0.3981	1.9889	4.4211	S4
B3PW91	1.0	0.4312	2.8524	4.4693	S10
B3P86	1.0	0.4601	3.3211	4.9294	this work
BHLYP	1.0	0.2793	1.0354	4.9615	S10
B1P86	1.0	0.4724	3.5681	4.9858	this work
B1LYP	1.0	0.1986	2.1167	5.3875	this work
B1B95	1.0	0.2092	1.4507	5.5545	S10
MPW1B95	1.0	0.1955	1.0508	6.4177	S10
PW6B95	1.0	0.2076	0.7257	6.3750	S4
MPWB1K	1.0	0.1474	0.9499	6.6223	S10
MPW1PW91	1.0	0.3342	1.8744	4.9819	this work
MPW1KCIS	1.0	0.0576	1.0893	5.5314	this work
MPWKCIS1K	1.0	0.0855	1.2875	5.8961	this work
PBE0	1.0	0.4145	1.2177	4.8593	S4
PBEh1PBE	1.0	0.0000	1.4877	7.0385	this work
PBE1KCIS	1.0	0.0000	0.7688	6.2794	this work
X3LYP	1.0	0.2022	1.5744	5.4184	this work
O3LYP	1.0	0.0963	1.8171	5.9940	this work
B97-1	1.0	0.0000	0.4814	6.2279	this work
B97-2	1.0	0.0000	0.9448	5.4603	this work
B98	1.0	0.0000	0.7086	6.0672	this work
HISS	1.0	0.0000	1.6112	7.3539	this work
HSE03	1.0	0.0000	1.1243	6.8889	this work
HSE06	1.0	0.3830	2.310	5.685	S13
TPSSh	1.0	0.4529	2.2382	4.6550	S10
revTPSSh	1.0	0.2660	1.4076	5.3761	this work
TPSS0	1.0	0.3768	1.2576	4.5865	S4
revTPSS0	1.0	0.2218	1.6151	5.7985	this work
TPSS1KCIS	1.0	0.0000	1.0542	6.0201	this work
BMK	1.0	0.1940	2.0860	5.9197	S10
τHCTHhyb	1.0	0.0000	0.9585	6.2303	this work
M11	1.0	0.0000	2.8112	10.1389	S12
SOGGA11X	1.0	0.1330	1.1426	5.7381	S12
N12SX	1.0	0.3283	2.4900	5.7898	S12
MN12SX	1.0	0.0983	1.1674	8.0259	S12
MN15	1.0	2.0971	0.7862	7.5923	this work
LC-ωhPBE	1.0	0.2746	1.1908	5.3157	this work
B2PLYP	0.64	0.3065	0.9147	5.0570	S10
B2GPPLYP	0.560	0.0000	0.2597	6.3332	S10
MPW2PLYP	0.66	0.4105	0.6223	5.0136	this work
PWPB95	0.820	0.0000	0.2904	7.3141	S10
DSD-BLYP	0.50	0.000	0.2130	6.0519	S10
DSD-PBEP86	0.418	0.000	0.000	5.6500	S14
DSD-PBEB95	0.61	0.000	0.000	6.2	S15

SI.2.2 Parameters for the DFT-D3 correcton with zero damping [DFT-D3(0)]

Tab. S4 shows all DFT-D3(0) parameters for all tested DFAs; a description of DFT-D3(0) and its parameters is given in Ref. S3. For those parameters that were determined in this work, s_6 was fixed to unity, while $s_{r,6}$ and s_8 were fitted as described in the main text. The only exception is the double hybrid MW2PLYP, for which an s_6 of 0.66 had been determined according to instructions outlined in Ref. S8 before the remaining parameters were fitted. Also note that the authors of ωB97X-D3 decided to fit the parameter $s_{r,8}$,[S16] which was set to unity in all other cases, as outlined in Ref. S3.
Any work using DFT-D3(BJ) should cite Ref. S3 as well as the work that presented the respective functional parameters for the first time (see last column of Tab. S4).

Table S4: Parameters for the DFT-D3 correcton with zero damping [DFT-D3(0)].

Functional	s_6	$s_{r,6}$	s_8	cite Ref.
PBE	1.0	1.217	0.722	S3
PBEhPBE	1.0	1.5703	1.4010	this work
revPBE	1.0	0.923	1.010	S3
RPBE	1.0	0.872	0.514	this work
BLYP	1.0	1.094	1.682	S3
BP86	1.0	1.139	1.683	S3
BPBE	1.0	1.087	2.033	S10
OPBE	1.0	0.837	2.055	S10
OLYP	1.0	0.806	1.764	S10
XLYP	1.0	0.9384	0.7447	this work
mPWLYP	1.0	1.239	1.098	S10
PW91P86	1.0	2.1040	0.8747	this work
mPWPW91	1.0	1.3725	1.9467	this work
rPW86PBE	1.0	1.224	0.901	S4
B97D3(0)	1.0	0.892	0.909	S3
HCTH/407	1.0	4.0426	2.7694	this work
N12	1.0	1.3493	2.3916	S12
PKZB	1.0	0.6327	0.000	this work
TPSS	1.0	1.166	1.105	S3
revTPSS	1.0	1.3491	1.3666	this work
SCAN	1.0	1.324	0.000	S11
τHCTH	1.0	0.9320	0.5662	this work
M06L	1.0	1.581	0.000	S10
M11L	1.0	2.3933	1.1129	S12
MN15L	1.0	3.3388	0.000	this work
B3LYP	1.0	1.261	1.703	S3
B3PW91	1.0	1.176	1.775	S10
B3P86	1.0	1.1897	1.1961	this work
BHLYP	1.0	1.370	1.442	S10
B1P86	1.0	1.1815	1.1209	this work
B1LYP	1.0	1.3725	1.9467	this work
B1B95	1.0	1.613	1.868	S10
MPW1B95	1.0	1.605	1.118	S10
PW6B95	1.0	1.523	0.862	S3
MPWB1K	1.0	1.671	1.061	S10
mPW1LYP	1.0	2.0512	1.9529	this work
MPW1PW91	1.0	1.2892	1.4758	this work
PW1PW	1.0	1.4968	1.1786	this work
MPW1KCIS	1.0	1.7231	2.2917	this work
MPWKCIS1K	1.0	1.4853	1.7553	this work
PBE0	1.0	1.287	0.928	S3
PBEh1PBE	1.0	1.3719	1.0430	this work
PBE1KCIS	1.0	3.6355	1.7934	this work
X3LYP	1.0	1.0	0.2990	this work
O3LYP	1.0	1.4060	1.8058	this work
B97-1	1.0	3.7924	1.6418	this work
B97-2	1.0	1.7066	2.4661	this work
B98	1.0	2.6895	1.9078	this work
HISS	1.0	1.3338	0.7615	this work
HSE03	1.0	1.3944	1.0156	this work
HSE06	1.0	1.129	0.109	S13
TPSSh	1.0	1.223	1.219	S10
revTPSSh	1.0	1.3224	1.2504	this work
TPSS0	1.0	1.252	1.242	S3
revTPSS0	1.0	1.2881	1.0649	this work
TPSS1KCIS	1.0	1.7729	2.0902	this work
BMK	1.0	1.931	2.168	S10
τHCTHhyb	1.0	1.5001	1.6302	this work
M05	1.0	1.373	0.595	S10
M052X	1.0	1.417	0.000	S10
M06	1.0	1.325	0.000	S10
M062X	1.0	1.619	0.000	S10
M08HX	1.0	1.6247	0.000	this work
LC-ωhPBE	1.0	1.3846	1.2797	this work
ωB97X-D3[a]	1.0	1.281	1.0	S16
B2PLYP	0.64	1.427	1.022	S8
B2GPPLYP	0.56	1.586	0.760	S8
MPW2PLYP	0.66	1.5527	0.7529	this work
PWPB95	0.82	1.557	0.705	S8
DSD-BLYP	0.5	1.569	0.705	S8

[a] $s_{r,8}$=1.094

SI.3 Comparison between the new and old reference values for ALX6

Table S5: Mean absolute deviations (MADs) for ALX6 based on the new and old reference values for all 83 DFAs. The def2-QZVP atomic-orbital (AO) basis set was applied in all cases.

Functional	new	old	Functional	new	old
DSD-PBEP86-D3(BJ)	0.31	1.69	B97-1-D3(BJ)	2.52	3.91
DSD-BLYP-D3(BJ)	0.54	1.27	TPSS0-D3(BJ)	2.56	3.94
PW6B95-D3(BJ)	0.61	1.99	MPW2PLYP-D3(BJ)	2.66	1.88
M06L-D3(0)	0.62	1.27	BPBE-D3(BJ)	2.69	4.08
B2GPPLYP-D3(BJ)	0.63	1.01	mPWPW91-D3(BJ)	2.69	4.07
B3P86-D3(BJ)	0.66	2.04	OLYP-D3(BJ)	2.69	2.77
M052X-D3(0)	0.77	1.77	B3LYP-D3(BJ)	2.71	1.81
B1LYP-D3(BJ)	0.90	1.62	VV10	2.74	2.44
B1P86-D3(BJ)	0.90	2.29	MPWB1K-D3(BJ)	2.84	3.89
M062X-D3(0)	0.90	1.77	LC-ωhPBE-D3(BJ)	2.92	4.30
PWPB95-D3(BJ)	0.91	2.29	ωB97X-D3(0)	3.02	2.23
HSE06-D3(BJ)	0.93	2.32	B1B95-D3(BJ)	3.04	4.42
DSD-PBEB95-D3(BJ)	0.97	2.35	revTPSSh-D3(BJ)	3.13	4.51
X3LYP-D3(BJ)	0.98	1.14	BMK-D3(BJ)	3.15	4.20
PW1PW-D3(0)	1.04	2.12	revTPSS0-D3(BJ)	3.41	4.54
ωB97X-V	1.21	1.03	MN12L-D3(BJ)	3.44	4.49
APFD	1.34	1.40	PBE1KCIS-D3(BJ)	3.56	4.95
MN12SX-D3(BJ)	1.35	0.72	rPW86PBE-D3(BJ)	3.61	3.08
MN15L-D3(0)	1.35	2.31	PBEhPBE-D3(BJ)	3.69	5.08
N12-D3(0)	1.42	2.44	HSE03-D3(BJ)	3.71	4.82
MN15-D3(BJ)	1.47	2.59	B98-D3(BJ)	3.89	5.10
PBE0-D3(BJ)	1.48	2.87	HISS-D3(BJ)	4.01	5.06
BHLYP-D3(BJ)	1.56	0.76	PBEh1PBE-D3(BJ)	4.01	5.13
PBE-D3(BJ)	1.63	2.65	MPWKCIS1K-D3(BJ)	4.27	5.32
PW91P86-D3(0)	1.64	1.94	O3LYP-D3(BJ)	4.38	5.77
BP86-D3(BJ)	1.73	3.11	mPW1LYP-D3(0)	4.40	3.35
MPW1B95-D3(BJ)	1.77	3.16	BLYP-D3(BJ)	4.48	3.43
B3PW91-D3(BJ)	1.85	3.23	τHCTHhyb-D3(BJ)	4.48	5.61
PW91-D3(BJ)	1.93	2.29	XLYP-D3(BJ)	4.52	5.87
revPBE-D3(BJ)	2.07	2.55	PKZB-D3(0)	4.78	6.16
SOGGA11X-D3(BJ)	2.08	3.13	B97-D3(BJ)	4.99	3.94
SCAN-D3(BJ)	2.13	3.18	OPBE-D3(BJ)	5.46	6.84
B2PLYP-D3(BJ)	2.21	1.46	mPWLYP-D3(BJ)	6.05	5.00
TPSSh-D3(BJ)	2.21	3.59	M11L-D3(0)	6.09	5.04
N12SX-D3(BJ)	2.22	3.60	MPW1KCIS-D3(BJ)	6.14	7.36
TPSS-D3(BJ)	2.24	3.62	M05-D3(0)	6.25	5.20
MPW1PW91-D3(BJ)	2.28	3.66	RPBE-D3(BJ)	7.57	8.95
M08HX-D3(0)	2.38	3.43	TPSS1KCIS-D3(BJ)	7.77	8.82
M11-D3(BJ)	2.39	3.44	τHCTH-D3(BJ)	9.81	10.86
revTPSS-D3(BJ)	2.42	3.81	B97-2-D3(BJ)	11.21	12.26
M06-D3(0)	2.46	1.98	HCTH/407-D3(BJ)	11.75	12.80

SI.4 Dispersion-corrected vs. -uncorrected results

SI.4.1 WTMADs for four functionals

Table S6: WTMAD-1 and WTMAD-2 values (in parenthesis) for four DFAs with and without the DFT-D3 dispersion correction. All values were obtained with the (aug'-)def2-QZVP AO basis set and are in kcal/mol.

Functional	no DFT-D3	with DFT-D3
basic properties and reaction energies for small systems		
BLYP	7.54 (8.52)	5.67 (6.88)
M11L	5.01 (5.24)	4.54 (4.89)
B3LYP	5.32 (5.72)	3.85 (4.36)
PWPB95	2.17 (2.43)	2.08 (2.23)
reaction energies for large systems and isomerisation reactions		
BLYP	10.67 (23.22)	7.31 (14.56)
M11L	7.00 (12.92)	6.06 (10.46)
B3LYP	7.84 (17.53)	5.02 (10.28)
PWPB95	3.28 (7.38)	2.53 (5.41)
reaction barrier heights		
BLYP	5.19 (14.56)	5.53 (15.55)
M11L	2.99 (5.66)	2.88 (5.47)
B3LYP	3.23 (9.19)	3.12 (9.04)
PWPB95	1.52 (3.43)	1.50 (3.39)
Intermolecular noncovalent interactions		
BLYP	19.19 (34.90)	3.20 (7.10)
M11L	7.85 (21.01)	5.90 (15.17)
B3LYP	15.55 (28.23)	2.75 (5.56)
PWPB95	6.50 (12.28)	1.75 (4.02)
Intramolecular noncovalent interactions		
BLYP	17.71 (29.47)	4.38 (8.04)
M11L	5.28 (10.56)	7.19 (13.39)
B3LYP	15.27 (25.14)	3.20 (5.68)
PWPB95	4.73 (8.69)	2.95 (5.98)
all noncovalent interactions		
BLYP	18.56 (32.25)	3.70 (7.56)
M11L	6.75 (15.90)	6.45 (14.30)
B3LYP	15.43 (26.72)	2.94 (5.62)
PWPB95	5.74 (10.52)	2.27 (4.98)
GMTKN55		
BLYP	11.96 (21.05)	5.17 (9.51)
M11L	5.74 (10.75)	5.31 (9.58)
B3LYP	9.33 (16.38)	3.60 (6.42)
PWPB95	3.63 (6.56)	2.15 (3.98)

SI.4.2 WTMADs for Minnesota functionals

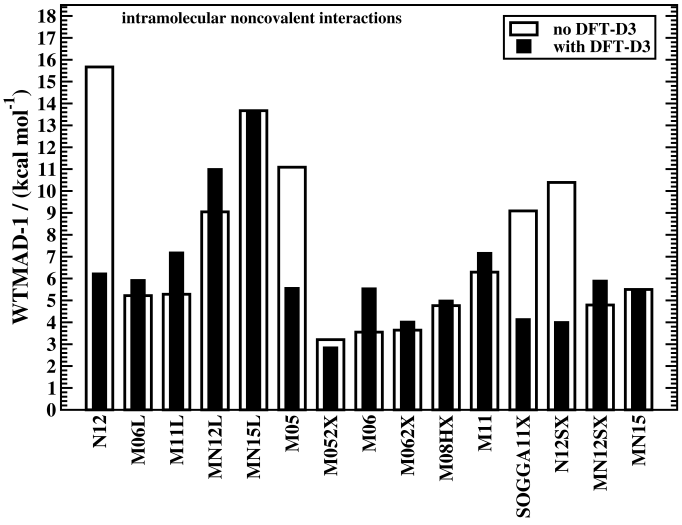

Figure S1: The effect of dispersion corrections on WTMAD-1 values (kcal/mol) of Minnesota-type DFAs for intramolecular noncovalent interactions.

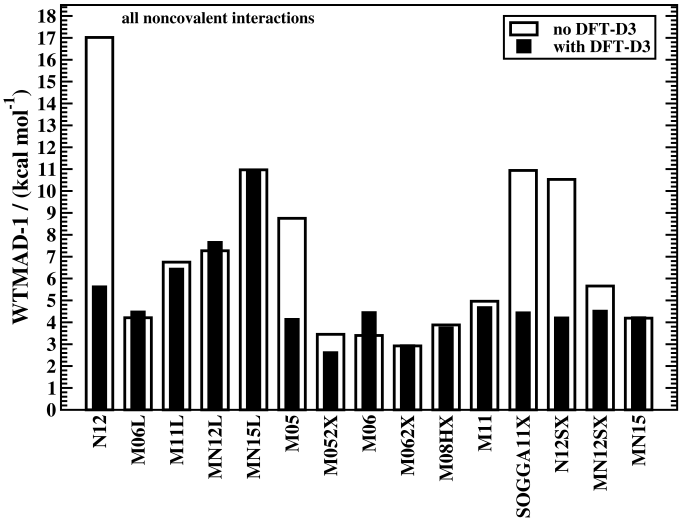

Figure S2: The effect of dispersion corrections on WTMAD-1 values (kcal/mol) of Minnesota-type DFAs for all noncovalent interaction benchmark sets in the GMTKN55 database.

Table S7: WTMAD-1 and WTMAD-2 values (in parenthesis) for Minnesota functionals with and without the DFT-D3 dispersion correction. All values were obtained with the (aug'-)def2-QZVP AO basis set and are in kcal/mol.

Functional	no DFT-D3	with DFT-D3
Intermolecular noncovalent interactions		
N12	18.02 (33.18)	5.19 (9.45)
M06L	3.45 (8.29)	3.41 (7.37)
M11L	7.85 (21.01)	5.90 (15.17)
MN12L	5.93 (16.00)	5.17 (12.92)
MN15L	8.95 (13.01)	8.95 (13.01)
M05	7.00 (11.35)	3.10 (6.00)
M052X	3.63 (6.80)	2.46 (5.46)
M06	3.29 (7.76)	3.64 (6.63)
M062X	2.38 (5.51)	2.13 (5.20)
M08HX	3.22 (7.11)	2.84 (6.75)
M11	3.96 (10.08)	2.82 (6.28)
SOGGA11X	12.33 (25.40)	4.69 (12.30)
N12SX	10.63 (19.83)	4.37 (8.65)
MN12SX	6.31 (14.30)	3.50 (8.89)
MN15	3.21 (5.55)	3.27 (5.63)
Intramolecular noncovalent interactions		
N12	15.67 (26.60)	6.23 (11.96)
M06L	5.22 (9.27)	5.93 (10.31)
M11L	5.28 (10.56)	7.19 (13.39)
MN12L	9.05 (18.43)	11.00 (21.72)
MN15L	13.67 (27.18)	13.65 (27.15)
M05	11.09 (17.95)	5.57 (8.83)
M052X	3.21 (5.79)	2.85 (5.52)
M06	3.55 (6.53)	5.55 (10.16)
M062X	3.64 (6.64)	4.03 (7.48)
M08HX	4.76 (8.55)	4.99 (9.22)
M11	6.29 (11.12)	7.17 (12.93)
SOGGA11X	9.09 (14.19)	4.14 (7.72)
N12SX	10.39 (17.27)	4.01 (8.05)
MN12SX	4.79 (10.16)	5.90 (12.29)
MN15	5.50 (10.84)	5.50 (10.86)
all noncovalent interactions		
N12	17.02 (29.96)	5.64 (10.68)
M06L	4.21 (8.77)	4.49 (8.81)
M11L	6.75 (15.90)	6.45 (14.30)
MN12L	7.27 (17.19)	7.67 (17.22)
MN15L	10.97 (19.94)	10.96 (19.92)
M05	8.75 (14.58)	4.15 (7.39)
M052X	3.45 (6.31)	2.63 (5.49)
M06	3.40 (7.16)	4.46 (8.36)
M062X	2.92 (6.06)	2.95 (6.31)
M08HX	3.88 (7.82)	3.76 (7.96)
M11	4.96 (10.59)	4.69 (9.53)
SOGGA11X	10.94 (19.92)	4.45 (10.06)
N12SX	10.53 (18.58)	4.22 (8.36)
MN12SX	5.66 (12.27)	4.53 (10.56)
MN15	4.19 (8.14)	4.23 (8.19)

SI.5 Analysis of best and worst mean absolute/root-mean-square deviations

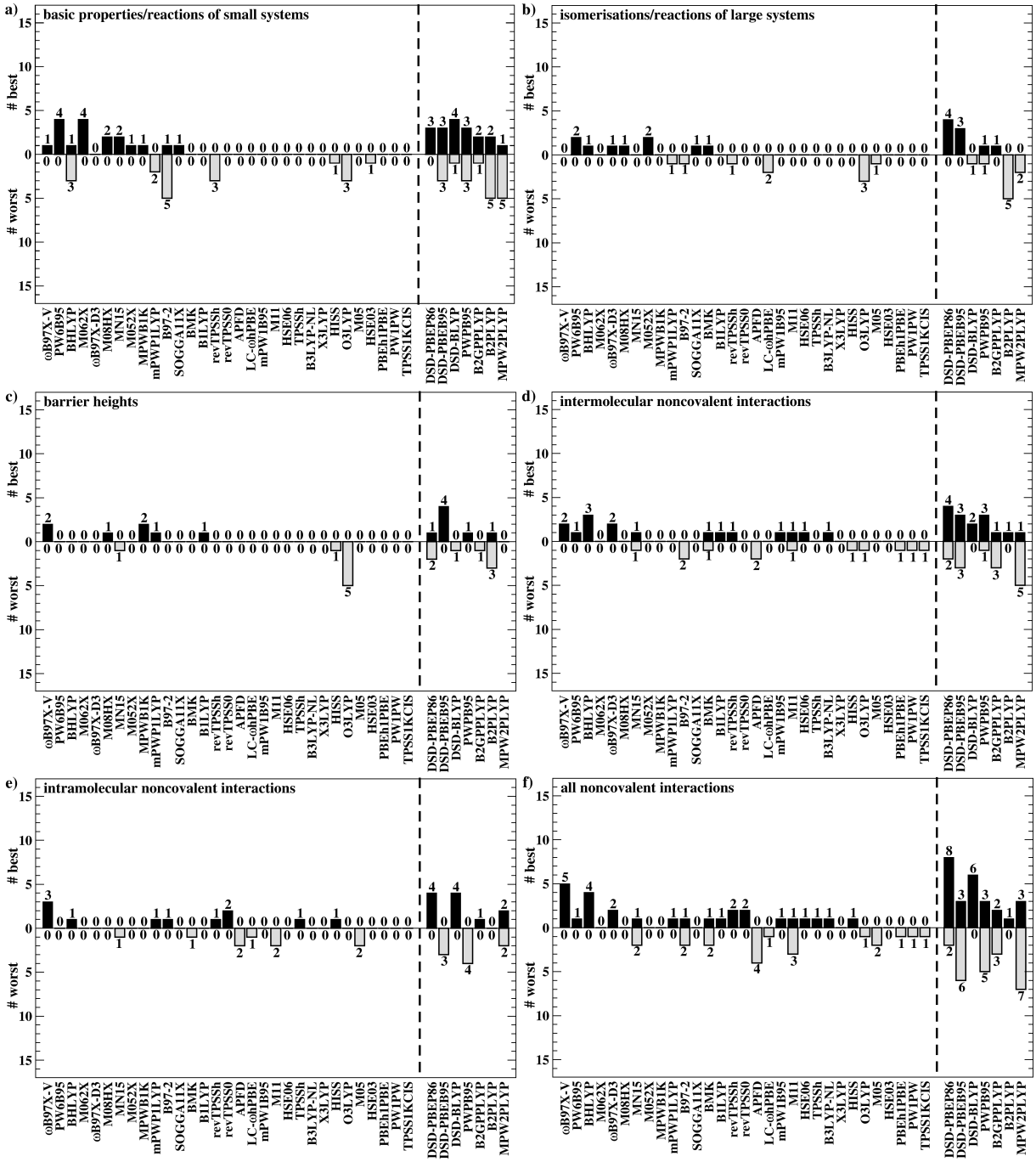

Figure S3: Analysis of how many times a DFA yielded the worst and best MAD in each of the categories of GMTKN55 (images a-f). The analysis was carried out separately for hybrid (left section in each image) and double-hybrid DFAs (right section in each image). All DFAs were dispersion corrected, but the suffix "D3" was omitted from the labels for better clarity.

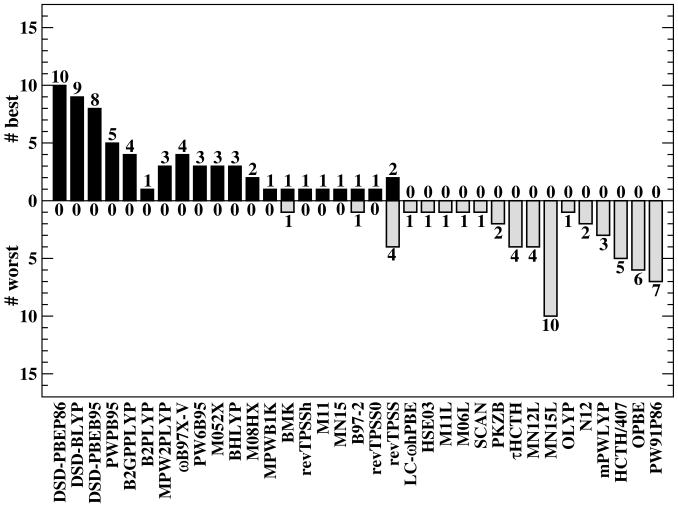

Figure S4: Analysis of how many times a DFA yielded the best and worst MAD for GMTKN55. All DFAs were dispersion corrected, but the suffix "D3" was omitted from the labels for better clarity.

Table S8: Best DFA for each benchmark set based on mean absolute deviations (kcal/mol). Results are analysed separately for each rung on Jacob's Ladder before the best of all 83 dispersion-corrected DFAs is shown.

	GGA/NGA	meta-GGA/meta-NGA	hybrid	double hybrid	all
W4-11	B97-D3(BJ) (4.73)	MN15L-D3(0) (3.41)	PW6B95-D3(BJ) (2.50)	PWPB95-D3(BJ) (1.86)	PWPB95-D3(BJ) (1.86)
G21EA	B97-D3(BJ) (2.34)	PKZB-D3(0) (2.15)	PW6B95-D3(BJ) (1.27)	B2PLYP-D3(BJ) (1.29)	PW6B95-D3(BJ) (1.27)
G21IP	B97-D3(BJ) (3.47)	MN15L-D3(0) (3.46)	B97-2-D3(BJ) (2.63)	PWPB95-D3(BJ) (1.94)	PWPB95-D3(BJ) (1.94)
DIPCS10	mPWPW91-D3(BJ) (3.76)	TPSS-D3(BJ) (3.69)	PW6B95-D3(BJ) (2.74)	B2GPPLYP-D3(BJ) (3.40)	PW6B95-D3(BJ) (2.74)
PA26	PW91P86-D3(0) (1.58)	MN15L-D3(0) (2.25)	M08HX-D3(0) (1.00)	DSD-BLYP-D3(BJ) (1.02)	M08HX-D3(0) (1.00)
SIE4x4	N12-D3(0) (21.63)	MN12L-D3(BJ) (9.26)	BHLYP-D3(BJ) (7.45)	DSD-PBEP86-D3(BJ) (5.04)	DSD-PBEP86-D3(BJ) (5.04)
ALKBDE10	OLYP-D3(BJ) (4.50)	TPSS-D3(BJ) (4.16)	MN15-D3(BJ) (2.88)	DSD-BLYP-D3(BJ) (2.78)	DSD-BLYP-D3(BJ) (2.78)
YBDE18	RPBE-D3(BJ) (3.22)	τHCTH-D3(BJ) (2.76)	M052X-D3(0) (0.93)	B2GPPLYP-D3(BJ) (0.93)	B2GPPLYP-D3(BJ) (0.93)
					M052X-D3(0) (0.93)
AL2X6	N12-D3(0) (1.42)	M06L-D3(0) (0.62)	PW6B95-D3(BJ) (0.61)	DSD-PBEP86-D3(BJ) (0.31)	DSD-PBEP86-D3(BJ) (0.31)
HEAVYSB11	revPBE-D3(BJ) (2.72)	M06L-D3(0) (2.56)	MPWB1K-D3(BJ) (0.45)	PWPB95-D3(BJ) (0.73)	MPWB1K-D3(BJ) (0.45)
NBPRC	BP86-D3(BJ) (1.79)	TPSS-D3(BJ) (1.46)	M062X-D3(0) (0.95)	DSD-PBEB95-D3(BJ) (0.73)	DSD-PBEB95-D3(BJ) (0.73)
ALK8	rPW86PBE-D3(BJ) (1.77)	revTPSS-D3(BJ) (2.87)	ωB97X-V (0.95)	B2PLYP-D3(BJ) (1.07)	ωB97X-V (0.95)
RC21	B97-D3(BJ) (3.75)	MN15L-D3(0) (2.00)	M08HX-D3(0) (1.52)	MPW2PLYP-D3(BJ) (1.05)	MPW2PLYP-D3(BJ) (1.05)
G2RC	rPW86PBE-D3(BJ) (4.70)	M11L-D3(0) (5.83)	M062X-D3(0) (1.92)	DSD-BLYP-D3(BJ) (1.03)	DSD-BLYP-D3(BJ) (1.03)
BH76RC	revPBE-D3(BJ) (2.76)	MN12L-D3(BJ) (2.35)	M062X-D3(0) (1.18)	DSD-BLYP-D3(BJ) (0.81)	DSD-BLYP-D3(BJ) (0.81)
FH51	N12-D3(0) (2.67)	M11L-D3(0) (2.10)	M062X-D3(0) (1.20)	DSD-PBEB95-D3(BJ) (0.69)	DSD-PBEB95-D3(BJ) (0.69)
TAUT15	revPBE-D3(BJ) (1.55)	MN15L-D3(0) (0.70)	SOGGA11X-D3(BJ) (0.44)	DSD-PBEB95-D3(BJ) (0.41)	DSD-PBEB95-D3(BJ) (0.41)
DC13	N12-D3(0) (7.77)	SCAN-D3(BJ) (6.87)	MN15-D3(BJ) (5.09)	DSD-PBEP86-D3(BJ) (2.55)	DSD-PBEP86-D3(BJ) (2.55)
MB16-43	PW91P86-D3(0) (18.79)	SCAN-D3(BJ) (17.77)	PW6B95-D3(BJ) (8.97)	DSD-PBEP86-D3(BJ) (6.46)	DSD-PBEP86-D3(BJ) (6.46)
DARC	OLYP-D3(BJ) (1.82)	SCAN-D3(BJ) (2.01)	M052X-D3(0) (0.96)	DSD-PBEB95-D3(BJ) (1.09)	M052X-D3(0) (0.96)
RSE43	revPBE-D3(BJ) (2.31)	MN15L-D3(0) (1.23)	BHLYP-D3(BJ) (0.48)	B2GPPLYP-D3(BJ) (0.41)	B2GPPLYP-D3(BJ) (0.41)
	RPBE-D3(BJ) (2.31)				
BSR36	RPBE-D3(BJ) (0.61)	M11L-D3(0) (0.54)	BMK-D3(BJ) (0.39)	DSD-PBEB95-D3(BJ) (1.20)	BMK-D3(BJ) (0.39)
CDIE20	XLYP-D3(BJ) (1.20)	PKZB-D3(0) (1.24)	M052X-D3(0) (0.34)	DSD-PBEP86-D3(BJ) (0.47)	M052X-D3(0) (0.34)
ISO34	N12-D3(0) (1.29)	M11L-D3(0) (1.20)	M08HX-D3(0) (0.95)	DSD-PBEP86-D3(BJ) (0.41)	DSD-PBEP86-D3(BJ) (0.41)
	RPBE-D3(BJ) (1.29)				
ISOL24	OLYP-D3(BJ) (3.45)	SCAN-D3(BJ) (3.23)	SOGGA11X-D3(BJ) (1.60)	DSD-PBEB95-D3(BJ) (0.96)	DSD-PBEB95-D3(BJ) (0.96)
C60ISO	HCTH/407-D3(BJ) (6.06)	MN12L-D3(BJ) (3.40)	PW6B95-D3(BJ) (1.65)	PWPB95-D3(BJ) (3.48)	PW6B95-D3(BJ) (1.65)
PArel	VV10 (1.42)	SCAN-D3(BJ) (1.50)	ωB97X-D3(0) (0.58)	DSD-PBEP86-D3(BJ) (0.50)	DSD-PBEP86-D3(BJ) (0.50)
BH76	HCTH/407-D3(BJ) (7.14)	MN12L-D3(BJ) (1.75)	M08HX-D3(0) (0.99)	DSD-PBEB95-D3(BJ) (1.03)	M08HX-D3(0) (0.99)
BHPERI	mPWLYP-D3(BJ) (2.72)	MN15L-D3(0) (1.78)	B1LYP-D3(BJ) (0.94)	PWPB95-D3(BJ) (0.80)	PWPB95-D3(BJ) (0.80)
BHDIV10	B97-D3(BJ) (5.83)	MN12L-D3(BJ) (2.03)	ωB97X-V (0.85)	DSD-PBEB95-D3(BJ) (0.83)	DSD-PBEB95-D3(BJ) (0.83)
INV24	B97-D3(BJ) (1.80)	SCAN-D3(BJ) (1.16)	mPW1LYP-D3(0) (0.95)	B2PLYP-D3(BJ) (0.69)	B2PLYP-D3(BJ) (0.69)
BHROT27	revPBE-D3(BJ) (0.37)	revTPSS-D3(BJ) (0.51)	ωB97X-V (0.31)	DSD-PBEP86-D3(BJ) (0.21)	DSD-PBEP86-D3(BJ) (0.21)
PX13	HCTH/407-D3(BJ) (6.09)	M06L-D3(0) (0.94)	MPWB1K-D3(BJ) (0.57)	DSD-PBEB95-D3(BJ) (0.43)	DSD-PBEB95-D3(BJ) (0.43)
WCPT18	XLYP-D3(BJ) (5.22)	MN12L-D3(BJ) (1.52)	MPWB1K-D3(BJ) (0.91)	DSD-PBEB95-D3(BJ) (0.58)	DSD-PBEB95-D3(BJ) (0.58)
RG18	mPWPW91-D3(BJ) (0.09)	revTPSS-D3(BJ) (0.06)	BHLYP-D3(BJ) (0.06)	B2PLYP-D3(BJ) (0.15)	BHLYP-D3(BJ) (0.06)
	revPBE-D3(BJ) (0.09)		revTPSSh-D3(BJ) (0.06)	DSD-PBEP86-D3(BJ) (0.15)	revTPSSh-D3(BJ) (0.06)
					revTPSS-D3(BJ) (0.06)
ADIM6	OLYP-D3(BJ) (0.06)	revTPSS-D3(BJ) (0.12)	BHLYP-D3(BJ) (0.05)	DSD-PBEP86-D3(BJ) (0.06)	BHLYP-D3(BJ) (0.05)
S22	BLYP-D3(BJ) (0.25)	revTPSS-D3(BJ) (0.27)	ωB97X-D3(0) (0.21)	B2GPPLYP-D3(BJ) (0.14)	B2GPPLYP-D3(BJ) (0.14)
S66	BLYP-D3(BJ) (0.17)	revTPSS-D3(BJ) (0.20)	ωB97X-V (0.12)	DSD-BLYP-D3(BJ) (0.17)	ωB97X-V (0.12)
HEAVY28	OLYP-D3(BJ) (0.23)	SCAN-D3(BJ) (0.27)	MPW1B95-D3(BJ) (0.17)	MPW2PLYP-D3(BJ) (0.12)	MPW2PLYP-D3(BJ) (0.12)
			PW6B95-D3(BJ) (0.17)		
WATER27	RPBE-D3(BJ) (1.28)	M06L-D3(0) (1.11)	BMK-D3(BJ) (1.02)	DSD-BLYP-D3(BJ) (0.94)	DSD-BLYP-D3(BJ) (0.94)
CARBHB12	OLYP-D3(BJ) (0.93)	M06L-D3(0) (0.44)	M11-D3(BJ) (0.22)	DSD-PBEB95-D3(BJ) (0.22)	DSD-PBEB95-D3(BJ) (0.22)
				PWPB95-D3(BJ) (0.22)	PWPB95-D3(BJ) (0.22)
					M11-D3(BJ) (0.22)
PNICO23	mPWLYP-D3(BJ) (0.50)	MN12L-D3(BJ) (0.25)	ωB97X-V (0.19)	PWPB95-D3(BJ) (0.14)	PWPB95-D3(BJ) (0.14)
HAL59	OLYP-D3(BJ) (0.59)	M06L-D3(0) (0.49)	BHLYP-D3(BJ) (0.29)	DSD-PBEB95-D3(BJ) (0.30)	BHLYP-D3(BJ) (0.29)
				PWPB95-D3(BJ) (0.30)	
AHB21	mPWLYP-D3(BJ) (0.65)	revTPSS-D3(BJ) (0.47)	B1LYP-D3(BJ) (0.30)	DSD-PBEB95-D3(BJ) (0.20)	DSD-PBEB95-D3(BJ) (0.20)
			ωB97X-D3(0) (0.30)		
CHB6	BP86-D3(BJ) (0.53)	SCAN-D3(BJ) (0.45)	MN15-D3(BJ) (0.32)	DSD-PBEP86-D3(BJ) (1.12)	MN15-D3(BJ) (0.32)
IL16	rPW86PBE-D3(BJ) (0.31)	TPSS-D3(BJ) (0.34)	HSE06-D3(BJ) (0.31)	DSD-PBEP86-D3(BJ) (0.23)	DSD-PBEP86-D3(BJ) (0.23)
			B3LYP-NL (0.31)		
IDISP	BPBE-D3(BJ) (2.45)	SCAN-D3(BJ) (2.05)	revTPSS0-D3(BJ) (1.12)	DSD-BLYP-D3(BJ) (1.02)	DSD-BLYP-D3(BJ) (1.02)
	OLYP-D3(BJ) (2.45)				
ICONF	BP86-D3(BJ) (0.27)	TPSS-D3(BJ) (0.19)	TPSSh-D3(BJ) (0.18)	DSD-PBEP86-D3(BJ) (0.14)	DSD-PBEP86-D3(BJ) (0.14)
	mPWPW91-D3(BJ) (0.27)				
ACONF	OLYP-D3(BJ) (0.04)	TPSS-D3(BJ) (0.09)	ωB97X-V (0.03)	MPW2PLYP-D3(BJ) (0.08)	ωB97X-V (0.03)
			revTPSS0-D3(BJ) (0.03)		revTPSS0-D3(BJ) (0.03)
			B97-2-D3(BJ) (0.03)		B97-2-D3(BJ) (0.03)
AMINO20x4	rPW86PBE-D3(BJ) (0.29)	SCAN-D3(BJ) (0.22)	ωB97X-V (0.19)	B2GPPLYP-D3(BJ) (0.13)	B2GPPLYP-D3(BJ) (0.13)
				DSD-BLYP-D3(BJ) (0.13)	DSD-BLYP-D3(BJ) (0.13)
				DSD-PBEP86-D3(BJ) (0.13)	DSD-PBEP86-D3(BJ) (0.13)
PCONF21	XLYP-D3(BJ) (0.66)	SCAN-D3(BJ) (0.47)	mPW1LYP-D3(0) (0.24)	DSD-BLYP-D3(BJ) (0.23)	DSD-BLYP-D3(BJ) (0.23)
MCONF	XLYP-D3(BJ) (0.33)	TPSS-D3(BJ) (0.42)	BHLYP-D3(BJ) (0.14)	MPW2PLYP-D3(BJ) (0.10)	MPW2PLYP-D3(BJ) (0.10)
SCONF	mPWLYP-D3(BJ) (0.36)	M11L-D3(0) (0.35)	HISS-D3(BJ) (0.13)	DSD-BLYP-D3(BJ) (0.06)	DSD-BLYP-D3(BJ) (0.06)
UPU23	VV10 (0.42)	revTPSS-D3(BJ) (0.33)	revTPSSh-D3(BJ) (0.35)	DSD-PBEP86-D3(BJ) (0.38)	revTPSS-D3(BJ) (0.33)
BUT14DIOL	RPBE-D3(BJ) (0.29)	revTPSS-D3(BJ) (0.18)	ωB97X-V (0.04)	DSD-PBEP86-D3(BJ) (0.05)	ωB97X-V (0.04)

Table S9: Worst DFA for each benchmark set based on mean absolute deviations (kcal/mol). Results are analysed separately for each rung on Jacob's Ladder before the worst of all 83 dispersion-corrected DFAs is shown.

	GGA/NGA	meta-GGA/meta-NGA	hybrid	double hybrid	all
W4-11	PW91P86-D3(0) (20.87)	PKZB-D3(0) (7.47)	BHLYP-D3(BJ) (20.20)	B2GPPLYP-D3(BJ) (2.77)	PW91P86-D3(0) (20.87)
G21EA	PW91P86-D3(0) (7.00)	M11L-D3(0) (5.66)	BHLYP-D3(BJ) (5.34)	DSD-PBEB95-D3(BJ) (2.89)	PW91P86-D3(0) (7.00)
G21IP	N12-D3(0) (4.87)	SCAN-D3(BJ) (4.69)	HSE03-D3(BJ) (6.04)	DSD-PBEB95-D3(BJ) (2.58)	HSE03-D3(BJ) (6.04)
DIPCS10	BLYP-D3(BJ) (7.87)	MN12L-D3(BJ) (14.64)	HSE03-D3(BJ) (10.23)	DSD-PBEB95-D3(BJ) (6.03)	MN12L-D3(BJ) (14.64)
PA26	OPBE-D3(BJ) (8.35)	PKZB-D3(0) (6.90)	B97-2-D3(BJ) (5.61)	PWPB95-D3(BJ) (1.90)	OPBE-D3(BJ) (8.35)
SIE4x4	OLYP-D3(BJ) (25.55)	PKZB-D3(0) (23.94)	O3LYP-D3(BJ) (21.38)	B2PLYP-D3(BJ) (10.08)	OLYP-D3(BJ) (25.55)
ALKBDE10	HCTH/407-D3(BJ) (9.06)	SCAN-D3(BJ) (19.27)	BHLYP-D3(BJ) (13.11)	MPW2PLYP-D3(BJ) (3.23)	SCAN-D3(BJ) (19.27)
YBDE18	mPWLYP-D3(BJ) (7.95)	MN12L-D3(BJ) (6.53)	mPW1LYP-D3(0) (5.66)	B2PLYP-D3(BJ) (2.12)	mPWLYP-D3(BJ) (7.95)
AL2X6	HCTH/407-D3(BJ) (11.75)	τHCTH-D3(BJ) (9.81)	B97-2-D3(BJ) (11.21)	MPW2PLYP-D3(BJ) (2.66)	HCTH/407-D3(BJ) (11.75)
HEAVYSB11	HCTH/407-D3(BJ) (13.91)	τHCTH-D3(BJ) (13.37)	B97-2-D3(BJ) (15.00)	MPW2PLYP-D3(BJ) (2.44)	B97-2-D3(BJ) (15.00)
NBPRC	OPBE-D3(BJ) (6.82)	M06L-D3(0) (3.97)	HISS-D3(BJ) (3.78)	MPW2PLYP-D3(BJ) (1.71)	OPBE-D3(BJ) (6.82)
ALK8	HCTH/407-D3(BJ) (21.56)	τHCTH-D3(BJ) (18.55)	B97-2-D3(BJ) (19.44)	PWPB95-D3(BJ) (4.23)	HCTH/407-D3(BJ) (21.56)
RC21	OPBE-D3(BJ) (10.63)	PKZB-D3(0) (7.46)	O3LYP-D3(BJ) (7.93)	DSD-BLYP-D3(BJ) (1.84)	OPBE-D3(BJ) (10.63)
G2RC	OPBE-D3(BJ) (10.17)	revTPSS-D3(BJ) (10.36)	revTPSSh-D3(BJ) (8.98)	PWPB95-D3(BJ) (2.17)	revTPSS-D3(BJ) (10.36)
BH76RC	PBE-D3(BJ) (4.18)	revTPSS-D3(BJ) (4.72)	revTPSSh-D3(BJ) (4.51)	MPW2PLYP-D3(BJ) (1.26)	revTPSS-D3(BJ) (4.72)
FH51	XLYP-D3(BJ) (4.85)	revTPSS-D3(BJ) (5.19)	revTPSSh-D3(BJ) (4.16)	B2PLYP-D3(BJ) (1.50)	revTPSS-D3(BJ) (5.19)
TAUT15	N12-D3(0) (2.34)	MN12L-D3(BJ) (2.13)	O3LYP-D3(BJ) (1.68)	B2PLYP-D3(BJ) (0.72)	N12-D3(0) (2.34)
DC13	OPBE-D3(BJ) (19.74)	τHCTH-D3(BJ) (10.97)	mPW1LYP-D3(0) (11.91)	B2PLYP-D3(BJ) (6.77)	OPBE-D3(BJ) (19.74)
MB16-43	HCTH/407-D3(BJ) (76.52)	M06L-D3(0) (63.27)	B97-2-D3(BJ) (56.32)	MPW2PLYP-D3(BJ) (22.08)	HCTH/407-D3(BJ) (76.52)
DARC	mPWLYP-D3(BJ) (15.78)	M06L-D3(0) (8.07)	LC-ωhPBE-D3(BJ) (10.90)	B2PLYP-D3(BJ) (5.03)	mPWLYP-D3(BJ) (15.78)
RSE43	HCTH/407-D3(BJ) (3.15)	τHCTH-D3(BJ) (3.12)	O3LYP-D3(BJ) (2.87)	PWPB95-D3(BJ) (0.97)	HCTH/407-D3(BJ) (3.15)
BSR36	mPWLYP-D3(BJ) (5.65)	PKZB-D3(0) (8.14)	M05-D3(0) (7.30)	MPW2PLYP-D3(BJ) (3.76)	PKZB-D3(0) (8.14)
CDIE20	HCTH/407-D3(BJ) (1.84)	M06L-D3(0) (2.22)	O3LYP-D3(BJ) (1.62)	B2PLYP-D3(BJ) (0.75)	M06L-D3(0) (2.22)
ISO34	mPWLYP-D3(BJ) (2.84)	revTPSS-D3(BJ) (2.84)	revTPSSh-D3(BJ) (2.63)	B2PLYP-D3(BJ) (1.13)	revTPSS-D3(BJ) (2.84)
ISOL24	mPWLYP-D3(BJ) (10.11)	M06L-D3(0) (6.52)	mPW1LYP-D3(0) (6.47)	B2PLYP-D3(BJ) (3.83)	mPWLYP-D3(BJ) (10.11)
C60ISO	VV10 (10.87)	PKZB-D3(0) (10.03)	LC-ωhPBE-D3(BJ) (17.64)	DSD-BLYP-D3(BJ) (7.63)	LC-ωhPBE-D3(BJ) (17.64)
PArel	OPBE-D3(BJ) (2.31)	M11L-D3(0) (2.41)	O3LYP-D3(BJ) (1.74)	B2PLYP-D3(BJ) (0.74)	M11L-D3(0) (2.41)
BH76	PW91P86-D3(0) (11.47)	TPSS-D3(BJ) (9.22)	O3LYP-D3(BJ) (7.65)	B2PLYP-D3(BJ) (2.59)	PW91P86-D3(0) (11.47)
BHPERI	OPBE-D3(BJ) (10.34)	PKZB-D3(0) (8.98)	O3LYP-D3(BJ) (4.84)	DSD-PBEP86-D3(BJ) (2.45)	OPBE-D3(BJ) (10.34)
BHDIV10	OPBE-D3(BJ) (10.41)	PKZB-D3(0) (8.96)	O3LYP-D3(BJ) (7.00)	B2PLYP-D3(BJ) (2.13)	OPBE-D3(BJ) (10.41)
INV24	HCTH/407-D3(BJ) (2.87)	τHCTH-D3(BJ) (2.37)	MN15-D3(BJ) (2.68)	DSD-BLYP-D3(BJ) (0.80)	HCTH/407-D3(BJ) (2.87)
BHROT27	N12-D3(0) (0.80)	MN12L-D3(BJ) (1.16)	HISS-D3(BJ) (0.88)	B2GPPLYP-D3(BJ) (0.33)	MN12L-D3(BJ) (1.16)
PX13	PW91P86-D3(0) (13.59)	τHCTH-D3(BJ) (9.97)	O3LYP-D3(BJ) (10.28)	B2PLYP-D3(BJ) (2.74)	PW91P86-D3(0) (13.59)
WCPT18	PW91P86-D3(0) (10.19)	PKZB-D3(0) (9.33)	O3LYP-D3(BJ) (7.06)	DSD-PBEP86-D3(BJ) (1.77)	PW91P86-D3(0) (10.19)
RG18	HCTH/407-D3(BJ) (1.26)	M11L-D3(0) (1.29)	BMK-D3(BJ) (1.42)	MPW2PLYP-D3(BJ) (0.27)	BMK-D3(BJ) (1.42)
ADIM6	HCTH/407-D3(BJ) (1.38)	MN15L-D3(0) (3.88)	MN15-D3(BJ) (1.32)	DSD-PBEB95-D3(BJ) (0.49)	MN15L-D3(0) (3.88)
S22	PW91P86-D3(0) (1.07)	MN15L-D3(0) (1.82)	APFD (0.93)	DSD-PBEB95-D3(BJ) (0.51)	MN15L-D3(0) (1.82)
S66	PW91P86-D3(0) (0.86)	MN15L-D3(0) (1.66)	APFD (0.75)	MPW2PLYP-D3(BJ) (0.29) DSD-PBEB95-D3(BJ) (0.29)	MN15L-D3(0) (1.66)
HEAVY28	XLYP-D3(BJ) (1.50)	τHCTH-D3(BJ) (1.87)	PBEh1PBE-D3(BJ) (1.34)	B2GPPLYP-D3(BJ) (0.20)	τHCTH-D3(BJ) (1.87)
WATER27	PW91P86-D3(0) (17.43)	MN15L-D3(0) (12.00)	PW1PW-D3(0) (8.17)	MPW2PLYP-D3(BJ) (4.99)	PW91P86-D3(0) (17.43)
CARBHB12	PW91P86-D3(0) (2.47)	τHCTH-D3(BJ) (2.00)	O3LYP-D3(BJ) (1.71)	MPW2PLYP-D3(BJ) (0.75)	PW91P86-D3(0) (2.47)
PNICO23	HCTH/407-D3(BJ) (1.97)	τHCTH-D3(BJ) (2.59)	B97-2-D3(BJ) (1.86)	DSD-PBEP86-D3(BJ) (0.40)	τHCTH-D3(BJ) (2.59)
HAL59	XLYP-D3(BJ) (2.16)	τHCTH-D3(BJ) (2.36)	TPSS1KCIS-D3(BJ) (1.62)	DSD-PBEP86-D3(BJ) (0.44) B2GPPLYP-D3(BJ) (0.44)	τHCTH-D3(BJ) (2.36)
AHB21	PW91P86-D3(0) (2.07)	MN15L-D3(0) (2.29)	HISS-D3(BJ) (1.75)	MPW2PLYP-D3(BJ) (0.63)	MN15L-D3(0) (2.29)
CHB6	XLYP-D3(BJ) (4.14)	τHCTH-D3(BJ) (4.39)	B97-2-D3(BJ) (4.11)	B2GPPLYP-D3(BJ) (1.81)	τHCTH-D3(BJ) (4.39)
IL16	N12-D3(0) (1.81)	MN15L-D3(0) (2.40)	M11-D3(BJ) (1.53)	PWPB95-D3(BJ) (1.25)	MN15L-D3(0) (2.40)
IDISP	mPWLYP-D3(BJ) (7.17)	MN15L-D3(0) (7.54)	M05-D3(0) (7.09)	MPW2PLYP-D3(BJ) (2.78)	MN15L-D3(0) (7.54)
ICONF	HCTH/407-D3(BJ) (0.65)	PKZB-D3(0) (0.81)	M05-D3(0) (0.64)	MPW2PLYP-D3(BJ) (0.25)	PKZB-D3(0) (0.81)
ACONF	HCTH/407-D3(BJ) (0.41)	MN12L-D3(BJ) (0.75)	M11-D3(BJ) (0.72)	DSD-PBEB95-D3(BJ) (0.37)	MN12L-D3(BJ) (0.75)
AMINO20x4	OPBE-D3(BJ) (0.56)	MN15L-D3(0) (0.92)	MN15-D3(BJ) (0.52)	PWPB95-D3(BJ) (0.23)	MN15L-D3(0) (0.92)
PCONF21	PW91-D3(BJ) (1.66)	MN15L-D3(0) (4.10)	BMK-D3(BJ) (1.70)	DSD-PBEB95-D3(BJ) (0.68)	MN15L-D3(0) (4.10)
MCONF	BPBE-D3(BJ) (0.74)	MN12L-D3(BJ) (1.65)	M11-D3(BJ) (1.24)	DSD-PBEB95-D3(BJ) (0.57)	MN12L-D3(BJ) (1.65)
SCONF	N12-D3(0) (1.39)	PKZB-D3(0) (1.36)	APFD (1.28)	PWPB95-D3(BJ) (0.18)	N12-D3(0) (1.39)
UPU23	PW91P86-D3(0) (0.69)	MN15L-D3(0) (1.67)	LC-ωhPBE-D3(BJ) (0.86)	PWPB95-D3(BJ) (0.53)	MN15L-D3(0) (1.67)
BUT14DIOL	PW91P86-D3(0) (0.78)	MN15L-D3(0) (1.10)	APFD (0.58)	PWPB95-D3(BJ) (0.36)	MN15L-D3(0) (1.10)

Table S10: Best DFA for each benchmark set based on root-mean-square deviations (kcal/mol). Results are analysed separately for each rung on Jacob's Ladder before the best of all 83 dispersion-corrected DFAs is shown.

	GGA/NGA	meta-GGA/meta-NGA	hybrid	double hybrid	all
W4-11	B97-D3(BJ) (6.87)	MN15L-D3(0) (4.67)	B98-D3(BJ) (4.02)	B2PLYP-D3(BJ) (2.72)	B2PLYP-D3(BJ) (2.72)
G21EA	B97-D3(BJ) (2.97)	revTPSS-D3(BJ) (2.53)	PW6B95-D3(BJ) (1.67)	B2PLYP-D3(BJ) (1.65)	B2PLYP-D3(BJ) (1.65)
G21IP	B97-D3(BJ) (4.49)	MN15L-D3(0) (4.51)	B97-2-D3(BJ) (3.33)	PWPB95-D3(BJ) (2.37)	PWPB95-D3(BJ) (2.37)
DIPCS10	BP86-D3(BJ) (4.59)	TPSS-D3(BJ) (4.97)	PW6B95-D3(BJ) (3.35)	B2GPPLYP-D3(BJ) (4.20)	PW6B95-D3(BJ) (3.35)
PA26	PW91P86-D3(0) (2.19)	MN15L-D3(0) (2.91)	M08HX-D3(0) (1.26)	DSD-PBEP86-D3(BJ) (1.49)	M08HX-D3(0) (1.26)
SIE4x4	N12-D3(0) (24.22)	MN12L-D3(BJ) (11.51)	BHLYP-D3(BJ) (9.71)	DSD-PBEP86-D3(BJ) (5.78)	DSD-PBEP86-D3(BJ) (5.78)
ALKBDE10	B97-D3(BJ) (8.03)	MN15L-D3(0) (5.13)	MN15-D3(BJ) (4.31)	DSD-BLYP-D3(BJ) (3.17)	DSD-BLYP-D3(BJ) (3.17)
	revPBE-D3(BJ) (8.03)				
YBDE18	RPBE-D3(BJ) (3.93)	SCAN-D3(BJ) (3.43)	M052X-D3(0) (1.08)	B2GPPLYP-D3(BJ) (1.29)	M052X-D3(0) (1.08)
AL2X6	PW91P86-D3(0) (2.05)	M06L-D3(0) (0.98)	PW6B95-D3(BJ) (0.71)	DSD-PBEP86-D3(BJ) (0.46)	DSD-PBEP86-D3(BJ) (0.46)
HEAVYSB11	BP86-D3(BJ) (3.14)	TPSS-D3(BJ) (2.92)	MPWB1K-D3(BJ) (0.57)	PWPB95-D3(BJ) (1.00)	MPWB1K-D3(BJ) (0.57)
NBPRC	BP86-D3(BJ) (2.18)	TPSS-D3(BJ) (1.93)	M062X-D3(0) (1.13)	DSD-PBEB95-D3(BJ) (0.81)	DSD-PBEB95-D3(BJ) (0.81)
ALK8	PW91P86-D3(0) (2.55)	revTPSS-D3(BJ) (4.11)	ωB97X-V (1.30)	B2PLYP-D3(BJ) (1.30)	B2PLYP-D3(BJ) (1.30)
					ωB97X-V (1.30)
RC21	B97-D3(BJ) (4.36)	MN15L-D3(0) (2.55)	M08HX-D3(0) (1.89)	MPW2PLYP-D3(BJ) (1.35)	MPW2PLYP-D3(BJ) (1.35)
G2RC	B97-D3(BJ) (6.30)	M06L-D3(0) (7.56)	M062X-D3(0) (2.51)	DSD-BLYP-D3(BJ) (1.46)	DSD-BLYP-D3(BJ) (1.46)
BH76RC	B97-D3(BJ) (4.03)	MN15L-D3(0) (3.44)	M08HX-D3(0) (1.54)	DSD-BLYP-D3(BJ) (1.21)	DSD-BLYP-D3(BJ) (1.21)
FH51	N12-D3(0) (4.19)	M11L-D3(0) (2.98)	M062X-D3(0) (1.55)	DSD-PBEB95-D3(BJ) (0.98)	DSD-PBEB95-D3(BJ) (0.98)
TAUT15	revPBE-D3(BJ) (1.78)	MN15L-D3(0) (0.96)	SOGGA11X-D3(BJ) (0.61)	DSD-PBEB95-D3(BJ) (0.49)	DSD-PBEB95-D3(BJ) (0.49)
DC13	N12-D3(0) (10.00)	MN15L-D3(0) (10.28)	MN15-D3(BJ) (7.19)	DSD-PBEP86-D3(BJ) (3.65)	DSD-PBEP86-D3(BJ) (3.65)
MB16-43	PW91P86-D3(0) (24.62)	SCAN-D3(BJ) (22.69)	PW6B95-D3(BJ) (11.26)	PWPB95-D3(BJ) (10.59)	PWPB95-D3(BJ) (10.59)
DARC	N12-D3(0) (2.28)	SCAN-D3(BJ) (2.66)	M052X-D3(0) (1.26)	DSD-PBEB95-D3(BJ) (1.24)	DSD-PBEB95-D3(BJ) (1.24)
RSE43	RPBE-D3(BJ) (2.55)	MN15L-D3(0) (1.53)	BHLYP-D3(BJ) (0.62)	MPW2PLYP-D3(BJ) (0.64)	BHLYP-D3(BJ) (0.62)
BSR36	RPBE-D3(BJ) (0.68)	M11L-D3(0) (0.82)	BMK-D3(BJ) (0.51)	DSD-PBEB95-D3(BJ) (1.26)	BMK-D3(BJ) (0.51)
CDIE20	XLYP-D3(BJ) (1.27)	PKZB-D3(0) (1.34)	BMK-D3(BJ) (0.49)	DSD-PBEP86-D3(BJ) (0.54)	BMK-D3(BJ) (0.49)
ISO34	N12-D3(0) (1.72)	M11L-D3(0) (1.64)	M08HX-D3(0) (1.31)	DSD-PBEP86-D3(BJ) (0.65)	DSD-PBEP86-D3(BJ) (0.65)
ISOL24	OLYP-D3(BJ) (4.84)	SCAN-D3(BJ) (4.68)	SOGGA11X-D3(BJ) (2.03)	DSD-PBEB95-D3(BJ) (1.33)	DSD-PBEB95-D3(BJ) (1.33)
				DSD-PBEP86-D3(BJ) (1.33)	DSD-PBEP86-D3(BJ) (1.33)
C60ISO	HCTH/407-D3(BJ) (8.11)	MN12L-D3(BJ) (4.59)	PW6B95-D3(BJ) (2.11)	PWPB95-D3(BJ) (4.81)	PW6B95-D3(BJ) (2.11)
PArel	OLYP-D3(BJ) (2.22)	revTPSS-D3(BJ) (2.04)	ωB97X-D3(0) (0.88)	DSD-PBEP86-D3(BJ) (0.76)	DSD-PBEP86-D3(BJ) (0.76)
BH76	B97-D3(BJ) (8.17)	MN12L-D3(BJ) (2.44)	M08HX-D3(0) (1.29)	DSD-PBEB95-D3(BJ) (1.65)	M08HX-D3(0) (1.29)
BHPERI	mPWLYP-D3(BJ) (3.76)	MN15L-D3(0) (2.12)	B1LYP-D3(BJ) (1.24)	PWPB95-D3(BJ) (0.90)	PWPB95-D3(BJ) (0.90)
BHDIV10	B97-D3(BJ) (6.84)	MN12L-D3(BJ) (2.17)	ωB97X-V (1.16)	DSD-PBEB95-D3(BJ) (1.02)	DSD-PBEB95-D3(BJ) (1.02)
INV24	B97-D3(BJ) (2.30)	SCAN-D3(BJ) (1.68)	B97-1-D3(BJ) (1.27)	MPW2PLYP-D3(BJ) (0.96)	MPW2PLYP-D3(BJ) (0.96)
BHROT27	revPBE-D3(BJ) (0.51)	revTPSS-D3(BJ) (0.69)	ωB97X-V (0.42)	DSD-PBEP86-D3(BJ) (0.27)	DSD-PBEP86-D3(BJ) (0.27)
PX13	HCTH/407-D3(BJ) (6.20)	M06L-D3(0) (1.17)	MPWB1K-D3(BJ) (0.66)	DSD-PBEB95-D3(BJ) (0.51)	DSD-PBEB95-D3(BJ) (0.51)
WCPT18	XLYP-D3(BJ) (5.78)	MN12L-D3(BJ) (1.87)	MN12SX-D3(BJ) (1.28)	DSD-PBEB95-D3(BJ) (0.76)	DSD-PBEB95-D3(BJ) (0.76)
RG18	revPBE-D3(BJ) (0.11)	revTPSS-D3(BJ) (0.08)	BHLYP-D3(BJ) (0.08)	B2PLYP-D3(BJ) (0.18)	BHLYP-D3(BJ) (0.08)
			revTPSSh-D3(BJ) (0.08)		revTPSSh-D3(BJ) (0.08)
		revTPSS-D3(BJ) (0.08)			revTPSS-D3(BJ) (0.08)
ADIM6	OLYP-D3(BJ) (0.07)	revTPSS-D3(BJ) (0.13)	BHLYP-D3(BJ) (0.06)	DSD-PBEP86-D3(BJ) (0.07)	BHLYP-D3(BJ) (0.06)
		SCAN-D3(BJ) (0.13)	PBE0-D3(BJ) (0.06)		PBE0-D3(BJ) (0.06)
S22	BLYP-D3(BJ) (0.32)	revTPSS-D3(BJ) (0.33)	ωB97X-D3(0) (0.29)	B2GPPLYP-D3(BJ) (0.20)	B2GPPLYP-D3(BJ) (0.20)
				B2PLYP-D3(BJ) (0.20)	B2PLYP-D3(BJ) (0.20)
S66	BLYP-D3(BJ) (0.24)	revTPSS-D3(BJ) (0.26)	ωB97X-V (0.16)	DSD-BLYP-D3(BJ) (0.21)	ωB97X-V (0.16)
HEAVY28	OLYP-D3(BJ) (0.30)	SCAN-D3(BJ) (0.32)	PW6B95-D3(BJ) (0.21)	MPW2PLYP-D3(BJ) (0.16)	MPW2PLYP-D3(BJ) (0.16)
WATER27	RPBE-D3(BJ) (2.04)	M06L-D3(0) (1.70)	MN15-D3(BJ) (1.48)	DSD-BLYP-D3(BJ) (1.29)	DSD-BLYP-D3(BJ) (1.29)
CARBHB12	BLYP-D3(BJ) (1.28)	M06L-D3(0) (0.67)	M11-D3(BJ) (0.28)	DSD-PBEB95-D3(BJ) (0.28)	DSD-PBEB95-D3(BJ) (0.28)
				PWPB95-D3(BJ) (0.28)	PWPB95-D3(BJ) (0.28)
					M11-D3(BJ) (0.28)
PNICO23	mPWLYP-D3(BJ) (0.68)	MN12L-D3(BJ) (0.35)	ωB97X-V (0.24cd ..)	PWPB95-D3(BJ) (0.22)	PWPB95-D3(BJ) (0.22)
HAL59	OLYP-D3(BJ) (0.97)	M06L-D3(0) (0.65)	BHLYP-D3(BJ) (0.40)	DSD-PBEB95-D3(BJ) (0.40)	DSD-PBEB95-D3(BJ) (0.40)
				PWPB95-D3(BJ) (0.40)	PWPB95-D3(BJ) (0.40)
					BHLYP-D3(BJ) (0.40)
AHB21	B97-D3(BJ) (0.98)	M06L-D3(0) (0.62)	B1LYP-D3(BJ) (0.37)	DSD-PBEB95-D3(BJ) (0.24)	DSD-PBEB95-D3(BJ) (0.24)
	mPWLYP-D3(BJ) (0.98)				
CHB6	VV10 (0.59)	SCAN-D3(BJ) (0.57)	MN15-D3(BJ) (0.41)	DSD-PBEP86-D3(BJ) (1.22)	MN15-D3(BJ) (0.41)
IL16	rPW86PBE-D3(BJ) (0.39)	TPSS-D3(BJ) (0.43)	B3LYP-NL (0.37)	DSD-PBEP86-D3(BJ) (0.28)	DSD-PBEP86-D3(BJ) (0.28)
IDISP	mPWPW91-D3(BJ) (3.34)	SCAN-D3(BJ) (3.45)	TPSS0-D3(BJ) (1.46)	DSD-BLYP-D3(BJ) (1.31)	DSD-BLYP-D3(BJ) (1.31)
	BP86-D3(BJ) (3.34)				
ICONF	BP86-D3(BJ) (0.32)	TPSS-D3(BJ) (0.22)	TPSSh-D3(BJ) (0.21)	DSD-PBEP86-D3(BJ) (0.18)	DSD-PBEP86-D3(BJ) (0.18)
ACONF	OLYP-D3(BJ) (0.05)	TPSS-D3(BJ) (0.11)	ωB97X-V (0.03)	MPW2PLYP-D3(BJ) (0.10)	ωB97X-V (0.03))
AMINO20x4	rPW86PBE-D3(BJ) (0.38)	SCAN-D3(BJ) (0.30)	ωB97X-V (0.24)	DSD-PBEP86-D3(BJ) (0.16)	DSD-PBEP86-D3(BJ) (0.16)
PCONF21	XLYP-D3(BJ) (0.76)	SCAN-D3(BJ) (0.53)	mPW1LYP-D3(0) (0.29)	DSD-BLYP-D3(BJ) (0.29)	DSD-BLYP-D3(BJ) (0.29)
					mPW1LYP-D3(0) (0.29)
MCONF	XLYP-D3(BJ) (0.42)	TPSS-D3(BJ) (0.50)	BHLYP-D3(BJ) (0.16)	MPW2PLYP-D3(BJ) (0.13)	MPW2PLYP-D3(BJ) (0.13)
SCONF	OLYP-D3(BJ) (0.55)	M11L-D3(0) (0.43)	HISS-D3(BJ) (0.19)	DSD-BLYP-D3(BJ) (0.12)	DSD-BLYP-D3(BJ) (0.12)
UPU23	VV10 (0.57)	revTPSS-D3(BJ) (0.43)	revTPSSh-D3(BJ) (0.44)	DSD-PBEP86-D3(BJ) (0.48)	revTPSS-D3(BJ) (0.43)
BUT14DIOL	RPBE-D3(BJ) (0.35)	revTPSS-D3(BJ) (0.23)	ωB97X-V (0.05)	DSD-PBEP86-D3(BJ) (0.07)	ωB97X-V (0.05)

Table S11: Worst DFA for each benchmark set based on root-mean-square deviations (kcal/mol). Results are analysed separately for each rung on Jacob's Ladder before the worst of all 83 dispersion-corrected DFAs is shown.

	GGA/NGA	meta-GGA/meta-NGA	hybrid	double hybrid	all
W4-11	PW91P86-D3(0) (24.32)	PKZB-D3(0) (9.79)	BHLYP-D3(BJ) (24.29)	B2GPPLYP-D3(BJ) (3.88)	PW91P86-D3(0) (24.32)
G21EA	PW91P86-D3(0) (7.55)	M11L-D3(0) (6.55)	BHLYP-D3(BJ) (6.09)	DSD-PBEB95-D3(BJ) (2.97)	PW91P86-D3(0) (7.55)
G21IP	N12-D3(0) (6.20)	MN12L-D3(BJ) (5.74)	HSE03-D3(BJ) (7.21)	DSD-PBEB95-D3(BJ) (2.89)	HSE03-D3(BJ) (7.21)
DIPCS10	N12-D3(0) (9.29)	MN12L-D3(BJ) (16.40)	HSE03-D3(BJ) (10.80)	DSD-PBEB95-D3(BJ) (6.33)	MN12L-D3(BJ) (16.40)
PA26	OPBE-D3(BJ) (8.77)	PKZB-D3(0) (7.69)	B97-2-D3(BJ) (6.00)	PWPB95-D3(BJ) (2.30)	OPBE-D3(BJ) (8.77)
SIE4x4	OLYP-D3(BJ) (28.58)	PKZB-D3(0) (26.96)	O3LYP-D3(BJ) (23.95)	PWPB95-D3(BJ) (11.44)	OLYP-D3(BJ) (28.58)
	mPWLYP-D3(BJ) (28.58)				mPWLYP-D3(BJ) (28.58)
ALKBDE10	HCTH/407-D3(BJ) (12.86)	SCAN-D3(BJ) (21.05)	BHLYP-D3(BJ) (14.86)	B2PLYP-D3(BJ) (3.80)	SCAN-D3(BJ) (21.05)
YBDE18	mPWLYP-D3(BJ) (10.09)	MN12L-D3(BJ) (7.01)	mPW1LYP-D3(0) (6.53)	B2PLYP-D3(BJ) (2.59)	mPWLYP-D3(BJ) (10.09)
AL2X6	HCTH/407-D3(BJ) (12.51)	τHCTH-D3(BJ) (10.53)	B97-2-D3(BJ) (11.72)	MPW2PLYP-D3(BJ) (2.77)	HCTH/407-D3(BJ) (12.51)
HEAVYSB11	HCTH/407-D3(BJ) (14.98)	τHCTH-D3(BJ) (15.91)	B97-2-D3(BJ) (16.63)	MPW2PLYP-D3(BJ) (2.62)	B97-2-D3(BJ) (16.63)
NBPRC	OPBE-D3(BJ) (7.69)	M06L-D3(0) (4.89)	M05-D3(0) (4.94)	MPW2PLYP-D3(BJ) (2.26)	OPBE-D3(BJ) (7.69)
ALK8	HCTH/407-D3(BJ) (29.98)	τHCTH-D3(BJ) (23.69)	B97-2-D3(BJ) (25.12)	PWPB95-D3(BJ) (6.65)	HCTH/407-D3(BJ) (29.98)
RC21	OPBE-D3(BJ) (11.82)	SCAN-D3(BJ) (8.45)	O3LYP-D3(BJ) (9.08)	DSD-BLYP-D3(BJ) (2.24)	OPBE-D3(BJ) (11.82)
G2RC	OPBE-D3(BJ) (13.20)	MN12L-D3(BJ) (13.54)	revTPSSh-D3(BJ) (11.14)	PWPB95-D3(BJ) (2.80)	MN12L-D3(BJ) (13.54)
BH76RC	OPBE-D3(BJ) (6.15)	revTPSS-D3(BJ) (6.10)	revTPSSh-D3(BJ) (5.49)	PWPB95-D3(BJ) (1.61)	OPBE-D3(BJ) (6.15)
FH51	XLYP-D3(BJ) (6.54)	revTPSS-D3(BJ) (6.89)	revTPSSh-D3(BJ) (5.65)	B2PLYP-D3(BJ) (2.04)	revTPSS-D3(BJ) (6.89)
TAUT15	N12-D3(0) (2.83)	MN12L-D3(BJ) (2.80)	O3LYP-D3(BJ) (2.45)	B2PLYP-D3(BJ) (0.85)	N12-D3(0) (2.83)
DC13	OPBE-D3(BJ) (25.06)	PKZB-D3(0) (13.81)	mPW1LYP-D3(0) (15.56)	MPW2PLYP-D3(BJ) (8.11)	OPBE-D3(BJ) (25.06)
MB16-43	HCTH/407-D3(BJ) (92.24)	M06L-D3(0) (68.15)	B97-2-D3(BJ) (66.75)	MPW2PLYP-D3(BJ) (26.72)	HCTH/407-D3(BJ) (92.24)
DARC	mPWLYP-D3(BJ) (15.98)	M06L-D3(0) (8.62)	LC-ωhPBE-D3(BJ) (10.99)	B2PLYP-D3(BJ) (5.16)	mPWLYP-D3(BJ) (15.98)
RSE43	HCTH/407-D3(BJ) (3.40)	τHCTH-D3(BJ) (3.36)	O3LYP-D3(BJ) (3.21)	DSD-PBEP86-D3(BJ) (1.72)	HCTH/407-D3(BJ) (3.40)
BSR36	mPWLYP-D3(BJ) (6.75)	PKZB-D3(0) (9.72)	M05-D3(0) (8.83)	MPW2PLYP-D3(BJ) (4.38)	PKZB-D3(0) (9.72)
CDIE20	HCTH/407-D3(BJ) (2.02)	M06L-D3(0) (2.47)	O3LYP-D3(BJ) (1.81)	PWPB95-D3(BJ) (0.84)	M06L-D3(0) (2.47)
ISO34	mPWLYP-D3(BJ) (4.05)	revTPSS-D3(BJ) (4.09)	revTPSSh-D3(BJ) (3.56)	B2PLYP-D3(BJ) (1.74)	revTPSS-D3(BJ) (4.09)
ISOL24	mPWLYP-D3(BJ) (14.36)	M06L-D3(0) (8.76)	mPW1LYP-D3(0) (9.19)	MPW2PLYP-D3(BJ) (5.42)	mPWLYP-D3(BJ) (14.36)
C60ISO	VV10 (12.98)	PKZB-D3(0) (12.53)	LC-ωhPBE-D3(BJ) (19.31)	DSD-BLYP-D3(BJ) (10.12)	LC-ωhPBE-D3(BJ) (19.31)
PArel	mPWLYP-D3(BJ) (2.73)	M11L-D3(0) (3.18)	MN12SX-D3(BJ) (2.38)	B2PLYP-D3(BJ) (1.16)	M11L-D3(0) (3.18)
BH76	PW91P86-D3(0) (12.58)	TPSS-D3(BJ) (10.09)	O3LYP-D3(BJ) (8.65)	B2PLYP-D3(BJ) (2.93)	PW91P86-D3(0) (12.58)
BHPERI	OPBE-D3(BJ) (11.42)	PKZB-D3(0) (9.56)	O3LYP-D3(BJ) (5.29)	DSD-PBEP86-D3(BJ) (2.61)	OPBE-D3(BJ) (11.42)
BHDIV10	OPBE-D3(BJ) (11.78)	PKZB-D3(0) (9.98)	O3LYP-D3(BJ) (7.76)	B2PLYP-D3(BJ) (2.60)	OPBE-D3(BJ) (11.78)
INV24	HCTH/407-D3(BJ) (3.98)	MN15L-D3(0) (3.74)	LC-ωhPBE-D3(BJ) (3.91)	DSD-PBEB95-D3(BJ) (1.20)	HCTH/407-D3(BJ) (3.98)
BHROT27	N12-D3(0) (1.13)	MN12L-D3(BJ) (1.57)	HISS-D3(BJ) (1.21)	B2GPPLYP-D3(BJ) (0.48)	MN12L-D3(BJ) (1.57)
PX13	PW91P86-D3(0) (13.83)	τHCTH-D3(BJ) (10.19)	O3LYP-D3(BJ) (10.56)	B2PLYP-D3(BJ) (2.83)	PW91P86-D3(0) (13.83)
WCPT18	PW91P86-D3(0) (10.86)	PKZB-D3(0) (10.04)	O3LYP-D3(BJ) (7.61)	B2PLYP-D3(BJ) (2.09)	PW91P86-D3(0) (10.86)
RG18	HCTH/407-D3(BJ) (1.56)	M11L-D3(0) (1.95)	BMK-D3(BJ) (2.03)	MPW2PLYP-D3(BJ) (0.40)	BMK-D3(BJ) (2.03)
ADIM6	HCTH/407-D3(BJ) (1.39)	MN15L-D3(0) (4.35)	MN15-D3(BJ) (1.47)	DSD-PBEB95-D3(BJ) (0.58)	MN15L-D3(0) (4.35)
S22	PW91P86-D3(0) (1.31)	MN15L-D3(0) (2.40)	BMK-D3(BJ) (1.32)	PWPB95-D3(BJ) (0.63)	MN15L-D3(0) (2.40)
				DSD-PBEB95-D3(BJ) (0.63)	
S66	PW91P86-D3(0) (1.11)	MN15L-D3(0) (1.97)	APFD (0.91)	MPW2PLYP-D3(BJ) (0.43)	MN15L-D3(0) (1.97)
HEAVY28	XLYP-D3(BJ) (1.70)	τHCTH-D3(BJ) (2.06)	PBEh1PBE-D3(BJ) (1.53)	B2GPPLYP-D3(BJ) (0.26)	τHCTH-D3(BJ) (2.06)
WATER27	PW91P86-D3(0) (23.99)	MN15L-D3(0) (16.73)	mPW1LYP-D3(0) (11.53)	MPW2PLYP-D3(BJ) (6.97)	PW91P86-D3(0) (23.99)
CARBHB12	PW91P86-D3(0) (2.85)	τHCTH-D3(BJ) (2.41)	O3LYP-D3(BJ) (2.14)	MPW2PLYP-D3(BJ) (0.85)	PW91P86-D3(0) (2.85)
PNICO23	HCTH/407-D3(BJ) (3.13)	τHCTH-D3(BJ) (3.46)	B97-2-D3(BJ) (2.69)	DSD-PBEP86-D3(BJ) (0.52)	τHCTH-D3(BJ) (3.46)
HAL59	XLYP-D3(BJ) (2.70)	τHCTH-D3(BJ) (3.08)	TPSS1KCIS-D3(BJ) (2.16)	B2GPPLYP-D3(BJ) (0.62)	τHCTH-D3(BJ) (3.08)
AHB21	PW91P86-D3(0) (2.19)	MN15L-D3(0) (2.46)	HISS-D3(BJ) (2.14)	MPW2PLYP-D3(BJ) (0.72)	MN15L-D3(0) (2.46)
CHB6	HCTH/407-D3(BJ) (4.42)	τHCTH-D3(BJ) (4.86)	B97-2-D3(BJ) (4.59)	B2GPPLYP-D3(BJ) (1.90)	τHCTH-D3(BJ) (4.86)
IL16	N12-D3(0) (1.88)	MN15L-D3(0) (2.62)	M11-D3(BJ) (1.58)	PWPB95-D3(BJ) (1.28)	MN15L-D3(0) (2.62)
IDISP	mPWLYP-D3(BJ) (10.79)	M06L-D3(0) (9.30)	mPW1LYP-D3(0) (8.92)	MPW2PLYP-D3(BJ) (3.81)	mPWLYP-D3(BJ) (10.79)
ICONF	HCTH/407-D3(BJ) (0.83)	PKZB-D3(0) (1.06)	M05-D3(0) (1.02)	MPW2PLYP-D3(BJ) (0.35)	PKZB-D3(0) (1.06)
ACONF	HCTH/407-D3(BJ) (0.46)	MN12L-D3(BJ) (0.86)	M11-D3(BJ) (0.81)	DSD-PBEB95-D3(BJ) (0.39)	MN12L-D3(BJ) (0.86)
AMINO20x4	OPBE-D3(BJ) (0.71)	MN15L-D3(0) (1.18)	MN15-D3(BJ) (0.68)	PWPB95-D3(BJ) (0.31)	MN15L-D3(0) (1.18)
PCONF21	PW91-D3(BJ) (1.87)	MN15L-D3(0) (4.59)	BMK-D3(BJ) (2.02)	DSD-PBEB95-D3(BJ) (0.83)	MN15L-D3(0) (4.59)
MCONF	BPBE-D3(BJ) (0.88)	MN12L-D3(BJ) (1.89)	M11-D3(BJ) (1.38)	DSD-PBEB95-D3(BJ) (0.65)	MN12L-D3(BJ) (1.89)
			BMK-D3(BJ) (1.38)		
SCONF	N12-D3(0) (1.68)	PKZB-D3(0) (1.49)	APFD (1.61)	PWPB95-D3(BJ) (0.28)	N12-D3(0) (1.68)
UPU23	PW91P86-D3(0) (0.94)	MN15L-D3(0) (2.44)	BMK-D3(BJ) (1.12)	PWPB95-D3(BJ) (0.65)	MN15L-D3(0) (2.44)
BUT14DIOL	PW91P86-D3(0) (0.82)	MN15L-D3(0) (1.16)	APFD (0.65)	PWPB95-D3(BJ) (0.37)	MN15L-D3(0) (1.16)

SI.6 Weighted total mean absolute deviations

SI.6.1 WTMAD-1 diagrams for all assessed methods

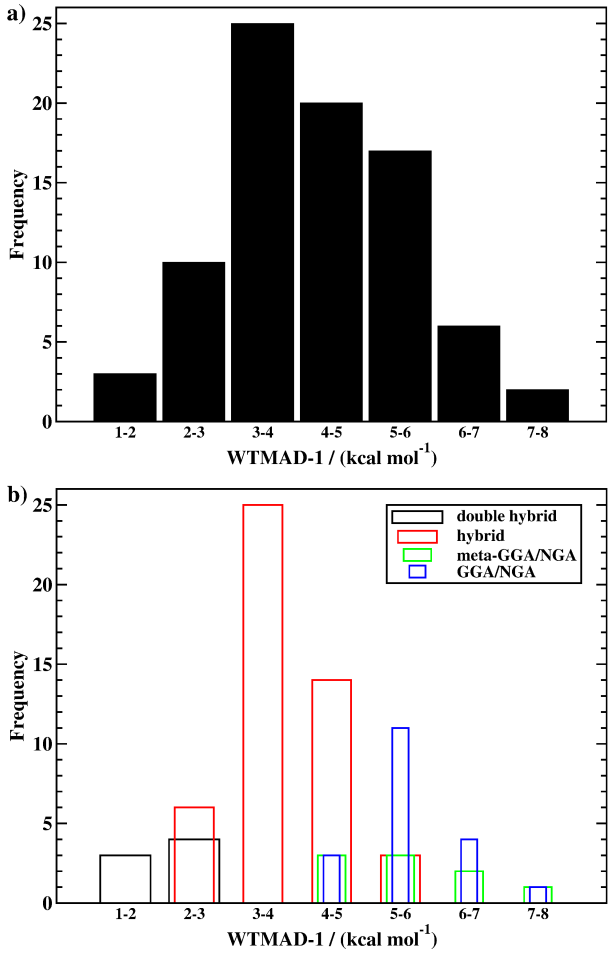

Figure S5: Histograms (1 kcal/mol bins) showing the WTMAD-1 distributions for all 83 dispersion-corrected DFAs (a) and for each rung of Jacob's Ladder (b).

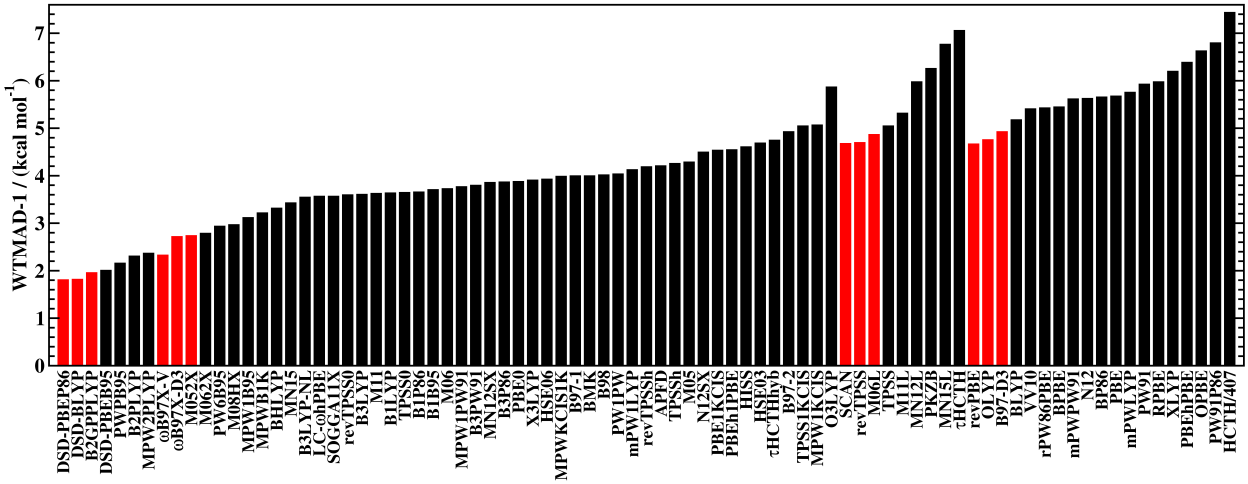

Figure S6: Final WTMAD-1 values over the entire GMTKN55 for all assessed 83 dispersion-corrected DFAs (kcal/mol). The red bars indicate the three best approaches on their respective rung of Jacob's Ladder. The suffix "D3" was omitted in all cases.

SI.6.2 Averaged WTMADs for each considered rung on Jacob's Ladder

Table S12: Average WTMAD-1 and WTMAD-2 values for the four highest rungs on Jacob's Ladder (kcal/mol).

Rung	WTMAD-1	WTMAD-2
Basic properties and reactions of small systems		
GGA/NGA	5.70	6.60
meta-GGA/NGA	4.91	5.43
hybrid	3.83	4.29
double hybrid	1.87	2.09
Isomerisations and reactions of large systems		
GGA/NGA	6.24	12.57
meta-GGA/NGA	6.16	11.95
hybrid	4.10	8.40
double hybrid	2.50	4.94
Barrier heights		
GGA/NGA	6.72	16.80
meta-GGA/NGA	5.05	11.64
hybrid	3.43	7.75
double hybrid	1.59	3.51
Intermolecular noncovalent interactions		
GGA/NGA	5.40	11.47
meta-GGA/NGA	5.54	11.39
hybrid	4.03	8.70
double hybrid	2.02	4.13
Intramolecular noncovalent interactions		
GGA/NGA	5.13	9.73
meta-GGA/NGA	7.05	13.05
hybrid	3.83	7.05
double hybrid	2.39	4.28
All noncovalent interactions		
GGA/NGA	5.28	10.62
meta-GGA/NGA	6.19	12.21
hybrid	3.95	7.89
double hybrid	2.18	4.20
GMTKN55		
GGA/NGA	5.76	10.47
meta-GGA/NGA	5.62	9.96
hybrid	3.87	6.82
double hybrid	2.05	3.57

SI.6.3 The worst density functional approximations according to WTMADs

Table S13: The worst three DFAs for each of the four highest rungs on Jacob's Ladder for basic properties and reactions of small systems according to WTMAD-1 and WTMAD-2 values (kcal/mol).

Rung	WTMAD-1	WTMAD-2
GGA/NGA	HCTH/407-D3(BJ) (7.77)	OPBE-D3(BJ) (8.23)
	OPBE-D3(BJ) (7.01)	HCTH/407-D3(BJ) (7.52)
	XLYP-D3(BJ) (6.60)	mPWLYP-D3(BJ) (7.29)
meta-GGA/NGA	τHCTH-D3(BJ) (6.82)	PKZB-D3(0) (6.71)
	PKZB-D3(0) (5.84)	τHCTH-D3(BJ) (6.37)
	MN12L-D3(BJ) (4.82)	revTPSS-D3(BJ) (6.31)
hybrid	B97-2-D3(BJ) (6.07)	O3LYP-D3(BJ) (6.72)
	O3LYP-D3(BJ) (5.92)	revTPSSh-D3(BJ) (5.69)
	MPW1KCIS-D3(BJ) (5.44)	revTPSS0-D3(BJ) (5.42)
double hybrid	MPW2PLYP-D3(BJ) (2.24)	B2PLYP-D3(BJ) (2.51)
	B2PLYP-D3(BJ) (2.24)	MPW2PLYP-D3(BJ) (2.46)
	PWPB95-D3(BJ) (2.08)	PWPB95-D3(BJ) (2.23)

Table S14: The worst three DFAs for each of the four highest rungs on Jacob's Ladder for isomerisatons and reactions of large systems according to WTMAD-1 and WTMAD-2 values (kcal/mol).

Rung	WTMAD-1	WTMAD-2
GGA/NGA	mPWLYP-D3(BJ) (8.17)	mPWLYP-D3(BJ) (17.13)
	OPBE-D3(BJ) (8.10)	rPW86PBE-D3(BJ) (14.95)
	BLYP-D3(BJ) (7.31)	BLYP-D3(BJ) (14.56)
meta-GGA/NGA	M06L-D3(0) (7.79)	M06L-D3(0) (15.81)
	PKZB-D3(0) (6.64)	PKZB-D3(0) (15.18)
	τHCTH-D3(BJ) (6.50)	τHCTH-D3(BJ) (13.57)
hybrid	M05-D3(0) (5.66)	M05-D3(0) (12.82)
	O3LYP-D3(BJ) (5.56)	mPW1LYP-D3(0) (11.69)
	mPW1LYP-D3(0) (5.50)	O3LYP-D3(BJ) (10.98)
double hybrid	MPW2PLYP-D3(BJ) (3.36)	MPW2PLYP-D3(BJ) (6.76)
	B2PLYP-D3(BJ) (3.36)	B2PLYP-D3(BJ) (6.28)
	PWPB95-D3(BJ) (2.53)	PWPB95-D3(BJ) (5.41)

Table S15: The worst three DFAs for each of the four highest rungs on Jacob's Ladder for barrier heights according to WTMAD-1 and WTMAD-2 values (kcal/mol).

Rung	WTMAD-1	WTMAD-2
GGA/NGA	PW91P86-D3(0) (8.33)	PW91P86-D3(0) (21.07)
	OPBE-D3(BJ) (8.25)	BP86-D3(BJ) (18.51)
	PBE-D3(BJ) (7.62)	PW91-D3(BJ) (18.44)
meta-GGA/NGA	PKZB-D3(0) (7.21)	PKZB-D3(0) (17.98)
	τHCTH-D3(BJ) (6.61)	TPSS-D3(BJ) (16.53)
	SCAN-D3(BJ) (6.29)	revTPSS-D3(BJ) (15.78)
hybrid	O3LYP-D3(BJ) (6.50)	O3LYP-D3(BJ) (14.87)
	MPW1KCIS-D3(BJ) (5.33)	TPSSh-D3(BJ) (12.85)
	TPSSh-D3(BJ) (4.93)	MPW1KCIS-D3(BJ) (12.62)
double hybrid	B2PLYP-D3(BJ) (2.02)	B2PLYP-D3(BJ) (4.90)
	DSD-PBEP86-D3(BJ) (1.80)	MPW2PLYP-D3(BJ) (4.22)
	MPW2PLYP-D3(BJ) (1.77)	DSD-PBEP86-D3(BJ) (3.52)

Table S16: The worst three DFAs for each of the four highest rungs on Jacob's Ladder for intermolecular noncovalent interactions according to WTMAD-1 and WTMAD-2 values (kcal/mol).

Rung	WTMAD-1	WTMAD-2
GGA/NGA	HCTH/407-D3(BJ) (9.22)	HCTH/407-D3(BJ) (22.29)
	PW91P86-D3(0) (8.50)	PW91P86-D3(0) (18.79)
	PBEhPBE-D3(BJ) (7.60)	PBEhPBE-D3(BJ) (17.52)
meta-GGA/NGA	τHCTH-D3(BJ) (9.34)	τHCTH-D3(BJ) (22.24)
	MN15L-D3(0) (8.95)	M11L-D3(0) (15.17)
	M11L-D3(0) (5.90)	MN15L-D3(0) (13.01)
hybrid	O3LYP-D3(BJ) (6.95)	O3LYP-D3(BJ) (16.32)
	TPSS1KCIS-D3(BJ) (6.49)	BMK-D3(BJ) (15.71)
	HSE03-D3(BJ) (6.36)	TPSS1KCIS-D3(BJ) (14.73)
double hybrid	MPW2PLYP-D3(BJ) (2.23)	MPW2PLYP-D3(BJ) (4.75)
	B2GPPLYP-D3(BJ) (2.16)	B2GPPLYP-D3(BJ) (4.28)
	DSD-PBEP86-D3(BJ) (2.12)	DSD-PBEP86-D3(BJ) (4.25)

Table S17: The worst three DFAs for each of the four highest rungs on Jacob's Ladder for intramolecular noncovalent interactions according to WTMAD-1 and WTMAD-2 values (kcal/mol).

Rung	WTMAD-1	WTMAD-2
GGA/NGA	HCTH/407-D3(BJ) (6.55)	PW91P86-D3(0) (12.34)
	PW91P86-D3(0) (6.43)	OPBE-D3(BJ) (12.02)
	N12-D3(0) (6.23)	N12-D3(0) (11.96)
meta-GGA/NGA	MN15L-D3(0) (13.65)	MN15L-D3(0) (27.15)
	MN12L-D3(BJ) (11.00)	MN12L-D3(BJ) (21.72)
	PKZB-D3(0) (7.62)	M11L-D3(0) (13.39)
hybrid	M11-D3(BJ) (7.17)	M11-D3(BJ) (12.93)
	BMK-D3(BJ) (6.59)	MN12SX-D3(BJ) (12.29)
	MN12SX-D3(BJ) (5.90)	BMK-D3(BJ) (12.08)
double hybrid	DSD-PBEB95-D3(BJ) (3.47)	DSD-PBEB95-D3(BJ) (6.70)
	PWPB95-D3(BJ) (2.95)	PWPB95-D3(BJ) (5.98)
	MPW2PLYP-D3(BJ) (2.23)	B2PLYP-D3(BJ) (3.78)

Table S18: The worst three DFAs for each of the four highest rungs on Jacob's Ladder for all noncovalent interactions test sets in GMTKN55 according to WTMAD-1 and WTMAD-2 values (kcal/mol).

Rung	WTMAD-1	WTMAD-2
GGA/NGA	HCTH/407-D3(BJ) (8.08)	HCTH/407-D3(BJ) (17.21)
	PW91P86-D3(0) (7.61)	PW91P86-D3(0) (15.64)
	PBEhPBE-D3(BJ) (6.55)	PBEhPBE-D3(BJ) (13.86)
meta-GGA/NGA	MN15L-D3(0) (10.96)	MN15L-D3(0) (19.92)
	MN12L-D3(BJ) (7.67)	MN12L-D3(BJ) (17.22)
	τHCTH-D3(BJ) (7.62)	τHCTH-D3(BJ) (16.25)
hybrid	O3LYP-D3(BJ) (5.72)	BMK-D3(BJ) (13.93)
	BMK-D3(BJ) (5.61)	O3LYP-D3(BJ) (12.44)
	TPSS1KCIS-D3(BJ) (5.18)	MN12SX-D3(BJ) (10.56)
double hybrid	DSD-PBEB95-D3(BJ) (2.67)	DSD-PBEB95-D3(BJ) (5.27)
	PWPB95-D3(BJ) (2.27)	PWPB95-D3(BJ) (4.98)
	MPW2PLYP-D3(BJ) (2.23)	MPW2PLYP-D3(BJ) (4.24)

Table S19: The worst three DFAs for each of the four highest rungs on Jacob's Ladder for GMTKN55 according to WTMAD-1 and WTMAD-2 values (kcal/mol)

Rung	WTMAD-1	WTMAD-2
GGA/NGA	HCTH/407-D3(BJ) (7.43)	PW91P86-D3(0) (13.29)
	PW91P86-D3(0) (6.79)	HCTH/407-D3(BJ) (13.09)
	OPBE-D3(BJ) (6.62)	PBEhPBE-D3(BJ) (11.91)
meta-GGA/NGA	τHCTH-D3(BJ) (7.05)	τHCTH-D3(BJ) (12.59)
	MN15L-D3(0) (6.76)	MN15L-D3(0) (11.55)
	PKZB-D3(0) (6.25)	PKZB-D3(0) (11.20)
hybrid	O3LYP-D3(BJ) (5.86)	O3LYP-D3(BJ) (10.72)
	MPW1KCIS-D3(BJ) (5.06)	TPSS1KCIS-D3(BJ) (8.70)
	TPSS1KCIS-D3(BJ) (5.04)	MPW1KCIS-D3(BJ) (8.67)
double hybrid	MPW2PLYP-D3(BJ) (2.36)	MPW2PLYP-D3(BJ) (4.08)
	B2PLYP-D3(BJ) (2.30)	PWPB95-D3(BJ) (3.98)
	PWPB95-D3(BJ) (2.15)	B2PLYP-D3(BJ) (3.93)

SI.6.4 WTMADs for dispersion-corrected density functional theory approximations

Table S20: WTMAD-1 values (kcal/mol) for dispersion-corrected DFAs for GMTKN55 and its categories (basic properties and reactions of small systems, isomerisations and reactions of large systems, barrier heights, intermolecular noncovalent interactions (NCIs), intramolecular NCIs, and all NCIs)

	basic + small	iso. + large	barriers	intermol. NCIs	intramol. NCIs	all NCIs	GMTKN55
PBE-D3(BJ)	5.29	5.93	7.62	5.40	5.04	5.25	5.67
PBEhPBE-D3(BJ)	5.95	6.00	7.45	7.60	5.15	6.55	6.38
revPBE-D3(BJ)	4.70	5.32	6.33	3.56	4.10	3.80	4.66
RPBE-D3(BJ)	6.38	5.17	7.21	6.41	4.48	5.58	5.98
PW91-D3(BJ)	5.25	6.28	7.56	5.79	5.79	5.79	5.92
BLYP-D3(BJ)	5.67	7.31	5.53	3.20	4.38	3.70	5.17
BP86-D3(BJ)	5.11	5.54	7.49	5.43	5.71	5.55	5.65
BPBE-D3(BJ)	5.03	5.39	7.22	5.05	5.46	5.23	5.44
OPBE-D3(BJ)	7.01	8.10	8.25	4.57	5.80	5.10	6.62
OLYP-D3(BJ)	5.16	4.81	6.56	3.33	4.35	3.77	4.75
XLYP-D3(BJ)	6.60	6.97	5.72	6.86	4.06	5.66	6.19
mPWLYP-D3(BJ)	6.04	8.17	5.61	3.89	5.32	4.50	5.75
PW91P86-D3(0)	5.57	6.10	8.33	8.50	6.43	7.61	6.79
mPWPW91-D3(BJ)	5.33	5.56	7.44	5.52	4.93	5.27	5.61
rPW86PBE-D3(BJ)	5.48	7.26	5.56	4.50	4.60	4.54	5.42
B97-D3(BJ)	5.26	6.76	5.15	3.42	4.20	3.75	4.92
HCTH/407-D3(BJ)	7.77	6.54	5.78	9.22	6.55	8.08	7.43
N12-D3(0)	5.43	5.10	6.74	5.19	6.23	5.64	5.62
VV10	5.18	6.17	6.17	5.09	4.88	5.00	5.40
PKZB-D3(0)	5.84	6.64	7.21	4.97	7.62	6.11	6.25
TPSS-D3(BJ)	4.76	6.15	6.28	4.15	4.74	4.40	5.04
revTPSS-D3(BJ)	4.79	5.52	5.65	3.58	4.43	3.94	4.69
SCAN-D3(BJ)	4.81	4.55	6.29	4.40	3.61	4.06	4.67
τHCTH-D3(BJ)	6.82	6.50	6.61	9.34	5.31	7.62	7.05
M06L-D3(0)	4.42	7.79	3.31	3.41	5.93	4.49	4.86
M11L-D3(0)	4.54	6.06	2.88	5.90	7.19	6.45	5.31
MN12L-D3(BJ)	4.82	6.07	3.69	5.17	11.00	7.67	5.97
MN15L-D3(0)	3.42	6.15	3.51	8.95	13.65	10.96	6.76
B3LYP-D3(BJ)	3.85	5.02	3.12	2.75	3.20	2.94	3.60
B3LYP-NL	3.82	4.00	3.67	2.94	3.21	3.06	3.54
B3PW91-D3(BJ)	3.53	3.81	4.39	3.77	3.83	3.80	3.79
B3P86-D3(BJ)	3.54	4.05	4.66	3.65	3.97	3.79	3.86
BHLYP-D3(BJ)	3.63	3.86	3.42	2.42	3.22	2.76	3.31
B1P86-D3(BJ)	3.38	3.73	4.21	3.59	3.77	3.67	3.65
B1LYP-D3(BJ)	3.71	4.65	2.39	3.90	3.04	3.53	3.63
B1B95-D3(BJ)	3.60	3.90	3.31	3.30	4.56	3.84	3.70
MPW1B95-D3(BJ)	3.27	3.80	2.83	2.17	3.57	2.77	3.11
PW6B95-D3(BJ)	3.00	3.99	2.47	2.01	3.29	2.56	2.93
MPWB1K-D3(BJ)	3.38	4.06	2.22	2.29	4.01	3.03	3.21
mPW1LYP-D3(0)	4.20	5.50	2.60	4.39	3.43	3.98	4.12
MPW1PW91-D3(BJ)	3.64	3.90	4.07	4.01	3.28	3.70	3.76
PW1PW-D3(0)	3.61	3.98	4.20	4.98	3.52	4.36	4.03
MPW1KCIS-D3(BJ)	5.44	4.58	5.33	6.00	3.31	4.84	5.06
MPWKCIS1K-D3(BJ)	4.29	4.26	2.68	4.65	3.21	4.03	3.98
PBE0-D3(BJ)	3.74	4.26	4.42	3.86	3.30	3.62	3.87
PBEh1PBE-D3(BJ)	4.34	4.14	4.17	6.20	3.40	5.00	4.54
PBE1KCIS-D3(BJ)	4.57	4.30	4.27	5.79	3.22	4.69	4.53
X3LYP-D3(BJ)	3.67	4.76	3.08	4.59	3.20	3.99	3.90
O3LYP-D3(BJ)	5.92	5.56	6.50	6.95	4.08	5.72	5.86
B97-1-D3(BJ)	3.88	3.81	3.40	5.56	2.77	4.37	3.99
B97-2-D3(BJ)	6.07	4.15	3.89	5.81	2.99	4.61	4.92
B98-D3(BJ)	4.03	3.73	3.46	5.44	2.77	4.30	4.01
HISS-D3(BJ)	4.54	5.00	3.18	6.04	3.53	4.96	4.60
HSE03-D3(BJ)	4.48	4.30	4.20	6.36	3.60	5.18	4.68
HSE06-D3(BJ)	3.56	4.21	4.14	4.26	3.73	4.03	3.92
TPSSh-D3(BJ)	4.14	5.15	4.93	3.63	3.86	3.73	4.25
revTPSSh-D3(BJ)	4.40	4.53	4.40	3.97	3.48	3.76	4.18
TPSS0-D3(BJ)	3.82	3.90	3.55	3.51	3.22	3.39	3.64
revTPSS0-D3(BJ)	3.99	3.92	2.95	3.77	2.69	3.31	3.59
TPSS1KCIS-D3(BJ)	5.21	4.75	4.51	6.49	3.43	5.18	5.04
BMK-D3(BJ)	3.50	2.74	2.00	4.87	6.59	5.61	3.99
τHCTHhyb-D3(BJ)	4.68	4.20	4.75	6.10	3.60	5.02	4.74
M05-D3(0)	4.29	5.66	2.84	3.10	5.57	4.15	4.28
M052X-D3(0)	2.82	2.62	2.97	2.46	2.85	2.63	2.73
M06-D3(0)	3.15	4.02	2.59	3.64	5.55	4.46	3.72
M062X-D3(0)	2.66	2.96	2.40	2.13	4.03	2.95	2.78
M08HX-D3(0)	2.48	2.82	1.99	2.84	4.99	3.76	2.96
M11-D3(BJ)	2.94	3.17	2.70	2.82	7.17	4.69	3.62
SOGGA11X-D3(BJ)	3.28	3.46	1.77	4.69	4.14	4.45	3.56
N12SX-D3(BJ)	4.61	4.89	4.45	4.37	4.01	4.22	4.49
MN12SX-D3(BJ)	3.30	4.60	2.24	3.50	5.90	4.53	3.85
MN15-D3(BJ)	3.00	3.31	2.21	3.27	5.50	4.23	3.42
LC-ωhPBE-D3(BJ)	3.89	4.65	3.01	2.50	3.61	2.98	3.56
ωB97X-D3(0)	2.96	3.07	2.08	2.17	3.06	2.56	2.71
ωB97X-V	2.63	3.20	1.91	1.45	2.29	1.81	2.32
APFD	3.57	3.95	4.12	4.41	5.47	4.87	4.20
B2PLYP-D3(BJ)	2.24	3.36	2.02	1.86	2.20	2.00	2.30
B2GPPLYP-D3(BJ)	1.72	2.44	1.60	2.16	1.90	2.05	1.95
MPW2PLYP-D3(BJ)	2.24	3.36	1.77	2.23	2.23	2.23	2.36
PWPB95-D3(BJ)	2.08	2.53	1.50	1.75	2.95	2.27	2.15
DSD-BLYP-D3(BJ)	1.63	2.22	1.45	1.94	1.87	1.91	1.81
DSD-PBEP86-D3(BJ)	1.46	1.80	1.80	2.12	2.08	2.10	1.80
DSD-PBEB95-D3(BJ)	1.70	1.78	1.02	2.08	3.47	2.67	2.00

Table S21: WTMAD-2 values (kcal/mol) for dispersion-corrected DFAs for GMTKN55 and its categories (basic properties and reactions of small systems, isomerisations and reactions of large systems, barrier heights, intermolecular noncovalent interactions (NCIs), intramolecular NCIs, and all NCIs)

	basic + small	iso. + large	barriers	intermol. NCIs	intramol. NCIs	all NCIs	GMTKN55
PBE-D3(BJ)	6.51	12.36	18.36	10.21	9.58	9.90	10.32
PBEhPBE-D3(BJ)	6.62	12.39	18.22	17.52	10.04	13.86	11.91
revPBE-D3(BJ)	5.54	10.50	15.79	6.19	7.99	7.07	8.27
RPBE-D3(BJ)	6.64	10.02	17.74	14.17	8.18	11.24	10.43
PW91-D3(BJ)	6.51	13.37	18.44	12.01	10.80	11.42	11.09
BLYP-D3(BJ)	6.88	14.56	15.55	7.10	8.04	7.56	9.51
BP86-D3(BJ)	6.30	10.70	18.51	12.78	11.06	11.94	10.81
BPBE-D3(BJ)	5.82	10.41	17.08	11.53	10.31	10.93	10.03
OPBE-D3(BJ)	8.23	14.52	17.60	8.28	12.02	10.11	11.19
OLYP-D3(BJ)	5.99	9.67	16.32	7.03	8.99	7.99	8.71
XLYP-D3(BJ)	7.28	13.58	16.30	16.80	7.42	12.21	11.41
mPWLYP-D3(BJ)	7.29	17.13	16.07	8.83	9.58	9.20	10.77
PW91P86-D3(0)	7.20	13.17	21.07	18.79	12.34	15.64	13.29
mPWPW91-D3(BJ)	6.20	11.04	17.99	11.04	9.35	10.21	10.09
rPW86PBE-D3(BJ)	6.71	14.95	15.17	8.33	8.21	8.27	9.75
B97-D3(BJ)	5.98	13.97	13.15	5.95	7.84	6.87	8.55
HCTH/407-D3(BJ)	7.52	13.34	13.76	22.29	11.90	17.21	13.09
N12-D3(0)	5.76	10.30	15.63	9.45	11.96	10.68	9.71
VV10	6.33	12.76	16.43	9.71	9.33	9.52	9.93
PKZB-D3(0)	6.71	15.18	17.98	9.05	12.89	10.93	11.20
TPSS-D3(BJ)	5.77	12.44	16.53	7.59	8.36	7.96	9.10
revTPSS-D3(BJ)	6.31	10.94	15.78	6.70	7.06	6.88	8.50
SCAN-D3(BJ)	5.31	7.86	14.94	8.50	6.61	7.58	7.86
τHCTH-D3(BJ)	6.37	13.57	15.28	22.24	9.99	16.25	12.59
M06L-D3(0)	5.09	15.81	7.56	7.37	10.31	8.81	8.61
M11L-D3(0)	4.89	10.46	5.47	15.17	13.39	14.30	9.58
MN12L-D3(BJ)	4.44	10.75	5.74	12.92	21.72	17.22	10.68
MN15L-D3(0)	4.01	10.58	5.49	13.01	27.15	19.92	11.55
B3LYP-D3(BJ)	4.36	10.28	9.04	5.56	5.68	5.62	6.42
B3LYP-NL	4.27	8.58	9.92	5.86	6.21	6.03	6.39
B3PW91-D3(BJ)	3.88	7.32	9.76	8.12	7.14	7.64	6.68
B3P86-D3(BJ)	4.27	8.17	10.98	8.04	7.66	7.86	7.18
BHLYP-D3(BJ)	5.32	7.76	7.73	4.46	4.86	4.66	5.76
B1P86-D3(BJ)	4.10	7.33	9.53	8.19	7.22	7.71	6.75
B1LYP-D3(BJ)	4.44	9.27	6.94	9.73	5.10	7.47	6.74
B1B95-D3(BJ)	3.71	8.35	7.43	8.03	8.72	8.37	6.78
MPW1B95-D3(BJ)	3.51	8.40	6.18	4.49	7.22	5.82	5.56
PW6B95-D3(BJ)	3.28	9.06	6.70	4.22	6.69	5.43	5.50
MPWB1K-D3(BJ)	4.15	7.95	3.99	4.69	8.23	6.42	5.64
mPW1LYP-D3(0)	4.66	11.69	7.76	10.65	5.26	8.01	7.52
MPW1PW91-D3(BJ)	4.16	7.50	8.68	7.40	6.16	6.79	6.32
PW1PW-D3(0)	4.32	8.49	9.27	10.27	6.12	8.24	7.18
MPW1KCIS-D3(BJ)	5.41	9.34	12.62	13.01	6.23	9.69	8.67
MPWKCIS1K-D3(BJ)	4.96	7.80	5.17	10.05	5.56	7.85	6.59
PBE0-D3(BJ)	4.45	8.39	9.88	6.65	6.40	6.53	6.61
PBEh1PBE-D3(BJ)	4.48	8.27	8.99	13.89	6.63	10.34	7.99
PBE1KCIS-D3(BJ)	4.83	9.25	10.02	13.20	5.86	9.61	8.10
X3LYP-D3(BJ)	4.13	9.98	8.68	10.60	5.75	8.23	7.28
O3LYP-D3(BJ)	6.72	10.98	14.87	16.32	8.39	12.44	10.72
B97-1-D3(BJ)	4.10	9.33	8.48	12.37	4.82	8.68	7.32
B97-2-D3(BJ)	5.29	8.81	8.36	12.24	5.61	9.00	7.72
B98-D3(BJ)	3.97	8.82	8.49	12.40	4.89	8.72	7.22
HISS-D3(BJ)	5.29	8.76	5.19	13.14	6.46	9.87	7.65
HSE03-D3(BJ)	4.69	8.72	9.15	13.87	7.02	10.52	8.22
HSE06-D3(BJ)	4.14	8.67	9.01	7.79	7.07	7.44	6.80
TPSSh-D3(BJ)	4.96	10.48	12.85	6.48	6.83	6.65	7.54
revTPSSh-D3(BJ)	5.69	8.96	12.27	8.04	5.63	6.86	7.53
TPSS0-D3(BJ)	4.89	7.92	8.66	5.93	5.71	5.82	6.23
revTPSS0-D3(BJ)	5.42	7.43	7.82	7.70	4.77	6.27	6.39
TPSS1KCIS-D3(BJ)	5.00	9.59	11.22	14.73	5.98	10.45	8.70
BMK-D3(BJ)	3.66	5.45	3.73	15.71	12.08	13.93	8.02
τHCTHhyb-D3(BJ)	4.54	9.60	11.05	13.15	6.92	10.11	8.40
M05-D3(0)	4.54	12.82	5.58	6.00	8.83	7.39	7.14
M052X-D3(0)	3.13	5.20	4.78	5.46	5.52	5.49	4.61
M06-D3(0)	3.52	7.89	5.60	6.63	10.16	8.36	6.40
M062X-D3(0)	2.73	5.84	4.99	5.20	7.48	6.31	4.94
M08HX-D3(0)	2.75	5.40	3.33	6.75	9.22	7.96	5.31
M11-D3(BJ)	3.11	6.69	4.36	6.28	12.93	9.53	6.39
SOGGA11X-D3(BJ)	3.88	7.04	3.84	12.30	7.72	10.06	6.83
N12SX-D3(BJ)	5.15	10.28	8.58	8.65	8.05	8.36	7.69
MN12SX-D3(BJ)	3.34	8.58	3.74	8.89	12.29	10.56	7.09
MN15-D3(BJ)	2.95	6.37	4.02	5.63	10.86	8.19	5.71
LC-ωhPBE-D3(BJ)	4.74	7.59	5.03	4.90	6.22	5.55	5.56
ωB97X-D3(0)	3.32	7.85	4.67	4.54	4.86	4.70	4.77
ωB97X-V	3.34	6.68	4.21	3.03	3.62	3.32	3.98
APFD	4.18	8.24	8.87	6.58	9.66	8.09	6.98
B2PLYP-D3(BJ)	2.51	6.28	4.90	3.78	3.78	3.78	3.93
B2GPPLYP-D3(BJ)	1.95	4.62	3.24	4.28	3.21	3.75	3.26
MPW2PLYP-D3(BJ)	2.46	6.76	4.22	4.75	3.70	4.24	4.08
PWPB95-D3(BJ)	2.23	5.41	3.39	4.02	5.98	4.98	3.98
DSD-BLYP-D3(BJ)	1.88	4.32	3.04	3.92	3.15	3.55	3.08
DSD-PBEP86-D3(BJ)	1.69	3.91	3.52	4.25	3.46	3.86	3.14
DSD-PBEB95-D3(BJ)	1.89	3.28	2.26	3.90	6.70	5.27	3.50

SI.6.5 WTMADs for dispersion-uncorrected density functional theory approximations

Table S22: WTMAD-1 values (kcal/mol) for dispersion-uncorrected DFAs for GMTKN55 and its categories (basic properties and reactions of small systems, isomerisations and reactions of large systems, barrier heights, intermolecular noncovalent interactions (NCIs), intramolecular NCIs, and all NCIs)

	basic + small	iso. + large	barriers	intermol. NCIs	intramol. NCIs	all NCIs	GMTKN55
PBE	5.44	7.32	6.98	10.17	11.68	10.82	8.00
PBEhPBE	5.48	7.41	6.85	10.02	11.62	10.71	7.97
revPBE	5.95	8.89	5.07	20.08	19.48	19.82	11.62
RPBE	6.02	9.04	4.81	17.72	19.51	18.49	11.12
PW91	5.46	7.27	7.23	9.58	11.41	10.36	7.85
BLYP	7.54	10.67	5.19	19.19	17.71	18.56	11.96
BP86	5.89	8.05	6.55	16.96	14.49	15.90	10.15
BPBE	5.68	8.38	6.04	22.00	17.67	20.14	11.69
OPBE	6.38	9.38	5.41	32.21	28.70	30.70	16.03
OLYP	7.05	10.34	4.63	30.03	28.48	29.37	15.80
XLYP	7.69	11.04	5.03	16.65	17.52	17.02	11.46
mPWLYP	7.02	10.06	5.56	12.24	14.83	13.35	9.75
PW91P86	5.71	6.91	8.10	8.55	9.79	9.08	7.50
mPWPW91	5.54	7.90	6.38	14.40	14.56	14.47	9.44
rPW86PBE	6.16	8.98	5.19	10.39	11.94	11.06	8.37
B97d	7.25	10.73	4.53	20.53	20.56	20.54	12.55
HCTH/407	6.54	10.07	4.34	14.39	21.97	17.64	11.07
N12	5.55	7.28	6.17	18.02	15.67	17.02	10.29
PKZB	5.55	7.33	3.78	19.68	13.83	17.17	10.05
TPSS	5.17	8.32	5.56	13.20	13.59	13.37	8.87
revTPSS	5.01	7.35	4.95	11.74	11.19	11.50	7.87
SCAN	4.74	4.89	6.12	6.21	4.94	5.66	5.29
τHCTH	6.11	9.87	5.27	14.51	19.02	16.44	10.56
M06L	4.46	7.92	3.31	3.45	5.22	4.21	4.78
M11L	5.01	7.00	2.99	7.85	5.28	6.75	5.74
MN12L	4.84	6.18	3.76	5.93	9.05	7.27	5.85
MN15L	3.42	6.15	3.51	8.95	13.67	10.97	6.76
B3LYP	5.32	7.84	3.23	15.55	15.27	15.43	9.33
B3PW91	4.16	6.26	3.76	17.77	15.15	16.64	9.22
B3P86	4.28	5.94	4.24	13.94	12.48	13.31	8.00
BHLYP	4.73	6.09	4.25	12.66	13.39	12.98	8.04
B1P86	4.02	5.34	3.82	13.93	12.00	13.11	7.68
B1LYP	5.36	7.76	2.78	16.05	15.50	15.81	9.42
B1B95	3.57	5.42	3.02	14.71	9.79	12.60	7.25
MPW1B95	3.27	4.57	2.74	8.65	7.21	8.03	5.23
PW6B95	3.22	4.92	2.53	7.28	6.85	7.09	4.89
MPWB1K	3.24	4.34	2.35	7.95	6.71	7.42	4.90
mPW1LYP	4.96	7.29	2.86	10.74	13.15	11.77	7.68
MPW1PW91	3.80	5.38	3.48	13.04	12.94	13.00	7.53
PW1PW	3.68	5.05	3.91	8.70	10.21	9.34	6.10
MPW1KCIS	4.61	6.83	4.34	14.12	15.25	14.61	8.76
MPWKCIS1K	3.80	5.12	2.66	12.74	14.02	13.29	7.49
PBE0	3.75	5.09	3.93	9.55	10.65	10.02	6.39
PBEh1PBE	3.69	5.05	3.73	9.39	10.39	9.82	6.26
PBE1KCIS	4.08	5.73	3.81	9.57	12.47	10.81	6.89
X3LYP	4.97	7.32	3.19	12.37	13.60	12.89	8.15
O3LYP	5.10	6.85	5.62	13.15	14.77	13.84	8.79
B97-1	3.75	5.63	3.02	8.26	11.05	9.45	6.14
B97-2	4.05	6.65	2.89	15.78	16.33	16.02	8.89
B98	3.94	5.95	3.07	10.12	12.43	11.11	6.89
HISS	3.84	5.18	3.08	8.62	9.97	9.20	6.01
HSE03	3.89	5.26	3.77	9.13	10.45	9.70	6.31
HSE06	3.71	5.21	3.82	9.25	10.43	9.75	6.28
TPSSh	4.50	7.17	4.33	12.79	12.91	12.84	8.10
revTPSSh	4.40	6.37	3.74	11.38	10.68	11.08	7.19
TPSS0	3.95	5.71	3.07	12.34	12.16	12.27	7.30
revTPSS0	3.87	5.21	2.52	11.00	10.09	10.61	6.49
TPSS1KCIS	4.40	7.18	3.78	12.38	13.59	12.90	8.02
BMK	3.30	3.18	2.23	13.65	6.59	10.63	5.94
τHCTHhyb	4.20	6.27	4.03	11.19	12.18	11.62	7.35
M05	4.45	6.44	3.04	7.00	11.09	8.75	6.24
M052X	2.84	2.78	2.96	3.63	3.21	3.45	3.08
M06	3.23	4.33	2.67	3.29	3.55	3.40	3.41
M062X	2.66	3.04	2.41	2.38	3.64	2.92	2.79
M08HX	2.48	2.90	1.99	3.22	4.76	3.88	3.02
M11	2.92	3.37	2.74	3.96	6.29	4.96	3.75
SOGGA11X	3.06	4.76	2.03	12.33	9.09	10.94	6.22
N12SX	4.27	5.49	4.15	10.63	10.39	10.53	6.84
MN12SX	3.59	5.10	2.37	6.31	4.79	5.66	4.47
MN15	3.00	3.31	2.21	3.21	5.50	4.19	3.41
LC-ωhPBE	3.48	4.82	3.22	11.86	10.35	11.21	6.62
B2PLYP	3.04	4.75	1.85	8.44	7.65	8.10	5.10
B2GPPLYP	2.23	3.47	1.38	6.20	5.48	5.89	3.72
MPW2PLYP	2.68	4.23	1.72	5.71	6.49	6.05	4.10
PWPB95	2.17	3.28	1.52	6.50	4.73	5.74	3.63
DSD-BLYP	2.12	3.29	1.16	5.97	4.98	5.55	3.50
DSD-PBEP86	1.60	2.36	1.40	3.74	3.33	3.57	2.45
DSD-PBEB95	1.66	2.41	1.00	4.76	3.54	4.24	2.68

Table S23: WTMAD-2 values (kcal/mol) for dispersion-uncorrected DFAs for GMTKN55 and its categories (basic properties and reactions of small systems, isomerisations and reactions of large systems, barrier heights, intermolecular noncovalent interactions (NCIs), intramolecular NCIs, and all NCIs)

	basic + small	iso. + large	barriers	intermol. NCIs	intramol. NCIs	all NCIs	GMTKN55
PBE	6.59	16.23	16.72	15.68	19.70	17.65	13.83
PBEhPBE	6.55	16.33	16.73	15.48	19.59	17.49	13.77
revPBE	6.81	19.57	12.77	35.30	33.36	34.35	20.53
RPBE	6.95	19.91	12.56	29.77	33.49	31.59	19.50
PW91	6.65	16.11	17.51	15.09	19.36	17.18	13.74
BLYP	8.52	23.22	14.56	34.90	29.47	32.25	21.05
BP86	6.93	17.37	16.06	32.71	24.14	28.52	18.33
BPBE	6.49	18.19	14.05	42.02	29.90	36.10	21.06
OPBE	7.15	20.76	11.26	59.02	50.65	54.92	28.76
OLYP	7.60	23.21	11.99	53.23	49.30	51.31	27.97
XLYP	8.77	23.92	14.65	28.50	29.01	28.75	19.87
mPWLYP	8.12	22.13	15.79	20.26	24.57	22.37	17.00
PW91P86	7.29	15.21	20.31	15.04	17.52	16.26	13.79
mPWPW91	6.51	17.36	15.34	24.55	24.43	24.49	16.51
rPW86PBE	7.36	19.50	14.15	17.19	19.60	18.37	14.55
B97d	7.91	23.77	11.65	36.06	34.97	35.53	21.87
HCTH/407	7.14	22.57	10.93	25.21	37.69	31.31	19.68
N12	5.80	16.21	13.68	33.18	26.60	29.96	18.05
PKZB	6.71	14.16	10.08	36.12	26.76	31.54	18.17
TPSS	6.30	18.07	14.60	22.11	22.66	22.38	15.63
revTPSS	6.64	15.85	13.95	20.01	18.54	19.29	14.07
SCAN	5.23	8.95	14.50	10.67	8.29	9.50	8.72
τHCTH	6.54	22.60	12.32	22.63	32.41	27.41	18.13
M06L	5.11	16.20	7.57	8.29	9.27	8.77	8.67
M11L	5.24	12.92	5.66	21.01	10.56	15.90	10.75
MN12L	4.48	10.80	5.89	16.00	18.43	17.19	10.71
MN15L	4.01	10.57	5.49	13.01	27.18	19.94	11.56
B3LYP	5.72	17.53	9.19	28.23	25.14	26.72	16.38
B3PW91	4.37	14.14	8.20	33.82	25.52	29.76	16.48
B3P86	4.73	13.35	9.83	26.80	20.81	23.87	14.35
BHLYP	6.14	13.35	9.39	22.76	21.59	22.19	14.07
B1P86	4.41	12.10	8.50	27.21	19.98	23.68	13.80
B1LYP	6.02	17.33	7.63	29.18	25.45	27.36	16.49
B1B95	3.92	12.51	6.72	29.30	17.33	23.44	13.39
MPW1B95	3.59	10.78	5.93	16.35	12.99	14.71	9.45
PW6B95	3.55	11.54	6.78	13.07	12.19	12.64	8.85
MPWB1K	4.09	9.68	4.24	15.40	12.28	13.87	8.88
mPW1LYP	5.44	16.48	8.13	18.05	21.39	19.68	13.20
MPW1PW91	4.23	12.36	7.23	22.94	21.79	22.38	13.11
PW1PW	4.24	11.61	8.32	13.52	17.15	15.30	10.33
MPW1KCIS	5.12	15.66	10.43	24.15	25.64	24.88	15.32
MPWKCIS1K	4.60	11.84	5.43	22.49	23.37	22.92	13.12
PBE0	4.34	11.57	8.63	15.42	17.94	16.65	10.93
PBEh1PBE	4.21	11.49	7.93	14.96	17.47	16.19	10.60
PBE1KCIS	4.58	13.49	9.00	15.13	20.75	17.87	11.84
X3LYP	5.29	16.60	8.84	21.19	22.28	21.72	14.07
O3LYP	6.04	15.69	12.79	21.97	25.18	23.54	15.39
B97-1	4.23	14.14	7.55	12.78	18.26	15.46	10.70
B97-2	4.38	16.23	6.50	28.06	27.62	27.85	15.84
B98	4.23	14.65	7.56	16.43	20.65	18.49	11.98
HISS	4.91	10.67	5.02	13.68	16.50	15.06	9.87
HSE03	4.44	11.97	8.07	14.09	17.56	15.79	10.61
HSE06	4.22	11.75	8.15	14.49	17.52	15.97	10.59
TPSSh	5.45	15.83	11.24	21.72	21.80	21.76	14.32
revTPSSh	5.90	13.97	10.56	19.62	18.10	18.87	12.93
TPSS0	5.11	13.07	7.46	21.46	20.67	21.08	13.01
revTPSS0	5.48	11.67	6.75	19.31	17.45	18.40	11.75
TPSS1KCIS	5.06	16.21	9.53	20.39	22.97	21.65	14.00
BMK	3.42	8.18	4.26	31.61	10.15	21.11	11.29
τHCTHhyb	4.56	15.18	9.35	18.75	20.35	19.53	12.81
M05	4.71	15.04	5.93	11.35	17.95	14.58	10.44
M052X	3.12	5.80	4.72	6.80	5.79	6.31	5.02
M06	3.56	8.83	5.70	7.76	6.53	7.16	6.11
M062X	2.73	6.14	4.98	5.51	6.64	6.06	4.89
M08HX	2.75	5.67	3.32	7.11	8.55	7.82	5.30
M11	3.15	7.27	4.44	10.08	11.12	10.59	6.92
SOGGA11X	3.73	11.77	4.28	25.40	14.19	19.92	11.50
N12SX	4.80	13.05	7.76	19.83	17.27	18.58	11.96
MN12SX	3.54	9.96	4.01	14.30	10.16	12.27	8.09
MN15	2.95	6.37	4.02	5.55	10.84	8.14	5.69
LC-ωhPBE	4.32	10.01	5.83	22.02	17.55	19.83	11.57
B2PLYP	3.23	9.87	4.42	15.29	12.59	13.97	8.70
B2GPPLYP	2.44	7.26	2.73	11.11	8.91	10.03	6.26
MPW2PLYP	2.86	9.04	4.09	9.56	10.50	10.02	6.85
PWPB95	2.43	7.38	3.43	12.28	8.69	10.52	6.56
DSD-BLYP	2.39	7.02	2.41	10.79	8.21	9.53	5.96
DSD-PBEP86	1.78	5.62	2.77	6.45	5.59	6.03	4.21
DSD-PBEB95	2.00	5.26	2.31	9.05	6.69	7.90	4.90

SI.7 Statistical results for all test sets and DFAs

SI.7.1 Results for dispersion-corrected GGA/NGA functionals

Table S24: Statistical analysis for the PBE-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	14.31	15.68	19.26	0.05	72.12	54.18	−17.94
G21EA	2.96	3.43	4.11	0.10	10.49	7.72	−2.77
G21IP	−0.12	3.85	4.84	0.01	19.31	10.17	−9.14
DIPCS10	−2.54	4.50	5.99	0.01	19.94	7.11	−12.82
PA26	1.83	2.19	2.91	0.01	9.15	7.34	−1.82
SIE4x4	23.72	23.72	26.41	0.70	42.21	46.59	4.38
ALKBDE10	6.03	6.30	10.42	0.06	28.68	27.70	−0.99
YBDE18	0.00	4.93	5.77	0.10	20.78	11.05	−9.73
AL2X6	−0.72	1.63	2.50	0.05	7.27	1.51	−5.76
HEAVYSB11	0.85	3.55	3.97	0.06	12.54	6.59	−5.95
NBPRC	−0.80	2.41	3.00	0.09	10.35	3.37	−6.97
ALK8	3.66	4.14	5.70	0.07	13.46	12.21	−1.26
RC21	5.92	6.85	7.81	0.19	18.10	14.16	−3.94
G2RC	0.69	6.92	8.39	0.13	35.48	19.64	−15.84
BH76RC	0.82	4.18	6.12	0.20	30.51	22.80	−7.71
FH51	0.97	3.17	4.49	0.10	24.22	12.78	−11.44
TAUT15	0.22	1.84	2.32	0.60	7.68	5.26	−2.42
DC13	0.44	8.63	12.22	0.16	50.68	17.53	−33.15
MB16-43	8.05	24.26	30.59	0.06	141.32	72.41	−68.91
DARC	2.13	3.31	3.65	0.10	9.20	5.22	−3.98
RSE43	−2.94	2.94	3.25	0.39	6.52	−0.79	−7.31
BSR36	−3.17	3.17	3.79	0.20	7.97	−1.12	−9.09
CDIE20	1.65	1.65	1.78	0.41	2.66	2.86	0.19
ISO34	−0.74	1.49	2.08	0.10	10.91	4.65	−6.26
ISOL24	−1.92	4.39	6.37	0.20	30.34	16.18	−14.16
C60ISO	−10.72	10.72	12.80	0.11	20.57	−1.67	−22.23
PArel	0.27	1.81	2.53	0.39	12.52	6.68	−5.84
BH76	−9.59	9.62	10.83	0.52	32.19	1.44	−30.75
BHPERI	−6.69	6.69	6.91	0.32	6.52	−3.37	−9.88
BHDIV10	−8.43	8.87	9.87	0.20	18.01	2.20	−15.81
INV24	−1.72	2.07	2.66	0.06	9.35	2.33	−7.01
BHROT27	0.37	0.47	0.65	0.07	2.05	1.65	−0.40
PX13	−12.02	12.02	12.24	0.36	8.55	−9.15	−17.70
WCPT18	−9.34	9.34	9.85	0.27	12.17	−4.98	−17.14
RG18	0.26	0.26	0.32	0.45	0.77	0.81	0.04
ADIM6	0.21	0.21	0.22	0.06	0.16	0.29	0.13
S22	0.17	0.48	0.63	0.07	2.83	1.25	−1.57
S66	0.27	0.40	0.52	0.07	2.33	1.47	−0.86
HEAVY28	0.42	0.42	0.52	0.34	0.97	1.04	0.08
WATER27	8.10	8.92	11.86	0.11	41.22	30.19	−11.03
CARBHB12	1.91	1.91	2.30	0.32	3.89	4.51	0.62
PNICO23	1.32	1.32	1.94	0.31	6.63	6.75	0.12
HAL59	1.11	1.18	1.86	0.26	7.36	6.70	−0.66
AHB21	−0.98	1.15	1.37	0.05	4.56	1.76	−2.80
CHB6	−0.45	0.93	1.01	0.03	2.80	1.42	−1.39
IL16	−0.58	0.59	0.67	0.01	1.32	0.09	−1.23
IDISP	2.70	2.76	4.15	0.19	9.23	9.08	−0.15
ICONF	0.13	0.32	0.45	0.10	1.71	1.28	−0.43
ACONF	−0.01	0.07	0.09	0.04	0.38	0.21	−0.17
AMINO20x4	0.03	0.34	0.42	0.14	1.96	1.00	−0.96
PCONF21	−0.59	1.25	1.50	0.77	4.13	1.48	−2.65
MCONF	−0.10	0.49	0.54	0.10	1.80	0.88	−0.92
SCONF	0.30	0.80	1.00	0.17	3.90	1.15	−2.75
UPU23	0.29	0.53	0.66	0.09	2.40	1.61	−0.78
BUT14DIOL	0.45	0.46	0.52	0.16	1.45	1.25	−0.21

Table S25: Statistical analysis for the PBEhPBE-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	13.26	14.41	17.97	0.05	63.50	51.94	−11.56
G21EA	2.75	3.22	3.93	0.10	10.09	7.40	−2.69
G21IP	−0.01	3.89	4.93	0.02	20.13	11.05	−9.08
DIPCS10	−2.35	4.38	5.83	0.01	19.72	7.38	−12.34
PA26	1.54	2.04	2.74	0.01	9.00	7.07	−1.93
SIE4x4	23.56	23.56	26.28	0.70	42.31	46.46	4.15
ALKBDE10	6.50	6.83	10.62	0.07	29.17	28.19	−0.97
YBDE18	−0.13	4.65	5.44	0.09	20.08	10.89	−9.18
AL2X6	2.87	3.69	3.75	0.10	7.07	4.59	−2.49
HEAVYSB11	6.01	6.17	7.03	0.11	13.27	12.43	−0.84
NBPRC	−0.71	2.44	2.96	0.09	9.90	3.10	−6.80
ALK8	10.62	11.44	16.13	0.18	37.32	34.02	−3.30
RC21	5.25	6.22	7.12	0.17	17.17	13.17	−4.01
G2RC	1.24	6.72	8.15	0.13	33.63	19.63	−14.01
BH76RC	0.92	4.02	5.98	0.19	29.65	22.35	−7.30
FH51	1.27	3.18	4.54	0.10	23.79	12.72	−11.06
TAUT15	0.16	1.89	2.34	0.62	7.77	5.23	−2.54
DC13	0.46	9.75	13.01	0.18	51.27	16.29	−34.98
MB16-43	24.96	31.49	39.81	0.08	151.80	101.02	−50.78
DARC	3.52	4.03	4.56	0.12	9.31	6.55	−2.75
RSE43	−2.95	2.95	3.26	0.39	6.46	−0.84	−7.30
BSR36	−2.55	2.55	2.97	0.16	6.07	−0.96	−7.03
CDIE20	1.67	1.67	1.80	0.41	2.64	2.82	0.18
ISO34	−0.72	1.58	2.21	0.11	12.60	6.01	−6.59
ISOL24	−2.24	4.92	7.01	0.22	33.49	17.33	−16.16
C60ISO	−10.07	10.07	12.24	0.10	20.50	−1.06	−21.55
PArel	0.22	1.71	2.48	0.37	12.62	6.72	−5.90
BH76	−9.66	9.69	10.86	0.52	31.41	1.35	−30.06
BHPERI	−6.30	6.30	6.52	0.30	5.78	−3.64	−9.42
BHDIV10	−8.19	8.75	9.69	0.19	18.56	2.78	−15.78
INV24	−1.98	2.38	3.17	0.07	10.91	2.29	−8.62
BHROT27	0.39	0.49	0.68	0.08	2.14	1.71	−0.43
PX13	−11.24	11.24	11.41	0.34	7.50	−8.65	−16.15
WCPT18	−8.88	8.88	9.38	0.25	11.69	−4.55	−16.24
RG18	0.35	0.35	0.40	0.60	0.65	0.75	0.09
ADIM6	−0.09	0.10	0.14	0.03	0.34	0.02	−0.32
S22	0.28	0.47	0.61	0.06	2.46	1.42	−1.04
S66	0.28	0.39	0.54	0.07	2.27	1.68	−0.59
HEAVY28	1.40	1.40	1.55	1.13	3.19	3.39	0.20
WATER27	8.08	8.88	11.94	0.11	42.12	31.27	−10.85
CARBHB12	2.01	2.01	2.40	0.33	3.93	4.66	0.74
PNICO23	1.96	1.96	2.59	0.46	7.71	7.97	0.26
HAL59	1.99	1.99	2.59	0.43	7.14	7.00	−0.13
AHB21	−1.16	1.32	1.54	0.06	4.86	1.72	−3.13
CHB6	−2.24	2.24	2.43	0.08	2.40	−1.23	−3.62
IL16	−0.79	0.81	0.92	0.01	1.70	0.10	−1.59
IDISP	2.77	2.96	4.21	0.21	9.79	9.21	−0.58
ICONF	0.04	0.29	0.34	0.09	1.20	0.66	−0.54
ACONF	−0.02	0.08	0.10	0.04	0.43	0.22	−0.20
AMINO20x4	0.05	0.36	0.44	0.15	2.01	1.09	−0.92
PCONF21	−0.52	1.16	1.43	0.72	3.85	1.30	−2.55
MCONF	−0.01	0.48	0.54	0.10	1.89	0.90	−1.00
SCONF	0.33	0.91	1.12	0.20	4.31	1.20	−3.11
UPU23	0.30	0.49	0.64	0.09	2.39	1.67	−0.72
BUT14DIOL	0.56	0.57	0.61	0.20	1.44	1.31	−0.13

Table S26: Statistical analysis for the revPBE-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	3.27	7.57	10.09	0.02	61.64	34.25	−27.38
G21EA	1.66	2.75	3.28	0.08	10.49	6.14	−4.35
G21IP	−1.24	4.20	5.09	0.02	18.79	9.09	−9.70
DIPCS10	−3.88	4.81	6.36	0.01	16.65	4.14	−12.51
PA26	4.73	4.73	5.40	0.03	9.77	10.97	1.20
SIE4x4	23.43	23.43	26.21	0.69	42.68	48.14	5.46
ALKBDE10	1.33	5.16	8.03	0.05	28.83	22.88	−5.94
YBDE18	−2.85	4.41	5.31	0.09	16.55	5.60	−10.95
AL2X6	−1.95	2.07	3.73	0.06	9.33	0.36	−8.97
HEAVYSB11	−1.73	2.72	3.71	0.05	10.52	2.15	−8.37
NBPRC	0.28	1.98	2.43	0.07	9.08	4.53	−4.55
ALK8	3.25	3.61	5.09	0.06	11.64	10.91	−0.73
RC21	3.86	4.85	5.60	0.14	13.37	9.53	−3.84
G2RC	2.89	6.16	7.77	0.12	30.30	19.42	−10.88
BH76RC	0.89	2.76	4.71	0.13	25.03	18.30	−6.74
FH51	2.04	3.34	4.56	0.11	20.62	12.78	−7.83
TAUT15	−0.29	1.55	1.78	0.51	5.81	3.14	−2.68
DC13	2.48	8.44	10.95	0.15	40.32	15.43	−24.89
MB16-43	−5.43	27.11	35.27	0.07	171.13	78.22	−92.91
DARC	3.54	3.71	4.18	0.11	6.98	6.10	−0.88
RSE43	−2.31	2.31	2.58	0.30	5.74	−0.57	−6.31
BSR36	−1.80	1.80	2.01	0.11	3.95	−0.33	−4.29
CDIE20	1.50	1.50	1.60	0.37	2.35	2.72	0.37
ISO34	−0.77	1.50	2.13	0.10	11.67	4.88	−6.79
ISOL24	−2.04	4.56	6.34	0.21	29.30	15.44	−13.86
C60ISO	−9.82	9.82	12.15	0.10	20.78	−0.67	−21.45
PArel	0.08	1.53	2.35	0.33	12.70	5.68	−7.02
BH76	−8.30	8.32	9.21	0.45	26.19	0.88	−25.31
BHPERI	−6.29	6.29	6.56	0.30	6.62	−3.13	−9.76
BHDIV10	−7.48	7.83	8.73	0.17	15.55	1.73	−13.82
INV24	−1.25	2.18	2.88	0.07	11.22	3.87	−7.35
BHROT27	0.22	0.37	0.51	0.06	1.59	1.19	−0.41
PX13	−8.75	8.75	8.93	0.26	5.97	−6.59	−12.56
WCPT18	−7.22	7.22	7.72	0.21	10.65	−3.57	−14.22
RG18	0.09	0.09	0.11	0.16	0.25	0.23	−0.02
ADIM6	0.25	0.25	0.27	0.07	0.34	0.43	0.10
S22	−0.05	0.43	0.56	0.06	2.14	0.80	−1.34
S66	−0.01	0.28	0.37	0.05	1.53	0.60	−0.93
HEAVY28	0.27	0.29	0.37	0.23	0.92	0.81	−0.11
WATER27	−3.26	3.51	5.03	0.04	14.86	1.80	−13.06
CARBHB12	1.10	1.10	1.55	0.18	3.36	3.52	0.16
PNICO23	0.82	0.88	1.45	0.21	5.72	5.37	−0.36
HAL59	0.50	0.72	1.19	0.16	5.91	4.94	−0.96
AHB21	0.71	1.04	1.45	0.05	6.01	4.76	−1.26
CHB6	0.70	0.90	1.51	0.03	3.98	3.58	−0.39
IL16	0.70	0.77	0.88	0.01	2.48	1.92	−0.56
IDISP	3.14	3.14	4.02	0.22	6.30	6.66	0.36
ICONF	0.04	0.32	0.39	0.10	1.40	0.77	−0.62
ACONF	−0.06	0.09	0.12	0.05	0.36	0.09	−0.28
AMINO20x4	−0.11	0.37	0.46	0.15	2.34	1.22	−1.12
PCONF21	−0.62	0.87	1.09	0.54	2.97	0.76	−2.20
MCONF	−0.03	0.44	0.54	0.09	2.23	1.00	−1.23
SCONF	−0.02	0.51	0.76	0.11	3.22	0.94	−2.28
UPU23	0.26	0.47	0.62	0.08	2.32	1.57	−0.75
BUT14DIOL	−0.06	0.31	0.37	0.11	1.79	0.97	−0.82

Table S27: Statistical analysis for the RPBE-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	5.45	8.29	11.54	0.03	77.00	52.65	−24.34
G21EA	2.00	2.87	3.41	0.09	10.39	6.37	−4.01
G21IP	−0.97	4.19	5.09	0.02	18.92	9.28	−9.64
DIPCS10	−2.85	5.13	6.24	0.01	18.34	6.73	−11.61
PA26	5.20	5.20	5.89	0.03	11.44	11.56	0.12
SIE4x4	23.63	23.63	26.38	0.70	42.75	48.42	5.67
ALKBDE10	3.45	5.80	9.29	0.06	31.62	26.26	−5.37
YBDE18	1.36	3.22	3.93	0.07	13.06	7.53	−5.53
AL2X6	7.09	7.57	8.26	0.21	13.08	11.64	−1.44
HEAVYSB11	6.18	6.18	7.38	0.11	13.26	13.90	0.64
NBPRC	−1.89	3.91	4.54	0.14	14.34	5.68	−8.67
ALK8	16.47	17.02	22.46	0.27	46.22	44.04	−2.18
RC21	5.42	6.15	7.01	0.17	13.56	10.90	−2.66
G2RC	2.93	7.58	9.48	0.15	39.20	19.81	−19.39
BH76RC	1.13	3.08	4.87	0.14	25.50	18.25	−7.25
FH51	1.60	3.83	5.06	0.12	22.33	13.21	−9.13
TAUT15	0.03	1.58	1.86	0.52	6.07	3.70	−2.37
DC13	−0.98	11.16	15.43	0.20	56.45	16.31	−40.14
MB16-43	45.18	50.76	63.76	0.12	236.63	175.25	−61.38
DARC	0.10	2.19	2.72	0.07	7.99	2.82	−5.17
RSE43	−2.31	2.31	2.55	0.30	5.20	−0.54	−5.74
BSR36	−0.61	0.61	0.68	0.04	1.20	−0.02	−1.22
CDIE20	1.30	1.30	1.39	0.32	1.77	2.28	0.51
ISO34	−0.50	1.29	1.96	0.09	9.74	3.69	−6.06
ISOL24	−0.55	4.37	6.06	0.20	28.49	18.60	−9.88
C60ISO	−7.75	7.82	10.17	0.08	19.33	0.32	−19.01
PArel	0.10	1.69	2.38	0.37	10.98	5.29	−5.69
BH76	−8.97	8.98	9.84	0.48	26.40	0.48	−25.92
BHPERI	−8.42	8.42	8.83	0.40	10.76	−3.72	−14.48
BHDIV10	−9.12	9.40	10.38	0.21	18.92	1.43	−17.49
INV24	−0.53	2.47	3.24	0.08	14.21	7.82	−6.39
BHROT27	0.31	0.47	0.63	0.07	1.85	1.31	−0.54
PX13	−8.72	8.72	8.94	0.26	6.18	−6.22	−12.40
WCPT18	−7.81	7.81	8.39	0.22	11.81	−3.79	−15.61
RG18	0.45	0.45	0.57	0.78	1.56	1.62	0.06
ADIM6	0.24	0.24	0.26	0.07	0.24	0.29	0.05
S22	−0.12	0.47	0.57	0.06	2.22	0.66	−1.56
S66	0.03	0.28	0.34	0.05	1.44	0.67	−0.77
HEAVY28	0.95	0.95	1.06	0.77	2.20	2.26	0.06
WATER27	−0.22	1.28	2.04	0.02	11.30	3.30	−8.01
CARBHB12	1.48	1.48	1.88	0.25	3.55	4.01	0.46
PNICO23	1.86	1.86	2.96	0.44	10.79	10.78	−0.01
HAL59	1.51	1.56	2.27	0.34	7.05	6.30	−0.75
AHB21	0.17	1.11	1.51	0.05	7.01	4.77	−2.24
CHB6	−2.31	2.69	2.91	0.10	5.40	1.13	−4.27
IL16	−0.02	0.46	0.66	0.00	3.18	1.35	−1.82
IDISP	2.55	2.62	4.09	0.18	7.68	7.46	−0.23
ICONF	0.13	0.53	0.74	0.16	3.37	1.85	−1.52
ACONF	0.01	0.06	0.07	0.03	0.22	0.13	−0.09
AMINO20x4	−0.02	0.31	0.39	0.13	1.77	0.88	−0.89
PCONF21	−0.79	1.07	1.34	0.66	3.65	1.15	−2.50
MCONF	−0.24	0.47	0.59	0.09	1.93	0.80	−1.13
SCONF	0.16	0.47	0.62	0.10	2.42	0.90	−1.52
UPU23	0.34	0.57	0.71	0.10	2.53	1.68	−0.85
BUT14DIOL	−0.11	0.29	0.35	0.10	1.61	0.83	−0.78

Table S28: Statistical analysis for the PW91-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	14.76	15.59	19.07	0.05	64.55	54.09	−10.46
G21EA	3.64	3.84	4.56	0.11	9.56	8.22	−1.33
G21IP	1.17	3.90	4.97	0.02	19.55	11.96	−7.59
DIPCS10	0.21	4.19	5.06	0.01	18.24	8.86	−9.38
PA26	1.71	2.05	2.81	0.01	9.14	7.36	−1.78
SIE4x4	23.76	23.76	26.49	0.70	42.50	46.68	4.17
ALKBDE10	7.20	7.20	11.28	0.07	29.18	29.37	0.19
YBDE18	−0.88	5.24	6.09	0.11	21.90	11.06	−10.83
AL2X6	−1.55	1.93	2.70	0.05	6.90	1.15	−5.75
HEAVYSB11	0.27	3.57	3.98	0.06	12.53	6.32	−6.21
NBPRC	−0.33	2.40	2.91	0.09	10.54	4.35	−6.19
ALK8	2.31	2.74	4.03	0.04	10.38	9.22	−1.16
RC21	5.52	6.35	7.35	0.18	17.95	13.99	−3.96
G2RC	0.56	6.50	7.88	0.13	32.64	18.84	−13.80
BH76RC	0.69	4.13	5.99	0.19	29.91	21.91	−8.00
FH51	1.17	3.20	4.52	0.10	23.97	12.73	−11.24
TAUT15	0.25	1.87	2.39	0.61	7.88	5.36	−2.52
DC13	0.62	8.85	12.24	0.16	46.70	14.97	−31.73
MB16-43	1.56	20.30	26.02	0.05	125.19	58.62	−66.57
DARC	4.03	4.47	5.12	0.14	9.71	7.12	−2.59
RSE43	−2.97	2.97	3.29	0.39	6.50	−0.87	−7.37
BSR36	−4.52	4.52	5.34	0.28	11.49	−1.49	−12.99
CDIE20	1.66	1.66	1.79	0.41	2.63	2.84	0.21
ISO34	−0.72	1.53	2.19	0.11	12.28	5.73	−6.55
ISOL24	−2.46	5.23	7.65	0.24	38.57	19.18	−19.39
C60ISO	−10.11	10.11	12.23	0.10	20.35	−1.13	−21.48
PArel	0.23	1.82	2.55	0.39	12.73	6.84	−5.90
BH76	−9.83	9.87	11.04	0.53	31.74	1.67	−30.07
BHPERI	−5.92	5.92	6.12	0.28	5.37	−3.37	−8.74
BHDIV10	−7.98	8.51	9.48	0.19	17.66	2.64	−15.02
INV24	−2.27	2.46	3.28	0.08	11.30	2.22	−9.08
BHROT27	0.36	0.48	0.67	0.08	2.13	1.72	−0.41
PX13	−12.18	12.18	12.41	0.37	9.12	−8.96	−18.08
WCPT18	−9.15	9.15	9.67	0.26	12.01	−4.70	−16.71
RG18	0.57	0.57	0.77	0.98	2.28	2.42	0.14
ADIM6	0.06	0.14	0.16	0.04	0.44	0.21	−0.23
S22	0.07	0.67	0.91	0.09	4.10	1.46	−2.63
S66	0.24	0.50	0.66	0.09	3.28	1.72	−1.56
HEAVY28	0.31	0.35	0.46	0.28	1.23	0.97	−0.25
WATER27	9.33	10.22	13.68	0.13	47.90	35.90	−12.00
CARBHB12	2.00	2.00	2.37	0.33	3.81	4.50	0.68
PNICO23	1.21	1.21	1.77	0.28	6.11	6.16	0.05
HAL59	1.02	1.15	1.83	0.25	7.81	6.86	−0.95
AHB21	−1.34	1.41	1.61	0.06	3.82	0.79	−3.03
CHB6	−0.66	1.13	1.22	0.04	3.10	1.42	−1.68
IL16	−0.54	0.56	0.66	0.01	1.49	0.10	−1.39
IDISP	3.01	4.28	5.82	0.30	13.99	12.08	−1.92
ICONF	0.15	0.36	0.56	0.11	2.31	1.83	−0.48
ACONF	0.15	0.15	0.20	0.08	0.49	0.55	0.05
AMINO20x4	0.04	0.34	0.44	0.14	2.08	1.03	−1.05
PCONF21	−0.70	1.66	1.87	1.02	5.34	2.08	−3.25
MCONF	−0.28	0.49	0.58	0.10	1.71	0.57	−1.14
SCONF	0.26	0.71	0.91	0.15	3.68	1.09	−2.59
UPU23	0.32	0.60	0.74	0.10	2.54	1.70	−0.84
BUT14DIOL	0.46	0.47	0.53	0.17	1.43	1.31	−0.12

Table S29: Statistical analysis for the BLYP-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	6.23	8.10	11.14	0.03	61.50	39.09	−22.41
G21EA	1.75	3.27	3.93	0.10	11.90	8.53	−3.37
G21IP	−1.86	4.68	5.57	0.02	23.02	12.28	−10.74
DIPCS10	−5.88	7.87	9.04	0.01	23.45	9.92	−13.53
PA26	2.48	2.79	3.83	0.01	10.64	9.16	−1.47
SIE4x4	25.25	25.25	28.39	0.75	47.78	52.25	4.47
ALKBDE10	5.04	6.01	8.91	0.06	26.22	22.61	−3.62
YBDE18	−5.29	7.20	9.15	0.15	28.53	10.21	−18.32
AL2X6	−4.48	4.48	4.71	0.12	4.14	−3.29	−7.43
HEAVYSB11	−2.60	3.18	4.12	0.05	10.98	1.89	−9.08
NBPRC	2.02	3.31	4.78	0.12	16.09	12.70	−3.39
ALK8	−0.82	2.05	2.61	0.03	8.40	2.25	−6.15
RC21	1.64	4.39	5.15	0.12	19.42	9.00	−10.42
G2RC	4.47	5.42	6.74	0.11	23.84	15.54	−8.29
BH76RC	0.55	3.06	4.28	0.14	19.93	12.61	−7.32
FH51	3.77	4.72	6.25	0.15	30.57	19.16	−11.41
TAUT15	−0.38	1.66	1.94	0.54	6.44	3.58	−2.86
DC13	4.92	16.12	18.75	0.29	67.15	34.25	−32.90
MB16-43	−26.49	30.18	35.81	0.07	108.97	33.04	−75.93
DARC	13.82	13.82	13.97	0.43	6.64	15.54	8.91
RSE43	−2.82	2.82	3.13	0.37	6.06	−0.83	−6.89
BSR36	−2.78	2.78	3.22	0.17	6.29	−1.13	−7.41
CDIE20	1.28	1.28	1.36	0.32	1.89	1.98	0.09
ISO34	−0.51	2.68	3.83	0.18	20.79	11.72	−9.07
ISOL24	−4.18	9.02	12.40	0.41	60.10	29.19	−30.91
C60ISO	−9.49	9.49	11.48	0.10	18.95	−1.16	−20.11
PArel	−0.46	1.79	2.70	0.39	14.25	6.15	−8.09
BH76	−9.29	9.29	10.28	0.50	24.00	−0.01	−24.02
BHPERI	−3.62	3.62	4.32	0.17	11.08	−0.06	−11.14
BHDIV10	−5.20	6.16	7.11	0.14	16.32	4.79	−11.53
INV24	−1.21	2.01	2.51	0.06	10.39	3.50	−6.89
BHROT27	0.14	0.42	0.55	0.07	1.76	1.30	−0.46
PX13	−7.91	7.91	8.03	0.24	5.12	−6.11	−11.24
WCPT18	−5.53	5.53	6.03	0.16	9.45	−1.67	−11.12
RG18	−0.17	0.24	0.35	0.41	1.42	0.29	−1.12
ADIM6	0.01	0.09	0.11	0.03	0.35	0.19	−0.16
S22	0.11	0.25	0.32	0.03	1.15	0.80	−0.34
S66	0.09	0.17	0.24	0.03	1.09	0.72	−0.37
HEAVY28	0.38	0.39	0.44	0.31	0.98	0.81	−0.18
WATER27	2.35	2.94	4.15	0.04	18.18	10.89	−7.29
CARBHB12	0.97	0.97	1.28	0.16	2.61	2.84	0.23
PNICO23	0.58	0.62	0.87	0.15	2.86	2.56	−0.30
HAL59	0.84	0.89	1.37	0.19	5.78	5.43	−0.35
AHB21	0.58	0.77	1.25	0.03	5.38	4.67	−0.71
CHB6	−0.12	0.99	1.29	0.04	3.93	2.35	−1.58
IL16	0.85	0.88	1.04	0.01	2.08	1.93	−0.16
IDISP	4.90	4.90	7.82	0.34	17.81	18.20	0.38
ICONF	−0.14	0.33	0.43	0.10	1.51	0.45	−1.06
ACONF	−0.10	0.13	0.17	0.07	0.53	0.11	−0.42
AMINO20x4	−0.09	0.31	0.41	0.13	2.30	1.44	−0.86
PCONF21	−0.32	0.76	0.87	0.47	2.54	0.81	−1.72
MCONF	−0.05	0.36	0.45	0.07	2.01	0.84	−1.17
SCONF	0.02	0.58	0.93	0.13	3.84	0.84	−3.00
UPU23	0.34	0.56	0.68	0.10	2.59	1.58	−1.01
BUT14DIOL	0.41	0.42	0.48	0.15	1.47	1.16	−0.31

Table S30: Statistical analysis for the BP86-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	13.62	14.42	17.02	0.05	68.00	46.40	−21.60
G21EA	5.04	5.08	5.78	0.15	9.99	9.57	−0.42
G21IP	1.68	4.10	5.05	0.02	19.13	12.00	−7.13
DIPCS10	0.77	4.02	4.59	0.01	14.59	6.95	−7.65
PA26	2.66	2.74	3.53	0.01	9.26	8.38	−0.89
SIE4x4	24.61	24.61	27.79	0.73	47.75	52.17	4.42
ALKBDE10	5.56	5.97	9.81	0.06	27.89	26.95	−0.94
YBDE18	−1.60	4.47	5.27	0.09	19.28	8.61	−10.67
AL2X6	−0.14	1.73	2.45	0.05	6.80	1.20	−5.60
HEAVYSB11	0.65	2.90	3.14	0.05	8.61	4.37	−4.23
NBPRC	−0.46	1.79	2.18	0.06	7.66	2.64	−5.02
ALK8	2.67	3.24	4.50	0.05	9.29	8.34	−0.94
RC21	4.94	5.61	6.44	0.16	16.30	12.32	−3.98
G2RC	1.71	5.97	7.36	0.12	31.09	18.57	−12.52
BH76RC	−0.04	3.48	5.08	0.16	27.37	16.72	−10.65
FH51	1.60	3.17	4.49	0.10	22.68	12.83	−9.85
TAUT15	0.24	1.83	2.33	0.60	7.76	5.39	−2.37
DC13	1.52	8.51	10.47	0.15	39.33	14.05	−25.28
MB16-43	8.08	23.62	30.00	0.06	140.20	76.91	−63.29
DARC	3.47	3.81	4.24	0.12	8.08	6.18	−1.89
RSE43	−2.72	2.72	3.01	0.36	6.09	−0.77	−6.86
BSR36	−0.81	0.88	1.00	0.05	3.46	1.17	−2.29
CDIE20	1.55	1.55	1.66	0.38	2.26	2.51	0.25
ISO34	−0.62	1.40	2.09	0.10	12.87	6.08	−6.79
ISOL24	−1.69	4.38	6.16	0.20	26.96	16.27	−10.70
C60ISO	−10.20	10.20	12.32	0.10	20.27	−1.35	−21.62
PArel	0.15	1.78	2.53	0.38	12.55	6.59	−5.97
BH76	−9.81	9.86	10.82	0.53	29.28	1.65	−27.63
BHPERI	−6.80	6.80	7.04	0.33	6.11	−3.89	−10.01
BHDIV10	−8.14	8.68	9.62	0.19	18.94	2.70	−16.23
INV24	−1.42	1.98	2.51	0.06	8.52	2.63	−5.89
BHROT27	0.30	0.41	0.59	0.07	1.85	1.48	−0.37
PX13	−12.28	12.28	12.51	0.37	9.17	−8.95	−18.12
WCPT18	−8.73	8.73	9.22	0.25	11.59	−4.51	−16.10
RG18	−0.64	0.64	1.03	1.10	3.49	−0.02	−3.52
ADIM6	−0.21	0.21	0.27	0.06	0.49	0.02	−0.46
S22	0.39	0.51	0.70	0.07	2.09	1.73	−0.37
S66	0.15	0.31	0.42	0.06	1.76	1.33	−0.44
HEAVY28	0.59	0.61	0.71	0.49	1.66	1.41	−0.25
WATER27	3.54	4.43	5.76	0.05	26.23	14.40	−11.83
CARBHB12	1.46	1.46	1.99	0.24	4.07	4.31	0.24
PNICO23	1.25	1.30	1.88	0.30	6.52	6.14	−0.37
HAL59	1.20	1.31	1.90	0.29	7.00	6.23	−0.77
AHB21	−0.32	0.69	1.01	0.03	4.70	2.49	−2.21
CHB6	0.53	0.53	0.67	0.02	1.14	1.34	0.20
IL16	−0.46	0.52	0.60	0.00	1.58	0.43	−1.15
IDISP	2.77	2.77	3.51	0.19	5.70	6.39	0.70
ICONF	0.03	0.27	0.32	0.08	1.25	0.66	−0.59
ACONF	−0.23	0.23	0.27	0.13	0.51	−0.06	−0.58
AMINO20x4	0.02	0.44	0.54	0.18	2.61	1.40	−1.21
PCONF21	−0.39	1.02	1.22	0.63	3.64	1.38	−2.26
MCONF	0.37	0.61	0.76	0.12	2.62	1.52	−1.09
SCONF	0.41	1.19	1.46	0.26	5.33	1.41	−3.92
UPU23	0.19	0.50	0.65	0.09	3.09	1.54	−1.55
BUT14DIOL	0.59	0.60	0.65	0.21	1.52	1.33	−0.19

Table S31: Statistical analysis for the BPBE-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	8.26	10.24	13.28	0.03	56.72	42.61	−14.12
G21EA	1.72	2.71	3.27	0.08	10.50	6.72	−3.78
G21IP	−0.72	4.05	4.96	0.02	19.03	9.65	−9.38
DIPCS10	−3.68	4.30	5.68	0.01	13.85	1.69	−12.15
PA26	4.09	4.09	4.74	0.02	9.37	9.94	0.56
SIE4x4	23.23	23.23	25.90	0.69	41.72	46.95	5.23
ALKBDE10	4.15	5.77	9.92	0.06	32.02	28.25	−3.77
YBDE18	−1.35	3.95	4.65	0.08	16.90	7.58	−9.33
AL2X6	0.40	2.69	3.34	0.07	9.84	2.96	−6.88
HEAVYSB11	1.31	3.09	3.30	0.05	8.44	4.58	−3.86
NBPRC	−0.61	2.08	2.69	0.08	10.16	4.41	−5.74
ALK8	4.56	4.85	7.04	0.08	14.00	13.40	−0.60
RC21	4.80	5.79	6.53	0.16	15.51	11.69	−3.81
G2RC	1.87	6.35	7.81	0.12	33.43	19.36	−14.06
BH76RC	0.79	3.32	5.27	0.16	27.36	20.36	−7.00
FH51	1.48	3.11	4.41	0.10	22.73	12.78	−9.95
TAUT15	0.07	1.81	2.17	0.59	7.29	4.75	−2.54
DC13	1.14	8.35	10.97	0.15	43.84	15.92	−27.92
MB16-43	13.41	28.41	36.30	0.07	159.05	89.30	−69.75
DARC	1.50	2.51	2.74	0.08	7.68	4.39	−3.28
RSE43	−2.62	2.62	2.91	0.34	6.12	−0.64	−6.76
BSR36	0.08	1.03	1.28	0.06	6.04	3.97	−2.07
CDIE20	1.61	1.61	1.74	0.40	2.58	2.76	0.17
ISO34	−0.65	1.34	1.93	0.09	10.82	4.64	−6.18
ISOL24	−1.14	3.46	4.87	0.16	22.26	12.27	−9.99
C60ISO	−9.48	9.48	11.84	0.10	20.64	−0.49	−21.12
PArel	0.22	1.77	2.48	0.38	12.35	6.34	−6.00
BH76	−8.62	8.65	9.64	0.46	28.60	1.21	−27.39
BHPERI	−7.13	7.13	7.45	0.34	7.45	−3.77	−11.22
BHDIV10	−8.30	8.69	9.67	0.19	17.91	1.95	−15.96
INV24	−1.46	2.22	2.97	0.07	11.75	3.62	−8.13
BHROT27	0.32	0.41	0.58	0.07	1.79	1.50	−0.29
PX13	−11.43	11.43	11.67	0.34	8.54	−8.34	−16.88
WCPT18	−8.32	8.32	8.78	0.24	11.26	−4.44	−15.70
RG18	−0.63	0.63	0.98	1.09	3.12	−0.17	−3.29
ADIM6	−0.30	0.30	0.33	0.09	0.43	−0.09	−0.52
S22	0.26	0.59	0.80	0.08	2.82	2.21	−0.61
S66	−0.03	0.38	0.48	0.07	2.12	1.26	−0.86
HEAVY28	0.39	0.45	0.54	0.36	1.60	1.24	−0.36
WATER27	−2.24	2.88	4.26	0.04	14.27	2.59	−11.69
CARBHB12	1.21	1.22	1.84	0.20	4.22	4.19	−0.03
PNICO23	1.07	1.21	1.85	0.28	7.16	6.39	−0.77
HAL59	0.84	1.10	1.62	0.24	6.36	5.51	−0.85
AHB21	0.21	0.86	1.13	0.04	5.20	3.18	−2.02
CHB6	0.61	0.61	0.93	0.02	1.97	2.12	0.15
IL16	−0.06	0.39	0.49	0.00	2.10	1.13	−0.97
IDISP	2.45	2.45	3.96	0.17	8.89	9.22	0.33
ICONF	0.05	0.29	0.35	0.09	1.28	0.82	−0.46
ACONF	−0.21	0.21	0.26	0.11	0.52	−0.02	−0.54
AMINO20x4	−0.02	0.47	0.59	0.19	2.98	1.60	−1.38
PCONF21	−0.43	1.04	1.23	0.64	3.95	1.56	−2.39
MCONF	0.43	0.74	0.88	0.15	3.01	1.74	−1.28
SCONF	0.29	1.03	1.34	0.22	5.00	1.29	−3.71
UPU23	0.21	0.54	0.69	0.09	3.15	1.61	−1.53
BUT14DIOL	0.31	0.35	0.45	0.12	1.61	1.20	−0.41

Table S32: Statistical analysis for the OPBE-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	10.48	12.09	14.96	0.04	56.89	38.35	−18.54
G21EA	−0.79	3.11	3.81	0.09	15.81	6.49	−9.33
G21IP	−1.63	4.52	5.34	0.02	17.74	6.80	−10.93
DIPCS10	−3.39	4.91	6.07	0.01	17.74	4.40	−13.35
PA26	8.35	8.35	8.77	0.04	13.06	14.11	1.06
SIE4x4	23.48	23.48	26.07	0.70	41.15	48.72	7.57
ALKBDE10	0.91	6.05	10.30	0.06	37.95	29.55	−8.41
YBDE18	4.20	4.25	4.84	0.09	9.48	9.00	−0.48
AL2X6	2.18	5.46	6.20	0.15	18.61	8.77	−9.84
HEAVYSB11	1.29	4.80	5.42	0.08	15.55	8.53	−7.02
NBPRC	−3.11	6.82	7.69	0.25	22.35	8.11	−14.25
ALK8	8.58	8.83	11.94	0.14	22.54	21.54	−1.00
RC21	9.34	10.63	11.82	0.30	26.51	19.37	−7.14
G2RC	−0.56	10.17	13.20	0.20	59.88	24.28	−35.60
BH76RC	0.25	3.70	6.15	0.17	35.24	25.70	−9.54
FH51	−1.36	4.18	5.70	0.13	29.21	15.24	−13.98
TAUT15	0.05	1.75	2.05	0.57	6.70	4.11	−2.59
DC13	−0.64	19.74	25.06	0.36	85.40	51.36	−34.04
MB16-43	43.19	53.44	69.05	0.13	243.00	163.82	−79.18
DARC	−13.35	13.35	13.60	0.41	8.87	−9.53	−18.40
RSE43	−2.36	2.36	2.67	0.31	6.09	−0.24	−6.33
BSR36	2.84	2.84	4.31	0.18	13.78	13.85	0.07
CDIE20	1.71	1.71	1.92	0.42	3.42	3.58	0.16
ISO34	−0.69	2.61	3.68	0.18	17.71	7.82	−9.88
ISOL24	2.54	5.32	6.96	0.24	27.93	19.07	−8.86
C60ISO	−8.46	8.55	11.21	0.09	21.39	0.42	−20.96
PArel	0.96	2.31	2.71	0.50	9.34	5.49	−3.85
BH76	−7.46	7.59	8.76	0.41	34.58	2.78	−31.80
BHPERI	−10.23	10.34	11.42	0.50	20.27	1.26	−19.00
BHDIV10	−10.41	10.41	11.78	0.23	17.69	−1.35	−19.05
INV24	0.03	2.77	3.85	0.09	18.27	10.88	−7.40
BHROT27	0.55	0.60	0.77	0.10	1.93	1.70	−0.23
PX13	−11.21	11.21	11.61	0.34	9.05	−7.89	−16.94
WCPT18	−9.45	9.45	10.02	0.27	13.39	−5.16	−18.55
RG18	−0.05	0.10	0.19	0.17	0.87	0.22	−0.66
ADIM6	−0.11	0.11	0.11	0.03	0.05	−0.08	−0.14
S22	−0.07	0.71	0.87	0.10	3.08	1.16	−1.91
S66	−0.28	0.52	0.68	0.10	2.42	0.80	−1.62
HEAVY28	0.10	0.29	0.38	0.23	1.46	0.92	−0.54
WATER27	−11.68	11.83	17.59	0.15	46.48	1.87	−44.61
CARBHB12	1.03	1.24	2.00	0.21	5.28	4.76	−0.52
PNICO23	0.90	1.23	2.27	0.29	10.33	9.24	−1.09
HAL59	0.04	0.87	1.26	0.19	6.17	4.09	−2.08
AHB21	0.78	1.48	1.85	0.07	7.47	3.17	−4.30
CHB6	0.96	1.45	2.31	0.05	6.44	5.41	−1.04
IL16	0.03	0.65	0.88	0.01	3.83	1.48	−2.35
IDISP	0.02	5.24	8.43	0.37	29.14	14.40	−14.74
ICONF	0.35	0.55	0.75	0.17	2.48	1.60	−0.88
ACONF	−0.06	0.07	0.09	0.04	0.26	0.07	−0.19
AMINO20x4	−0.04	0.56	0.71	0.23	3.42	1.71	−1.71
PCONF21	−0.92	1.15	1.59	0.71	4.90	1.20	−3.70
MCONF	0.15	0.66	0.81	0.13	3.36	1.79	−1.56
SCONF	0.17	0.62	0.76	0.13	2.91	1.38	−1.54
UPU23	0.01	0.49	0.58	0.09	2.22	1.23	−0.99
BUT14DIOL	−0.46	0.60	0.70	0.21	2.11	0.88	−1.23

Table S33: Statistical analysis for the OLYP-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	8.87	9.88	11.92	0.03	51.67	34.29	−17.38
G21EA	−0.97	2.41	2.99	0.07	10.03	3.80	−6.24
G21IP	−3.04	4.33	5.33	0.02	17.09	5.50	−11.59
DIPCS10	−5.96	6.87	8.44	0.01	18.29	3.26	−15.03
PA26	6.95	6.95	7.44	0.04	10.79	13.49	2.70
SIE4x4	25.55	25.55	28.58	0.76	47.09	54.03	6.94
ALKBDE10	2.30	4.50	8.30	0.04	28.72	24.93	−3.80
YBDE18	0.74	3.66	4.37	0.07	14.10	7.56	−6.54
AL2X6	−2.25	2.69	4.20	0.07	11.10	1.33	−9.77
HEAVYSB11	−2.26	3.59	5.22	0.06	15.07	3.78	−11.29
NBPRC	−0.75	2.43	2.90	0.09	10.21	5.08	−5.13
ALK8	3.68	4.34	6.40	0.07	16.49	13.90	−2.59
RC21	6.26	6.96	7.75	0.19	15.35	11.97	−3.38
G2RC	1.93	6.80	8.60	0.13	39.74	20.44	−19.30
BH76RC	0.03	2.89	4.69	0.14	27.90	17.94	−9.96
FH51	0.85	3.19	4.23	0.10	21.97	13.02	−8.96
TAUT15	−0.33	1.69	1.92	0.55	6.12	3.31	−2.81
DC13	2.97	8.21	10.63	0.15	41.40	21.02	−20.38
MB16-43	5.59	29.04	37.15	0.07	168.69	89.86	−78.83
DARC	−1.16	1.82	2.52	0.06	7.06	1.55	−5.51
RSE43	−2.57	2.57	2.87	0.34	5.88	−0.53	−6.41
BSR36	0.35	0.74	1.03	0.05	5.05	3.73	−1.31
CDIE20	1.35	1.35	1.47	0.33	2.15	2.69	0.54
ISO34	−0.49	1.39	1.92	0.10	8.98	3.86	−5.12
ISOL24	−0.21	3.45	4.84	0.16	23.39	13.97	−9.41
C60ISO	−7.41	7.55	9.94	0.08	19.41	0.62	−18.79
PArel	0.31	1.62	2.22	0.35	10.95	5.23	−5.73
BH76	−8.41	8.44	9.29	0.45	28.35	1.40	−26.95
BHPERI	−6.98	6.98	7.48	0.33	9.45	−2.98	−12.43
BHDIV10	−7.49	7.85	8.77	0.17	15.98	1.83	−14.15
INV24	−0.02	2.56	3.57	0.08	18.00	10.53	−7.47
BHROT27	0.41	0.52	0.70	0.08	1.92	1.55	−0.37
PX13	−7.99	7.99	8.27	0.24	6.37	−5.32	−11.68
WCPT18	−6.87	6.87	7.46	0.20	11.21	−3.16	−14.37
RG18	0.31	0.32	0.41	0.55	1.26	1.19	−0.06
ADIM6	0.04	0.06	0.07	0.02	0.17	0.11	−0.06
S22	−0.17	0.44	0.58	0.06	1.93	0.62	−1.31
S66	−0.16	0.30	0.39	0.05	1.62	0.55	−1.07
HEAVY28	0.14	0.23	0.30	0.19	1.08	0.69	−0.38
WATER27	−6.63	6.79	9.75	0.08	26.25	1.70	−24.54
CARBHB12	0.85	0.93	1.46	0.15	3.77	3.53	−0.24
PNICO23	0.52	0.74	1.37	0.17	6.19	5.61	−0.58
HAL59	0.16	0.59	0.97	0.13	5.64	4.24	−1.40
AHB21	1.02	1.30	1.67	0.06	6.18	4.57	−1.61
CHB6	0.23	1.84	2.70	0.07	8.25	5.88	−2.37
IL16	0.71	0.94	1.14	0.01	3.82	2.02	−1.80
IDISP	2.45	2.45	3.99	0.17	9.14	9.31	0.17
ICONF	0.17	0.38	0.51	0.12	2.15	1.18	−0.97
ACONF	0.02	0.04	0.05	0.02	0.17	0.12	−0.05
AMINO20x4	−0.06	0.39	0.49	0.16	2.21	0.98	−1.23
PCONF21	−0.77	1.04	1.33	0.64	4.08	1.44	−2.63
MCONF	−0.22	0.49	0.61	0.10	2.25	0.92	−1.34
SCONF	0.05	0.44	0.55	0.10	2.12	0.95	−1.17
UPU23	0.22	0.46	0.58	0.08	2.01	1.23	−0.78
BUT14DIOL	−0.27	0.43	0.51	0.15	1.92	0.89	−1.03

Table S34: Statistical analysis for the XLYP-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	6.70	7.98	11.02	0.03	50.36	36.78	−13.58
G21EA	2.59	3.58	4.45	0.11	12.48	9.68	−2.81
G21IP	−1.06	4.53	5.55	0.02	24.03	14.09	−9.94
DIPCS10	−3.70	7.12	8.21	0.01	24.72	13.24	−11.48
PA26	2.53	2.86	3.92	0.02	11.01	9.45	−1.56
SIE4x4	25.29	25.29	28.45	0.75	47.93	52.33	4.40
ALKBDE10	6.89	7.27	10.07	0.07	27.51	25.60	−1.90
YBDE18	−3.29	5.93	7.29	0.12	24.73	10.50	−14.23
AL2X6	4.52	4.52	5.22	0.13	8.86	8.96	0.10
HEAVYSB11	7.23	7.30	9.55	0.13	18.89	18.50	−0.39
NBPRC	1.06	3.53	4.42	0.13	14.25	10.67	−3.58
ALK8	13.12	14.31	18.33	0.23	38.72	33.97	−4.76
RC21	1.61	4.29	4.93	0.12	17.53	6.89	−10.64
G2RC	5.12	6.21	7.33	0.12	23.36	15.22	−8.14
BH76RC	0.67	3.10	4.24	0.14	18.88	11.61	−7.27
FH51	3.84	4.85	6.54	0.16	31.86	21.11	−10.75
TAUT15	−0.36	1.62	1.89	0.53	6.28	3.46	−2.82
DC13	2.92	16.65	19.41	0.30	68.90	35.74	−33.16
MB16-43	20.28	28.77	35.86	0.07	129.93	92.09	−37.83
DARC	12.96	12.96	13.12	0.40	6.38	14.60	8.21
RSE43	−2.79	2.79	3.10	0.37	5.79	−0.81	−6.60
BSR36	−1.27	1.27	1.49	0.08	3.13	−0.15	−3.28
CDIE20	1.20	1.20	1.27	0.30	1.84	1.85	0.01
ISO34	−0.37	2.77	3.99	0.19	21.14	12.00	−9.14
ISOL24	−3.65	9.03	12.50	0.41	60.09	30.83	−29.27
C60ISO	−8.22	8.22	10.36	0.08	18.50	−0.18	−18.68
PArel	−0.48	1.82	2.65	0.39	13.22	5.97	−7.25
BH76	−9.62	9.62	10.58	0.52	23.73	−0.16	−23.90
BHPERI	−4.64	4.64	5.20	0.22	10.22	−1.05	−11.27
BHDIV10	−5.76	6.76	7.50	0.15	17.91	5.00	−12.91
INV24	−1.17	2.26	2.96	0.07	11.60	4.43	−7.18
BHROT27	0.18	0.45	0.60	0.07	1.74	1.24	−0.50
PX13	−7.02	7.02	7.12	0.21	4.22	−5.62	−9.84
WCPT18	−5.22	5.22	5.78	0.15	9.57	−1.21	−10.79
RG18	0.28	0.28	0.33	0.48	0.64	0.71	0.07
ADIM6	0.10	0.12	0.13	0.04	0.27	0.22	−0.05
S22	0.22	0.26	0.33	0.04	0.88	0.62	−0.26
S66	0.25	0.26	0.33	0.05	1.10	0.95	−0.15
HEAVY28	1.50	1.50	1.70	1.21	4.06	4.08	0.01
WATER27	3.29	3.83	5.58	0.05	21.40	15.03	−6.37
CARBHB12	1.28	1.28	1.55	0.21	2.72	3.19	0.47
PNICO23	1.83	1.83	2.43	0.43	6.77	6.96	0.19
HAL59	2.16	2.16	2.70	0.47	6.42	6.49	0.07
AHB21	0.25	0.78	1.27	0.03	5.96	4.71	−1.25
CHB6	−4.14	4.14	4.38	0.15	4.35	−2.63	−6.98
IL16	0.39	0.59	0.75	0.01	2.58	1.76	−0.82
IDISP	4.58	4.58	7.82	0.32	18.18	18.30	0.12
ICONF	−0.20	0.38	0.53	0.12	1.76	0.38	−1.38
ACONF	−0.11	0.13	0.17	0.07	0.46	0.06	−0.39
AMINO20x4	−0.08	0.30	0.40	0.12	2.18	1.31	−0.88
PCONF21	−0.38	0.66	0.76	0.41	2.25	0.64	−1.61
MCONF	−0.12	0.33	0.42	0.07	1.82	0.68	−1.13
SCONF	−0.02	0.48	0.82	0.10	3.37	0.70	−2.67
UPU23	0.44	0.55	0.68	0.10	2.07	1.65	−0.42
BUT14DIOL	0.35	0.37	0.42	0.13	1.35	1.02	−0.33

Table S35: Statistical analysis for the mPWLYP-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	9.02	10.01	13.16	0.03	60.30	44.33	−15.97
G21EA	2.72	3.60	4.51	0.11	12.47	9.80	−2.68
G21IP	−1.17	4.53	5.49	0.02	23.47	13.40	−10.08
DIPCS10	−4.20	7.40	8.58	0.01	25.91	13.44	−12.47
PA26	1.25	2.34	3.08	0.01	10.34	7.82	−2.51
SIE4x4	25.42	25.42	28.58	0.75	47.99	51.95	3.95
ALKBDE10	6.42	7.23	9.88	0.07	27.40	23.74	−3.66
YBDE18	−5.66	7.95	10.09	0.16	31.07	11.38	−19.69
AL2X6	−6.05	6.05	6.24	0.17	4.29	−3.61	−7.90
HEAVYSB11	−3.47	3.58	4.88	0.06	10.70	0.43	−10.26
NBPRC	2.55	3.92	5.60	0.14	17.09	14.41	−2.68
ALK8	−3.00	3.42	4.99	0.05	13.39	1.34	−12.05
RC21	1.61	4.42	5.20	0.12	19.41	8.25	−11.16
G2RC	3.95	5.07	6.44	0.10	23.46	15.34	−8.12
BH76RC	0.51	3.11	4.49	0.15	21.16	13.45	−7.71
FH51	3.79	4.85	6.30	0.16	30.58	17.57	−13.02
TAUT15	−0.30	1.66	1.96	0.54	6.52	3.75	−2.78
DC13	4.95	17.62	20.59	0.32	72.62	35.85	−36.77
MB16-43	−36.28	37.52	43.24	0.09	103.11	14.12	−88.99
DARC	15.78	15.78	15.98	0.49	8.05	17.84	9.79
RSE43	−3.01	3.01	3.33	0.40	6.31	−0.95	−7.26
BSR36	−5.65	5.65	6.75	0.35	14.68	−1.71	−16.38
CDIE20	1.37	1.37	1.45	0.34	1.95	2.20	0.25
ISO34	−0.62	2.84	4.05	0.19	21.79	12.32	−9.47
ISOL24	−5.16	10.11	14.36	0.46	72.90	32.44	−40.47
C60ISO	−9.47	9.47	11.53	0.10	19.21	−0.84	−20.05
PArel	−0.44	1.77	2.73	0.38	14.54	6.42	−8.12
BH76	−9.86	9.86	10.92	0.53	25.78	0.23	−25.54
BHPERI	−2.50	2.72	3.76	0.13	13.09	1.63	−11.45
BHDIV10	−4.87	5.98	6.94	0.13	15.89	5.04	−10.85
INV24	−2.14	2.50	3.26	0.08	12.29	3.40	−8.89
BHROT27	0.14	0.42	0.56	0.07	1.83	1.37	−0.45
PX13	−8.20	8.20	8.32	0.25	5.58	−6.24	−11.82
WCPT18	−5.80	5.80	6.29	0.17	9.49	−1.84	−11.32
RG18	0.49	0.49	0.66	0.84	1.92	2.01	0.09
ADIM6	0.12	0.19	0.19	0.06	0.42	0.21	−0.21
S22	−0.11	0.43	0.61	0.06	2.93	0.90	−2.03
S66	0.14	0.36	0.47	0.07	2.07	1.12	−0.95
HEAVY28	0.23	0.29	0.35	0.23	0.94	0.64	−0.30
WATER27	6.39	6.97	9.95	0.09	34.15	26.41	−7.74
CARBHB12	1.27	1.27	1.49	0.21	2.43	2.93	0.50
PNICO23	0.47	0.50	0.68	0.12	2.26	2.00	−0.26
HAL59	0.75	0.85	1.35	0.19	6.45	5.81	−0.63
AHB21	−0.01	0.65	0.98	0.03	4.98	3.62	−1.36
CHB6	−0.62	1.38	1.61	0.05	4.56	2.26	−2.31
IL16	0.95	0.95	1.08	0.01	1.54	1.70	0.16
IDISP	5.41	7.17	10.79	0.50	27.10	24.30	−2.80
ICONF	−0.09	0.44	0.63	0.13	2.91	1.38	−1.53
ACONF	0.19	0.19	0.26	0.10	0.64	0.67	0.03
AMINO20x4	−0.08	0.32	0.42	0.13	2.54	1.54	−0.99
PCONF21	−0.44	1.18	1.32	0.73	4.36	1.82	−2.54
MCONF	−0.47	0.48	0.57	0.10	1.38	0.19	−1.19
SCONF	−0.10	0.36	0.61	0.08	2.74	0.57	−2.17
UPU23	0.49	0.68	0.83	0.12	2.54	1.90	−0.64
BUT14DIOL	0.41	0.42	0.48	0.15	1.43	1.19	−0.23

Table S36: Statistical analysis for the PW91P86-D3(0) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	20.77	20.87	24.32	0.07	62.89	59.33	−3.56
G21EA	7.00	7.00	7.55	0.21	10.20	11.78	1.58
G21IP	3.02	4.67	5.64	0.02	19.90	13.91	−5.99
DIPCS10	3.63	5.45	6.52	0.01	20.14	13.93	−6.21
PA26	0.26	1.58	2.19	0.01	8.92	5.60	−3.33
SIE4x4	25.11	25.11	28.22	0.74	47.87	51.32	3.45
ALKBDE10	8.64	8.64	11.82	0.09	28.98	29.14	0.16
YBDE18	0.09	5.46	6.34	0.11	23.50	12.84	−10.66
AL2X6	−1.13	1.64	2.05	0.05	5.54	1.53	−4.01
HEAVYSB11	0.44	3.64	4.12	0.06	13.02	6.68	−6.34
NBPRC	−1.09	2.89	3.30	0.10	10.66	4.43	−6.23
ALK8	1.13	1.80	2.55	0.03	6.74	4.68	−2.05
RC21	6.44	7.15	8.17	0.20	19.76	15.62	−4.14
G2RC	0.18	6.75	8.07	0.13	32.75	18.44	−14.31
BH76RC	−0.05	3.89	5.74	0.18	30.73	19.20	−11.53
FH51	0.75	3.22	4.68	0.10	24.77	12.84	−11.94
TAUT15	0.31	1.92	2.57	0.63	8.76	5.99	−2.77
DC13	0.57	8.31	11.47	0.15	43.35	14.08	−29.27
MB16-43	3.99	18.79	24.62	0.05	117.71	60.19	−57.52
DARC	3.72	4.14	4.75	0.13	9.11	6.57	−2.54
RSE43	−2.94	2.94	3.25	0.39	6.31	−0.98	−7.29
BSR36	−4.64	4.64	6.04	0.29	16.54	−0.93	−17.46
CDIE20	1.49	1.49	1.58	0.37	1.94	2.39	0.46
ISO34	−0.69	1.46	2.14	0.10	12.76	6.12	−6.64
ISOL24	−2.24	5.40	7.78	0.25	39.23	20.93	−18.30
C60ISO	−10.56	10.56	12.73	0.11	20.77	−1.22	−21.99
PArel	0.22	1.85	2.60	0.40	12.93	7.06	−5.87
BH76	−11.42	11.47	12.58	0.62	33.09	1.89	−31.20
BHPERI	−6.96	6.96	7.17	0.33	6.77	−4.07	−10.84
BHDIV10	−8.39	8.95	9.98	0.20	19.31	2.78	−16.52
INV24	−2.32	2.54	3.39	0.08	12.00	2.43	−9.57
BHROT27	0.39	0.46	0.68	0.07	2.03	1.63	−0.40
PX13	−13.59	13.59	13.83	0.41	9.81	−10.18	−19.99
WCPT18	−10.19	10.19	10.86	0.29	13.51	−4.98	−18.49
RG18	0.69	0.69	0.87	1.19	2.29	2.50	0.21
ADIM6	0.26	0.26	0.29	0.08	0.41	0.40	0.00
S22	0.48	1.07	1.31	0.15	5.14	3.01	−2.13
S66	0.63	0.86	1.11	0.16	4.43	3.17	−1.26
HEAVY28	0.86	0.86	0.91	0.69	1.16	1.57	0.42
WATER27	16.57	17.43	23.99	0.21	69.62	57.99	−11.64
CARBHB12	2.47	2.47	2.85	0.41	4.29	5.16	0.87
PNICO23	1.64	1.64	2.10	0.38	6.29	6.41	0.12
HAL59	1.76	1.84	2.48	0.40	9.47	8.12	−1.35
AHB21	−2.05	2.07	2.19	0.09	3.52	0.20	−3.32
CHB6	−1.02	1.08	1.17	0.04	1.70	0.18	−1.52
IL16	−1.73	1.73	1.77	0.02	1.10	−1.09	−2.19
IDISP	3.14	4.17	6.59	0.29	17.86	15.20	−2.66
ICONF	0.18	0.34	0.50	0.10	2.16	1.41	−0.74
ACONF	0.06	0.09	0.12	0.05	0.41	0.29	−0.13
AMINO20x4	0.12	0.42	0.53	0.17	2.37	1.45	−0.92
PCONF21	−0.62	1.31	1.56	0.81	4.47	1.44	−3.03
MCONF	−0.27	0.54	0.66	0.11	2.08	0.90	−1.18
SCONF	0.53	1.20	1.40	0.26	4.99	1.55	−3.44
UPU23	0.48	0.69	0.94	0.12	2.79	2.19	−0.60
BUT14DIOL	0.77	0.78	0.82	0.28	1.67	1.51	−0.15

Table S37: Statistical analysis for the mPWPW91-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	11.60	12.72	15.86	0.04	57.05	47.44	−9.60
G21EA	3.07	3.43	4.13	0.10	9.88	7.69	−2.19
G21IP	0.52	3.93	4.90	0.02	19.23	11.18	−8.05
DIPCS10	−1.08	3.76	4.68	0.01	15.33	5.50	−9.83
PA26	3.14	3.16	3.90	0.02	9.17	8.94	−0.22
SIE4x4	23.61	23.61	26.31	0.70	42.36	47.12	4.76
ALKBDE10	6.17	6.59	10.81	0.07	30.84	29.65	−1.19
YBDE18	−0.56	4.29	4.98	0.09	18.58	9.50	−9.08
AL2X6	0.98	2.69	2.92	0.07	7.91	2.79	−5.12
HEAVYSB11	2.09	3.55	3.92	0.06	9.24	5.73	−3.50
NBPRC	−0.84	2.25	2.74	0.08	9.30	2.96	−6.34
ALK8	6.31	6.54	9.18	0.10	17.31	16.38	−0.93
RC21	5.25	6.12	7.01	0.17	16.56	12.71	−3.84
G2RC	1.36	6.42	7.81	0.13	33.53	18.96	−14.56
BH76RC	0.73	3.61	5.50	0.17	28.20	20.60	−7.60
FH51	1.31	3.12	4.47	0.10	23.33	12.78	−10.54
TAUT15	0.13	1.85	2.26	0.61	7.57	5.05	−2.52
DC13	0.50	8.71	11.77	0.16	45.96	14.52	−31.44
MB16-43	17.29	27.10	34.58	0.07	147.29	88.18	−59.11
DARC	2.33	3.18	3.49	0.10	8.43	5.26	−3.16
RSE43	−2.75	2.75	3.05	0.36	6.18	−0.73	−6.92
BSR36	−1.55	1.55	1.73	0.10	3.33	−0.43	−3.75
CDIE20	1.59	1.59	1.70	0.39	2.41	2.64	0.23
ISO34	−0.62	1.38	2.01	0.09	11.69	5.37	−6.32
ISOL24	−1.50	4.20	5.98	0.19	26.80	15.88	−10.92
C60ISO	−9.43	9.43	11.72	0.10	20.28	−0.58	−20.86
PArel	0.19	1.74	2.49	0.38	12.37	6.53	−5.85
BH76	−9.30	9.33	10.38	0.50	29.76	1.42	−28.34
BHPERI	−7.05	7.05	7.31	0.34	6.78	−3.94	−10.72
BHDIV10	−8.29	8.77	9.73	0.19	18.64	2.43	−16.21
INV24	−1.68	2.25	3.00	0.07	10.90	2.67	−8.24
BHROT27	0.36	0.45	0.64	0.07	1.90	1.61	−0.29
PX13	−11.56	11.56	11.78	0.35	8.51	−8.52	−17.03
WCPT18	−8.63	8.63	9.14	0.25	11.84	−4.34	−16.18
RG18	0.07	0.09	0.12	0.16	0.49	0.33	−0.16
ADIM6	−0.17	0.17	0.19	0.05	0.25	−0.10	−0.35
S22	0.26	0.33	0.46	0.05	1.58	1.16	−0.42
S66	0.16	0.27	0.37	0.05	1.62	1.20	−0.42
HEAVY28	0.84	0.84	0.93	0.68	1.56	1.57	0.01
WATER27	3.74	4.59	5.94	0.06	27.60	16.14	−11.46
CARBHB12	1.72	1.72	2.18	0.28	4.03	4.53	0.50
PNICO23	1.54	1.55	2.18	0.36	7.21	7.14	−0.07
HAL59	1.38	1.42	2.04	0.31	6.80	6.45	−0.34
AHB21	−0.65	0.92	1.22	0.04	4.84	2.08	−2.76
CHB6	−0.81	0.93	1.02	0.03	1.81	0.36	−1.45
IL16	−0.54	0.61	0.70	0.01	1.75	0.47	−1.28
IDISP	2.61	2.61	3.34	0.18	5.52	5.90	0.38
ICONF	0.05	0.27	0.32	0.08	1.24	0.76	−0.48
ACONF	−0.10	0.11	0.15	0.06	0.39	0.04	−0.35
AMINO20x4	0.02	0.39	0.49	0.16	2.21	1.28	−0.93
PCONF21	−0.55	1.02	1.31	0.63	3.44	0.99	−2.45
MCONF	0.09	0.47	0.57	0.09	2.24	1.12	−1.12
SCONF	0.32	0.97	1.23	0.21	4.59	1.22	−3.37
UPU23	0.40	0.52	0.66	0.09	2.39	1.78	−0.60
BUT14DIOL	0.42	0.43	0.51	0.15	1.51	1.25	−0.26

Table S38: Statistical analysis for the rPW86PBE-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	5.84	9.17	12.15	0.03	58.74	38.10	−20.64
G21EA	5.40	5.40	6.27	0.16	11.47	11.65	0.18
G21IP	2.56	4.54	6.09	0.02	25.87	19.40	−6.46
DIPCS10	3.47	4.59	6.23	0.01	18.73	14.91	−3.82
PA26	3.06	3.08	4.01	0.02	9.68	9.45	−0.23
SIE4x4	23.33	23.33	26.10	0.69	42.20	46.60	4.40
ALKBDE10	4.74	6.66	9.38	0.07	28.31	23.63	−4.68
YBDE18	−4.67	6.50	7.99	0.13	25.48	9.26	−16.21
AL2X6	−3.61	3.61	4.02	0.10	5.36	−1.14	−6.50
HEAVYSB11	−2.12	2.99	3.88	0.05	9.96	1.83	−8.12
NBPRC	1.53	2.96	4.14	0.11	12.54	10.32	−2.22
ALK8	1.32	1.77	2.98	0.03	9.12	7.84	−1.27
RC21	1.91	4.13	4.60	0.12	14.50	7.43	−7.07
G2RC	3.21	4.70	6.36	0.09	27.39	17.28	−10.11
BH76RC	1.09	2.98	4.79	0.14	22.06	16.40	−5.66
FH51	3.01	4.17	5.50	0.13	22.16	13.23	−8.93
TAUT15	−0.36	1.73	2.00	0.57	6.50	3.56	−2.94
DC13	3.60	15.92	17.82	0.29	54.64	26.39	−28.25
MB16-43	−22.67	26.56	32.41	0.06	114.24	34.88	−79.36
DARC	12.02	12.02	12.32	0.37	8.57	14.38	5.81
RSE43	−2.57	2.57	2.87	0.34	5.86	−0.87	−6.73
BSR36	−5.09	5.09	6.09	0.31	13.51	−1.69	−15.20
CDIE20	1.52	1.52	1.62	0.37	2.14	2.52	0.38
ISO34	−0.70	2.35	3.37	0.16	19.44	10.73	−8.71
ISOL24	−4.39	8.62	11.92	0.39	58.56	27.08	−31.48
C60ISO	−9.36	9.36	11.44	0.10	19.20	−0.82	−20.02
PArel	−0.27	1.59	2.57	0.34	14.39	6.20	−8.19
BH76	−8.86	8.88	9.96	0.48	24.82	0.77	−24.05
BHPERI	−3.67	3.67	4.08	0.18	7.51	−0.43	−7.94
BHDIV10	−5.61	6.52	7.47	0.14	16.88	4.55	−12.33
INV24	−1.97	2.37	3.09	0.07	11.58	3.10	−8.47
BHROT27	0.23	0.41	0.59	0.07	1.93	1.47	−0.47
PX13	−7.47	7.47	7.55	0.22	4.12	−5.92	−10.04
WCPT18	−5.93	5.93	6.45	0.17	9.76	−2.03	−11.78
RG18	0.02	0.11	0.17	0.19	0.78	0.44	−0.33
ADIM6	0.35	0.35	0.39	0.10	0.54	0.62	0.08
S22	0.14	0.33	0.42	0.05	1.89	0.91	−0.98
S66	0.28	0.33	0.42	0.06	1.54	1.03	−0.51
HEAVY28	0.43	0.43	0.51	0.35	1.05	1.08	0.04
WATER27	6.46	6.92	9.76	0.09	30.76	24.47	−6.28
CARBHB12	1.54	1.54	1.80	0.25	2.89	3.43	0.54
PNICO23	0.96	0.96	1.26	0.22	3.59	3.74	0.14
HAL59	1.07	1.11	1.66	0.24	6.51	6.19	−0.33
AHB21	−0.38	0.82	1.09	0.04	5.02	3.41	−1.61
CHB6	0.32	0.86	1.07	0.03	2.95	2.21	−0.74
IL16	0.07	0.31	0.39	0.00	1.37	0.94	−0.43
IDISP	4.81	5.07	8.38	0.36	20.28	19.50	−0.78
ICONF	−0.06	0.39	0.51	0.12	2.10	1.06	−1.04
ACONF	−0.05	0.12	0.16	0.07	0.59	0.22	−0.37
AMINO20x4	−0.05	0.29	0.38	0.12	2.24	1.39	−0.85
PCONF21	−0.38	0.84	1.03	0.52	3.10	1.07	−2.04
MCONF	−0.08	0.37	0.44	0.07	1.72	0.77	−0.95
SCONF	0.05	0.57	0.87	0.12	3.57	0.76	−2.81
UPU23	0.49	0.63	0.77	0.11	2.60	1.95	−0.66
BUT14DIOL	0.41	0.42	0.47	0.15	1.40	1.12	−0.28

Table S39: Statistical analysis for the B97-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	2.93	4.73	6.87	0.02	60.99	26.72	−34.27
G21EA	0.89	2.34	2.97	0.07	12.42	8.58	−3.84
G21IP	−1.26	3.47	4.49	0.01	17.35	8.49	−8.86
DIPCS10	−4.58	5.00	6.22	0.01	11.85	1.42	−10.43
PA26	6.12	6.12	6.68	0.03	10.05	12.60	2.55
SIE4x4	24.50	24.50	27.20	0.73	43.32	50.84	7.52
ALKBDE10	3.34	5.10	8.03	0.05	27.19	21.91	−5.28
YBDE18	−4.36	5.30	6.63	0.11	18.04	5.30	−12.74
AL2X6	−4.99	4.99	5.41	0.14	6.01	−3.51	−9.53
HEAVYSB11	−4.05	4.05	4.71	0.07	7.65	−1.08	−8.73
NBPRC	1.99	3.03	4.02	0.11	12.41	10.31	−2.09
ALK8	−2.01	2.61	3.36	0.04	9.07	1.79	−7.29
RC21	2.17	3.75	4.36	0.11	15.96	8.75	−7.22
G2RC	3.46	4.90	6.30	0.10	27.51	17.95	−9.56
BH76RC	−0.18	2.84	4.03	0.13	22.28	14.21	−8.07
FH51	2.62	3.71	5.04	0.12	25.42	16.90	−8.52
TAUT15	−0.26	1.61	1.85	0.53	6.20	3.60	−2.60
DC13	6.67	14.13	15.22	0.26	47.89	25.07	−22.82
MB16-43	−32.64	36.10	41.95	0.09	122.02	31.94	−90.08
DARC	10.73	10.73	10.97	0.33	7.53	12.93	5.40
RSE43	−2.95	2.95	3.21	0.39	5.47	−1.42	−6.89
BSR36	−2.90	2.90	3.31	0.18	6.15	−1.19	−7.34
CDIE20	1.48	1.48	1.59	0.36	2.35	2.66	0.31
ISO34	−0.54	2.17	3.06	0.15	16.40	10.53	−5.87
ISOL24	−3.70	7.90	10.80	0.36	51.80	25.17	−26.64
C60ISO	−8.63	8.63	10.68	0.09	18.60	−0.67	−19.27
PArel	−0.05	1.49	2.38	0.32	13.17	6.12	−7.05
BH76	−7.20	7.29	8.17	0.39	22.81	3.11	−19.70
BHPERI	−3.95	3.95	4.27	0.19	5.73	−1.51	−7.24
BHDIV10	−5.08	5.83	6.84	0.13	15.08	3.78	−11.29
INV24	−0.90	1.80	2.30	0.06	9.68	4.21	−5.48
BHROT27	0.30	0.40	0.60	0.06	1.64	1.41	−0.23
PX13	−7.80	7.80	7.96	0.23	5.97	−5.57	−11.54
WCPT18	−5.39	5.39	5.90	0.15	9.71	−1.64	−11.35
RG18	0.02	0.10	0.14	0.17	0.60	0.20	−0.40
ADIM6	0.37	0.37	0.40	0.11	0.46	0.59	0.13
S22	0.10	0.38	0.45	0.05	1.77	0.89	−0.88
S66	0.08	0.29	0.34	0.05	1.30	0.73	−0.57
HEAVY28	0.30	0.31	0.38	0.25	0.86	0.73	−0.13
WATER27	−2.38	2.71	4.00	0.03	12.18	1.88	−10.29
CARBHB12	1.01	1.01	1.40	0.17	3.04	3.18	0.14
PNICO23	0.62	0.68	0.92	0.16	2.98	2.69	−0.29
HAL59	0.44	0.67	1.07	0.15	5.45	4.46	−0.99
AHB21	0.49	0.74	0.98	0.03	4.07	3.09	−0.99
CHB6	1.81	1.81	2.47	0.07	4.72	4.78	0.07
IL16	0.72	0.79	0.92	0.01	2.39	1.85	−0.54
IDISP	4.58	4.58	6.79	0.32	14.77	15.26	0.49
ICONF	0.03	0.40	0.47	0.12	1.79	0.93	−0.86
ACONF	−0.06	0.07	0.10	0.04	0.30	0.08	−0.23
AMINO20x4	−0.13	0.36	0.47	0.15	2.33	1.34	−0.99
PCONF21	−0.56	0.83	1.05	0.51	2.96	0.90	−2.06
MCONF	−0.06	0.38	0.47	0.08	2.03	0.89	−1.14
SCONF	−0.11	0.45	0.69	0.10	3.08	0.83	−2.24
UPU23	0.30	0.53	0.66	0.09	2.27	1.42	−0.85
BUT14DIOL	−0.01	0.30	0.36	0.11	1.75	0.98	−0.77

Table S40: Statistical analysis for the HCTH/407-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	8.01	8.93	12.89	0.03	85.04	75.85	−9.19
G21EA	4.30	4.68	5.58	0.14	13.04	10.64	−2.40
G21IP	3.22	4.83	5.93	0.02	20.06	13.99	−6.07
DIPCS10	5.89	6.47	7.58	0.01	16.37	13.47	−2.90
PA26	5.41	5.78	6.15	0.03	16.29	11.42	−4.87
SIE4x4	24.20	24.20	26.88	0.72	42.32	49.42	7.10
ALKBDE10	9.06	9.06	12.86	0.09	31.62	32.80	1.18
YBDE18	3.01	4.69	5.11	0.10	15.93	8.33	−7.60
AL2X6	11.75	11.75	12.51	0.33	13.72	17.14	3.42
HEAVYSB11	13.91	13.91	14.98	0.24	18.62	25.12	6.50
NBPRC	−1.09	3.78	5.20	0.14	17.99	8.08	−9.91
ALK8	20.53	21.56	29.98	0.34	74.25	70.14	−4.11
RC21	5.65	6.19	7.19	0.17	14.79	12.77	−2.01
G2RC	1.95	8.47	10.72	0.17	47.77	26.60	−21.17
BH76RC	0.29	3.00	5.18	0.14	30.22	22.48	−7.73
FH51	0.62	3.73	5.26	0.12	25.03	13.99	−11.04
TAUT15	0.01	1.67	1.98	0.55	6.61	4.14	−2.47
DC13	−0.06	13.70	19.52	0.25	79.52	28.02	−51.50
MB16-43	75.40	76.52	92.24	0.18	279.27	257.01	−22.26
DARC	2.05	3.76	4.07	0.12	10.53	5.52	−5.01
RSE43	−3.15	3.15	3.40	0.41	5.56	−1.38	−6.95
BSR36	−1.13	1.13	1.47	0.07	3.73	0.03	−3.70
CDIE20	1.84	1.84	2.02	0.45	3.54	3.74	0.20
ISO34	−0.45	1.84	2.53	0.13	13.20	6.39	−6.81
ISOL24	−2.11	5.40	7.87	0.25	39.35	18.48	−20.88
C60ISO	−5.66	6.06	8.11	0.06	17.30	1.07	−16.23
PArel	0.40	1.69	2.42	0.37	10.50	6.26	−4.23
BH76	−7.05	7.14	8.21	0.38	30.01	3.23	−26.78
BHPERI	−4.58	4.61	5.05	0.22	10.51	0.46	−10.06
BHDIV10	−6.47	6.93	7.75	0.15	13.84	2.30	−11.54
INV24	−0.47	2.87	3.98	0.09	19.82	10.57	−9.26
BHROT27	0.67	0.70	0.94	0.11	2.31	2.12	−0.19
PX13	−6.09	6.09	6.20	0.18	4.23	−4.71	−8.93
WCPT18	−5.80	5.80	6.29	0.17	9.45	−2.68	−12.14
RG18	1.26	1.26	1.56	2.17	3.78	4.20	0.43
ADIM6	1.38	1.38	1.39	0.41	0.50	1.65	1.15
S22	0.22	0.61	0.73	0.08	2.82	1.06	−1.76
S66	0.57	0.63	0.70	0.12	1.66	1.30	−0.36
HEAVY28	1.33	1.33	1.39	1.07	2.06	2.51	0.46
WATER27	0.05	1.47	2.18	0.02	12.18	6.14	−6.05
CARBHB12	1.68	1.68	1.99	0.28	3.28	4.03	0.74
PNICO23	1.97	1.97	3.13	0.46	11.66	12.03	0.37
HAL59	1.70	1.70	2.26	0.37	5.92	5.82	−0.10
AHB21	−0.36	1.01	1.34	0.04	5.92	2.34	−3.58
CHB6	−3.84	3.85	4.42	0.14	6.77	0.03	−6.74
IL16	0.11	0.57	0.74	0.01	3.07	1.53	−1.53
IDISP	3.54	5.12	6.19	0.36	15.58	11.46	−4.12
ICONF	0.43	0.65	0.83	0.20	2.93	1.71	−1.21
ACONF	0.41	0.41	0.46	0.22	0.66	0.81	0.15
AMINO20x4	−0.05	0.42	0.53	0.17	2.37	1.10	−1.27
PCONF21	−0.61	1.43	1.58	0.88	5.04	2.81	−2.22
MCONF	−0.38	0.47	0.57	0.09	1.63	0.41	−1.22
SCONF	−0.50	0.93	1.11	0.20	3.79	2.16	−1.63
UPU23	−0.10	0.55	0.68	0.10	2.93	1.08	−1.85
BUT14DIOL	−0.42	0.52	0.59	0.19	1.78	0.75	−1.03

Table S41: Statistical analysis for the N12-D3(0) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	0.74	7.33	9.76	0.02	62.40	38.77	−23.63
G21EA	−2.83	3.53	4.13	0.10	12.56	5.07	−7.49
G21IP	−2.92	4.87	6.20	0.02	26.80	9.81	−17.00
DIPCS10	−7.78	7.78	9.29	0.01	14.10	−1.29	−15.39
PA26	3.80	3.85	4.63	0.02	11.03	10.60	−0.43
SIE4x4	21.63	21.63	24.22	0.64	40.42	43.58	3.17
ALKBDE10	0.17	6.83	8.94	0.07	32.24	20.96	−11.28
YBDE18	−0.32	4.00	4.72	0.08	18.31	10.52	−7.80
AL2X6	−0.97	1.42	2.14	0.04	5.08	0.70	−4.39
HEAVYSB11	5.37	5.78	6.42	0.10	12.59	10.32	−2.27
NBPRC	−0.97	2.11	2.47	0.08	7.95	3.07	−4.88
ALK8	3.38	4.89	6.84	0.08	16.53	14.14	−2.39
RC21	6.46	7.33	8.39	0.21	18.00	14.07	−3.92
G2RC	−1.55	6.36	7.80	0.12	32.78	15.31	−17.47
BH76RC	0.58	3.72	5.07	0.17	27.19	18.06	−9.14
FH51	−0.85	2.67	4.19	0.09	25.27	12.59	−12.68
TAUT15	−0.52	2.34	2.83	0.77	9.78	5.56	−4.22
DC13	−0.38	7.77	10.00	0.14	38.00	16.37	−21.64
MB16-43	29.67	30.46	36.34	0.07	89.14	77.01	−12.14
DARC	−0.05	1.89	2.28	0.06	7.45	2.73	−4.73
RSE43	−2.54	2.54	2.98	0.33	6.67	−0.48	−7.15
BSR36	−1.65	1.65	2.12	0.10	6.31	−0.40	−6.70
CDIE20	1.49	1.49	1.55	0.37	1.54	2.25	0.71
ISO34	−0.46	1.29	1.72	0.09	9.25	4.73	−4.52
ISOL24	−0.52	3.55	5.01	0.16	23.94	11.97	−11.97
C60ISO	−9.30	9.30	11.45	0.09	19.93	−0.59	−20.52
PArel	0.45	1.61	2.56	0.35	12.73	8.40	−4.32
BH76	−7.84	7.96	9.02	0.43	27.71	2.75	−24.96
BHPERI	−5.47	5.47	5.80	0.26	7.56	−0.94	−8.50
BHDIV10	−7.13	7.47	8.34	0.16	15.29	1.69	−13.60
INV24	−2.44	2.63	3.76	0.08	11.80	1.30	−10.50
BHROT27	0.78	0.80	1.13	0.13	2.72	2.62	−0.10
PX13	−8.69	8.69	8.84	0.26	5.95	−6.17	−12.12
WCPT18	−6.93	6.93	7.55	0.20	11.53	−2.16	−13.69
RG18	−0.17	0.30	0.39	0.52	1.58	0.48	−1.09
ADIM6	−0.21	0.28	0.31	0.08	0.68	0.20	−0.47
S22	0.80	0.87	1.31	0.12	4.13	3.55	−0.58
S66	0.54	0.66	0.99	0.12	4.31	3.65	−0.66
HEAVY28	0.09	0.26	0.31	0.21	1.20	0.60	−0.60
WATER27	8.41	9.02	12.02	0.11	36.82	28.60	−8.22
CARBHB12	1.74	1.75	2.34	0.29	4.66	4.62	−0.04
PNICO23	0.31	0.78	1.28	0.18	6.13	5.26	−0.86
HAL59	0.69	0.88	1.53	0.19	6.93	6.15	−0.77
AHB21	−1.78	1.79	2.12	0.08	4.39	0.10	−4.29
CHB6	−1.59	1.64	1.82	0.06	2.49	0.16	−2.33
IL16	−1.81	1.81	1.88	0.02	1.85	−0.90	−2.75
IDISP	2.86	2.86	3.42	0.20	5.80	6.57	0.77
ICONF	0.28	0.55	0.73	0.17	2.38	1.73	−0.65
ACONF	−0.11	0.13	0.17	0.07	0.46	0.07	−0.39
AMINO20x4	0.21	0.49	0.63	0.20	2.90	1.79	−1.11
PCONF21	−0.14	0.89	1.02	0.55	3.09	1.44	−1.65
MCONF	0.35	0.57	0.70	0.11	2.50	1.49	−1.00
SCONF	0.47	1.39	1.68	0.30	5.88	1.69	−4.19
UPU23	−0.06	0.56	0.66	0.10	2.46	1.08	−1.39
BUT14DIOL	0.73	0.74	0.79	0.26	1.63	1.40	−0.23

Table S42: Statistical analysis for the VV10 DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	8.06	10.50	13.65	0.03	61.50	42.70	−18.80
G21EA	3.57	3.88	4.69	0.12	11.21	9.53	−1.69
G21IP	0.45	4.04	5.42	0.02	25.35	16.99	−8.36
DIPCS10	−0.69	4.00	5.07	0.01	18.57	10.55	−8.02
PA26	2.10	2.37	3.20	0.01	9.05	8.28	−0.78
SIE4x4	23.37	23.37	26.13	0.69	42.36	46.60	4.24
ALKBDE10	5.32	6.93	9.72	0.07	28.50	24.27	−4.23
YBDE18	−3.35	6.12	7.38	0.12	25.68	10.89	−14.79
AL2X6	−2.74	2.74	3.06	0.08	4.09	−0.44	−4.53
HEAVYSB11	−0.82	3.02	3.47	0.05	9.76	3.35	−6.41
NBPRC	0.81	2.41	3.20	0.09	10.50	7.58	−2.92
ALK8	0.47	1.98	2.79	0.03	9.48	6.82	−2.66
RC21	2.99	4.62	5.22	0.13	13.71	9.28	−4.43
G2RC	2.80	5.11	6.78	0.10	28.59	17.96	−10.63
BH76RC	1.11	3.13	5.06	0.15	23.56	17.47	−6.09
FH51	2.45	3.79	5.08	0.12	21.07	12.42	−8.65
TAUT15	−0.13	1.73	2.03	0.57	6.86	4.15	−2.72
DC13	2.30	12.94	14.75	0.24	48.83	19.27	−29.56
MB16-43	−14.71	21.22	27.04	0.05	112.94	43.50	−69.44
DARC	8.72	8.72	9.03	0.27	7.41	10.79	3.39
RSE43	−2.55	2.55	2.85	0.34	5.89	−0.89	−6.78
BSR36	−3.46	3.46	4.14	0.21	9.50	−1.18	−10.68
CDIE20	1.45	1.45	1.53	0.36	1.79	2.27	0.48
ISO34	−0.76	2.03	2.92	0.14	17.79	8.87	−8.92
ISOL24	−3.56	6.82	9.32	0.31	45.00	22.83	−22.18
C60ISO	−10.87	10.87	12.98	0.11	20.52	−1.57	−22.09
PArel	−0.08	1.42	2.45	0.31	13.90	6.51	−7.40
BH76	−9.32	9.35	10.49	0.50	26.26	0.99	−25.27
BHPERI	−4.71	4.71	4.98	0.23	5.64	−2.32	−7.95
BHDIV10	−6.28	7.10	8.00	0.16	17.85	4.07	−13.79
INV24	−2.07	2.35	3.09	0.07	11.49	3.14	−8.35
BHROT27	0.27	0.43	0.62	0.07	2.00	1.52	−0.49
PX13	−8.56	8.56	8.65	0.26	5.10	−6.60	−11.70
WCPT18	−6.81	6.81	7.36	0.19	10.43	−2.60	−13.03
RG18	0.14	0.14	0.19	0.24	0.51	0.51	0.00
ADIM6	0.38	0.39	0.46	0.12	0.70	0.67	−0.03
S22	0.26	0.38	0.56	0.05	1.76	1.45	−0.31
S66	0.38	0.43	0.58	0.08	1.94	1.72	−0.21
HEAVY28	0.39	0.39	0.50	0.31	1.21	1.24	0.03
WATER27	9.69	10.21	14.40	0.13	41.69	34.68	−7.01
CARBHB12	1.64	1.64	1.92	0.27	3.22	3.67	0.46
PNICO23	1.05	1.05	1.40	0.25	4.31	4.26	−0.04
HAL59	1.40	1.41	2.03	0.31	7.07	6.89	−0.18
AHB21	−0.92	1.17	1.31	0.05	4.71	2.58	−2.13
CHB6	0.05	0.55	0.59	0.02	1.62	0.95	−0.67
IL16	−0.73	0.73	0.83	0.01	1.78	−0.07	−1.85
IDISP	3.94	3.94	6.55	0.28	15.09	15.48	0.38
ICONF	−0.04	0.32	0.41	0.10	1.72	1.10	−0.63
ACONF	−0.10	0.13	0.17	0.07	0.54	0.12	−0.42
AMINO20x4	0.02	0.31	0.40	0.13	2.19	1.35	−0.84
PCONF21	−0.38	0.74	0.84	0.46	2.50	0.82	−1.67
MCONF	0.19	0.42	0.51	0.08	1.79	1.02	−0.77
SCONF	0.32	0.99	1.23	0.22	4.51	1.15	−3.36
UPU23	0.19	0.42	0.57	0.07	2.71	1.52	−1.19
BUT14DIOL	0.66	0.67	0.70	0.24	1.19	1.12	−0.06

SI.7.2 Results for dispersion-corrected meta-GGA/meta-NGA functionals

Table S43: Statistical analysis for the PKZB-D3(0) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	4.40	7.47	9.79	0.02	64.15	28.99	−35.16
G21EA	−1.26	2.15	2.78	0.06	9.26	2.49	−6.77
G21IP	−3.86	4.32	5.65	0.02	15.19	3.91	−11.27
DIPCS10	−8.69	8.69	10.25	0.01	14.11	−1.53	−15.64
PA26	6.90	6.90	7.69	0.04	14.12	14.95	0.84
SIE4x4	23.94	23.94	26.96	0.71	46.79	51.29	4.50
ALKBDE10	−2.44	5.78	7.29	0.06	26.24	16.68	−9.56
YBDE18	0.42	4.07	4.72	0.08	16.00	8.03	−7.97
AL2X6	4.05	4.78	5.85	0.13	12.89	10.69	−2.20
HEAVYSB11	−0.56	3.86	4.75	0.07	14.15	4.03	−10.12
NBPRC	−1.55	3.61	4.07	0.13	13.27	5.10	−8.17
ALK8	10.24	11.32	15.30	0.18	35.03	32.66	−2.37
RC21	6.93	7.46	8.37	0.21	15.86	13.41	−2.45
G2RC	3.84	8.78	10.87	0.17	45.71	25.69	−20.03
BH76RC	0.53	4.04	5.01	0.19	22.66	13.51	−9.15
FH51	1.38	4.07	5.25	0.13	24.08	14.49	−9.59
TAUT15	0.41	1.35	1.83	0.44	5.64	4.13	−1.51
DC13	1.05	10.17	13.81	0.18	56.17	33.48	−22.69
MB16-43	14.00	32.60	44.78	0.08	232.38	148.56	−83.82
DARC	−4.86	4.86	5.24	0.15	6.63	−2.56	−9.19
RSE43	−2.87	2.87	3.19	0.38	7.07	−1.06	−8.13
BSR36	8.14	8.14	9.72	0.50	20.84	23.21	2.37
CDIE20	1.24	1.24	1.34	0.31	1.85	2.05	0.20
ISO34	−0.59	2.03	2.74	0.14	14.82	5.18	−9.64
ISOL24	1.34	3.64	5.13	0.17	21.58	13.79	−7.80
C60ISO	−10.03	10.03	12.53	0.10	22.19	−0.59	−22.77
PArel	0.64	2.16	2.69	0.47	10.23	3.90	−6.34
BH76	−9.03	9.03	9.94	0.49	23.48	−0.99	−24.47
BHPERI	−8.98	8.98	9.56	0.43	11.85	−2.99	−14.84
BHDIV10	−8.96	8.96	9.98	0.20	14.12	−1.16	−15.28
INV24	0.19	2.08	2.82	0.07	12.74	7.67	−5.08
BHROT27	0.34	0.65	0.92	0.10	3.23	2.09	−1.15
PX13	−4.44	5.57	6.16	0.17	12.93	4.23	−8.70
WCPT18	−9.33	9.33	10.04	0.27	12.50	−4.62	−17.13
RG18	0.24	0.29	0.46	0.50	1.82	1.56	−0.26
ADIM6	1.45	1.45	1.60	0.43	1.98	2.54	0.56
S22	−0.02	0.45	0.55	0.06	1.94	0.79	−1.15
S66	0.11	0.44	0.56	0.08	2.65	1.71	−0.93
HEAVY28	−0.46	0.46	0.50	0.37	0.78	−0.02	−0.80
WATER27	−1.32	1.55	2.77	0.02	9.13	0.91	−8.21
CARBHB12	0.01	0.75	0.91	0.12	2.69	1.94	−0.75
PNICO23	0.06	0.78	1.35	0.18	6.81	5.65	−1.16
HAL59	−0.13	0.90	1.21	0.20	6.06	4.32	−1.74
AHB21	1.10	1.24	1.93	0.06	8.35	7.22	−1.13
CHB6	−2.06	2.99	3.51	0.11	9.14	2.81	−6.33
IL16	−0.79	0.99	1.29	0.01	4.05	0.71	−3.34
IDISP	−0.16	6.15	7.33	0.43	20.24	7.98	−12.26
ICONF	0.01	0.81	1.06	0.25	4.62	2.65	−1.97
ACONF	−0.52	0.52	0.60	0.28	0.93	−0.10	−1.02
AMINO20x4	0.09	0.53	0.73	0.22	4.71	2.49	−2.22
PCONF21	−0.93	1.26	1.49	0.78	3.63	0.91	−2.72
MCONF	0.57	0.81	1.01	0.16	3.35	2.39	−0.96
SCONF	0.81	1.36	1.49	0.30	4.18	1.91	−2.28
UPU23	−0.48	0.61	0.77	0.11	2.16	0.55	−1.62
BUT14DIOL	0.03	0.34	0.43	0.12	2.02	0.89	−1.13

Table S44: Statistical analysis for the TPSS-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	4.46	5.91	7.48	0.02	43.57	25.78	−17.80
G21EA	0.42	2.20	2.66	0.07	9.63	5.80	−3.83
G21IP	−0.96	3.95	4.83	0.02	19.84	11.95	−7.89
DIPCS10	−3.57	3.69	4.97	0.01	10.08	0.60	−9.48
PA26	4.87	4.87	5.45	0.03	9.81	11.72	1.91
SIE4x4	21.91	21.91	24.66	0.65	40.65	45.69	5.04
ALKBDE10	1.93	4.16	7.56	0.04	26.60	22.77	−3.83
YBDE18	−4.32	4.67	5.34	0.09	11.57	1.77	−9.80
AL2X6	0.89	2.24	2.41	0.06	6.38	2.32	−4.07
HEAVYSB11	−0.31	2.57	2.92	0.04	8.38	3.37	−5.01
NBPRC	−0.84	1.46	1.93	0.05	5.78	1.09	−4.69
ALK8	3.73	3.73	5.15	0.06	8.52	9.11	0.59
RC21	3.39	4.44	4.95	0.12	12.67	8.60	−4.07
G2RC	3.43	7.11	9.21	0.14	33.57	20.70	−12.87
BH76RC	0.44	3.57	4.95	0.17	22.48	13.07	−9.40
FH51	2.67	4.30	5.65	0.14	24.79	15.17	−9.62
TAUT15	0.07	1.63	1.90	0.53	6.12	3.72	−2.40
DC13	0.72	8.91	11.75	0.16	39.40	14.91	−24.49
MB16-43	−22.33	25.88	31.77	0.06	123.50	41.13	−82.38
DARC	5.42	5.42	5.98	0.17	7.22	8.10	0.88
RSE43	−1.97	1.97	2.24	0.26	4.90	−0.74	−5.64
BSR36	−4.32	4.32	4.79	0.27	9.57	−1.11	−10.67
CDIE20	1.67	1.67	1.76	0.41	2.10	2.72	0.62
ISO34	−1.64	2.31	3.17	0.16	16.97	5.01	−11.96
ISOL24	−3.21	5.84	7.94	0.27	40.00	19.35	−20.65
C60ISO	−8.40	8.40	10.61	0.09	18.86	−0.28	−19.14
PArel	0.16	1.54	2.19	0.33	11.32	5.42	−5.90
BH76	−9.21	9.22	10.09	0.50	23.57	0.46	−23.12
BHPERI	−5.51	5.51	5.73	0.26	5.43	−2.98	−8.41
BHDIV10	−6.64	6.90	7.55	0.15	13.80	1.29	−12.51
INV24	−1.51	1.79	2.28	0.06	7.94	2.82	−5.12
BHROT27	0.34	0.53	0.70	0.08	2.18	1.54	−0.64
PX13	−8.92	8.92	9.05	0.27	6.50	−6.05	−12.55
WCPT18	−6.34	6.34	6.76	0.18	8.75	−2.60	−11.35
RG18	0.13	0.13	0.16	0.22	0.43	0.41	−0.02
ADIM6	−0.16	0.16	0.20	0.05	0.33	−0.08	−0.40
S22	0.04	0.32	0.48	0.04	2.31	1.12	−1.19
S66	0.02	0.29	0.38	0.05	2.01	1.20	−0.81
HEAVY28	0.34	0.35	0.45	0.28	1.03	0.98	−0.05
WATER27	3.64	4.43	5.88	0.05	27.79	17.21	−10.57
CARBHB12	1.42	1.42	1.76	0.24	3.11	3.54	0.44
PNICO23	1.11	1.11	1.56	0.26	5.04	4.95	−0.09
HAL59	0.86	0.99	1.64	0.22	6.54	6.07	−0.46
AHB21	−0.34	0.67	0.87	0.03	3.60	2.01	−1.59
CHB6	−0.37	0.94	1.11	0.04	3.19	1.73	−1.47
IL16	0.25	0.34	0.43	0.00	1.19	0.83	−0.37
IDISP	3.21	3.22	4.84	0.23	10.90	10.87	−0.03
ICONF	0.00	0.19	0.22	0.06	0.75	0.39	−0.35
ACONF	−0.04	0.09	0.11	0.05	0.34	0.12	−0.23
AMINO20x4	0.04	0.34	0.41	0.14	1.58	0.91	−0.66
PCONF21	−0.59	1.08	1.36	0.67	3.63	1.17	−2.46
MCONF	−0.07	0.42	0.50	0.08	1.84	0.79	−1.06
SCONF	0.34	1.05	1.31	0.23	4.56	1.21	−3.34
UPU23	0.33	0.49	0.61	0.09	2.10	1.49	−0.61
BUT14DIOL	0.26	0.28	0.34	0.10	1.21	0.95	−0.26

Table S45: Statistical analysis for the revTPSS-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	3.32	5.70	7.51	0.02	46.14	26.51	−19.63
G21EA	−0.60	2.32	2.53	0.07	7.75	3.86	−3.89
G21IP	−1.59	3.99	4.90	0.02	20.04	11.49	−8.56
DIPCS10	−4.45	4.45	5.64	0.01	10.60	−0.54	−11.14
PA26	4.65	4.65	5.34	0.02	10.50	11.73	1.24
SIE4x4	21.33	21.33	24.07	0.63	39.65	44.33	4.68
ALKBDE10	−0.30	4.23	6.62	0.04	23.84	18.61	−5.22
YBDE18	−3.56	3.86	4.55	0.08	11.04	2.64	−8.40
AL2X6	1.55	2.42	2.44	0.07	5.55	2.92	−2.63
HEAVYSB11	0.87	2.75	3.02	0.05	8.46	4.69	−3.77
NBPRC	−1.47	1.62	2.19	0.06	5.48	0.69	−4.79
ALK8	2.61	2.87	4.11	0.05	8.86	8.34	−0.52
RC21	3.93	5.07	5.76	0.14	14.55	10.70	−3.85
G2RC	5.70	10.36	13.32	0.20	47.16	30.29	−16.87
BH76RC	0.95	4.72	6.10	0.22	23.25	14.74	−8.50
FH51	3.12	5.19	6.89	0.17	30.69	20.16	−10.53
TAUT15	0.04	1.31	1.66	0.43	5.31	3.18	−2.13
DC13	−0.14	8.25	11.92	0.15	47.18	18.67	−28.51
MB16-43	−32.80	36.75	43.07	0.09	128.15	32.00	−96.14
DARC	2.38	3.09	3.35	0.10	7.62	5.04	−2.58
RSE43	−1.73	1.73	2.01	0.23	4.74	−0.53	−5.27
BSR36	−2.25	2.25	2.42	0.14	4.13	−0.22	−4.35
CDIE20	1.49	1.49	1.54	0.37	1.42	2.35	0.93
ISO34	−2.26	2.84	4.09	0.19	18.21	2.90	−15.31
ISOL24	−2.86	4.93	6.23	0.22	29.63	16.03	−13.60
C60ISO	−9.51	9.51	11.71	0.10	20.21	−0.78	−20.99
PArel	0.39	1.53	2.04	0.33	10.12	4.75	−5.37
BH76	−8.88	8.88	9.97	0.48	24.35	−0.61	−24.95
BHPERI	−6.14	6.14	6.44	0.29	7.11	−2.27	−9.38
BHDIV10	−6.19	6.21	6.93	0.14	12.12	0.10	−12.02
INV24	−1.05	1.49	1.95	0.05	7.84	3.31	−4.53
BHROT27	0.34	0.51	0.69	0.08	1.99	1.47	−0.52
PX13	−6.25	6.25	6.36	0.19	4.50	−4.42	−8.92
WCPT18	−5.50	5.50	5.87	0.16	7.03	−2.34	−9.37
RG18	0.03	0.06	0.08	0.10	0.33	0.20	−0.13
ADIM6	−0.12	0.12	0.13	0.04	0.11	−0.09	−0.19
S22	0.06	0.27	0.33	0.04	1.23	0.73	−0.50
S66	0.04	0.20	0.26	0.04	1.22	0.78	−0.44
HEAVY28	0.32	0.34	0.45	0.27	1.30	1.23	−0.07
WATER27	3.01	3.48	4.63	0.04	19.43	13.14	−6.29
CARBHB12	0.99	0.99	1.18	0.16	2.07	2.42	0.36
PNICO23	1.15	1.15	1.57	0.27	4.77	4.78	0.01
HAL59	0.89	1.00	1.65	0.22	6.41	5.97	−0.44
AHB21	0.05	0.47	0.75	0.02	3.69	2.77	−0.93
CHB6	−0.32	0.80	0.98	0.03	3.05	1.42	−1.63
IL16	0.37	0.55	0.65	0.01	1.76	1.11	−0.64
IDISP	2.97	3.34	4.94	0.23	10.43	9.31	−1.12
ICONF	0.02	0.23	0.31	0.07	1.23	0.62	−0.61
ACONF	−0.14	0.14	0.16	0.08	0.29	−0.01	−0.29
AMINO20x4	0.09	0.27	0.36	0.11	1.80	1.23	−0.57
PCONF21	−0.40	0.71	0.88	0.44	2.51	0.77	−1.73
MCONF	0.24	0.55	0.65	0.11	2.02	1.04	−0.98
SCONF	0.55	1.24	1.43	0.27	4.49	1.51	−2.98
UPU23	0.04	0.33	0.43	0.06	1.65	0.93	−0.72
BUT14DIOL	0.08	0.18	0.23	0.06	1.02	0.64	−0.38

Table S46: Statistical analysis for the SCAN-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	0.02	4.08	5.76	0.01	42.03	13.65	−28.38
G21EA	0.27	3.64	4.20	0.11	13.52	8.04	−5.48
G21IP	0.01	4.69	5.68	0.02	24.45	12.51	−11.94
DIPCS10	−2.82	4.92	5.99	0.01	16.69	4.67	−12.02
PA26	3.11	3.18	4.03	0.02	11.05	10.39	−0.66
SIE4x4	17.99	17.99	20.51	0.53	35.81	39.29	3.48
ALKBDE10	19.27	19.27	21.05	0.19	31.10	39.29	8.19
YBDE18	−2.58	3.12	3.43	0.06	8.85	3.01	−5.83
AL2X6	2.13	2.13	2.37	0.06	2.93	3.18	0.25
HEAVYSB11	3.37	6.64	8.73	0.11	21.98	16.90	−5.08
NBPRC	−1.67	2.51	2.99	0.09	9.23	3.04	−6.18
ALK8	2.77	3.45	4.59	0.06	10.55	8.46	−2.08
RC21	6.08	6.69	8.45	0.19	28.98	25.94	−3.05
G2RC	−1.27	6.39	7.85	0.12	32.67	13.18	−19.49
BH76RC	−0.27	3.38	4.41	0.16	18.69	9.45	−9.24
FH51	−0.79	2.75	4.07	0.09	22.06	10.89	−11.17
TAUT15	0.42	1.74	2.34	0.57	7.96	5.49	−2.47
DC13	−0.21	6.87	10.70	0.12	43.52	11.84	−31.68
MB16-43	14.03	17.77	22.69	0.04	99.79	75.95	−23.85
DARC	−1.01	2.01	2.66	0.06	8.08	1.73	−6.35
RSE43	−1.28	1.29	1.79	0.17	5.47	0.08	−5.39
BSR36	−1.28	1.28	1.68	0.08	4.84	−0.13	−4.97
CDIE20	1.45	1.45	1.57	0.36	2.31	2.27	−0.04
ISO34	−0.24	1.30	1.85	0.09	10.51	6.13	−4.38
ISOL24	−0.46	3.23	4.68	0.15	24.26	14.62	−9.64
C60ISO	−5.93	6.01	7.98	0.06	15.82	0.39	−15.43
PArel	0.71	1.50	2.24	0.32	10.03	7.63	−2.40
BH76	−7.48	7.77	8.48	0.42	23.84	6.01	−17.84
BHPERI	−5.50	5.50	5.81	0.26	7.88	−0.57	−8.45
BHDIV10	−5.69	6.62	7.15	0.15	16.00	4.65	−11.36
INV24	−0.51	1.16	1.68	0.04	8.18	2.36	−5.81
BHROT27	0.83	0.84	1.16	0.13	2.46	2.35	−0.11
PX13	−8.34	8.34	8.53	0.25	6.95	−5.48	−12.43
WCPT18	−6.22	6.22	6.98	0.18	10.47	−2.32	−12.79
RG18	0.11	0.18	0.25	0.31	1.06	0.77	−0.30
ADIM6	−0.12	0.12	0.13	0.04	0.13	−0.04	−0.17
S22	0.45	0.47	0.74	0.06	2.73	2.63	−0.10
S66	0.38	0.43	0.64	0.08	3.20	2.78	−0.43
HEAVY28	−0.13	0.27	0.32	0.22	1.24	0.72	−0.52
WATER27	9.57	10.15	13.44	0.13	38.63	30.73	−7.90
CARBHB12	1.38	1.38	1.89	0.23	3.91	4.02	0.11
PNICO23	1.07	1.08	1.60	0.25	5.74	5.63	−0.11
HAL59	0.95	1.03	1.71	0.22	6.58	6.19	−0.39
AHB21	−1.67	1.67	1.92	0.07	3.98	−0.27	−4.25
CHB6	−0.13	0.45	0.57	0.02	1.78	0.89	−0.89
IL16	−0.98	0.98	1.08	0.01	1.54	−0.14	−1.68
IDISP	1.77	2.05	3.45	0.14	8.95	8.16	−0.79
ICONF	0.27	0.31	0.44	0.09	1.53	1.34	−0.19
ACONF	0.13	0.13	0.15	0.07	0.22	0.27	0.05
AMINO20x4	0.11	0.22	0.30	0.09	1.46	0.94	−0.52
PCONF21	−0.06	0.47	0.53	0.29	1.58	0.74	−0.84
MCONF	0.36	0.46	0.60	0.09	1.43	1.05	−0.38
SCONF	0.37	0.66	0.73	0.14	2.34	0.81	−1.53
UPU23	−0.22	0.39	0.49	0.07	1.76	0.50	−1.26
BUT14DIOL	0.39	0.40	0.42	0.14	0.80	0.65	−0.15

Table S47: Statistical analysis for the τHCTH-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	4.79	5.91	8.62	0.02	57.44	43.63	−13.81
G21EA	2.65	3.03	3.84	0.09	11.03	9.09	−1.93
G21IP	2.08	4.06	5.08	0.02	17.27	11.71	−5.56
DIPCS10	2.94	4.23	5.28	0.01	12.03	9.48	−2.55
PA26	5.58	5.58	6.15	0.03	11.02	12.02	1.00
SIE4x4	23.42	23.42	25.76	0.69	39.41	46.90	7.49
ALKBDE10	7.56	7.85	11.99	0.08	33.46	32.03	−1.43
YBDE18	0.86	2.76	3.47	0.06	14.06	6.17	−7.89
AL2X6	9.81	9.81	10.53	0.27	12.37	15.18	2.80
HEAVYSB11	13.37	13.37	15.91	0.23	26.93	28.89	1.96
NBPRC	−0.40	2.85	3.61	0.10	11.69	5.33	−6.35
ALK8	17.25	18.55	23.69	0.30	50.24	45.03	−5.21
RC21	4.59	5.11	6.10	0.14	15.27	12.32	−2.96
G2RC	2.05	6.86	8.59	0.13	36.75	20.58	−16.17
BH76RC	0.12	2.66	4.66	0.12	28.08	19.86	−8.21
FH51	1.34	3.37	4.62	0.11	22.39	12.77	−9.62
TAUT15	0.31	1.73	2.16	0.57	7.12	4.95	−2.18
DC13	1.71	10.97	13.38	0.20	49.47	19.32	−30.15
MB16-43	47.96	49.41	60.04	0.12	171.19	154.35	−16.84
DARC	3.83	4.43	4.90	0.14	9.87	6.83	−3.04
RSE43	−3.12	3.12	3.36	0.41	5.85	−1.58	−7.43
BSR36	−2.80	2.80	3.07	0.17	4.64	−1.17	−5.81
CDIE20	1.83	1.83	2.00	0.45	3.28	3.44	0.16
ISO34	−0.65	1.67	2.34	0.11	12.60	8.01	−4.59
ISOL24	−2.35	5.73	8.10	0.26	39.31	18.92	−20.39
C60ISO	−7.18	7.23	9.41	0.07	18.03	0.20	−17.83
PArel	0.36	1.68	2.33	0.36	10.74	6.74	−4.00
BH76	−7.48	7.64	8.61	0.41	27.65	3.94	−23.71
BHPERI	−6.17	6.17	6.47	0.30	7.91	−3.34	−11.25
BHDIV10	−7.29	7.83	8.68	0.17	18.18	2.72	−15.46
INV24	−1.23	2.37	3.08	0.07	13.61	5.81	−7.80
BHROT27	0.48	0.55	0.75	0.09	1.95	1.69	−0.26
PX13	−9.97	9.97	10.19	0.30	8.71	−6.27	−14.98
WCPT18	−6.82	6.82	7.38	0.19	10.86	−2.54	−13.40
RG18	0.57	0.57	0.68	0.98	1.31	1.47	0.15
ADIM6	−0.13	0.24	0.32	0.07	0.89	0.18	−0.71
S22	0.32	0.55	0.70	0.08	3.17	1.66	−1.51
S66	0.25	0.40	0.53	0.07	2.50	1.74	−0.76
HEAVY28	1.87	1.87	2.06	1.51	4.43	4.62	0.19
WATER27	3.49	4.37	5.79	0.05	29.41	17.55	−11.86
CARBHB12	2.00	2.00	2.41	0.33	3.97	4.79	0.82
PNICO23	2.59	2.59	3.46	0.61	10.43	10.40	−0.03
HAL59	2.36	2.36	3.08	0.51	8.04	8.00	−0.04
AHB21	−1.31	1.38	1.75	0.06	5.05	0.41	−4.63
CHB6	−4.39	4.39	4.86	0.16	5.81	−2.22	−8.03
IL16	−0.90	0.94	1.14	0.01	2.31	0.29	−2.02
IDISP	3.25	4.52	5.26	0.32	12.65	9.14	−3.51
ICONF	0.11	0.46	0.54	0.14	1.93	1.02	−0.91
ACONF	0.14	0.14	0.17	0.08	0.45	0.46	0.01
AMINO20x4	−0.05	0.39	0.49	0.16	2.59	1.27	−1.33
PCONF21	−0.80	1.53	1.79	0.94	5.25	2.06	−3.19
MCONF	−0.36	0.44	0.54	0.09	1.54	0.39	−1.15
SCONF	−0.07	0.48	0.75	0.10	3.32	0.76	−2.56
UPU23	0.33	0.57	0.72	0.10	2.45	1.64	−0.81
BUT14DIOL	0.27	0.32	0.42	0.11	1.63	1.27	−0.36

Table S48: Statistical analysis for the M06L-D3(0) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.22	4.46	6.09	0.01	47.60	18.28	−29.32
G21EA	−3.39	3.80	4.64	0.11	14.32	4.07	−10.25
G21IP	−2.77	4.46	5.49	0.02	23.24	8.35	−14.89
DIPCS10	−8.12	8.42	10.87	0.01	23.19	1.51	−21.67
PA26	5.10	5.11	5.83	0.03	12.50	12.35	−0.15
SIE4x4	17.96	17.96	20.13	0.53	31.54	36.44	4.89
ALKBDE10	1.38	5.59	7.02	0.06	23.97	16.20	−7.77
YBDE18	−4.51	4.82	6.05	0.10	13.82	1.53	−12.28
AL2X6	−0.49	0.62	0.98	0.02	2.61	0.31	−2.29
HEAVYSB11	−1.77	2.56	3.32	0.04	10.38	2.58	−7.80
NBPRC	1.28	3.97	4.89	0.14	17.41	11.17	−6.24
ALK8	2.14	3.70	6.23	0.06	18.58	16.51	−2.06
RC21	2.38	3.11	3.73	0.09	11.28	8.39	−2.89
G2RC	0.06	5.90	7.56	0.12	32.53	18.31	−14.21
BH76RC	1.44	2.92	4.22	0.14	22.70	17.14	−5.56
FH51	0.61	2.64	3.53	0.09	16.23	8.56	−7.67
TAUT15	−0.49	1.44	1.77	0.47	5.88	3.23	−2.65
DC13	2.07	10.41	13.25	0.19	55.13	24.61	−30.52
MB16-43[a]	−63.27	63.27	68.15	0.15	108.55	−13.62	−122.17
DARC	8.07	8.07	8.62	0.25	9.51	11.46	1.95
RSE43	−2.67	2.67	3.06	0.35	7.85	−0.98	−8.83
BSR36	−5.09	5.09	5.84	0.31	11.32	−2.17	−13.49
CDIE20	2.19	2.22	2.47	0.55	4.17	3.87	−0.30
ISO34	−1.09	2.32	3.00	0.16	14.81	8.63	−6.18
ISOL24	−4.31	6.52	8.76	0.30	36.05	15.76	−20.29
C60ISO	−7.07	7.07	8.68	0.07	14.73	−1.23	−15.96
PArel	0.79	1.62	2.31	0.35	11.65	6.65	−5.00
BH76	−3.29	3.93	4.92	0.21	23.52	8.03	−15.49
BHPERI	1.02	1.86	2.13	0.09	7.86	4.30	−3.57
BHDIV10	−2.08	3.08	3.66	0.07	9.86	2.75	−7.11
INV24	−0.65	1.46	2.15	0.05	10.98	3.94	−7.04
BHROT27	0.90	0.98	1.32	0.16	3.97	3.12	−0.85
PX13	0.59	0.94	1.17	0.03	3.78	2.59	−1.19
WCPT18	−1.86	2.10	2.56	0.06	5.28	0.74	−4.54
RG18	−0.15	0.32	0.38	0.55	1.45	0.75	−0.70
ADIM6	0.94	0.94	1.09	0.28	1.70	1.86	0.16
S22	−0.40	0.44	0.52	0.06	1.48	0.43	−1.04
S66	−0.18	0.35	0.43	0.06	1.99	1.05	−0.94
HEAVY28	−0.44	0.53	0.57	0.43	1.37	0.44	−0.93
WATER27	−0.54	1.11	1.70	0.01	9.38	2.71	−6.67
CARBHB12	0.22	0.44	0.67	0.07	2.00	1.59	−0.41
PNICO23	−0.24	0.33	0.39	0.08	1.15	0.44	−0.70
HAL59	−0.04	0.49	0.65	0.11	3.75	2.84	−0.91
AHB21	0.15	0.49	0.62	0.02	2.89	0.99	−1.90
CHB6	1.90	1.90	2.22	0.07	2.82	3.42	0.59
IL16	−0.47	0.75	0.88	0.01	2.56	0.94	−1.62
IDISP	3.13	6.33	9.30	0.45	29.05	19.65	−9.41
ICONF	−0.04	0.30	0.35	0.09	1.18	0.58	−0.61
ACONF	−0.50	0.50	0.55	0.27	0.75	−0.16	−0.91
AMINO20x4	0.01	0.35	0.43	0.14	2.02	1.10	−0.92
PCONF21	0.25	1.28	1.55	0.79	5.14	2.17	−2.97
MCONF	0.66	0.90	1.13	0.18	3.11	2.25	−0.85
SCONF	−0.07	0.42	0.66	0.09	2.63	0.66	−1.97
UPU23	−0.66	0.73	1.07	0.13	4.01	0.49	−3.52
BUT14DIOL	0.09	0.22	0.26	0.08	0.99	0.61	−0.39

[a] Systems **6** and **16** did not converge and were omitted from the statistics

Table S49: Statistical analysis for the M11L-D3(0) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−3.45	6.46	8.26	0.02	45.89	20.33	−25.56
G21EA	2.72	5.66	6.55	0.17	26.43	12.63	−13.80
G21IP	−1.01	3.87	5.08	0.02	23.32	10.25	−13.08
DIPCS10	−4.29	7.37	8.61	0.01	20.77	4.70	−16.07
PA26	3.91	4.22	5.09	0.02	14.21	11.88	−2.34
SIE4x4	11.54	11.54	13.59	0.34	25.03	25.79	0.76
ALKBDE10	−10.78	10.78	12.57	0.11	19.80	−2.97	−22.77
YBDE18	−0.86	4.80	5.49	0.10	18.88	7.66	−11.22
AL2X6	−6.09	6.09	6.53	0.17	6.66	−1.82	−8.48
HEAVYSB11	0.06	2.62	3.23	0.05	10.89	5.39	−5.50
NBPRC	2.67	3.84	4.78	0.14	14.64	10.93	−3.71
ALK8	−2.36	9.52	13.10	0.15	45.85	27.77	−18.08
RC21	1.28	2.16	2.75	0.06	9.61	6.09	−3.52
G2RC	1.40	5.83	7.80	0.11	37.79	23.91	−13.89
BH76RC	0.22	3.27	4.68	0.15	23.73	7.86	−15.87
FH51	0.43	2.10	2.98	0.07	15.48	10.46	−5.02
TAUT15	0.91	1.29	1.59	0.42	5.11	3.14	−1.98
DC13	4.79	8.18	11.49	0.15	38.43	27.53	−10.90
MB16-43	−41.31	41.68	47.47	0.10	103.44	5.67	−97.77
DARC	2.16	2.30	2.78	0.07	4.58	3.97	−0.61
RSE43	−2.24	2.25	2.67	0.30	8.34	0.14	−8.20
BSR36	−0.29	0.54	0.82	0.03	4.19	1.21	−2.98
CDIE20	1.58	1.58	1.82	0.39	3.26	3.41	0.15
ISO34	0.54	1.20	1.64	0.08	6.52	3.14	−3.38
ISOL24	−1.09	3.51	4.96	0.16	25.03	16.50	−8.52
C60ISO	−6.80	6.85	8.89	0.07	17.07	0.22	−16.85
PArel	1.87	2.41	3.18	0.52	8.71	7.36	−1.35
BH76	−1.32	2.26	3.11	0.12	16.70	7.40	−9.31
BHPERI	−0.10	2.01	2.39	0.10	9.13	4.24	−4.89
BHDIV10	−0.38	3.32	3.86	0.07	13.14	6.33	−6.81
INV24	−0.14	2.04	3.48	0.06	18.84	6.78	−12.06
BHROT27	0.52	0.64	0.95	0.10	3.36	2.88	−0.48
PX13	1.60	1.88	2.23	0.06	5.96	4.35	−1.62
WCPT18	−1.43	2.28	2.88	0.07	8.08	2.53	−5.54
RG18	−1.29	1.29	1.95	2.22	6.17	−0.02	−6.19
ADIM6	1.44	1.44	1.75	0.43	2.75	2.81	0.06
S22	0.41	0.73	1.02	0.10	3.63	2.51	−1.12
S66	0.38	0.73	0.86	0.13	3.34	2.16	−1.18
HEAVY28	0.27	0.41	0.52	0.33	2.00	1.33	−0.67
WATER27	−5.63	6.14	8.68	0.08	34.11	6.96	−27.14
CARBHB12	−0.95	0.95	1.11	0.16	1.88	−0.32	−2.19
PNICO23	0.04	0.46	0.57	0.11	2.47	0.95	−1.51
HAL59	−0.49	0.81	1.08	0.18	5.99	1.65	−4.34
AHB21	0.82	1.17	1.63	0.05	5.95	4.73	−1.23
CHB6	0.71	0.71	0.79	0.03	1.04	1.46	0.42
IL16	−1.02	1.17	1.38	0.01	2.93	0.49	−2.44
IDISP	2.83	4.51	5.60	0.32	13.70	10.52	−3.18
ICONF	0.18	0.46	0.59	0.14	2.56	1.37	−1.20
ACONF	−0.16	0.17	0.22	0.09	0.52	0.05	−0.46
AMINO20x4	−0.03	0.55	0.69	0.23	3.05	1.29	−1.76
PCONF21	0.81	1.88	2.14	1.16	5.77	3.59	−2.18
MCONF	0.67	0.86	1.04	0.17	3.25	2.22	−1.03
SCONF	−0.12	0.35	0.43	0.08	1.63	0.59	−1.05
UPU23	−1.39	1.39	1.69	0.24	4.52	−0.14	−4.66
BUT14DIOL	−0.35	0.36	0.38	0.13	0.85	0.08	−0.77

Table S50: Statistical analysis for the MN12L-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.54	4.17	5.59	0.01	40.87	15.77	−25.10
G21EA	−1.63	3.41	4.58	0.10	17.74	5.35	−12.39
G21IP	−2.64	4.65	5.74	0.02	22.22	10.30	−11.92
DIPCS10	−14.64	14.64	16.40	0.02	22.12	−1.14	−23.26
PA26	2.31	3.14	3.82	0.02	10.86	6.99	−3.88
SIE4x4	7.50	9.26	11.51	0.27	30.63	24.24	−6.39
ALKBDE10	−7.60	7.60	10.45	0.08	20.09	−0.36	−20.45
YBDE18	0.03	6.53	7.01	0.13	20.64	12.02	−8.62
AL2X6	3.44	3.44	3.60	0.10	3.09	4.32	1.23
HEAVYSB11	−6.68	6.79	7.84	0.12	11.76	0.56	−11.20
NBPRC	−0.55	2.35	2.98	0.08	10.64	4.36	−6.28
ALK8	−0.11	8.90	13.83	0.14	47.66	13.51	−34.15
RC21	1.21	2.23	2.76	0.06	9.34	5.89	−3.45
G2RC	1.72	6.61	13.54	0.13	70.98	59.71	−11.26
BH76RC	0.59	2.35	3.45	0.11	16.95	6.06	−10.89
FH51	1.06	2.32	3.44	0.07	16.74	11.10	−5.64
TAUT15	1.00	2.13	2.80	0.70	9.06	6.02	−3.05
DC13	−1.02	7.91	10.84	0.14	41.28	11.55	−29.73
MB16-43	16.87	20.89	25.64	0.05	86.90	61.05	−25.85
DARC	4.74	4.74	5.46	0.15	7.86	8.03	0.17
RSE43	−2.33	2.33	2.79	0.31	8.31	−0.34	−8.65
BSR36	0.69	1.27	1.83	0.08	6.66	5.10	−1.57
CDIE20	1.83	1.83	2.05	0.45	3.32	3.47	0.16
ISO34	0.05	1.40	2.02	0.10	9.47	5.27	−4.21
ISOL24	−0.91	4.08	5.70	0.19	27.64	18.80	−8.84
C60ISO	−1.97	3.40	4.59	0.03	12.13	2.05	−10.08
PArel	1.69	2.01	3.15	0.43	10.87	9.22	−1.65
BH76	−0.88	1.75	2.44	0.09	13.41	4.80	−8.61
BHPERI	1.39	2.30	2.65	0.11	9.14	5.07	−4.08
BHDIV10	−0.49	2.03	2.17	0.04	5.70	2.83	−2.87
INV24	0.48	2.10	3.60	0.07	18.67	12.07	−6.60
BHROT27	1.14	1.16	1.57	0.19	3.84	3.59	−0.25
PX13	4.36	4.55	5.34	0.14	10.18	9.51	−0.67
WCPT18	0.03	1.52	1.87	0.04	7.05	3.04	−4.01
RG18	−0.88	0.88	1.20	1.52	3.12	−0.24	−3.36
ADIM6	0.87	1.08	1.37	0.32	3.08	2.60	−0.47
S22	0.04	1.01	1.45	0.14	6.24	3.85	−2.39
S66	0.00	0.79	0.92	0.14	3.38	1.72	−1.66
HEAVY28	0.25	0.52	0.71	0.42	2.93	2.07	−0.86
WATER27	−9.49	9.82	14.41	0.12	40.01	4.54	−35.47
CARBHB12	−0.76	0.76	0.85	0.13	1.48	−0.11	−1.59
PNICO23	0.09	0.25	0.35	0.06	1.53	1.09	−0.45
HAL59	−0.24	0.61	0.72	0.13	2.77	1.41	−1.36
AHB21	1.30	1.35	1.51	0.06	3.56	3.04	−0.52
CHB6	−0.59	0.64	0.74	0.02	1.43	0.13	−1.30
IL16	1.23	1.25	1.44	0.01	2.51	2.38	−0.13
IDISP	2.51	7.08	8.46	0.50	22.50	13.17	−9.32
ICONF	−0.02	0.58	0.72	0.18	2.53	1.30	−1.23
ACONF	−0.75	0.75	0.86	0.41	1.33	−0.19	−1.52
AMINO20x4	0.14	0.79	1.02	0.32	4.75	2.79	−1.96
PCONF21	1.38	3.18	3.69	1.96	11.09	5.95	−5.14
MCONF	1.53	1.65	1.89	0.33	4.41	3.62	−0.78
SCONF	0.16	0.62	0.90	0.13	4.03	1.69	−2.35
UPU23	−0.74	0.98	1.51	0.17	6.16	0.91	−5.25
BUT14DIOL	−0.64	0.64	0.72	0.23	1.40	−0.14	−1.53

Table S51: Statistical analysis for the MN15L-D3(0) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	0.05	3.41	4.67	0.01	33.14	11.22	−21.92
G21EA	0.97	2.40	2.88	0.07	11.74	6.23	−5.51
G21IP	−1.89	3.46	4.51	0.01	20.87	8.64	−12.24
DIPCS10	−10.18	10.46	12.05	0.02	20.95	1.40	−19.55
PA26	0.92	2.25	2.91	0.01	12.29	7.37	−4.92
SIE4x4	10.81	10.99	13.42	0.33	26.10	24.92	−1.18
ALKBDE10	−4.48	4.48	5.13	0.04	9.80	−0.06	−9.86
YBDE18	−4.11	4.20	5.04	0.09	9.63	0.81	−8.82
AL2X6	1.03	1.35	1.46	0.04	2.92	1.97	−0.95
HEAVYSB11	−5.72	6.47	7.54	0.11	17.18	2.87	−14.31
NBPRC	−0.47	1.93	2.98	0.07	11.76	2.92	−8.85
ALK8	−1.12	3.23	4.29	0.05	14.95	7.84	−7.10
RC21	0.75	2.00	2.55	0.06	8.51	5.92	−2.58
G2RC	2.29	6.73	8.33	0.13	28.84	18.58	−10.26
BH76RC	0.98	2.43	3.44	0.11	19.58	10.35	−9.23
FH51	0.82	2.55	3.67	0.08	19.78	13.91	−5.87
TAUT15	0.46	0.70	0.96	0.23	3.20	2.03	−1.17
DC13	3.18	7.83	10.28	0.14	32.39	25.31	−7.08
MB16-43	−9.44	20.42	25.52	0.05	103.56	44.64	−58.92
DARC	2.39	2.78	3.12	0.09	6.11	4.62	−1.49
RSE43	−0.99	1.23	1.53	0.16	7.24	1.92	−5.32
BSR36	3.55	3.55	4.40	0.22	10.87	11.29	0.42
CDIE20	1.78	1.78	1.94	0.44	2.91	3.34	0.43
ISO34	−0.82	1.88	2.34	0.13	9.49	4.80	−4.69
ISOL24	−2.29	3.55	4.70	0.16	20.32	10.33	−10.00
C60ISO	−5.79	5.94	7.93	0.06	16.54	0.67	−15.87
PArel	1.66	2.19	2.93	0.47	10.13	7.04	−3.10
BH76	−1.10	1.81	2.64	0.10	13.59	3.53	−10.06
BHPERI	0.85	1.78	2.12	0.09	8.41	4.20	−4.21
BHDIV10	−0.03	2.08	2.49	0.05	8.96	4.82	−4.15
INV24	1.26	2.02	3.74	0.06	19.16	13.52	−5.63
BHROT27	0.82	0.87	1.17	0.14	3.39	2.85	−0.54
PX13	6.38	6.38	6.87	0.19	9.00	11.11	2.10
WCPT18	1.08	1.81	2.41	0.05	6.84	4.70	−2.14
RG18	0.10	0.17	0.29	0.29	1.02	0.77	−0.25
ADIM6	3.88	3.88	4.35	1.15	5.39	6.62	1.24
S22	0.03	1.82	2.40	0.25	9.45	5.26	−4.19
S66	0.60	1.66	1.97	0.30	8.03	4.72	−3.31
HEAVY28	0.06	0.58	0.71	0.47	2.66	1.21	−1.45
WATER27	−11.26	12.00	16.73	0.15	56.04	10.09	−45.94
CARBHB12	−1.20	1.20	1.42	0.20	2.63	−0.19	−2.82
PNICO23	−0.18	0.40	0.48	0.09	1.80	0.55	−1.25
HAL59	−0.18	0.59	0.78	0.13	3.96	2.06	−1.90
AHB21	2.28	2.29	2.46	0.10	4.33	4.20	−0.12
CHB6	0.64	0.64	0.75	0.02	0.91	1.03	0.12
IL16	2.40	2.40	2.62	0.02	3.32	4.17	0.86
IDISP	2.99	7.54	8.62	0.53	22.52	14.06	−8.46
ICONF	0.11	0.53	0.65	0.16	2.50	1.43	−1.07
ACONF	−0.69	0.69	0.81	0.38	1.35	−0.15	−1.51
AMINO20x4	−0.04	0.92	1.18	0.38	6.10	3.19	−2.91
PCONF21	1.28	4.10	4.59	2.53	13.43	7.42	−6.00
MCONF	1.52	1.60	1.81	0.32	4.07	3.27	−0.80
SCONF	−0.37	0.92	1.14	0.20	3.86	1.87	−1.99
UPU23	−1.47	1.67	2.44	0.29	8.92	0.87	−8.05
BUT14DIOL	−1.10	1.10	1.16	0.39	1.76	−0.36	−2.12

SI.7.3 Results for dispersion-corrected hybrid functionals

Table S52: Statistical analysis for the B3LYP-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−1.25	3.40	5.53	0.01	40.94	9.79	−31.15
G21EA	0.55	1.91	2.48	0.06	10.01	7.45	−2.56
G21IP	−0.15	3.55	4.38	0.01	16.75	9.59	−7.16
DIPCS10	−2.19	4.73	5.93	0.01	19.90	9.22	−10.68
PA26	2.80	2.87	3.62	0.02	9.93	9.06	−0.88
SIE4x4	18.06	18.06	20.57	0.54	36.88	40.25	3.38
ALKBDE10	−1.39	4.39	4.99	0.04	15.97	7.51	−8.46
YBDE18	−4.37	4.72	5.74	0.10	13.44	2.64	−10.81
AL2X6	−2.71	2.71	2.78	0.08	1.47	−2.01	−3.48
HEAVYSB11	−3.30	3.30	3.69	0.06	6.29	−0.19	−6.48
NBPRC	1.32	2.00	3.03	0.07	9.59	7.97	−1.63
ALK8	0.55	2.48	3.14	0.04	10.29	5.58	−4.70
RC21	1.49	2.44	2.97	0.07	10.00	4.50	−5.50
G2RC	0.74	2.73	3.32	0.05	13.00	7.82	−5.18
BH76RC	−0.38	2.25	2.79	0.11	11.61	4.25	−7.36
FH51	1.45	2.61	3.51	0.08	17.38	8.87	−8.51
TAUT15	−0.16	1.16	1.38	0.38	4.54	2.71	−1.82
DC13	2.34	10.57	13.11	0.19	47.67	21.27	−26.40
MB16-43	−23.19	24.84	28.92	0.06	85.74	19.81	−65.92
DARC	8.03	8.03	8.26	0.25	6.85	9.66	2.81
RSE43	−1.72	1.72	1.96	0.23	3.78	−0.62	−4.40
BSR36	−3.35	3.35	3.87	0.21	7.54	−1.23	−8.76
CDIE20	0.98	1.00	1.12	0.25	2.18	2.02	−0.15
ISO34	−0.14	1.78	2.64	0.12	14.53	10.46	−4.08
ISOL24	−2.32	5.80	8.15	0.26	39.18	19.03	−20.15
C60ISO	0.00	2.22	2.56	0.02	7.12	2.22	−4.90
PArel	0.00	1.18	1.71	0.25	8.38	5.40	−2.98
BH76	−4.81	5.70	6.45	0.31	27.22	16.19	−11.03
BHPERI	−0.84	1.18	1.55	0.06	6.15	1.87	−4.28
BHDIV10	−2.12	3.22	3.78	0.07	10.63	5.18	−5.45
INV24	−0.37	1.05	1.37	0.03	6.39	3.25	−3.14
BHROT27	0.36	0.41	0.60	0.07	1.49	1.31	−0.17
PX13	−4.33	4.33	4.46	0.13	3.95	−2.61	−6.56
WCPT18	−2.13	2.27	2.94	0.06	7.29	1.08	−6.21
RG18	−0.08	0.13	0.20	0.22	0.88	0.25	−0.62
ADIM6	0.09	0.11	0.13	0.03	0.29	0.24	−0.05
S22	0.29	0.31	0.43	0.04	1.22	1.16	−0.05
S66	0.25	0.26	0.39	0.05	1.50	1.38	−0.12
HEAVY28	0.33	0.34	0.38	0.27	0.77	0.63	−0.14
WATER27	3.74	4.07	5.48	0.05	18.31	13.89	−4.42
CARBHB12	0.88	0.88	1.07	0.15	1.95	2.20	0.25
PNICO23	0.48	0.48	0.58	0.11	1.31	1.33	0.02
HAL59	0.51	0.57	0.84	0.12	3.54	3.22	−0.32
AHB21	−0.18	0.33	0.44	0.01	1.72	0.58	−1.14
CHB6	−0.97	1.41	1.48	0.05	3.54	1.30	−2.24
IL16	0.70	0.76	0.92	0.01	1.82	1.50	−0.32
IDISP	3.30	3.57	5.53	0.25	13.19	12.38	−0.81
ICONF	−0.03	0.29	0.40	0.09	1.85	0.83	−1.02
ACONF	−0.02	0.05	0.07	0.03	0.30	0.13	−0.17
AMINO20x4	−0.02	0.21	0.29	0.09	1.92	1.12	−0.80
PCONF21	−0.06	0.53	0.61	0.33	1.84	0.73	−1.12
MCONF	−0.02	0.22	0.27	0.04	1.22	0.51	−0.71
SCONF	−0.12	0.30	0.51	0.07	2.18	0.35	−1.83
UPU23	0.43	0.61	0.72	0.11	2.50	1.46	−1.05
BUT14DIOL	0.30	0.31	0.34	0.11	0.96	0.82	−0.14

Table S53: Statistical analysis for the B3LYP-NL DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	1.97	3.84	5.16	0.01	40.03	13.97	−26.06
G21EA	−1.76	2.47	2.85	0.07	8.92	4.34	−4.58
G21IP	−3.06	4.46	5.25	0.02	16.30	6.45	−9.85
DIPCS10	−7.52	8.24	9.08	0.01	18.27	3.58	−14.69
PA26	1.36	1.64	2.41	0.01	8.45	7.29	−1.16
SIE4x4	18.10	18.10	20.61	0.54	37.13	40.25	3.12
ALKBDE10	−0.73	4.29	4.88	0.04	15.67	8.10	−7.57
YBDE18	−3.28	4.12	5.24	0.08	14.66	4.63	−10.04
AL2X6	−2.97	2.97	3.10	0.08	2.49	−1.90	−4.39
HEAVYSB11	−2.56	2.56	3.14	0.04	5.77	−0.07	−5.84
NBPRC	0.87	1.71	2.30	0.06	7.33	5.71	−1.62
ALK8	−2.61	3.37	4.73	0.05	12.87	2.40	−10.47
RC21	2.81	3.33	3.89	0.09	9.30	6.56	−2.74
G2RC	0.16	3.14	4.02	0.06	16.82	8.66	−8.16
BH76RC	−0.37	2.28	2.92	0.11	13.16	5.19	−7.97
FH51	0.86	2.34	3.21	0.08	15.01	8.66	−6.35
TAUT15	0.16	1.15	1.55	0.38	5.08	3.48	−1.60
DC13	1.02	8.55	9.65	0.16	29.68	12.59	−17.09
MB16-43	−21.17	23.47	28.18	0.06	83.82	14.54	−69.27
DARC	4.80	4.80	5.10	0.15	5.94	6.20	0.26
RSE43	−1.69	1.69	1.93	0.22	3.78	−0.65	−4.43
BSR36	−2.70	2.70	3.04	0.17	5.55	−1.18	−6.73
CDIE20	0.92	0.92	1.02	0.23	1.76	1.82	0.06
ISO34	−0.28	1.43	2.09	0.10	12.71	8.15	−4.57
ISOL24	−1.62	4.02	5.56	0.18	26.74	14.74	−12.00
C60ISO	−1.87	2.77	3.61	0.03	8.81	1.26	−7.55
PArel	0.26	0.95	1.66	0.21	7.89	5.86	−2.03
BH76	−5.95	6.01	6.61	0.32	14.27	1.67	−12.60
BHPERI	−1.53	1.58	1.92	0.08	4.32	0.32	−4.00
BHDIV10	−2.81	3.72	4.17	0.08	11.23	4.56	−6.66
INV24	−0.82	0.99	1.25	0.03	4.11	1.11	−3.00
BHROT27	0.39	0.43	0.63	0.07	1.63	1.40	−0.23
PX13	−5.84	5.84	5.99	0.18	5.37	−3.50	−8.88
WCPT18	−3.22	3.24	4.00	0.09	7.80	0.18	−7.62
RG18	−0.04	0.11	0.14	0.19	0.55	0.20	−0.35
ADIM6	−0.17	0.17	0.18	0.05	0.18	−0.10	−0.28
S22	0.06	0.48	0.63	0.07	2.50	1.78	−0.72
S66	0.09	0.43	0.56	0.08	2.55	2.01	−0.54
HEAVY28	−0.17	0.26	0.30	0.21	1.00	0.39	−0.61
WATER27	6.91	7.34	9.95	0.09	30.17	24.34	−5.83
CARBHB12	0.83	0.83	1.05	0.14	2.06	2.10	0.04
PNICO23	0.18	0.37	0.45	0.09	1.79	1.25	−0.54
HAL59	0.46	0.63	1.01	0.14	4.45	3.89	−0.56
AHB21	−0.72	0.72	0.84	0.03	1.47	−0.18	−1.65
CHB6	−0.82	1.00	1.09	0.04	2.21	0.53	−1.67
IL16	0.13	0.31	0.37	0.00	1.27	0.84	−0.43
IDISP	2.45	2.91	4.25	0.20	10.99	9.61	−1.37
ICONF	0.03	0.25	0.36	0.08	1.58	0.84	−0.74
ACONF	−0.01	0.06	0.08	0.03	0.29	0.18	−0.11
AMINO20x4	0.05	0.21	0.28	0.09	1.68	1.12	−0.56
PCONF21	−0.10	0.36	0.45	0.22	1.70	0.64	−1.07
MCONF	0.09	0.19	0.24	0.04	0.88	0.42	−0.45
SCONF	0.16	0.57	0.73	0.12	2.81	0.67	−2.13
UPU23	0.22	0.43	0.58	0.08	2.53	1.19	−1.34
BUT14DIOL	0.53	0.53	0.54	0.19	0.77	0.78	0.01

Table S54: Statistical analysis for the B3PW91-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	0.47	3.32	4.68	0.01	33.86	9.08	−24.78
G21EA	1.03	2.14	2.70	0.06	7.87	5.68	−2.19
G21IP	1.07	3.64	4.37	0.01	17.95	10.56	−7.38
DIPCS10	0.47	3.13	3.38	0.00	10.05	5.10	−4.95
PA26	4.14	4.14	4.59	0.02	8.31	9.73	1.42
SIE4x4	16.47	16.47	18.55	0.49	32.17	36.16	3.99
ALKBDE10	−1.74	5.13	6.09	0.05	21.85	12.38	−9.47
YBDE18	−1.40	1.67	2.12	0.03	6.43	1.66	−4.77
AL2X6	0.69	1.85	2.03	0.05	5.71	2.24	−3.46
HEAVYSB11	−0.51	1.18	1.49	0.02	4.10	1.23	−2.87
NBPRC	−0.60	2.12	2.30	0.08	7.05	2.79	−4.26
ALK8	4.43	4.43	5.89	0.07	9.22	9.46	0.24
RC21	4.01	4.45	5.16	0.12	11.87	9.50	−2.37
G2RC	−1.27	5.11	6.43	0.10	28.18	10.62	−17.55
BH76RC	−0.24	2.04	3.00	0.10	16.59	9.37	−7.21
FH51	−0.27	2.08	3.00	0.07	17.26	8.60	−8.66
TAUT15	0.16	1.27	1.59	0.42	5.25	3.53	−1.72
DC13	−0.53	5.45	8.21	0.10	37.26	16.93	−20.33
MB16-43	6.34	15.80	20.24	0.04	111.15	73.44	−37.70
DARC	−1.20	1.76	2.44	0.05	7.66	1.35	−6.31
RSE43	−1.54	1.54	1.77	0.20	3.81	−0.37	−4.18
BSR36	−1.70	1.70	1.80	0.10	2.73	−0.74	−3.46
CDIE20	1.22	1.23	1.42	0.30	2.78	2.63	−0.15
ISO34	−0.24	1.10	1.54	0.08	8.47	5.07	−3.40
ISOL24	−0.01	2.19	3.06	0.10	14.08	6.30	−7.78
C60ISO	−0.04	2.47	2.93	0.03	8.43	2.76	−5.67
PArel	0.48	1.19	1.72	0.26	7.09	5.51	−1.59
BH76	−4.78	4.88	5.35	0.26	16.49	2.28	−14.21
BHPERI	−3.53	3.53	3.92	0.17	6.57	−0.26	−6.83
BHDIV10	−4.45	5.06	5.52	0.11	11.88	3.04	−8.84
INV24	−0.36	1.14	1.64	0.04	7.54	4.06	−3.48
BHROT27	0.49	0.52	0.70	0.08	1.57	1.44	−0.14
PX13	−6.80	6.80	7.00	0.20	6.26	−4.23	−10.49
WCPT18	−4.15	4.15	4.76	0.12	8.59	−1.00	−9.59
RG18	−0.43	0.43	0.65	0.74	2.11	−0.11	−2.22
ADIM6	−0.24	0.24	0.25	0.07	0.24	−0.10	−0.35
S22	0.33	0.44	0.55	0.06	1.51	1.17	−0.34
S66	0.10	0.29	0.36	0.05	1.69	1.23	−0.46
HEAVY28	0.30	0.34	0.42	0.27	1.26	0.92	−0.34
WATER27	−0.13	1.40	2.12	0.02	10.09	2.46	−7.63
CARBHB12	1.04	1.04	1.44	0.17	3.09	3.16	0.07
PNICO23	0.79	0.89	1.26	0.21	4.62	4.11	−0.51
HAL59	0.45	0.70	1.01	0.15	4.06	3.24	−0.82
AHB21	−0.43	0.63	0.87	0.03	3.15	0.61	−2.54
CHB6	−0.32	0.76	0.88	0.03	2.54	1.26	−1.28
IL16	0.11	0.39	0.44	0.00	1.55	0.89	−0.66
IDISP	1.50	1.69	1.95	0.12	4.10	3.53	−0.57
ICONF	0.10	0.25	0.37	0.08	1.44	1.11	−0.33
ACONF	−0.17	0.17	0.18	0.09	0.31	−0.01	−0.32
AMINO20x4	0.02	0.33	0.43	0.14	2.06	1.19	−0.87
PCONF21	−0.16	0.72	0.87	0.44	2.91	1.12	−1.79
MCONF	0.30	0.49	0.58	0.10	1.96	1.16	−0.80
SCONF	0.07	0.51	0.75	0.11	3.04	0.71	−2.32
UPU23	0.41	0.59	0.71	0.10	2.66	1.56	−1.10
BUT14DIOL	0.19	0.22	0.29	0.08	1.08	0.82	−0.26

Table S55: Statistical analysis for the B3P86-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	4.87	6.52	8.26	0.02	48.48	23.80	−24.68
G21EA	3.37	3.37	4.14	0.10	7.95	8.05	0.09
G21IP	2.54	3.86	4.81	0.01	16.33	11.91	−4.42
DIPCS10	3.20	3.88	4.73	0.01	9.89	7.96	−1.93
PA26	2.83	2.83	3.41	0.01	7.67	8.25	0.59
SIE4x4	17.47	17.47	20.01	0.52	36.48	39.84	3.36
ALKBDE10	−0.88	4.27	5.46	0.04	20.38	11.49	−8.89
YBDE18	−1.79	2.17	2.71	0.04	7.39	1.76	−5.63
AL2X6	−0.35	0.66	1.25	0.02	3.37	0.34	−3.03
HEAVYSB11	−1.36	1.48	1.98	0.03	4.06	0.40	−3.66
NBPRC	−0.30	1.72	2.00	0.06	6.64	3.03	−3.61
ALK8	1.61	1.79	2.37	0.03	4.58	4.28	−0.29
RC21	4.11	4.49	5.16	0.13	11.25	8.77	−2.49
G2RC	−1.43	5.08	6.24	0.10	26.53	10.24	−16.29
BH76RC	−0.83	2.60	3.55	0.12	17.06	7.12	−9.94
FH51	−0.16	2.12	3.04	0.07	17.17	8.70	−8.46
TAUT15	0.33	1.28	1.77	0.42	5.92	4.06	−1.86
DC13	−0.06	5.75	7.68	0.10	32.30	15.06	−17.24
MB16-43	−2.01	13.91	18.31	0.03	96.27	58.24	−38.03
DARC	0.42	2.04	2.35	0.06	8.15	2.88	−5.27
RSE43	−1.67	1.67	1.89	0.22	3.82	−0.50	−4.32
BSR36	−2.70	2.70	2.99	0.17	5.07	−1.31	−6.38
CDIE20	1.21	1.22	1.40	0.30	2.66	2.54	−0.13
ISO34	−0.28	1.10	1.62	0.08	9.44	5.98	−3.46
ISOL24	−0.56	2.77	3.81	0.13	17.73	9.10	−8.63
C60ISO	−0.42	2.46	2.99	0.03	8.39	2.35	−6.05
PArel	0.47	1.23	1.80	0.27	7.75	5.72	−2.03
BH76	−5.79	5.91	6.48	0.32	17.44	2.67	−14.77
BHPERI	−3.04	3.04	3.29	0.15	4.98	−0.61	−5.58
BHDIV10	−4.36	5.06	5.52	0.11	12.23	3.48	−8.76
INV24	−0.69	1.11	1.50	0.03	6.11	2.58	−3.53
BHROT27	0.47	0.50	0.68	0.08	1.57	1.38	−0.19
PX13	−7.81	7.81	8.02	0.23	7.17	−4.91	−12.08
WCPT18	−4.66	4.66	5.29	0.13	8.79	−1.33	−10.11
RG18	−0.48	0.48	0.75	0.83	2.46	−0.08	−2.54
ADIM6	−0.12	0.15	0.18	0.04	0.40	0.08	−0.33
S22	0.36	0.43	0.59	0.06	1.86	1.60	−0.26
S66	0.20	0.28	0.44	0.05	2.11	1.79	−0.32
HEAVY28	0.19	0.25	0.32	0.20	1.00	0.76	−0.24
WATER27	3.57	4.19	5.35	0.05	22.20	13.88	−8.32
CARBHB12	1.16	1.16	1.51	0.19	2.95	3.16	0.21
PNICO23	0.73	0.78	1.11	0.18	3.86	3.60	−0.27
HAL59	0.49	0.68	1.04	0.15	4.28	3.63	−0.65
AHB21	−0.75	0.79	1.00	0.04	2.72	0.28	−2.43
CHB6	−0.04	0.49	0.66	0.02	1.97	1.32	−0.65
IL16	−0.02	0.34	0.38	0.00	1.11	0.43	−0.68
IDISP	1.83	1.83	2.00	0.13	2.13	2.82	0.69
ICONF	0.13	0.27	0.38	0.08	1.49	0.98	−0.51
ACONF	−0.09	0.09	0.11	0.05	0.25	0.03	−0.22
AMINO20x4	0.05	0.32	0.40	0.13	2.08	1.23	−0.85
PCONF21	−0.16	0.83	0.95	0.51	2.64	0.91	−1.73
MCONF	0.26	0.39	0.48	0.08	1.64	0.98	−0.66
SCONF	0.12	0.55	0.74	0.12	2.96	0.67	−2.30
UPU23	0.36	0.58	0.70	0.10	2.87	1.59	−1.28
BUT14DIOL	0.36	0.36	0.40	0.13	1.05	0.93	−0.12

Table S56: Statistical analysis for the BHLYP-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−20.11	20.20	24.29	0.07	65.30	3.12	−62.18
G21EA	−4.34	5.34	6.09	0.16	17.42	5.43	−12.00
G21IP	−1.54	4.53	5.53	0.02	22.38	11.35	−11.03
DIPCS10	−3.76	7.12	8.80	0.01	26.55	8.15	−18.40
PA26	3.65	3.75	4.47	0.02	11.24	9.93	−1.30
SIE4x4	7.45	7.45	9.71	0.22	21.54	22.16	0.63
ALKBDE10	−13.11	13.11	14.86	0.13	26.44	−4.27	−30.70
YBDE18	−5.64	5.64	6.01	0.11	8.16	−2.79	−10.95
AL2X6	−1.12	1.56	1.70	0.04	3.90	1.32	−2.58
HEAVYSB11	−5.88	5.88	6.33	0.10	7.08	−3.29	−10.37
NBPRC	1.05	2.39	2.88	0.09	8.11	4.99	−3.12
ALK8	1.80	4.23	5.22	0.07	15.22	9.73	−5.48
RC21	1.29	2.55	3.21	0.07	14.11	8.88	−5.22
G2RC	−3.22	4.29	5.40	0.08	19.88	7.64	−12.24
BH76RC	−1.22	3.90	4.90	0.18	22.27	9.33	−12.94
FH51	−1.07	1.96	2.59	0.06	11.37	3.94	−7.43
TAUT15	−0.09	0.57	0.79	0.19	3.14	0.93	−2.21
DC13	−0.59	9.55	11.87	0.17	41.00	16.20	−24.80
MB16-43	−27.85	31.73	41.48	0.08	147.92	30.28	−117.65
DARC	2.40	2.80	2.94	0.09	6.32	3.51	−2.81
RSE43	−0.30	0.48	0.62	0.06	2.22	0.90	−1.33
BSR36	−4.47	4.47	5.17	0.28	10.41	−1.49	−11.90
CDIE20	0.50	0.63	0.85	0.16	2.73	1.90	−0.84
ISO34	0.30	1.24	2.05	0.09	12.90	9.38	−3.53
ISOL24	−0.49	3.56	4.49	0.16	19.23	9.01	−10.22
C60ISO	13.09	13.09	14.03	0.13	16.04	21.75	5.71
PArel	0.52	1.14	1.64	0.25	6.18	4.60	−1.59
BH76	1.25	3.37	8.42	0.18	60.52	51.13	−9.39
BHPERI	4.18	4.18	4.34	0.20	4.90	6.33	1.44
BHDIV10	2.68	2.68	3.31	0.06	5.47	5.65	0.18
INV24	1.07	2.17	3.57	0.07	19.72	13.23	−6.49
BHROT27	0.58	0.59	0.85	0.09	1.89	1.79	−0.10
PX13	2.08	2.08	2.34	0.06	3.59	3.77	0.18
WCPT18	3.55	3.55	4.19	0.10	7.82	8.88	1.06
RG18	0.00	0.06	0.08	0.10	0.34	0.21	−0.13
ADIM6	−0.05	0.05	0.06	0.01	0.11	−0.02	−0.13
S22	0.31	0.53	0.75	0.07	3.01	2.19	−0.83
S66	0.28	0.40	0.62	0.07	2.71	2.30	−0.41
HEAVY28	0.25	0.26	0.31	0.21	0.74	0.59	−0.15
WATER27	4.12	4.12	5.52	0.05	12.69	13.11	0.43
CARBHB12	0.60	0.60	0.70	0.10	1.15	1.35	0.20
PNICO23	0.26	0.33	0.43	0.08	1.83	1.05	−0.78
HAL59	0.12	0.29	0.40	0.06	2.34	1.61	−0.73
AHB21	−0.79	0.91	1.30	0.04	4.50	0.56	−3.94
CHB6	−2.44	2.44	2.73	0.09	3.68	−0.35	−4.03
IL16	0.94	1.06	1.22	0.01	2.66	2.04	−0.62
IDISP	1.48	3.88	4.86	0.27	13.93	7.06	−6.87
ICONF	0.07	0.43	0.59	0.13	2.26	1.21	−1.05
ACONF	0.13	0.13	0.15	0.07	0.20	0.24	0.04
AMINO20x4	0.04	0.24	0.30	0.10	1.56	0.81	−0.75
PCONF21	0.28	0.31	0.43	0.19	1.08	0.95	−0.13
MCONF	−0.09	0.14	0.16	0.03	0.54	0.18	−0.36
SCONF	−0.35	0.41	0.45	0.09	1.22	0.54	−0.68
UPU23	0.65	0.73	0.91	0.13	2.35	1.65	−0.70
BUT14DIOL	0.12	0.12	0.15	0.04	0.38	0.35	−0.03

Table S57: Statistical analysis for the B1P86-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	0.00	4.81	6.79	0.02	48.37	18.09	−30.28
G21EA	1.97	2.75	3.54	0.08	9.81	7.18	−2.62
G21IP	1.64	3.78	4.58	0.01	16.50	11.24	−5.26
DIPCS10	1.93	3.67	4.13	0.01	11.12	7.05	−4.07
PA26	3.03	3.03	3.59	0.02	8.11	8.40	0.29
SIE4x4	15.38	15.38	17.79	0.46	33.15	36.41	3.27
ALKBDE10	−3.93	5.28	6.42	0.05	19.96	6.07	−13.90
YBDE18	−2.01	2.03	2.32	0.04	4.61	0.22	−4.40
AL2X6	0.11	0.90	1.12	0.03	3.09	0.72	−2.37
HEAVYSB11	−2.10	2.10	2.32	0.04	3.04	−1.09	−4.12
NBPRC	−0.49	2.13	2.32	0.08	7.67	4.00	−3.68
ALK8	1.68	1.81	2.50	0.03	5.35	5.06	−0.29
RC21	4.12	4.54	5.23	0.13	12.72	10.72	−2.01
G2RC	−2.19	5.51	6.82	0.11	29.20	10.55	−18.64
BH76RC	−0.94	2.73	3.54	0.13	14.54	4.71	−9.83
FH51	−0.69	2.23	3.05	0.07	16.04	7.75	−8.29
TAUT15	0.39	1.12	1.63	0.37	5.44	3.74	−1.70
DC13	−0.65	5.45	7.65	0.10	32.41	16.89	−15.53
MB16-43	−2.03	13.99	18.56	0.03	96.90	61.71	−35.18
DARC	−1.54	1.88	2.70	0.06	7.92	0.84	−7.09
RSE43	−1.30	1.30	1.49	0.17	3.17	−0.38	−3.55
BSR36	−2.68	2.68	2.93	0.17	4.79	−1.36	−6.15
CDIE20	1.12	1.14	1.34	0.28	2.73	2.53	−0.20
ISO34	−0.22	1.17	1.59	0.08	8.35	5.13	−3.21
ISOL24	0.03	2.06	2.91	0.09	13.58	5.74	−7.84
C60ISO	1.58	2.67	2.79	0.03	6.43	3.69	−2.73
PArel	0.59	1.14	1.70	0.25	7.57	5.46	−2.11
BH76	−4.80	4.98	5.49	0.27	14.32	2.75	−11.57
BHPERI	−2.65	2.69	2.99	0.13	5.60	0.45	−5.15
BHDIV10	−3.86	4.52	4.91	0.10	10.92	3.29	−7.63
INV24	−0.78	1.17	1.60	0.04	6.34	2.40	−3.94
BHROT27	0.49	0.52	0.70	0.08	1.53	1.37	−0.16
PX13	−6.96	6.96	7.18	0.21	6.74	−4.17	−10.91
WCPT18	−3.92	3.92	4.63	0.11	8.47	−0.59	−9.06
RG18	−0.57	0.57	0.85	0.98	2.68	−0.16	−2.84
ADIM6	−0.19	0.19	0.23	0.06	0.39	0.00	−0.39
S22	0.36	0.44	0.60	0.06	1.97	1.66	−0.31
S66	0.17	0.28	0.44	0.05	2.21	1.83	−0.37
HEAVY28	0.11	0.22	0.28	0.18	0.97	0.67	−0.29
WATER27	2.87	3.44	4.30	0.04	18.80	11.13	−7.67
CARBHB12	1.08	1.08	1.42	0.18	2.80	2.97	0.16
PNICO23	0.68	0.75	1.06	0.18	3.78	3.42	−0.37
HAL59	0.35	0.61	0.91	0.13	3.80	3.07	−0.73
AHB21	−0.78	0.83	1.09	0.04	2.95	0.32	−2.63
CHB6	−0.07	0.50	0.65	0.02	2.00	1.21	−0.79
IL16	0.01	0.36	0.40	0.00	1.20	0.49	−0.71
IDISP	1.30	1.30	1.60	0.09	2.39	2.41	0.02
ICONF	0.16	0.28	0.39	0.09	1.45	1.02	−0.43
ACONF	−0.10	0.10	0.12	0.05	0.24	0.03	−0.21
AMINO20x4	0.05	0.31	0.39	0.13	1.93	1.11	−0.82
PCONF21	−0.11	0.76	0.88	0.47	2.64	0.97	−1.67
MCONF	0.29	0.41	0.49	0.08	1.58	1.00	−0.58
SCONF	0.11	0.50	0.67	0.11	2.67	0.59	−2.08
UPU23	0.37	0.59	0.72	0.10	2.93	1.56	−1.36
BUT14DIOL	0.31	0.31	0.35	0.11	0.96	0.84	−0.11

Table S58: Statistical analysis for the B1LYP-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−7.06	7.32	9.22	0.02	37.74	4.17	−33.56
G21EA	−1.53	2.60	3.07	0.08	11.07	6.46	−4.62
G21IP	−1.94	4.23	4.96	0.02	17.21	7.88	−9.33
DIPCS10	−4.78	6.27	7.83	0.01	22.26	7.30	−14.96
PA26	2.87	2.96	3.71	0.02	10.43	9.25	−1.18
SIE4x4	16.07	16.07	18.44	0.48	33.68	36.89	3.21
ALKBDE10	−4.02	4.64	5.93	0.05	15.50	2.55	−12.95
YBDE18	−4.78	4.78	5.43	0.10	9.52	−0.37	−9.88
AL2X6	−0.07	0.90	1.17	0.03	3.41	2.50	−0.91
HEAVYSB11	−1.41	2.67	3.18	0.05	9.53	4.45	−5.08
NBPRC	1.33	2.17	3.20	0.08	9.95	8.44	−1.51
ALK8	5.65	5.98	7.66	0.10	15.24	13.95	−1.29
RC21	0.79	2.18	2.57	0.06	9.66	3.40	−6.25
G2RC	0.73	2.60	3.04	0.05	10.11	5.55	−4.56
BH76RC	−0.34	2.26	2.72	0.11	11.77	5.26	−6.51
FH51	1.39	2.49	3.38	0.08	18.64	9.24	−9.40
TAUT15	−0.20	0.97	1.15	0.32	3.84	2.08	−1.76
DC13	1.90	9.91	12.76	0.18	49.00	21.36	−27.64
MB16-43	−12.13	15.52	18.82	0.04	81.06	33.42	−47.64
DARC	7.80	7.80	7.99	0.24	6.29	9.13	2.84
RSE43	−1.34	1.34	1.56	0.18	3.28	−0.31	−3.59
BSR36	−3.22	3.22	3.62	0.20	6.50	−1.38	−7.88
CDIE20	0.87	0.91	1.03	0.22	2.24	1.92	−0.33
ISO34	−0.05	1.80	2.70	0.12	14.63	10.84	−3.79
ISOL24	−2.12	5.62	7.77	0.26	36.71	17.28	−19.43
C60ISO	2.50	2.94	3.21	0.03	6.25	5.23	−1.02
PArel	0.02	1.11	1.57	0.24	6.93	5.10	−1.83
BH76	−4.28	4.33	4.86	0.23	11.70	1.03	−10.68
BHPERI	0.08	0.94	1.24	0.05	6.08	2.92	−3.16
BHDIV10	−1.22	2.32	2.95	0.05	9.72	5.45	−4.27
INV24	−0.02	1.04	1.49	0.03	6.93	3.89	−3.04
BHROT27	0.36	0.40	0.58	0.06	1.47	1.31	−0.17
PX13	−2.52	2.52	2.65	0.08	2.72	−1.17	−3.89
WCPT18	−0.67	1.60	1.91	0.05	6.12	2.18	−3.94
RG18	0.01	0.15	0.20	0.26	0.89	0.36	−0.53
ADIM6	−0.03	0.06	0.07	0.02	0.21	0.10	−0.11
S22	0.29	0.31	0.41	0.04	1.07	0.97	−0.10
S66	0.22	0.24	0.35	0.04	1.31	1.16	−0.16
HEAVY28	1.01	1.02	1.18	0.82	2.75	2.57	−0.19
WATER27	1.86	2.11	2.95	0.03	11.26	8.23	−3.03
CARBHB12	0.75	0.75	0.92	0.12	1.70	1.86	0.16
PNICO23	0.83	0.84	1.01	0.20	1.91	1.87	−0.04
HAL59	0.98	0.99	1.24	0.22	3.16	3.04	−0.12
AHB21	−0.07	0.30	0.37	0.01	1.23	0.35	−0.88
CHB6	−2.61	2.61	2.72	0.10	2.31	−1.49	−3.80
IL16	0.86	0.89	1.04	0.01	1.90	1.64	−0.26
IDISP	3.10	3.22	4.99	0.23	11.51	11.14	−0.37
ICONF	−0.11	0.34	0.44	0.10	1.66	0.80	−0.86
ACONF	−0.09	0.10	0.12	0.05	0.27	0.04	−0.23
AMINO20x4	−0.04	0.22	0.30	0.09	1.93	1.18	−0.75
PCONF21	0.06	0.37	0.43	0.23	1.54	0.80	−0.74
MCONF	0.01	0.23	0.28	0.05	1.25	0.57	−0.68
SCONF	−0.26	0.28	0.43	0.06	1.59	0.12	−1.47
UPU23	0.51	0.66	0.79	0.12	2.67	1.55	−1.11
BUT14DIOL	0.20	0.21	0.25	0.07	0.81	0.63	−0.18

Table S59: Statistical analysis for the B1B95-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	1.60	3.33	4.99	0.01	48.77	26.82	−21.94
G21EA	−1.72	2.01	2.34	0.06	6.66	1.20	−5.46
G21IP	−1.75	2.91	3.62	0.01	14.22	4.57	−9.65
DIPCS10	−5.37	5.37	6.08	0.01	7.90	−2.14	−10.04
PA26	2.70	2.70	3.22	0.01	7.49	7.68	0.19
SIE4x4	16.29	16.29	18.43	0.48	32.73	35.90	3.17
ALKBDE10	−1.89	4.35	5.32	0.04	19.27	10.05	−9.22
YBDE18	−0.75	2.69	2.96	0.05	9.53	4.34	−5.19
AL2X6	2.71	3.04	3.28	0.08	5.72	4.72	−1.00
HEAVYSB11	1.94	2.16	2.54	0.04	4.65	3.96	−0.69
NBPRC	−0.76	1.33	1.66	0.05	4.97	0.88	−4.09
ALK8	7.40	7.76	11.31	0.12	24.54	23.60	−0.94
RC21	3.20	3.67	4.38	0.10	11.24	8.15	−3.08
G2RC	−0.17	3.94	5.07	0.08	22.55	11.11	−11.44
BH76RC	0.21	1.65	2.45	0.08	14.00	9.43	−4.57
FH51	0.37	1.65	2.44	0.05	13.89	7.67	−6.22
TAUT15	0.29	0.96	1.36	0.31	4.65	3.32	−1.33
DC13	−0.71	7.16	9.23	0.13	39.13	21.84	−17.29
MB16-43	23.24	24.87	31.36	0.06	91.70	80.69	−11.01
DARC	0.22	1.55	1.95	0.05	6.09	2.96	−3.13
RSE43	−2.30	2.30	2.59	0.30	5.01	−0.70	−5.71
BSR36	−0.37	1.28	1.62	0.08	6.88	4.65	−2.24
CDIE20	1.21	1.24	1.45	0.31	3.02	2.79	−0.23
ISO34	−0.68	1.27	1.65	0.09	6.92	2.43	−4.49
ISOL24	−0.69	2.16	2.90	0.10	12.57	5.23	−7.35
C60ISO	0.00	2.43	2.87	0.02	8.54	3.21	−5.33
PArel	0.65	1.14	1.68	0.25	6.76	5.35	−1.41
BH76	−3.77	3.80	4.27	0.20	13.51	1.29	−12.22
BHPERI	−2.00	2.31	2.77	0.11	6.82	1.24	−5.59
BHDIV10	−3.99	4.04	4.42	0.09	6.46	0.27	−6.18
INV24	−0.55	1.15	1.57	0.04	6.14	2.41	−3.73
BHROT27	0.51	0.58	0.76	0.09	1.87	1.45	−0.42
PX13	−3.32	3.32	3.35	0.10	1.71	−2.48	−4.19
WCPT18	−2.73	2.73	3.05	0.08	5.27	−1.06	−6.34
RG18	−0.42	0.42	0.48	0.72	0.95	−0.16	−1.12
ADIM6	−0.05	0.40	0.43	0.12	1.12	0.62	−0.50
S22	−0.27	0.59	0.76	0.08	2.89	1.25	−1.64
S66	−0.32	0.44	0.53	0.08	1.70	0.58	−1.12
HEAVY28	0.29	0.35	0.49	0.28	1.64	1.18	−0.47
WATER27	−6.40	6.46	9.91	0.08	25.71	0.70	−25.02
CARBHB12	0.14	0.38	0.53	0.06	1.59	1.20	−0.39
PNICO23	0.34	0.52	0.85	0.12	3.82	3.14	−0.68
HAL59	0.15	0.58	0.75	0.13	3.05	2.01	−1.04
AHB21	0.47	0.59	0.69	0.03	2.11	1.17	−0.93
CHB6	−1.40	1.42	1.87	0.05	3.36	0.07	−3.28
IL16	1.22	1.22	1.29	0.01	1.53	1.99	0.46
IDISP	1.40	2.36	2.74	0.17	6.86	4.27	−2.58
ICONF	0.01	0.34	0.49	0.10	2.15	0.96	−1.19
ACONF	−0.37	0.37	0.43	0.20	0.77	−0.04	−0.81
AMINO20x4	0.05	0.40	0.53	0.16	2.85	1.97	−0.89
PCONF21	0.38	0.74	0.92	0.46	3.13	2.02	−1.11
MCONF	0.45	0.62	0.77	0.12	2.49	1.64	−0.85
SCONF	0.06	0.48	0.70	0.10	2.86	0.85	−2.01
UPU23	0.44	0.62	0.73	0.11	2.09	1.36	−0.73
BUT14DIOL	−0.29	0.30	0.34	0.11	0.84	0.06	−0.78

Table S60: Statistical analysis for the MPW1B95-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	0.35	2.78	4.39	0.01	46.44	20.57	−25.87
G21EA	−1.74	2.10	2.51	0.06	7.09	1.55	−5.54
G21IP	−1.16	2.80	3.39	0.01	14.71	5.98	−8.73
DIPCS10	−3.91	3.91	4.94	0.01	9.32	−0.28	−9.61
PA26	2.05	2.10	2.68	0.01	7.22	6.86	−0.35
SIE4x4	14.30	14.30	16.23	0.42	29.50	32.07	2.58
ALKBDE10	−3.23	4.58	5.57	0.05	18.10	5.57	−12.53
YBDE18	−0.80	2.40	2.66	0.05	8.75	3.73	−5.02
AL2X6	1.63	1.77	1.90	0.05	3.12	2.69	−0.42
HEAVYSB11	0.42	1.32	1.53	0.02	4.71	2.61	−2.10
NBPRC	−0.70	1.60	1.90	0.06	6.28	2.41	−3.87
ALK8	5.23	5.54	7.77	0.09	16.23	15.31	−0.91
RC21	3.39	3.82	4.56	0.11	12.43	9.39	−3.04
G2RC	−1.60	4.28	5.34	0.08	23.99	10.98	−13.01
BH76RC	−0.03	1.77	2.39	0.08	12.10	7.32	−4.77
FH51	−0.32	1.51	2.19	0.05	12.74	6.48	−6.25
TAUT15	0.38	0.93	1.38	0.30	4.49	3.19	−1.30
DC13	−1.37	7.46	9.59	0.14	38.29	22.64	−15.66
MB16-43	14.42	15.60	20.21	0.04	62.93	53.02	−9.91
DARC	−0.30	1.74	2.13	0.05	6.67	2.40	−4.27
RSE43	−2.06	2.06	2.33	0.27	4.55	−0.67	−5.23
BSR36	−2.46	2.46	2.64	0.15	4.40	−0.30	−4.69
CDIE20	1.14	1.17	1.41	0.29	3.11	2.79	−0.32
ISO34	−0.63	1.36	1.76	0.09	7.32	2.81	−4.51
ISOL24	−0.73	2.36	3.12	0.11	13.38	5.75	−7.63
C60ISO	2.30	2.82	3.07	0.03	5.82	4.59	−1.23
PArel	0.76	1.07	1.66	0.23	6.84	5.31	−1.53
BH76	−3.02	3.13	3.54	0.17	11.18	1.61	−9.57
BHPERI	−0.64	1.56	1.81	0.07	6.65	2.85	−3.80
BHDIV10	−2.91	3.02	3.33	0.07	5.56	0.53	−5.04
INV24	−0.48	1.23	1.79	0.04	8.51	4.59	−3.93
BHROT27	0.56	0.64	0.84	0.10	2.04	1.64	−0.39
PX13	−2.47	2.47	2.53	0.07	1.95	−1.32	−3.27
WCPT18	−1.99	2.02	2.35	0.06	5.42	0.21	−5.20
RG18	0.08	0.20	0.33	0.34	1.39	1.11	−0.28
ADIM6	0.16	0.30	0.39	0.09	0.89	0.70	−0.19
S22	−0.24	0.32	0.48	0.04	1.67	0.35	−1.32
S66	−0.15	0.22	0.27	0.04	0.92	0.28	−0.64
HEAVY28	0.15	0.17	0.23	0.14	0.83	0.64	−0.19
WATER27	−2.55	2.83	4.62	0.03	13.96	1.13	−12.83
CARBHB12	0.36	0.38	0.56	0.06	1.43	1.34	−0.09
PNICO23	0.26	0.34	0.57	0.08	2.48	2.25	−0.23
HAL59	0.02	0.41	0.55	0.09	2.72	1.72	−1.00
AHB21	−0.16	0.50	0.62	0.02	2.01	0.65	−1.36
CHB6	−1.71	1.71	2.17	0.06	3.85	−0.21	−4.05
IL16	1.10	1.10	1.16	0.01	1.22	1.80	0.58
IDISP	1.22	1.64	2.03	0.12	4.58	3.57	−1.01
ICONF	0.08	0.28	0.39	0.09	1.52	1.01	−0.50
ACONF	−0.21	0.21	0.25	0.11	0.54	0.03	−0.51
AMINO20x4	0.07	0.36	0.48	0.15	2.33	1.50	−0.82
PCONF21	0.35	0.58	0.67	0.36	2.33	1.23	−1.10
MCONF	0.24	0.44	0.54	0.09	1.78	1.14	−0.63
SCONF	−0.01	0.26	0.41	0.06	1.91	0.66	−1.25
UPU23	0.51	0.62	0.76	0.11	1.92	1.47	−0.45
BUT14DIOL	−0.30	0.30	0.33	0.11	0.68	−0.04	−0.73

Table S61: Statistical analysis for the PW6B95-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.36	2.50	4.81	0.01	49.33	15.11	−34.23
G21EA	0.29	1.27	1.67	0.04	6.73	4.59	−2.15
G21IP	0.97	2.77	3.47	0.01	14.45	8.06	−6.39
DIPCS10	0.26	2.74	3.35	0.00	11.25	5.09	−6.16
PA26	2.48	2.52	3.06	0.01	8.33	7.80	−0.53
SIE4x4	15.36	15.36	17.47	0.46	31.55	34.28	2.73
ALKBDE10	−2.27	3.96	4.89	0.04	16.98	6.37	−10.61
YBDE18	−2.45	3.26	3.98	0.07	10.03	2.74	−7.28
AL2X6	0.22	0.61	0.71	0.02	2.16	0.98	−1.18
HEAVYSB11	−1.01	1.38	1.85	0.02	5.25	1.10	−4.15
NBPRC	0.08	1.46	1.71	0.05	5.56	3.17	−2.39
ALK8	4.30	4.48	6.18	0.07	11.12	10.70	−0.42
RC21	2.29	2.83	3.36	0.08	8.51	6.72	−1.79
G2RC	−0.53	3.08	3.83	0.06	16.43	8.56	−7.87
BH76RC	−0.01	1.48	2.06	0.07	10.65	5.79	−4.86
FH51	0.57	1.67	2.31	0.05	11.65	7.00	−4.65
TAUT15	0.18	0.88	1.19	0.29	4.29	2.76	−1.53
DC13	−0.35	6.90	8.52	0.13	32.16	17.21	−14.94
MB16-43	2.90	8.97	11.26	0.02	49.26	33.14	−16.12
DARC	3.58	3.66	4.16	0.11	6.53	5.99	−0.53
RSE43	−2.16	2.16	2.41	0.28	4.40	−0.87	−5.26
BSR36	−3.20	3.20	3.50	0.20	7.26	−0.54	−7.80
CDIE20	1.13	1.14	1.33	0.28	2.66	2.50	−0.16
ISO34	−0.64	1.28	1.60	0.09	7.16	3.90	−3.26
ISOL24	−1.91	3.67	4.86	0.17	21.74	10.02	−11.72
C60ISO	−0.37	1.65	2.11	0.02	5.86	1.48	−4.38
PArel	0.55	0.95	1.56	0.21	6.34	5.35	−0.99
BH76	−2.67	4.02	5.51	0.22	33.26	24.54	−8.72
BHPERI	−0.08	1.06	1.29	0.05	5.16	2.10	−3.05
BHDIV10	−2.38	2.62	2.78	0.06	5.53	1.19	−4.34
INV24	−0.74	1.15	1.59	0.04	6.81	3.29	−3.52
BHROT27	0.49	0.56	0.75	0.09	1.74	1.46	−0.28
PX13	−1.45	1.45	1.60	0.04	2.55	−0.16	−2.71
WCPT18	−1.36	1.39	1.76	0.04	4.40	0.27	−4.14
RG18	0.22	0.22	0.30	0.38	0.83	0.85	0.02
ADIM6	0.32	0.32	0.35	0.10	0.46	0.61	0.15
S22	−0.21	0.32	0.46	0.04	1.58	0.26	−1.32
S66	−0.07	0.19	0.24	0.03	1.06	0.43	−0.63
HEAVY28	0.16	0.17	0.21	0.14	0.57	0.55	−0.03
WATER27	−1.90	2.19	3.71	0.03	11.71	0.93	−10.78
CARBHB12	0.38	0.38	0.52	0.06	1.14	1.20	0.06
PNICO23	0.19	0.25	0.39	0.06	1.71	1.48	−0.23
HAL59	0.08	0.34	0.50	0.07	2.76	1.81	−0.95
AHB21	−0.07	0.37	0.45	0.02	1.46	0.62	−0.83
CHB6	−1.51	1.51	1.84	0.06	3.04	−0.40	−3.44
IL16	1.28	1.28	1.33	0.01	1.19	1.90	0.71
IDISP	2.06	2.90	3.88	0.20	11.00	8.46	−2.53
ICONF	0.01	0.23	0.33	0.07	1.29	0.85	−0.44
ACONF	−0.13	0.13	0.17	0.07	0.31	−0.01	−0.31
AMINO20x4	0.04	0.32	0.42	0.13	2.00	1.16	−0.85
PCONF21	0.40	0.51	0.62	0.31	1.68	1.20	−0.47
MCONF	0.17	0.37	0.44	0.07	1.57	0.96	−0.61
SCONF	−0.08	0.19	0.30	0.04	1.44	0.53	−0.90
UPU23	0.39	0.58	0.67	0.10	1.77	1.25	−0.52
BUT14DIOL	−0.34	0.34	0.36	0.12	0.50	−0.11	−0.61

Table S62: Statistical analysis for the MPWB1K-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−6.44	6.89	9.42	0.02	51.49	14.52	−36.96
G21EA	−3.24	3.57	4.36	0.11	10.47	1.87	−8.61
G21IP	−1.19	3.10	3.84	0.01	17.53	8.55	−8.97
DIPCS10	−3.47	4.20	5.28	0.01	15.10	3.66	−11.44
PA26	2.52	2.56	3.16	0.01	7.53	7.19	−0.34
SIE4x4	9.72	9.72	11.35	0.29	22.27	24.34	2.07
ALKBDE10	−7.79	7.79	9.33	0.08	20.21	−1.48	−21.69
YBDE18	−0.64	1.23	1.92	0.02	6.58	1.58	−5.00
AL2X6	2.84	2.84	2.94	0.08	2.46	4.03	1.57
HEAVYSB11	0.01	0.45	0.57	0.01	2.07	1.20	−0.88
NBPRC	−1.16	2.45	2.72	0.09	8.43	4.47	−3.97
ALK8	6.34	6.34	8.88	0.10	17.50	17.51	0.01
RC21	3.61	4.10	5.04	0.11	16.92	13.80	−3.12
G2RC	−3.57	5.38	6.75	0.10	29.96	12.73	−17.23
BH76RC	−0.47	2.45	2.79	0.11	9.37	3.22	−6.15
FH51	−1.65	2.19	2.73	0.07	10.98	4.01	−6.97
TAUT15	0.43	0.89	1.22	0.29	4.03	2.57	−1.46
DC13	−2.99	8.77	11.54	0.16	42.43	24.88	−17.55
MB16-43	17.02	18.01	21.92	0.04	65.79	59.26	−6.53
DARC	−3.93	3.93	4.34	0.12	6.21	−1.47	−7.68
RSE43	−1.37	1.37	1.59	0.18	3.42	−0.42	−3.83
BSR36	−2.47	2.47	2.61	0.15	3.83	−0.64	−4.47
CDIE20	0.93	1.02	1.29	0.25	3.34	2.87	−0.47
ISO34	−0.40	1.55	2.04	0.11	7.82	3.11	−4.71
ISOL24	0.44	2.44	3.25	0.11	14.07	8.16	−5.92
C60ISO	7.69	7.69	8.15	0.08	9.33	13.00	3.67
PArel	1.00	1.20	1.77	0.26	6.25	4.93	−1.31
BH76	−0.72	1.44	1.77	0.08	8.28	3.63	−4.65
BHPERI	0.96	1.65	2.36	0.08	9.91	6.96	−2.95
BHDIV10	−1.11	1.72	2.01	0.04	4.54	1.02	−3.51
INV24	0.43	1.93	3.01	0.06	16.05	9.81	−6.24
BHROT27	0.68	0.73	0.98	0.12	2.27	2.00	−0.27
PX13	−0.01	0.57	0.66	0.02	2.36	1.32	−1.04
WCPT18	0.20	0.91	1.30	0.03	6.03	3.98	−2.05
RG18	0.08	0.19	0.33	0.33	1.37	1.05	−0.32
ADIM6	0.33	0.39	0.54	0.12	1.12	1.01	−0.11
S22	0.03	0.30	0.39	0.04	1.67	0.67	−1.00
S66	0.06	0.20	0.25	0.04	1.18	0.72	−0.46
HEAVY28	0.21	0.24	0.32	0.19	1.10	0.88	−0.23
WATER27	−2.09	2.41	4.12	0.03	12.58	1.11	−11.47
CARBHB12	0.33	0.35	0.49	0.06	1.32	1.24	−0.08
PNICO23	0.32	0.35	0.52	0.08	1.90	1.68	−0.22
HAL59	−0.01	0.39	0.51	0.08	2.60	1.50	−1.10
AHB21	−0.50	0.75	1.10	0.03	3.95	0.60	−3.35
CHB6	−2.29	2.29	2.76	0.09	4.56	−0.44	−5.00
IL16	0.96	0.96	1.05	0.01	1.66	1.84	0.18
IDISP	0.24	1.66	2.02	0.12	5.97	3.95	−2.03
ICONF	0.12	0.40	0.53	0.12	1.88	1.22	−0.66
ACONF	−0.27	0.27	0.31	0.15	0.54	0.01	−0.53
AMINO20x4	0.10	0.41	0.55	0.17	2.66	1.69	−0.97
PCONF21	0.51	0.66	0.79	0.41	2.39	1.55	−0.85
MCONF	0.39	0.48	0.59	0.10	1.73	1.24	−0.49
SCONF	−0.07	0.20	0.30	0.04	1.46	0.50	−0.96
UPU23	0.52	0.67	0.80	0.12	2.07	1.48	−0.58
BUT14DIOL	−0.35	0.35	0.36	0.12	0.59	−0.14	−0.74

Table S63: Statistical analysis for the mPW1LYP-D3(0) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−5.90	6.28	8.12	0.02	36.66	3.84	−32.82
G21EA	−0.81	2.24	2.80	0.07	11.39	7.34	−4.06
G21IP	−1.35	4.08	4.78	0.02	17.06	8.46	−8.60
DIPCS10	−3.59	5.98	7.44	0.01	23.67	9.96	−13.71
PA26	2.04	2.27	3.09	0.01	10.11	8.30	−1.81
SIE4x4	16.37	16.37	18.67	0.49	34.13	36.90	2.77
ALKBDE10	−3.88	4.61	6.13	0.05	14.27	1.58	−12.69
YBDE18	−5.54	5.66	6.53	0.11	12.41	1.06	−11.35
AL2X6	−4.40	4.40	4.54	0.12	3.03	−3.15	−6.18
HEAVYSB11	−5.63	5.63	5.79	0.10	4.59	−3.59	−8.18
NBPRC	1.57	3.40	4.24	0.12	13.93	9.13	−4.79
ALK8	−2.23	3.61	4.85	0.06	13.33	3.15	−10.17
RC21	1.00	2.36	2.88	0.07	10.85	3.94	−6.90
G2RC	0.17	2.63	2.95	0.05	9.38	5.25	−4.13
BH76RC	−0.42	2.16	2.66	0.10	11.10	4.40	−6.70
FH51	0.99	2.34	3.22	0.08	17.99	7.62	−10.37
TAUT15	−0.47	1.05	1.22	0.34	3.83	1.72	−2.11
DC13	2.83	11.91	15.56	0.22	55.08	24.87	−30.22
MB16-43	−37.67	37.86	44.01	0.09	114.90	2.84	−112.05
DARC	9.57	9.57	9.72	0.29	6.03	10.93	4.90
RSE43	−1.17	1.17	1.42	0.15	3.33	−0.15	−3.48
BSR36	−6.56	6.56	8.18	0.40	20.55	−1.69	−22.24
CDIE20	0.78	0.82	0.93	0.20	2.36	1.90	−0.46
ISO34	−0.21	1.87	2.79	0.13	15.11	11.01	−4.10
ISOL24	−2.96	6.47	9.19	0.30	45.87	20.23	−25.64
C60ISO	1.30	2.30	2.43	0.02	5.95	3.65	−2.30
PArel	0.04	1.16	1.68	0.25	8.14	5.40	−2.74
BH76	−4.76	4.82	5.40	0.26	11.97	1.05	−10.92
BHPERI	0.80	1.43	1.81	0.07	7.51	3.69	−3.82
BHDIV10	−0.58	2.29	2.81	0.05	9.28	5.08	−4.21
INV24	−0.46	0.95	1.29	0.03	5.35	2.71	−2.64
BHROT27	0.39	0.41	0.60	0.07	1.70	1.47	−0.23
PX13	−2.63	2.63	2.75	0.08	2.53	−1.32	−3.85
WCPT18	−1.05	1.98	2.39	0.06	7.08	2.35	−4.73
RG18	0.59	0.59	0.75	1.02	1.92	2.06	0.14
ADIM6	0.33	0.33	0.33	0.10	0.09	0.37	0.28
S22	0.38	0.74	0.87	0.10	3.32	1.98	−1.34
S66	0.51	0.65	0.80	0.12	2.99	2.10	−0.88
HEAVY28	0.53	0.53	0.57	0.43	1.00	1.02	0.02
WATER27	8.09	8.20	11.53	0.10	28.66	27.19	−1.47
CARBHB12	1.08	1.08	1.21	0.18	1.65	2.08	0.44
PNICO23	0.11	0.40	0.46	0.09	1.66	0.92	−0.74
HAL59	0.55	0.61	0.82	0.13	4.12	3.32	−0.79
AHB21	−0.68	0.68	0.81	0.03	1.66	0.05	−1.60
CHB6	−1.71	1.80	1.98	0.07	3.03	0.28	−2.74
IL16	0.08	0.74	0.83	0.01	2.56	1.54	−1.02
IDISP	3.90	6.18	8.92	0.43	25.83	19.39	−6.44
ICONF	0.07	0.53	0.66	0.16	2.35	1.17	−1.19
ACONF	0.09	0.10	0.12	0.05	0.27	0.25	−0.03
AMINO20x4	0.03	0.21	0.28	0.09	1.65	1.07	−0.58
PCONF21	0.04	0.24	0.29	0.15	1.07	0.66	−0.40
MCONF	−0.27	0.31	0.36	0.06	0.93	0.32	−0.61
SCONF	−0.17	0.29	0.44	0.06	1.69	0.28	−1.41
UPU23	0.49	0.59	0.79	0.10	2.29	1.80	−0.49
BUT14DIOL	0.19	0.20	0.24	0.07	0.83	0.69	−0.14

Table S64: Statistical analysis for the MPW1PW91-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−3.14	3.95	5.62	0.01	36.01	7.06	−28.96
G21EA	−0.17	2.66	2.98	0.08	9.53	4.79	−4.74
G21IP	0.44	3.73	4.43	0.01	17.90	10.01	−7.89
DIPCS10	−0.18	3.01	3.49	0.00	10.88	4.39	−6.48
PA26	3.78	3.78	4.26	0.02	8.86	9.25	0.40
SIE4x4	14.31	14.31	16.09	0.42	27.97	31.64	3.67
ALKBDE10	−3.81	5.79	6.66	0.06	21.22	8.01	−13.22
YBDE18	−1.07	1.25	1.69	0.03	5.43	0.90	−4.53
AL2X6	1.63	2.28	2.32	0.06	4.93	2.98	−1.95
HEAVYSB11	−0.51	0.96	1.21	0.02	3.07	0.96	−2.11
NBPRC	−0.94	2.78	3.02	0.10	9.25	4.32	−4.93
ALK8	5.92	5.92	7.73	0.09	12.84	12.96	0.13
RC21	4.32	4.78	5.65	0.13	14.10	12.20	−1.90
G2RC	−2.44	5.97	7.50	0.12	32.14	11.41	−20.73
BH76RC	−0.23	2.15	2.91	0.10	15.00	8.20	−6.80
FH51	−0.97	2.38	3.28	0.08	16.66	7.65	−9.01
TAUT15	0.26	1.12	1.49	0.37	4.95	3.35	−1.60
DC13	−1.65	6.90	9.24	0.13	40.42	19.01	−21.42
MB16-43	10.06	16.40	21.37	0.04	108.11	79.17	−28.93
DARC	−3.10	3.10	3.82	0.10	7.96	−0.54	−8.49
RSE43	−1.26	1.26	1.46	0.17	3.24	−0.29	−3.53
BSR36	−2.72	2.72	2.96	0.17	4.93	−1.31	−6.24
CDIE20	1.16	1.18	1.39	0.29	2.90	2.68	−0.22
ISO34	−0.20	1.24	1.65	0.09	7.84	4.24	−3.60
ISOL24	0.36	1.88	2.75	0.09	13.21	5.58	−7.63
C60ISO	1.87	2.82	2.95	0.03	6.52	4.12	−2.40
PArel	0.63	1.12	1.66	0.24	7.11	5.37	−1.74
BH76	−3.99	4.18	4.54	0.22	14.35	2.37	−11.98
BHPERI	−3.05	3.21	3.54	0.15	7.48	1.15	−6.33
BHDIV10	−4.00	4.59	5.00	0.10	10.59	2.94	−7.65
INV24	−0.19	1.21	1.75	0.04	7.51	4.31	−3.20
BHROT27	0.53	0.56	0.75	0.09	1.58	1.48	−0.11
PX13	−6.04	6.04	6.25	0.18	5.92	−3.57	−9.49
WCPT18	−3.65	3.65	4.39	0.10	8.38	−0.51	−8.90
RG18	0.03	0.07	0.11	0.12	0.53	0.30	−0.22
ADIM6	−0.20	0.20	0.22	0.06	0.27	−0.11	−0.37
S22	0.33	0.37	0.51	0.05	1.77	1.51	−0.26
S66	0.19	0.28	0.40	0.05	2.03	1.62	−0.41
HEAVY28	0.55	0.56	0.63	0.45	1.24	1.12	−0.12
WATER27	2.12	2.64	3.27	0.03	16.06	8.99	−7.08
CARBHB12	1.27	1.27	1.58	0.21	2.85	3.21	0.36
PNICO23	1.03	1.06	1.42	0.25	4.66	4.46	−0.19
HAL59	0.65	0.74	1.09	0.16	3.76	3.24	−0.51
AHB21	−0.95	0.99	1.29	0.04	3.58	0.31	−3.27
CHB6	−1.36	1.36	1.64	0.05	2.79	−0.08	−2.87
IL16	−0.08	0.34	0.41	0.00	1.15	0.49	−0.66
IDISP	0.97	1.24	1.47	0.09	3.49	2.68	−0.81
ICONF	0.13	0.25	0.38	0.08	1.48	1.13	−0.36
ACONF	−0.08	0.09	0.10	0.05	0.16	0.02	−0.14
AMINO20x4	0.04	0.29	0.37	0.12	1.87	1.02	−0.85
PCONF21	−0.18	0.77	0.92	0.48	2.83	1.04	−1.80
MCONF	0.13	0.30	0.37	0.06	1.51	0.81	−0.71
SCONF	0.02	0.34	0.53	0.07	2.26	0.52	−1.74
UPU23	0.51	0.61	0.73	0.11	2.01	1.62	−0.39
BUT14DIOL	0.16	0.18	0.24	0.06	0.93	0.73	−0.20

Table S65: Statistical analysis for the PW1PW-D3(0) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.80	3.28	4.74	0.01	34.02	6.67	−27.35
G21EA	0.50	2.46	2.89	0.07	9.07	5.29	−3.78
G21IP	0.90	3.68	4.40	0.01	17.25	10.20	−7.05
DIPCS10	0.71	3.09	3.52	0.00	10.11	4.74	−5.37
PA26	2.77	2.82	3.37	0.01	8.72	8.07	−0.65
SIE4x4	14.55	14.55	16.29	0.43	28.27	31.50	3.23
ALKBDE10	−3.02	5.24	6.15	0.05	20.24	8.04	−12.19
YBDE18	−0.91	1.21	1.66	0.02	5.34	1.45	−3.90
AL2X6	0.03	1.04	1.17	0.03	3.43	1.31	−2.12
HEAVYSB11	−1.73	1.77	2.25	0.03	4.08	0.18	−3.90
NBPRC	−1.02	3.16	3.39	0.11	9.86	5.04	−4.82
ALK8	3.28	3.31	4.43	0.05	7.68	7.54	−0.13
RC21	4.78	5.27	6.12	0.15	13.95	11.86	−2.09
G2RC	−3.04	6.42	7.90	0.13	30.89	11.18	−19.71
BH76RC	−0.27	2.35	3.18	0.11	16.22	9.15	−7.08
FH51	−1.37	2.83	3.77	0.09	17.06	7.58	−9.49
TAUT15	0.18	1.15	1.54	0.38	5.27	3.42	−1.85
DC13	−1.54	7.33	9.53	0.13	40.36	19.25	−21.11
MB16-43	1.25	14.25	18.42	0.03	89.42	57.10	−32.32
DARC	−2.24	2.33	3.26	0.07	8.03	0.28	−7.75
RSE43	−1.25	1.25	1.46	0.16	3.24	−0.42	−3.66
BSR36	−4.83	4.83	5.83	0.30	13.59	−1.51	−15.10
CDIE20	1.12	1.12	1.34	0.28	2.75	2.67	−0.08
ISO34	−0.30	1.30	1.72	0.09	8.06	4.32	−3.74
ISOL24	−0.13	2.30	3.27	0.10	15.27	6.64	−8.63
C60ISO	1.09	2.41	2.56	0.02	6.45	3.28	−3.17
PArel	0.67	1.09	1.73	0.24	7.45	5.67	−1.78
BH76	−4.51	4.70	5.13	0.25	15.78	2.46	−13.32
BHPERI	−2.65	2.82	3.04	0.14	6.52	1.27	−5.25
BHDIV10	−3.83	4.38	4.84	0.10	10.01	2.77	−7.23
INV24	−0.55	1.09	1.64	0.03	8.15	4.03	−4.12
BHROT27	0.58	0.58	0.78	0.09	1.54	1.50	−0.03
PX13	−6.43	6.43	6.62	0.19	5.97	−3.96	−9.93
WCPT18	−4.18	4.18	5.00	0.12	9.10	−0.66	−9.76
RG18	0.45	0.45	0.59	0.78	1.70	1.76	0.06
ADIM6	0.21	0.21	0.21	0.06	0.09	0.26	0.17
S22	0.37	0.79	0.95	0.11	3.84	2.33	−1.51
S66	0.44	0.59	0.76	0.11	3.38	2.44	−0.94
HEAVY28	0.44	0.44	0.49	0.35	0.82	0.90	0.09
WATER27	8.17	8.64	11.46	0.11	35.37	28.92	−6.44
CARBHB12	1.62	1.62	1.88	0.27	2.92	3.43	0.52
PNICO23	0.78	0.79	1.09	0.19	3.72	3.57	−0.15
HAL59	0.63	0.69	1.08	0.15	4.67	3.85	−0.82
AHB21	−1.57	1.57	1.77	0.07	3.05	−0.33	−3.38
CHB6	−1.50	1.50	1.79	0.06	3.13	−0.03	−3.16
IL16	−0.77	0.77	0.85	0.01	1.13	−0.22	−1.35
IDISP	1.43	2.91	3.47	0.20	9.55	5.12	−4.43
ICONF	0.24	0.35	0.53	0.11	1.72	1.31	−0.41
ACONF	0.06	0.07	0.08	0.04	0.20	0.14	−0.06
AMINO20x4	0.10	0.23	0.32	0.09	1.55	0.93	−0.62
PCONF21	−0.26	0.83	0.97	0.51	2.60	0.96	−1.65
MCONF	−0.06	0.27	0.33	0.05	1.20	0.59	−0.61
SCONF	0.11	0.39	0.51	0.08	2.04	0.56	−1.48
UPU23	0.42	0.54	0.68	0.09	2.20	1.64	−0.56
BUT14DIOL	0.19	0.20	0.25	0.07	0.88	0.76	−0.11

Table S66: Statistical analysis for the MPW1KCIS-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	9.69	10.57	12.57	0.03	55.76	42.10	−13.67
G21EA	0.58	1.75	2.12	0.05	7.53	4.25	−3.29
G21IP	−0.77	3.34	4.15	0.01	15.82	7.51	−8.32
DIPCS10	−3.12	4.21	5.15	0.01	14.09	3.64	−10.45
PA26	2.30	2.72	3.25	0.01	11.40	7.60	−3.80
SIE4x4	19.32	19.32	21.77	0.57	37.98	41.30	3.32
ALKBDE10	2.91	4.32	6.68	0.04	20.89	18.15	−2.74
YBDE18	1.46	3.04	3.82	0.06	13.11	7.04	−6.07
AL2X6	6.14	6.14	6.75	0.17	8.52	9.01	0.49
HEAVYSB11	7.80	7.80	8.69	0.13	11.73	15.04	3.31
NBPRC	−0.72	3.37	3.87	0.12	11.76	4.35	−7.42
ALK8	15.40	16.24	21.38	0.26	39.89	36.57	−3.32
RC21	4.83	5.33	6.10	0.15	13.20	10.48	−2.72
G2RC	−1.21	6.12	7.41	0.12	30.25	12.55	−17.71
BH76RC	−0.10	2.73	3.77	0.13	20.46	12.34	−8.12
FH51	−0.19	2.36	3.34	0.08	18.87	9.80	−9.07
TAUT15	0.21	1.35	1.78	0.44	5.77	4.07	−1.70
DC13	−1.22	7.74	12.86	0.14	53.75	18.44	−35.30
MB16-43	50.00	50.67	60.48	0.12	175.91	161.53	−14.38
DARC	−0.43	1.88	2.45	0.06	8.31	2.24	−6.07
RSE43	−2.44	2.44	2.70	0.32	5.24	−0.55	−5.79
BSR36	−0.26	0.41	0.56	0.03	2.65	0.82	−1.83
CDIE20	1.35	1.37	1.56	0.34	2.98	2.80	−0.18
ISO34	0.01	1.31	1.75	0.09	9.22	5.43	−3.79
ISOL24	−0.34	3.14	4.11	0.14	18.27	9.66	−8.61
C60ISO	−2.54	3.62	4.64	0.04	11.41	1.54	−9.88
PArel	0.43	1.29	1.93	0.28	8.45	6.03	−2.42
BH76	−6.52	6.58	7.25	0.35	21.12	2.21	−18.92
BHPERI	−4.56	4.56	4.95	0.22	7.99	−1.15	−9.14
BHDIV10	−6.21	6.81	7.49	0.15	14.10	2.98	−11.12
INV24	−0.68	1.55	2.12	0.05	10.29	5.13	−5.16
BHROT27	0.47	0.50	0.68	0.08	1.60	1.42	−0.17
PX13	−7.27	7.27	7.45	0.22	5.60	−5.32	−10.92
WCPT18	−5.57	5.57	6.12	0.16	9.75	−2.28	−12.03
RG18	0.17	0.17	0.19	0.29	0.36	0.42	0.06
ADIM6	−0.25	0.25	0.29	0.07	0.45	−0.06	−0.50
S22	0.17	0.26	0.34	0.04	1.23	0.75	−0.48
S66	0.12	0.23	0.30	0.04	1.40	0.96	−0.44
HEAVY28	1.18	1.18	1.35	0.95	3.21	3.20	−0.01
WATER27	1.49	2.04	2.77	0.03	15.14	7.74	−7.41
CARBHB12	1.45	1.45	1.81	0.24	3.36	3.81	0.45
PNICO23	1.73	1.74	2.50	0.41	8.27	8.20	−0.08
HAL59	1.49	1.49	2.01	0.32	5.60	5.39	−0.21
AHB21	−0.67	0.81	1.13	0.04	3.91	0.59	−3.32
CHB6	−3.22	3.22	3.52	0.12	3.80	−1.73	−5.53
IL16	−0.22	0.50	0.57	0.00	1.93	0.85	−1.09
IDISP	1.32	1.56	1.87	0.11	3.86	3.16	−0.70
ICONF	0.08	0.35	0.44	0.11	1.69	1.07	−0.62
ACONF	−0.02	0.04	0.05	0.02	0.17	0.09	−0.08
AMINO20x4	−0.01	0.27	0.35	0.11	1.94	0.99	−0.95
PCONF21	−0.30	0.80	0.97	0.49	2.97	1.11	−1.86
MCONF	−0.03	0.32	0.38	0.06	1.57	0.72	−0.85
SCONF	−0.02	0.30	0.48	0.07	2.15	0.49	−1.66
UPU23	0.40	0.53	0.66	0.09	2.02	1.53	−0.49
BUT14DIOL	0.17	0.21	0.28	0.07	1.19	0.86	−0.33

Table S67: Statistical analysis for the MPWKCIS1K-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−5.38	7.54	10.31	0.02	52.50	15.59	−36.91
G21EA	−2.52	3.40	4.17	0.10	11.04	2.52	−8.52
G21IP	−0.86	3.45	4.29	0.01	17.40	8.56	−8.84
DIPCS10	−2.26	3.67	4.82	0.01	14.80	4.65	−10.14
PA26	3.05	3.31	3.82	0.02	10.83	8.08	−2.75
SIE4x4	9.88	9.88	11.68	0.29	23.34	25.54	2.21
ALKBDE10	−7.42	7.42	9.11	0.07	20.57	−1.06	−21.64
YBDE18	0.00	2.17	2.65	0.04	9.02	3.52	−5.50
AL2X6	4.27	4.27	4.55	0.12	4.88	6.45	1.57
HEAVYSB11	2.36	2.86	3.67	0.05	9.06	7.28	−1.78
NBPRC	−0.47	3.47	3.88	0.13	12.41	6.14	−6.27
ALK8	12.76	13.10	17.43	0.21	34.94	33.58	−1.36
RC21	4.21	4.79	5.85	0.13	16.99	15.14	−1.85
G2RC	−5.15	7.49	9.63	0.15	36.74	13.93	−22.81
BH76RC	−1.09	2.43	3.37	0.11	12.47	2.89	−9.58
FH51	−2.48	3.23	3.92	0.10	14.94	4.57	−10.38
TAUT15	0.27	0.85	1.20	0.28	3.98	2.44	−1.54
DC13	−3.05	9.06	11.50	0.16	45.39	22.77	−22.62
MB16-43	31.86	32.75	38.62	0.08	107.74	95.60	−12.13
DARC	−5.45	5.45	5.84	0.17	7.73	−3.28	−11.00
RSE43	−1.12	1.12	1.30	0.15	2.83	−0.21	−3.04
BSR36	−1.63	1.63	1.75	0.10	2.74	−0.68	−3.41
CDIE20	1.01	1.08	1.40	0.27	3.69	3.08	−0.61
ISO34	0.35	1.68	2.16	0.12	8.50	4.56	−3.94
ISOL24	1.17	2.70	3.34	0.12	13.66	8.09	−5.57
C60ISO	8.48	8.48	8.94	0.09	9.32	14.02	4.70
PArel	0.88	1.08	1.71	0.23	6.16	5.23	−0.93
BH76	−1.32	2.16	2.55	0.12	10.12	5.09	−5.03
BHPERI	0.05	1.80	2.29	0.09	10.45	6.89	−3.56
BHDIV10	−1.68	2.67	3.04	0.06	8.97	3.37	−5.60
INV24	0.71	2.10	3.14	0.07	15.75	9.78	−5.97
BHROT27	0.64	0.65	0.88	0.10	1.74	1.71	−0.04
PX13	−1.78	1.78	2.05	0.05	3.27	−0.15	−3.42
WCPT18	−0.62	1.78	2.14	0.05	7.51	2.81	−4.70
RG18	0.11	0.12	0.16	0.21	0.51	0.43	−0.08
ADIM6	−0.26	0.26	0.30	0.08	0.41	−0.08	−0.49
S22	0.29	0.34	0.46	0.05	1.62	1.36	−0.26
S66	0.18	0.28	0.39	0.05	1.91	1.51	−0.41
HEAVY28	1.04	1.05	1.21	0.85	2.91	2.85	−0.06
WATER27	0.26	1.20	1.54	0.01	6.13	2.68	−3.45
CARBHB12	1.08	1.08	1.33	0.18	2.31	2.65	0.34
PNICO23	1.14	1.18	1.53	0.28	4.73	4.45	−0.28
HAL59	0.78	0.84	1.15	0.18	3.79	3.40	−0.39
AHB21	−1.00	1.05	1.49	0.05	4.06	0.31	−3.75
CHB6	−3.10	3.10	3.38	0.12	3.39	−1.41	−4.79
IL16	0.23	0.47	0.55	0.00	1.51	0.95	−0.56
IDISP	−0.23	2.46	2.92	0.17	8.01	4.40	−3.61
ICONF	0.13	0.35	0.51	0.11	2.03	1.46	−0.57
ACONF	0.10	0.10	0.12	0.05	0.18	0.20	0.02
AMINO20x4	0.03	0.30	0.38	0.12	1.92	0.97	−0.95
PCONF21	0.08	0.56	0.72	0.35	2.61	1.38	−1.23
MCONF	0.04	0.17	0.21	0.03	0.99	0.51	−0.48
SCONF	−0.31	0.39	0.45	0.08	1.36	0.67	−0.69
UPU23	0.52	0.64	0.77	0.11	2.03	1.49	−0.54
BUT14DIOL	−0.02	0.13	0.16	0.05	0.70	0.45	−0.25

Table S68: Statistical analysis for the PBE0-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.94	3.70	5.66	0.01	38.86	8.16	−30.70
G21EA	−0.40	2.62	2.91	0.08	8.81	4.03	−4.77
G21IP	−0.02	3.68	4.35	0.01	17.03	9.00	−8.03
DIPCS10	−1.50	2.99	3.76	0.00	10.36	3.06	−7.29
PA26	2.79	2.88	3.40	0.02	9.17	8.00	−1.16
SIE4x4	14.39	14.39	16.12	0.43	27.78	31.21	3.42
ALKBDE10	−3.96	5.66	6.53	0.06	19.42	6.49	−12.93
YBDE18	−0.33	0.98	1.42	0.02	5.91	2.33	−3.57
AL2X6	0.80	1.48	1.56	0.04	3.83	1.77	−2.06
HEAVYSB11	−1.05	1.37	1.72	0.02	3.94	0.80	−3.15
NBPRC	−1.07	3.18	3.50	0.11	10.68	5.03	−5.65
ALK8	4.59	4.61	5.98	0.07	9.68	9.60	−0.08
RC21	4.96	5.50	6.45	0.15	15.80	13.61	−2.19
G2RC	−2.98	6.75	8.45	0.13	34.71	12.30	−22.40
BH76RC	−0.15	2.46	3.30	0.12	17.05	10.18	−6.87
FH51	−1.29	2.77	3.72	0.09	17.31	7.64	−9.67
TAUT15	0.36	1.13	1.60	0.37	5.27	3.59	−1.68
DC13	−1.89	8.01	10.48	0.15	44.85	21.69	−23.16
MB16-43	5.87	15.86	20.79	0.04	106.67	71.79	−34.88
DARC	−3.76	3.76	4.52	0.12	8.53	−1.04	−9.57
RSE43	−1.45	1.45	1.65	0.19	3.45	−0.40	−3.85
BSR36	−3.25	3.25	3.73	0.20	6.98	−1.25	−8.24
CDIE20	1.21	1.24	1.46	0.31	3.05	2.80	−0.24
ISO34	−0.29	1.42	1.87	0.10	7.79	3.45	−4.35
ISOL24	0.21	2.11	2.93	0.10	14.59	6.34	−8.25
C60ISO	0.98	2.35	2.50	0.02	6.52	3.07	−3.45
PArel	0.71	1.21	1.76	0.26	7.66	5.48	−2.18
BH76	−3.58	5.00	6.18	0.27	38.92	24.82	−14.10
BHPERI	−3.04	3.27	3.53	0.16	7.56	1.68	−5.87
BHDIV10	−4.26	4.81	5.29	0.11	10.55	2.71	−7.84
INV24	−0.50	1.17	1.69	0.04	7.86	4.08	−3.78
BHROT27	0.55	0.58	0.77	0.09	1.60	1.47	−0.13
PX13	−6.55	6.55	6.75	0.20	6.12	−4.15	−10.27
WCPT18	−4.33	4.33	5.03	0.12	8.73	−1.12	−9.85
RG18	0.11	0.11	0.13	0.19	0.25	0.25	0.00
ADIM6	0.05	0.06	0.06	0.02	0.12	0.09	−0.03
S22	0.30	0.48	0.64	0.07	2.79	1.76	−1.03
S66	0.27	0.36	0.51	0.07	2.44	1.90	−0.54
HEAVY28	0.31	0.31	0.40	0.25	0.84	0.85	0.01
WATER27	5.42	5.92	7.53	0.07	26.24	19.45	−6.79
CARBHB12	1.44	1.44	1.72	0.24	2.85	3.31	0.46
PNICO23	0.94	0.94	1.32	0.22	4.32	4.45	0.12
HAL59	0.52	0.61	1.00	0.13	3.73	3.37	−0.36
AHB21	−1.24	1.24	1.50	0.06	3.43	−0.03	−3.46
CHB6	−1.22	1.37	1.62	0.05	3.47	0.45	−3.02
IL16	−0.21	0.34	0.42	0.00	1.03	0.32	−0.71
IDISP	0.87	1.54	2.08	0.11	5.91	3.92	−2.00
ICONF	0.19	0.28	0.44	0.09	1.37	1.11	−0.25
ACONF	0.06	0.06	0.07	0.03	0.16	0.17	0.01
AMINO20x4	0.07	0.28	0.35	0.11	1.71	0.80	−0.91
PCONF21	−0.21	0.90	1.07	0.56	3.36	1.44	−1.91
MCONF	0.01	0.27	0.31	0.05	1.09	0.58	−0.51
SCONF	0.04	0.27	0.40	0.06	1.77	0.44	−1.33
UPU23	0.39	0.54	0.65	0.09	2.03	1.46	−0.57
BUT14DIOL	0.21	0.22	0.27	0.08	0.89	0.76	−0.13

Table S69: Statistical analysis for the PBEh1PBE-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−1.72	3.61	5.24	0.01	41.39	14.36	−27.03
G21EA	−0.54	2.68	2.97	0.08	8.93	4.11	−4.82
G21IP	0.05	3.71	4.40	0.01	17.19	9.25	−7.94
DIPCS10	−1.37	3.00	3.73	0.00	10.53	3.24	−7.29
PA26	2.57	2.67	3.22	0.01	9.20	7.83	−1.37
SIE4x4	14.25	14.25	16.01	0.42	27.86	31.09	3.23
ALKBDE10	−3.62	5.39	6.26	0.05	19.44	6.82	−12.62
YBDE18	−0.47	0.99	1.53	0.02	6.00	1.82	−4.18
AL2X6	4.01	4.01	4.32	0.11	5.20	5.99	0.79
HEAVYSB11	3.56	3.83	4.88	0.07	10.66	9.18	−1.49
NBPRC	−0.99	3.02	3.33	0.11	10.16	4.64	−5.52
ALK8	11.39	11.89	16.57	0.19	38.55	36.56	−1.98
RC21	4.44	4.93	5.84	0.14	14.48	12.49	−1.99
G2RC	−2.56	6.57	8.10	0.13	34.26	13.29	−20.96
BH76RC	−0.08	2.35	3.15	0.11	16.40	9.82	−6.57
FH51	−1.05	2.50	3.44	0.08	17.05	7.60	−9.45
TAUT15	0.31	1.17	1.61	0.38	5.19	3.55	−1.64
DC13	−1.91	7.58	10.26	0.14	45.36	20.74	−24.62
MB16-43	21.04	23.68	29.13	0.06	104.85	86.17	−18.69
DARC	−2.64	2.65	3.62	0.08	8.62	0.02	−8.61
RSE43	−1.48	1.48	1.68	0.19	3.42	−0.44	−3.86
BSR36	−2.92	2.92	3.26	0.18	5.63	−1.19	−6.81
CDIE20	1.23	1.26	1.48	0.31	3.07	2.82	−0.25
ISO34	−0.29	1.32	1.77	0.09	8.59	4.50	−4.09
ISOL24	−0.06	2.23	3.08	0.10	13.56	5.46	−8.10
C60ISO	1.50	2.64	2.73	0.03	6.54	3.63	−2.91
PArel	0.67	1.14	1.70	0.25	7.30	5.51	−1.80
BH76	−4.28	4.46	4.90	0.24	15.83	2.28	−13.55
BHPERI	−2.66	2.89	3.15	0.14	7.53	1.73	−5.81
BHDIV10	−4.09	4.72	5.17	0.10	10.77	3.16	−7.61
INV24	−0.42	1.17	1.71	0.04	7.70	4.03	−3.67
BHROT27	0.56	0.60	0.79	0.10	1.63	1.48	−0.15
PX13	−5.97	5.97	6.12	0.18	5.35	−3.76	−9.12
WCPT18	−3.97	3.97	4.68	0.11	8.33	−0.79	−9.12
RG18	0.19	0.19	0.25	0.33	0.65	0.68	0.03
ADIM6	−0.28	0.28	0.32	0.08	0.43	−0.11	−0.53
S22	0.33	0.46	0.64	0.06	2.66	1.86	−0.80
S66	0.23	0.37	0.53	0.07	2.60	2.02	−0.57
HEAVY28	1.34	1.34	1.53	1.08	3.42	3.50	0.08
WATER27	5.15	5.66	7.22	0.07	26.33	19.52	−6.81
CARBHB12	1.52	1.52	1.80	0.25	2.88	3.45	0.57
PNICO23	1.50	1.50	1.91	0.35	5.42	5.47	0.05
HAL59	1.30	1.31	1.71	0.29	4.29	4.10	−0.19
AHB21	−1.34	1.34	1.60	0.06	3.70	0.00	−3.70
CHB6	−2.81	2.81	3.08	0.10	2.97	−1.27	−4.23
IL16	−0.33	0.42	0.48	0.00	1.19	0.26	−0.92
IDISP	0.91	1.50	1.98	0.11	5.06	3.86	−1.20
ICONF	0.10	0.25	0.37	0.08	1.62	1.05	−0.57
ACONF	0.07	0.07	0.09	0.04	0.21	0.22	0.01
AMINO20x4	0.08	0.27	0.35	0.11	1.78	0.89	−0.89
PCONF21	−0.16	0.90	1.07	0.56	3.21	1.42	−1.79
MCONF	0.05	0.27	0.32	0.05	1.22	0.64	−0.58
SCONF	0.06	0.31	0.46	0.07	1.98	0.46	−1.52
UPU23	0.42	0.56	0.68	0.10	2.02	1.52	−0.50
BUT14DIOL	0.27	0.28	0.31	0.10	0.87	0.79	−0.08

Table S70: Statistical analysis for the PBE1KCIS-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	7.52	8.76	10.55	0.03	46.72	29.06	−17.66
G21EA	−0.15	1.67	2.03	0.05	7.30	3.44	−3.87
G21IP	−0.83	3.34	3.99	0.01	14.39	6.24	−8.15
DIPCS10	−3.31	4.32	5.29	0.01	14.51	4.77	−9.74
PA26	1.51	2.04	2.61	0.01	10.59	6.54	−4.05
SIE4x4	16.91	16.91	19.14	0.50	34.33	37.00	2.68
ALKBDE10	−0.12	3.95	4.83	0.04	17.45	10.20	−7.25
YBDE18	0.87	2.64	3.29	0.05	12.44	6.00	−6.44
AL2X6	3.46	3.56	3.88	0.10	5.12	4.81	−0.31
HEAVYSB11	4.53	4.53	5.28	0.08	8.27	9.13	0.86
NBPRC	−0.26	3.06	3.53	0.11	12.28	5.78	−6.49
ALK8	11.92	12.68	16.70	0.20	32.55	29.52	−3.03
RC21	4.61	5.09	5.88	0.14	12.68	10.13	−2.54
G2RC	−2.64	6.34	7.88	0.12	30.32	12.16	−18.16
BH76RC	−0.36	2.52	3.42	0.12	17.99	10.01	−7.98
FH51	−0.86	2.35	3.19	0.08	16.98	8.31	−8.67
TAUT15	0.22	1.16	1.59	0.38	5.21	3.56	−1.64
DC13	−1.17	7.10	11.40	0.13	52.14	20.74	−31.40
MB16-43	32.00	33.49	40.96	0.08	123.32	106.91	−16.41
DARC	−0.76	1.96	2.63	0.06	8.69	1.84	−6.84
RSE43	−2.17	2.17	2.42	0.29	4.75	−0.50	−5.25
BSR36	−2.17	2.17	2.51	0.13	4.93	−0.69	−5.62
CDIE20	1.33	1.36	1.59	0.33	3.34	3.00	−0.34
ISO34	−0.02	1.42	1.90	0.10	9.42	5.35	−4.08
ISOL24	−0.64	2.91	3.90	0.13	15.20	6.73	−8.47
C60ISO	−0.16	2.30	2.80	0.02	8.18	2.57	−5.62
PArel	0.56	1.09	1.76	0.24	7.16	5.88	−1.28
BH76	−5.25	5.40	5.99	0.29	18.24	2.61	−15.63
BHPERI	−2.52	2.63	2.99	0.13	7.02	1.28	−5.74
BHDIV10	−4.61	5.31	5.84	0.12	12.07	3.23	−8.84
INV24	−0.64	1.38	1.82	0.04	8.47	3.74	−4.73
BHROT27	0.50	0.52	0.70	0.08	1.53	1.40	−0.13
PX13	−5.62	5.62	5.76	0.17	4.65	−3.99	−8.63
WCPT18	−4.36	4.36	4.92	0.12	8.67	−1.40	−10.07
RG18	0.35	0.35	0.40	0.60	0.67	0.77	0.10
ADIM6	0.22	0.22	0.23	0.07	0.19	0.30	0.11
S22	0.29	0.39	0.46	0.05	1.83	1.03	−0.79
S66	0.34	0.36	0.44	0.07	1.44	1.27	−0.17
HEAVY28	1.09	1.09	1.20	0.88	2.44	2.60	0.16
WATER27	4.00	4.40	5.79	0.05	21.24	15.84	−5.39
CARBHB12	1.48	1.48	1.74	0.25	2.78	3.43	0.64
PNICO23	1.42	1.42	1.91	0.33	5.90	6.09	0.19
HAL59	1.21	1.21	1.55	0.26	4.10	4.05	−0.05
AHB21	−0.97	0.97	1.23	0.04	3.33	0.02	−3.32
CHB6	−2.79	2.79	3.00	0.10	2.92	−1.48	−4.39
IL16	−0.10	0.39	0.43	0.00	1.38	0.62	−0.77
IDISP	1.30	2.67	3.16	0.19	8.11	5.08	−3.03
ICONF	0.10	0.25	0.38	0.08	1.56	1.14	−0.42
ACONF	0.10	0.10	0.12	0.05	0.28	0.31	0.03
AMINO20x4	0.00	0.25	0.33	0.10	1.85	0.79	−1.06
PCONF21	−0.14	0.79	0.93	0.49	2.99	1.55	−1.44
MCONF	−0.07	0.24	0.29	0.05	1.08	0.45	−0.63
SCONF	−0.20	0.28	0.35	0.06	1.17	0.38	−0.79
UPU23	0.34	0.54	0.64	0.09	2.11	1.51	−0.60
BUT14DIOL	0.15	0.18	0.24	0.06	1.01	0.75	−0.26

Table S71: Statistical analysis for the X3LYP-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.77	3.02	4.66	0.01	37.53	9.45	−28.08
G21EA	0.11	1.87	2.42	0.06	10.03	7.01	−3.01
G21IP	−0.74	3.73	4.49	0.01	16.40	8.88	−7.52
DIPCS10	−2.84	5.16	6.45	0.01	21.09	9.50	−11.59
PA26	2.14	2.28	3.06	0.01	9.57	8.27	−1.30
SIE4x4	17.47	17.47	19.90	0.52	35.81	38.87	3.07
ALKBDE10	−1.23	4.23	4.79	0.04	16.09	7.21	−8.88
YBDE18	−3.65	4.05	5.01	0.08	12.24	2.67	−9.57
AL2X6	−0.69	0.98	1.03	0.03	2.27	0.87	−1.40
HEAVYSB11	−1.19	2.15	2.40	0.04	7.33	3.26	−4.07
NBPRC	0.99	1.85	2.74	0.07	8.82	7.04	−1.79
ALK8	4.18	4.52	5.62	0.07	12.41	11.05	−1.36
RC21	1.75	2.59	3.10	0.07	9.57	4.78	−4.79
G2RC	0.31	2.89	3.47	0.06	13.28	7.12	−6.17
BH76RC	−0.37	2.11	2.66	0.10	11.08	3.72	−7.36
FH51	1.17	2.45	3.33	0.08	16.69	8.53	−8.16
TAUT15	−0.07	1.14	1.39	0.37	4.53	2.86	−1.68
DC13	1.61	9.92	12.28	0.18	45.30	20.07	−25.24
MB16-43	−11.58	15.91	18.86	0.04	76.91	32.65	−44.26
DARC	7.39	7.39	7.65	0.23	7.06	9.01	1.96
RSE43	−1.67	1.67	1.90	0.22	3.73	−0.60	−4.33
BSR36	−3.77	3.77	4.39	0.23	8.91	−1.37	−10.27
CDIE20	0.97	0.98	1.11	0.24	2.14	2.02	−0.12
ISO34	−0.11	1.72	2.58	0.12	14.24	10.45	−3.80
ISOL24	−2.20	5.60	7.90	0.26	38.42	18.30	−20.12
C60ISO	0.96	2.37	2.56	0.02	6.38	2.92	−3.46
PArel	0.06	1.11	1.66	0.24	7.71	5.46	−2.25
BH76	−5.35	5.41	5.95	0.29	11.97	1.33	−10.64
BHPERI	−0.72	1.09	1.41	0.05	5.76	2.02	−3.73
BHDIV10	−2.08	3.15	3.68	0.07	10.51	5.32	−5.20
INV24	−0.43	1.00	1.35	0.03	6.21	3.10	−3.11
BHROT27	0.38	0.43	0.62	0.07	1.56	1.33	−0.23
PX13	−4.31	4.31	4.45	0.13	4.08	−2.54	−6.62
WCPT18	−2.11	2.31	3.01	0.07	7.26	1.12	−6.14
RG18	0.22	0.22	0.27	0.38	0.53	0.59	0.06
ADIM6	0.20	0.20	0.21	0.06	0.23	0.34	0.11
S22	0.41	0.41	0.56	0.06	1.57	1.52	−0.05
S66	0.40	0.40	0.53	0.07	1.67	1.71	0.04
HEAVY28	0.88	0.88	0.98	0.71	1.97	1.95	−0.02
WATER27	5.53	5.86	8.14	0.07	25.28	20.76	−4.52
CARBHB12	1.08	1.08	1.24	0.18	1.91	2.36	0.45
PNICO23	0.92	0.92	1.06	0.22	2.03	2.28	0.24
HAL59	1.04	1.04	1.30	0.23	3.47	3.48	0.00
AHB21	−0.55	0.55	0.68	0.02	1.44	−0.02	−1.46
CHB6	−2.39	2.39	2.50	0.09	1.84	−1.36	−3.20
IL16	0.43	0.59	0.68	0.01	1.75	1.16	−0.59
IDISP	3.15	3.71	5.53	0.26	13.94	12.27	−1.67
ICONF	−0.05	0.28	0.37	0.09	1.68	0.82	−0.86
ACONF	−0.04	0.08	0.09	0.04	0.31	0.13	−0.18
AMINO20x4	0.00	0.21	0.28	0.09	1.99	1.20	−0.80
PCONF21	−0.04	0.53	0.60	0.33	1.95	0.76	−1.18
MCONF	−0.04	0.19	0.23	0.04	1.03	0.39	−0.64
SCONF	−0.15	0.26	0.45	0.06	1.90	0.25	−1.66
UPU23	0.49	0.63	0.75	0.11	2.41	1.58	−0.83
BUT14DIOL	0.33	0.33	0.36	0.12	0.85	0.78	−0.06

Table S72: Statistical analysis for the O3LYP-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	19.47	19.66	22.55	0.06	56.19	45.51	−10.68
G21EA	0.65	1.90	2.41	0.06	9.32	4.72	−4.61
G21IP	−0.23	3.12	3.95	0.01	14.76	7.37	−7.39
DIPCS10	−1.90	3.92	4.88	0.01	15.77	5.79	−9.98
PA26	1.84	2.06	2.66	0.01	9.12	6.94	−2.18
SIE4x4	21.38	21.38	23.95	0.63	40.57	44.59	4.02
ALKBDE10	6.48	6.50	9.75	0.06	25.92	25.82	−0.09
YBDE18	3.80	4.39	5.52	0.09	14.36	9.78	−4.57
AL2X6	4.29	4.38	4.88	0.12	7.26	6.97	−0.29
HEAVYSB11	6.62	6.62	7.05	0.11	8.40	10.45	2.05
NBPRC	−1.74	3.75	4.13	0.14	11.03	3.51	−7.52
ALK8	11.39	12.03	15.85	0.19	33.61	31.04	−2.57
RC21	7.30	7.93	9.08	0.22	18.46	15.51	−2.95
G2RC	−2.24	7.42	9.43	0.14	39.92	15.39	−24.53
BH76RC	−0.62	3.39	4.99	0.16	28.73	18.17	−10.56
FH51	−1.10	2.86	4.18	0.09	23.43	10.48	−12.95
TAUT15	0.50	1.68	2.45	0.55	8.17	5.64	−2.54
DC13	−1.29	10.12	13.62	0.18	52.50	23.98	−28.53
MB16-43	45.06	45.35	51.83	0.11	122.03	115.78	−6.25
DARC	−3.53	3.53	4.51	0.11	9.58	−0.21	−9.79
RSE43	−2.87	2.87	3.21	0.38	6.30	−0.77	−7.07
BSR36	−0.96	0.96	1.14	0.06	2.98	−0.24	−3.22
CDIE20	1.60	1.62	1.81	0.40	3.37	3.25	−0.12
ISO34	−0.34	1.55	2.00	0.11	9.00	4.06	−4.94
ISOL24	0.03	2.58	3.73	0.12	18.29	7.63	−10.66
C60ISO	−3.30	4.31	5.55	0.04	12.92	1.46	−11.45
PArel	0.74	1.74	2.33	0.38	10.04	6.69	−3.35
BH76	−7.52	7.65	8.65	0.41	29.39	3.19	−26.20
BHPERI	−4.84	4.84	5.29	0.23	9.12	−0.13	−9.25
BHDIV10	−6.43	7.00	7.76	0.15	14.31	2.82	−11.48
INV24	−0.91	1.77	2.39	0.06	10.58	4.95	−5.63
BHROT27	0.65	0.69	0.92	0.11	2.25	2.09	−0.16
PX13	−10.28	10.28	10.56	0.31	9.41	−6.70	−16.11
WCPT18	−7.06	7.06	7.61	0.20	10.30	−3.42	−13.72
RG18	0.47	0.47	0.58	0.81	1.25	1.43	0.17
ADIM6	−0.18	0.20	0.27	0.06	0.61	0.04	−0.57
S22	0.43	0.47	0.68	0.06	2.39	1.92	−0.46
S66	0.31	0.38	0.57	0.07	2.49	2.10	−0.40
HEAVY28	1.33	1.33	1.51	1.07	3.35	3.46	0.11
WATER27	5.26	6.07	7.88	0.07	32.79	21.78	−11.02
CARBHB12	1.71	1.71	2.14	0.28	3.93	4.43	0.51
PNICO23	1.64	1.64	2.28	0.38	7.44	7.51	0.07
HAL59	1.54	1.54	2.04	0.34	5.44	5.47	0.03
AHB21	−1.37	1.39	1.75	0.06	4.76	0.24	−4.52
CHB6	−3.93	3.93	4.22	0.15	4.13	−1.86	−5.99
IL16	−0.68	0.68	0.81	0.01	1.44	−0.02	−1.46
IDISP	1.26	1.79	2.33	0.13	5.83	4.38	−1.46
ICONF	0.18	0.29	0.44	0.09	1.93	1.27	−0.67
ACONF	0.14	0.14	0.16	0.08	0.33	0.33	0.00
AMINO20x4	0.10	0.33	0.44	0.14	2.31	1.29	−1.02
PCONF21	−0.30	1.20	1.42	0.74	4.26	2.01	−2.26
MCONF	−0.01	0.35	0.41	0.07	1.50	0.66	−0.84
SCONF	0.10	0.34	0.52	0.07	2.34	0.67	−1.67
UPU23	0.26	0.46	0.58	0.08	2.12	1.46	−0.65
BUT14DIOL	0.38	0.38	0.43	0.14	1.19	1.09	−0.11

Table S73: Statistical analysis for the B97-1-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	0.97	3.67	4.98	0.01	39.74	15.38	−24.36
G21EA	−0.40	1.44	1.75	0.04	6.82	4.04	−2.78
G21IP	−0.37	2.86	3.52	0.01	13.68	6.81	−6.87
DIPCS10	−3.72	4.55	5.69	0.01	14.20	2.58	−11.62
PA26	3.81	3.81	4.42	0.02	9.55	10.01	0.46
SIE4x4	16.83	16.83	18.61	0.50	29.83	34.25	4.42
ALKBDE10	−0.11	3.25	4.65	0.03	17.83	10.89	−6.94
YBDE18	−0.76	3.27	3.72	0.07	12.08	4.76	−7.31
AL2X6	2.21	2.52	2.64	0.07	4.44	3.48	−0.96
HEAVYSB11	3.88	3.94	4.55	0.07	8.30	7.95	−0.35
NBPRC	0.10	1.75	1.96	0.06	6.05	3.00	−3.04
ALK8	7.98	8.40	10.67	0.13	20.93	19.23	−1.70
RC21	3.68	4.12	4.84	0.12	10.72	7.95	−2.77
G2RC	−0.54	4.83	5.81	0.09	26.29	12.43	−13.87
BH76RC	0.36	2.18	2.81	0.10	13.51	8.67	−4.83
FH51	0.36	2.20	2.99	0.07	14.82	8.73	−6.09
TAUT15	−0.14	0.97	1.16	0.32	3.96	2.24	−1.72
DC13	−1.23	6.78	7.99	0.12	26.07	9.29	−16.78
MB16-43	5.31	13.57	17.76	0.03	93.86	61.60	−32.26
DARC	1.95	2.66	2.93	0.08	7.33	4.07	−3.26
RSE43	−2.18	2.18	2.38	0.29	3.90	−0.99	−4.89
BSR36	−4.31	4.31	5.03	0.27	10.21	−1.59	−11.80
CDIE20	0.96	0.96	1.07	0.24	1.63	1.72	0.09
ISO34	−0.20	1.06	1.58	0.07	9.29	5.76	−3.54
ISOL24	−0.99	3.68	5.13	0.17	23.93	12.07	−11.86
C60ISO	−0.62	2.25	2.86	0.02	8.00	2.03	−5.97
PArel	0.26	0.92	1.50	0.20	6.89	5.13	−1.76
BH76	−4.51	4.65	5.30	0.25	12.84	2.27	−10.57
BHPERI	−2.67	2.67	2.94	0.13	5.24	−0.57	−5.81
BHDIV10	−3.63	4.34	4.56	0.10	10.78	3.52	−7.27
INV24	−0.57	1.01	1.27	0.03	5.18	2.17	−3.01
BHROT27	0.34	0.39	0.55	0.06	1.47	1.30	−0.17
PX13	−4.12	4.12	4.25	0.12	3.46	−2.97	−6.43
WCPT18	−3.14	3.14	3.80	0.09	7.74	−0.01	−7.75
RG18	0.34	0.34	0.38	0.59	0.65	0.74	0.09
ADIM6	0.46	0.46	0.47	0.14	0.32	0.64	0.31
S22	0.29	0.38	0.45	0.05	1.77	0.98	−0.79
S66	0.40	0.41	0.46	0.07	1.25	1.14	−0.11
HEAVY28	0.98	0.98	1.05	0.79	1.91	2.05	0.14
WATER27	4.06	4.34	5.78	0.05	19.08	15.32	−3.76
CARBHB12	1.36	1.36	1.55	0.23	2.20	2.88	0.68
PNICO23	1.30	1.30	1.61	0.30	4.38	4.67	0.29
HAL59	1.09	1.10	1.40	0.24	3.63	3.56	−0.07
AHB21	−0.81	0.81	1.00	0.04	2.42	−0.07	−2.50
CHB6	−2.17	2.17	2.32	0.08	2.16	−1.21	−3.37
IL16	0.20	0.37	0.44	0.00	1.24	0.91	−0.33
IDISP	2.23	3.12	4.15	0.22	10.25	8.02	−2.24
ICONF	−0.01	0.19	0.25	0.06	1.02	0.66	−0.36
ACONF	0.00	0.05	0.08	0.03	0.33	0.21	−0.12
AMINO20x4	−0.04	0.22	0.28	0.09	1.70	0.73	−0.97
PCONF21	−0.16	0.55	0.65	0.34	2.10	0.97	−1.12
MCONF	−0.07	0.19	0.25	0.04	0.98	0.41	−0.57
SCONF	−0.27	0.29	0.39	0.06	1.28	0.15	−1.13
UPU23	0.34	0.54	0.66	0.09	2.18	1.48	−0.70
BUT14DIOL	0.09	0.15	0.20	0.05	0.97	0.63	−0.34

Table S74: Statistical analysis for the B97-2-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	3.40	4.85	8.50	0.02	86.47	65.71	−20.76
G21EA	−1.73	2.07	2.47	0.06	8.05	1.91	−6.13
G21IP	−0.83	2.63	3.33	0.01	13.25	6.27	−6.98
DIPCS10	−4.37	4.70	5.97	0.01	13.05	1.34	−11.71
PA26	5.47	5.61	6.00	0.03	13.31	11.56	−1.76
SIE4x4	16.55	16.55	18.21	0.49	28.57	33.96	5.39
ALKBDE10	1.44	4.79	6.71	0.05	23.31	16.56	−6.75
YBDE18	3.85	4.31	4.84	0.09	11.73	8.58	−3.14
AL2X6	11.21	11.21	11.72	0.31	10.01	15.19	5.18
HEAVYSB11	15.00	15.00	16.63	0.26	22.53	27.81	5.28
NBPRC	−1.20	3.48	4.18	0.13	13.59	5.22	−8.37
ALK8	18.57	19.44	25.12	0.31	52.13	48.66	−3.47
RC21	4.90	5.21	6.23	0.15	13.10	11.43	−1.66
G2RC	−0.66	6.39	8.15	0.12	40.54	19.20	−21.35
BH76RC	0.39	2.10	3.05	0.10	16.42	11.73	−4.69
FH51	−0.48	2.32	3.26	0.07	16.76	8.46	−8.31
TAUT15	0.16	1.06	1.31	0.35	4.25	2.94	−1.31
DC13	−2.60	8.35	13.29	0.15	51.21	20.61	−30.61
MB16-43	56.32	56.32	66.75	0.14	173.00	173.84	0.84
DARC	−2.53	2.53	3.40	0.08	7.75	−0.01	−7.77
RSE43	−2.42	2.42	2.64	0.32	4.49	−1.05	−5.54
BSR36	−0.34	0.57	0.69	0.04	3.15	1.61	−1.54
CDIE20	1.20	1.21	1.40	0.30	2.78	2.75	−0.03
ISO34	−0.14	1.07	1.61	0.07	9.25	5.01	−4.24
ISOL24	0.33	2.32	3.28	0.11	14.58	7.28	−7.30
C60ISO	1.72	2.97	3.09	0.03	7.35	3.98	−3.37
PArel	0.60	1.04	1.65	0.22	6.75	5.17	−1.58
BH76	−3.66	3.88	4.58	0.21	14.96	3.15	−11.81
BHPERI	−3.72	3.86	4.36	0.18	10.87	1.75	−9.12
BHDIV10	−4.39	4.96	5.35	0.11	11.56	2.84	−8.72
INV24	0.30	1.52	2.18	0.05	10.74	6.91	−3.83
BHROT27	0.58	0.59	0.78	0.09	1.65	1.58	−0.07
PX13	−4.23	4.23	4.39	0.13	4.21	−2.43	−6.64
WCPT18	−2.84	2.85	3.54	0.08	7.78	0.07	−7.71
RG18	0.03	0.09	0.13	0.16	0.63	0.32	−0.32
ADIM6	−0.32	0.32	0.35	0.10	0.45	−0.12	−0.57
S22	0.11	0.23	0.31	0.03	1.34	0.79	−0.55
S66	0.02	0.21	0.26	0.04	1.36	0.88	−0.49
HEAVY28	1.12	1.13	1.30	0.91	3.35	3.19	−0.16
WATER27	−1.65	2.21	3.35	0.03	11.20	1.74	−9.47
CARBHB12	1.18	1.18	1.52	0.20	2.93	3.19	0.26
PNICO23	1.82	1.86	2.69	0.44	9.24	8.96	−0.27
HAL59	1.40	1.44	2.01	0.31	6.25	5.94	−0.32
AHB21	−0.59	0.80	1.13	0.04	4.29	0.56	−3.73
CHB6	−4.11	4.11	4.59	0.15	5.17	−2.18	−7.35
IL16	0.00	0.48	0.59	0.00	2.23	1.07	−1.16
IDISP	1.15	1.34	1.83	0.09	4.47	3.91	−0.56
ICONF	0.16	0.46	0.61	0.14	2.16	1.31	−0.85
ACONF	−0.02	0.03	0.04	0.02	0.13	0.03	−0.11
AMINO20x4	−0.01	0.27	0.34	0.11	1.88	1.07	−0.81
PCONF21	−0.24	0.57	0.73	0.35	2.43	0.80	−1.63
MCONF	0.01	0.27	0.33	0.05	1.43	0.67	−0.76
SCONF	−0.13	0.24	0.34	0.05	1.44	0.37	−1.07
UPU23	0.42	0.52	0.66	0.09	1.96	1.54	−0.42
BUT14DIOL	−0.09	0.20	0.24	0.07	1.00	0.51	−0.48

Table S75: Statistical analysis for the B98-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	0.34	2.57	4.02	0.01	40.78	13.13	−27.64
G21EA	0.34	1.44	1.91	0.04	7.46	5.37	−2.09
G21IP	0.57	2.97	3.64	0.01	15.00	8.71	−6.29
DIPCS10	−1.88	3.62	4.76	0.01	14.72	4.63	−10.09
PA26	3.93	3.93	4.53	0.02	9.84	10.14	0.30
SIE4x4	16.64	16.64	18.53	0.49	30.85	35.09	4.24
ALKBDE10	0.07	3.21	4.67	0.03	18.89	11.08	−7.81
YBDE18	−1.34	2.71	3.19	0.05	10.20	3.20	−6.99
AL2X6	3.89	3.89	4.25	0.11	5.58	6.09	0.51
HEAVYSB11	5.21	5.23	6.44	0.09	10.90	10.78	−0.12
NBPRC	0.02	1.71	1.89	0.06	5.61	2.62	−2.99
ALK8	9.52	10.10	12.78	0.16	24.54	22.25	−2.30
RC21	3.37	3.67	4.36	0.10	9.34	6.82	−2.53
G2RC	−0.43	4.57	5.63	0.09	26.49	13.22	−13.26
BH76RC	−0.08	1.76	2.33	0.08	12.28	6.34	−5.94
FH51	0.40	2.10	2.85	0.07	14.45	8.59	−5.86
TAUT15	−0.07	0.99	1.22	0.32	4.29	2.50	−1.79
DC13	−1.12	7.18	8.21	0.13	26.98	10.74	−16.25
MB16-43	13.12	17.40	21.65	0.04	92.36	69.22	−23.14
DARC	2.26	2.79	3.07	0.09	7.12	4.30	−2.82
RSE43	−2.01	2.01	2.21	0.26	3.70	−0.87	−4.58
BSR36	−3.50	3.50	3.99	0.22	7.35	−1.41	−8.76
CDIE20	0.90	0.90	1.00	0.22	1.57	1.55	−0.02
ISO34	−0.06	1.16	1.67	0.08	9.89	6.35	−3.53
ISOL24	−0.71	3.84	5.27	0.18	23.71	12.93	−10.78
C60ISO	0.26	2.27	2.57	0.02	7.25	2.57	−4.68
PArel	0.25	0.93	1.54	0.20	7.34	5.19	−2.15
BH76	−4.46	4.61	5.08	0.25	12.32	2.35	−9.97
BHPERI	−2.71	2.71	3.04	0.13	5.96	−0.53	−6.48
BHDIV10	−3.47	4.23	4.45	0.09	11.10	3.80	−7.29
INV24	−0.40	1.02	1.32	0.03	5.76	2.67	−3.09
BHROT27	0.37	0.42	0.59	0.07	1.50	1.34	−0.16
PX13	−4.47	4.47	4.64	0.13	4.20	−2.99	−7.19
WCPT18	−2.95	2.98	3.69	0.09	7.76	0.25	−7.50
RG18	0.27	0.27	0.30	0.47	0.50	0.56	0.06
ADIM6	0.23	0.23	0.24	0.07	0.17	0.34	0.16
S22	0.28	0.35	0.42	0.05	1.69	1.08	−0.61
S66	0.32	0.33	0.40	0.06	1.35	1.23	−0.12
HEAVY28	1.08	1.08	1.19	0.87	2.52	2.58	0.06
WATER27	3.18	3.52	4.53	0.04	17.13	12.48	−4.64
CARBHB12	1.28	1.28	1.50	0.21	2.30	2.88	0.58
PNICO23	1.40	1.40	1.77	0.33	4.90	5.05	0.15
HAL59	1.19	1.20	1.55	0.26	4.06	3.94	−0.11
AHB21	−0.77	0.78	0.99	0.03	2.58	0.07	−2.52
CHB6	−2.75	2.75	2.95	0.10	2.95	−1.51	−4.46
IL16	0.24	0.41	0.49	0.00	1.35	1.01	−0.34
IDISP	2.10	2.69	3.70	0.19	8.53	7.40	−1.13
ICONF	−0.02	0.20	0.27	0.06	1.10	0.71	−0.40
ACONF	−0.01	0.05	0.06	0.03	0.26	0.16	−0.10
AMINO20x4	−0.04	0.23	0.29	0.09	1.73	0.79	−0.95
PCONF21	−0.18	0.56	0.66	0.35	2.11	0.89	−1.22
MCONF	−0.06	0.19	0.24	0.04	1.00	0.40	−0.60
SCONF	−0.23	0.28	0.39	0.06	1.50	0.20	−1.29
UPU23	0.38	0.56	0.68	0.10	2.09	1.46	−0.62
BUT14DIOL	0.10	0.15	0.20	0.05	0.95	0.64	−0.31

Table S76: Statistical analysis for the HISS-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−7.06	7.32	9.54	0.02	48.48	4.88	−43.59
G21EA	−1.83	3.65	4.22	0.11	12.53	4.41	−8.12
G21IP	1.03	4.19	5.17	0.02	19.89	10.53	−9.36
DIPCS10	0.04	4.42	5.09	0.01	17.36	9.69	−7.67
PA26	3.43	3.44	4.03	0.02	8.68	8.63	−0.05
SIE4x4	8.78	8.78	10.30	0.26	19.37	21.96	2.60
ALKBDE10	−4.78	5.72	7.33	0.06	22.21	4.03	−18.18
YBDE18	−0.57	3.19	3.63	0.06	11.35	4.33	−7.02
AL2X6	4.01	4.01	4.18	0.11	3.98	5.84	1.86
HEAVYSB11	1.48	3.13	3.95	0.05	12.63	9.35	−3.29
NBPRC	−1.36	3.78	4.15	0.14	12.88	7.34	−5.54
ALK8	11.37	11.55	15.80	0.18	35.26	34.54	−0.73
RC21	4.34	4.97	6.25	0.14	20.89	17.72	−3.17
G2RC	−5.92	7.99	10.17	0.16	37.59	11.81	−25.79
BH76RC	−1.05	2.44	3.16	0.11	10.56	3.91	−6.65
FH51	−3.04	3.88	4.88	0.13	18.59	4.85	−13.74
TAUT15	0.10	1.16	1.52	0.38	4.89	2.91	−1.98
DC13	−4.20	10.31	12.73	0.19	45.08	24.06	−21.03
MB16-43	24.67	28.22	34.02	0.07	124.88	93.67	−31.21
DARC	−7.26	7.26	7.61	0.22	8.23	−4.88	−13.11
RSE43	−0.60	0.62	0.81	0.08	2.40	0.24	−2.17
BSR36	−3.72	3.72	4.14	0.23	7.07	−1.47	−8.53
CDIE20	1.21	1.26	1.57	0.31	3.65	3.26	−0.39
ISO34	−0.01	1.82	2.36	0.12	8.99	4.35	−4.64
ISOL24	1.41	2.91	4.02	0.13	17.31	10.22	−7.09
C60ISO	5.51	5.51	6.04	0.06	8.85	10.56	1.70
PArel	0.96	1.27	1.96	0.27	7.74	6.12	−1.62
BH76	−1.02	1.73	2.11	0.09	10.05	5.13	−4.92
BHPERI	0.16	1.86	2.45	0.09	10.92	7.87	−3.05
BHDIV10	−1.12	2.23	2.69	0.05	8.11	2.98	−5.13
INV24	0.10	2.07	3.44	0.06	20.17	12.30	−7.86
BHROT27	0.87	0.88	1.21	0.14	2.42	2.31	−0.11
PX13	−3.03	3.03	3.31	0.09	4.65	−0.48	−5.13
WCPT18	−0.70	2.54	2.78	0.07	8.81	4.44	−4.37
RG18	0.14	0.15	0.22	0.26	0.69	0.66	−0.03
ADIM6	−0.37	0.37	0.40	0.11	0.49	−0.15	−0.64
S22	0.40	0.55	0.80	0.08	3.30	2.45	−0.85
S66	0.28	0.43	0.63	0.08	3.16	2.52	−0.63
HEAVY28	1.29	1.29	1.48	1.04	3.26	3.33	0.07
WATER27	5.46	5.77	7.26	0.07	23.31	19.08	−4.24
CARBHB12	1.44	1.44	1.67	0.24	2.43	2.99	0.56
PNICO23	1.36	1.36	1.64	0.32	4.14	4.13	−0.01
HAL59	1.11	1.13	1.50	0.25	4.12	3.94	−0.18
AHB21	−1.75	1.75	2.14	0.08	4.44	−0.13	−4.57
CHB6	−2.89	2.89	3.10	0.11	2.97	−1.42	−4.39
IL16	−0.07	0.39	0.45	0.00	1.57	0.85	−0.72
IDISP	−0.03	2.53	3.07	0.18	9.28	4.73	−4.55
ICONF	0.15	0.38	0.56	0.12	2.03	1.47	−0.55
ACONF	0.16	0.16	0.18	0.09	0.30	0.34	0.04
AMINO20x4	0.14	0.31	0.42	0.13	2.04	1.21	−0.83
PCONF21	0.10	0.89	1.10	0.55	3.32	1.77	−1.55
MCONF	0.10	0.24	0.27	0.05	0.92	0.54	−0.39
SCONF	−0.09	0.13	0.19	0.03	0.81	0.32	−0.49
UPU23	0.59	0.68	0.83	0.12	1.79	1.45	−0.35
BUT14DIOL	0.12	0.13	0.16	0.05	0.51	0.45	−0.06

Table S77: Statistical analysis for the HSE03-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.84	3.44	4.95	0.01	40.71	14.15	−26.56
G21EA	4.45	4.45	5.31	0.13	9.19	9.70	0.50
G21IP	5.71	6.04	7.21	0.02	18.36	15.03	−3.32
DIPCS10	10.23	10.23	10.80	0.02	10.25	14.57	4.32
PA26	3.10	3.12	3.67	0.02	8.93	8.64	−0.29
SIE4x4	14.49	14.49	16.23	0.43	27.75	31.22	3.47
ALKBDE10	−1.66	4.66	5.73	0.05	21.01	10.23	−10.78
YBDE18	−0.40	1.03	1.60	0.02	6.33	1.98	−4.35
AL2X6	3.71	3.71	3.96	0.10	4.55	5.35	0.80
HEAVYSB11	3.35	3.65	4.52	0.06	9.72	8.09	−1.64
NBPRC	−1.01	2.96	3.32	0.11	10.34	4.82	−5.52
ALK8	11.24	11.63	15.97	0.19	35.10	33.53	−1.57
RC21	4.54	5.01	5.93	0.14	14.69	12.61	−2.08
G2RC	−2.88	6.43	8.03	0.13	33.57	12.11	−21.46
BH76RC	−0.14	2.33	3.17	0.11	16.54	9.73	−6.81
FH51	−1.10	2.54	3.54	0.08	17.82	8.04	−9.78
TAUT15	0.29	1.21	1.65	0.40	5.30	3.64	−1.65
DC13	−2.10	7.63	10.74	0.14	48.00	20.20	−27.80
MB16-43	20.42	22.92	27.92	0.06	100.85	84.64	−16.21
DARC	−2.32	2.44	3.49	0.08	9.04	0.41	−8.63
RSE43	−1.50	1.50	1.70	0.20	3.45	−0.48	−3.93
BSR36	−3.48	3.48	3.94	0.21	7.34	−1.34	−8.68
CDIE20	1.32	1.34	1.55	0.33	3.06	2.86	−0.19
ISO34	−0.25	1.32	1.80	0.09	9.09	5.15	−3.94
ISOL24	−0.15	2.50	3.46	0.11	15.46	6.96	−8.50
C60ISO	0.47	2.48	2.81	0.03	7.93	3.00	−4.93
PArel	0.67	1.15	1.75	0.25	7.47	5.78	−1.68
BH76	−4.39	4.58	5.02	0.25	16.05	2.52	−13.53
BHPERI	−2.68	2.88	3.14	0.14	7.16	1.44	−5.73
BHDIV10	−4.00	4.70	5.18	0.10	11.46	3.48	−7.98
INV24	−0.44	1.20	1.76	0.04	8.17	4.13	−4.05
BHROT27	0.59	0.63	0.84	0.10	1.83	1.63	−0.21
PX13	−5.87	5.87	6.04	0.18	5.45	−3.57	−9.02
WCPT18	−3.86	3.86	4.63	0.11	8.47	−0.53	−9.00
RG18	0.22	0.22	0.27	0.38	0.56	0.61	0.05
ADIM6	−0.25	0.25	0.30	0.07	0.47	−0.06	−0.53
S22	0.36	0.54	0.76	0.07	3.16	2.14	−1.02
S66	0.28	0.42	0.61	0.08	2.89	2.28	−0.62
HEAVY28	1.21	1.21	1.36	0.98	2.96	3.06	0.09
WATER27	6.40	6.89	8.87	0.08	29.97	23.32	−6.65
CARBHB12	1.65	1.65	1.93	0.27	3.01	3.63	0.61
PNICO23	1.51	1.51	1.91	0.35	5.34	5.49	0.14
HAL59	1.31	1.32	1.72	0.29	4.26	4.09	−0.17
AHB21	−1.63	1.63	1.90	0.07	4.04	−0.15	−4.18
CHB6	−2.71	2.71	2.92	0.10	2.70	−1.30	−4.00
IL16	−0.60	0.62	0.73	0.01	1.49	0.11	−1.38
IDISP	1.17	2.04	2.47	0.14	6.17	4.28	−1.89
ICONF	0.11	0.23	0.36	0.07	1.50	1.06	−0.44
ACONF	0.07	0.07	0.09	0.04	0.24	0.23	−0.01
AMINO20x4	0.08	0.28	0.36	0.11	1.79	0.88	−0.91
PCONF21	−0.19	0.96	1.14	0.59	3.36	1.51	−1.85
MCONF	−0.01	0.27	0.31	0.05	1.13	0.55	−0.58
SCONF	0.06	0.34	0.49	0.07	2.14	0.50	−1.64
UPU23	0.45	0.58	0.70	0.10	2.05	1.56	−0.49
BUT14DIOL	0.31	0.31	0.34	0.11	0.90	0.83	−0.07

Table S78: Statistical analysis for the HSE06-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−1.98	3.56	5.18	0.01	33.26	6.45	−26.81
G21EA	−0.60	2.68	2.99	0.08	9.09	4.21	−4.88
G21IP	−0.08	3.70	4.39	0.01	17.28	9.14	−8.14
DIPCS10	−1.63	3.05	3.88	0.00	10.73	3.14	−7.58
PA26	2.59	2.65	3.24	0.01	8.68	7.98	−0.70
SIE4x4	14.49	14.49	16.26	0.43	28.04	31.29	3.25
ALKBDE10	−3.94	5.57	6.40	0.06	18.69	6.05	−12.64
YBDE18	−1.23	1.41	1.95	0.03	6.30	1.51	−4.80
AL2X6	0.25	0.93	1.11	0.03	3.33	1.29	−2.04
HEAVYSB11	−0.79	1.14	1.54	0.02	4.41	0.66	−3.76
NBPRC	−0.53	2.57	2.91	0.09	9.43	4.60	−4.83
ALK8	4.62	4.67	6.11	0.07	10.35	10.12	−0.23
RC21	4.28	4.75	5.63	0.13	13.82	11.73	−2.09
G2RC	−2.64	6.21	7.72	0.12	30.97	11.00	−19.96
BH76RC	−0.09	2.35	3.16	0.11	16.56	9.94	−6.62
FH51	−0.94	2.47	3.41	0.08	17.30	8.11	−9.18
TAUT15	0.29	1.19	1.65	0.39	5.40	3.59	−1.81
DC13	−1.17	6.67	9.61	0.12	43.39	20.23	−23.16
MB16-43	1.61	14.27	18.67	0.03	97.25	62.43	−34.82
DARC	−1.53	2.11	3.04	0.06	8.93	1.15	−7.78
RSE43	−1.49	1.49	1.69	0.20	3.54	−0.43	−3.97
BSR36	−3.83	3.83	4.38	0.24	8.51	−1.41	−9.92
CDIE20	1.30	1.32	1.53	0.33	3.03	2.85	−0.18
ISO34	−0.30	1.34	1.81	0.09	8.92	4.97	−3.96
ISOL24	−0.42	2.64	3.65	0.12	16.58	7.76	−8.83
C60ISO	−0.04	2.43	2.90	0.02	8.30	2.63	−5.67
PArel	0.66	1.16	1.76	0.25	7.49	5.78	−1.71
BH76	−4.41	4.58	5.04	0.25	16.09	2.25	−13.84
BHPERI	−2.36	2.52	2.76	0.12	5.99	1.11	−4.88
BHDIV10	−3.90	4.56	5.03	0.10	10.73	3.33	−7.40
INV24	−0.60	1.16	1.69	0.04	7.95	3.86	−4.10
BHROT27	0.57	0.61	0.81	0.10	1.75	1.57	−0.18
PX13	−6.02	6.02	6.18	0.18	5.38	−3.83	−9.22
WCPT18	−4.01	4.01	4.70	0.11	8.39	−0.79	−9.18
RG18	0.13	0.13	0.15	0.22	0.20	0.24	0.04
ADIM6	−0.14	0.14	0.17	0.04	0.27	−0.05	−0.32
S22	0.25	0.52	0.71	0.07	3.21	1.83	−1.37
S66	0.23	0.39	0.55	0.07	2.74	2.01	−0.73
HEAVY28	0.44	0.44	0.51	0.35	0.93	1.01	0.08
WATER27	5.78	6.29	8.15	0.08	28.52	21.72	−6.79
CARBHB12	1.47	1.47	1.73	0.24	2.80	3.30	0.50
PNICO23	0.97	0.97	1.31	0.23	4.06	4.16	0.10
HAL59	0.66	0.73	1.11	0.16	3.93	3.57	−0.35
AHB21	−1.32	1.32	1.55	0.06	3.36	0.00	−3.36
CHB6	−1.24	1.29	1.54	0.05	2.93	0.15	−2.78
IL16	−0.17	0.31	0.38	0.00	1.16	0.47	−0.69
IDISP	1.35	2.55	3.06	0.18	7.82	4.95	−2.86
ICONF	0.18	0.30	0.46	0.09	1.60	1.12	−0.48
ACONF	0.14	0.14	0.16	0.08	0.32	0.36	0.04
AMINO20x4	0.07	0.27	0.36	0.11	1.88	0.94	−0.94
PCONF21	−0.24	1.05	1.22	0.65	3.63	1.68	−1.95
MCONF	−0.03	0.27	0.30	0.05	1.03	0.50	−0.53
SCONF	0.04	0.26	0.40	0.06	1.82	0.45	−1.37
UPU23	0.37	0.55	0.65	0.10	2.13	1.48	−0.64
BUT14DIOL	0.25	0.26	0.30	0.09	0.90	0.82	−0.07

Table S79: Statistical analysis for the TPSSh-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.53	4.44	6.13	0.01	43.62	17.69	−25.93
G21EA	−0.64	2.71	2.96	0.08	9.97	5.41	−4.56
G21IP	−0.89	3.91	4.68	0.02	19.79	11.55	−8.24
DIPCS10	−3.01	3.39	4.70	0.01	11.67	1.40	−10.27
PA26	4.89	4.89	5.37	0.03	9.02	11.48	2.46
SIE4x4	18.39	18.39	20.89	0.55	35.66	40.15	4.49
ALKBDE10	−1.71	4.66	6.12	0.05	22.36	14.47	−7.89
YBDE18	−4.18	4.21	4.63	0.09	7.38	0.31	−7.08
AL2X6	1.24	2.21	2.24	0.06	5.34	2.42	−2.92
HEAVYSB11	−0.98	1.85	2.26	0.03	6.02	1.43	−4.59
NBPRC	−0.88	1.61	2.00	0.06	6.46	2.04	−4.42
ALK8	3.98	3.98	5.17	0.06	7.87	8.69	0.81
RC21	3.20	3.92	4.32	0.11	10.25	7.74	−2.50
G2RC	1.66	6.18	7.68	0.12	28.78	16.31	−12.46
BH76RC	0.00	3.38	4.39	0.16	17.66	8.42	−9.23
FH51	1.62	3.33	4.49	0.11	21.05	12.27	−8.78
TAUT15	0.13	1.34	1.56	0.44	4.92	3.10	−1.82
DC13	−0.10	7.25	10.13	0.13	38.11	16.86	−21.26
MB16-43	−21.18	23.62	28.68	0.06	111.05	42.93	−68.12
DARC	2.94	3.41	3.74	0.11	7.02	5.49	−1.53
RSE43	−1.48	1.48	1.71	0.19	3.87	−0.54	−4.41
BSR36	−4.39	4.39	4.84	0.27	9.32	−1.32	−10.64
CDIE20	1.48	1.48	1.61	0.36	2.35	2.73	0.38
ISO34	−1.37	2.01	2.69	0.14	13.69	4.57	−9.12
ISOL24	−2.29	4.32	5.89	0.20	29.17	13.98	−15.19
C60ISO	−3.89	4.42	5.94	0.04	12.93	1.06	−11.87
PArel	0.34	1.31	1.78	0.28	8.66	5.02	−3.64
BH76	−7.20	7.22	7.94	0.39	17.93	0.92	−17.00
BHPERI	−4.02	4.02	4.24	0.19	5.32	−1.33	−6.65
BHDIV10	−5.09	5.40	5.80	0.12	10.85	1.57	−9.29
INV24	−0.93	1.17	1.51	0.04	5.05	1.11	−3.94
BHROT27	0.41	0.53	0.70	0.08	1.97	1.47	−0.50
PX13	−6.87	6.87	6.99	0.21	5.57	−4.25	−9.81
WCPT18	−4.51	4.51	4.98	0.13	7.55	−1.23	−8.78
RG18	0.11	0.11	0.13	0.19	0.28	0.29	0.00
ADIM6	−0.12	0.12	0.15	0.04	0.26	−0.05	−0.31
S22	0.12	0.33	0.45	0.05	2.15	1.24	−0.91
S66	0.07	0.27	0.36	0.05	1.87	1.31	−0.56
HEAVY28	0.30	0.31	0.40	0.25	0.90	0.83	−0.07
WATER27	2.75	3.40	4.47	0.04	22.28	13.43	−8.85
CARBHB12	1.26	1.26	1.54	0.21	2.68	3.08	0.40
PNICO23	0.95	0.97	1.33	0.23	4.26	4.12	−0.14
HAL59	0.62	0.78	1.28	0.17	5.25	4.70	−0.54
AHB21	−0.46	0.60	0.77	0.03	2.30	0.53	−1.77
CHB6	−0.66	1.10	1.26	0.04	3.39	1.33	−2.06
IL16	0.36	0.41	0.50	0.00	1.16	0.93	−0.24
IDISP	2.46	2.46	3.43	0.17	7.23	7.36	0.13
ICONF	0.03	0.18	0.21	0.06	0.78	0.48	−0.30
ACONF	−0.04	0.07	0.09	0.04	0.25	0.09	−0.16
AMINO20x4	0.05	0.29	0.35	0.12	1.51	0.83	−0.69
PCONF21	−0.43	0.95	1.15	0.59	3.06	0.98	−2.08
MCONF	−0.02	0.35	0.41	0.07	1.63	0.72	−0.90
SCONF	0.20	0.74	0.97	0.16	3.48	0.87	−2.61
UPU23	0.34	0.47	0.60	0.08	1.98	1.41	−0.58
BUT14DIOL	0.16	0.18	0.24	0.06	0.99	0.75	−0.24

Table S80: Statistical analysis for the revTPSSh-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−1.34	5.14	7.05	0.02	51.75	24.23	−27.51
G21EA	−1.44	2.90	3.22	0.09	9.18	3.69	−5.49
G21IP	−1.23	3.94	4.75	0.02	20.00	11.22	−8.78
DIPCS10	−3.64	3.74	5.24	0.01	12.16	0.54	−11.62
PA26	4.64	4.64	5.22	0.02	9.73	11.44	1.71
SIE4x4	17.95	17.95	20.42	0.53	34.88	39.02	4.15
ALKBDE10	−3.52	5.71	6.45	0.06	21.25	10.94	−10.31
YBDE18	−3.29	3.44	4.01	0.07	8.78	1.10	−7.68
AL2X6	2.84	3.13	3.33	0.09	5.08	4.22	−0.86
HEAVYSB11	1.11	1.96	2.33	0.03	6.74	4.05	−2.69
NBPRC	−1.55	1.70	2.13	0.06	4.88	0.75	−4.13
ALK8	5.02	5.02	7.22	0.08	14.92	15.39	0.47
RC21	3.66	4.47	5.05	0.13	13.16	9.57	−3.59
G2RC	3.82	8.98	11.14	0.18	37.29	22.79	−14.50
BH76RC	0.45	4.51	5.49	0.21	19.90	10.94	−8.96
FH51	2.06	4.16	5.65	0.13	26.41	16.69	−9.71
TAUT15	0.13	1.05	1.34	0.34	4.19	2.64	−1.56
DC13	−1.06	8.19	10.91	0.15	42.72	20.15	−22.56
MB16-43	−24.54	28.52	33.86	0.07	118.75	43.16	−75.59
DARC	0.15	1.77	2.15	0.05	6.80	2.70	−4.10
RSE43	−1.30	1.30	1.55	0.17	3.71	−0.39	−4.10
BSR36	−2.14	2.14	2.28	0.13	3.61	−0.30	−3.90
CDIE20	1.33	1.33	1.41	0.33	1.63	2.37	0.74
ISO34	−1.94	2.63	3.56	0.18	15.33	3.12	−12.20
ISOL24	−1.95	3.46	4.44	0.16	19.93	11.00	−8.93
C60ISO	−4.83	5.03	6.80	0.05	14.20	0.69	−13.51
PArel	0.55	1.28	1.69	0.28	7.51	4.43	−3.08
BH76	−6.94	6.94	7.90	0.37	18.04	−0.05	−18.09
BHPERI	−4.67	4.67	5.02	0.22	7.61	−0.50	−8.11
BHDIV10	−4.77	4.87	5.34	0.11	9.56	0.51	−9.05
INV24	−0.48	1.02	1.36	0.03	5.44	2.04	−3.40
BHROT27	0.41	0.52	0.68	0.08	1.92	1.52	−0.41
PX13	−4.41	4.41	4.54	0.13	3.84	−2.73	−6.57
WCPT18	−3.71	3.71	4.11	0.11	5.97	−0.96	−6.93
RG18	0.03	0.06	0.08	0.10	0.33	0.16	−0.17
ADIM6	−0.30	0.30	0.32	0.09	0.29	−0.17	−0.46
S22	0.08	0.25	0.32	0.03	1.35	0.87	−0.48
S66	0.01	0.21	0.27	0.04	1.44	0.91	−0.53
HEAVY28	0.65	0.65	0.73	0.52	1.36	1.28	−0.08
WATER27	1.82	2.20	2.83	0.03	13.81	8.75	−5.06
CARBHB12	0.89	0.89	1.06	0.15	1.76	2.12	0.36
PNICO23	1.21	1.22	1.57	0.29	4.57	4.49	−0.08
HAL59	0.93	1.00	1.50	0.22	5.09	4.69	−0.39
AHB21	−0.12	0.37	0.49	0.02	2.03	1.18	−0.85
CHB6	−1.18	1.18	1.45	0.04	2.48	−0.25	−2.73
IL16	0.44	0.55	0.63	0.01	1.51	1.08	−0.43
IDISP	2.16	2.32	3.56	0.16	8.08	7.58	−0.51
ICONF	0.01	0.24	0.28	0.07	0.98	0.54	−0.44
ACONF	−0.10	0.10	0.11	0.05	0.21	0.00	−0.21
AMINO20x4	0.09	0.24	0.31	0.10	1.40	0.95	−0.45
PCONF21	−0.23	0.56	0.71	0.35	2.10	0.64	−1.46
MCONF	0.08	0.36	0.45	0.07	1.78	0.90	−0.87
SCONF	0.38	0.91	1.06	0.20	3.41	1.14	−2.26
UPU23	0.12	0.35	0.44	0.06	1.60	1.01	−0.59
BUT14DIOL	0.01	0.14	0.17	0.05	0.79	0.47	−0.33

Table S81: Statistical analysis for the TPSS0-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−7.29	9.54	11.95	0.03	56.23	18.58	−37.65
G21EA	−2.11	3.66	4.36	0.11	13.35	4.78	−8.57
G21IP	−0.77	4.07	4.82	0.02	19.74	10.96	−8.78
DIPCS10	−2.17	3.93	5.10	0.01	15.95	4.56	−11.39
PA26	5.07	5.07	5.49	0.03	8.97	11.29	2.32
SIE4x4[a]	13.64	13.64	15.88	0.40	28.30	32.04	3.74
ALKBDE10	−6.69	7.30	8.41	0.07	21.20	3.08	−18.12
YBDE18	−3.42	3.44	4.21	0.07	7.74	0.14	−7.60
AL2X6	2.29	2.56	2.68	0.07	3.93	3.13	−0.80
HEAVYSB11	−1.57	1.57	1.92	0.03	3.74	−0.11	−3.85
NBPRC	−1.34	2.70	2.92	0.10	8.74	4.47	−4.27
ALK8	5.22	5.22	6.48	0.08	9.49	10.55	1.07
RC21	3.56	4.00	4.64	0.11	12.83	10.92	−1.91
G2RC	−1.06	5.58	7.02	0.11	29.62	11.52	−18.10
BH76RC	−0.63	3.53	4.41	0.17	18.47	9.25	−9.22
FH51	−0.16	2.53	3.43	0.08	16.08	8.06	−8.02
TAUT15	0.22	0.99	1.18	0.32	3.56	2.42	−1.14
DC13	−1.77	7.50	9.51	0.14	37.51	19.81	−17.70
MB16-43	−14.48	19.53	23.84	0.05	108.58	54.71	−53.86
DARC	−1.71	1.89	2.65	0.06	6.75	0.63	−6.11
RSE43	−0.81	0.82	1.02	0.11	2.82	0.10	−2.72
BSR36	−4.13	4.13	4.53	0.25	8.16	−1.62	−9.78
CDIE20	1.18	1.18	1.37	0.29	2.54	2.63	0.09
ISO34	−0.92	1.83	2.17	0.13	8.24	3.50	−4.75
ISOL24	−0.57	2.27	3.01	0.10	13.44	6.09	−7.35
C60ISO	2.68	3.16	3.46	0.03	6.67	5.55	−1.12
PArel	0.62	1.01	1.44	0.22	6.22	4.54	−1.68
BH76	−4.54	4.64	5.34	0.25	14.50	1.50	−13.00
BHPERI	−2.38	2.66	2.94	0.13	7.65	2.25	−5.41
BHDIV10	−3.16	3.53	3.73	0.08	7.36	1.84	−5.52
INV24	0.09	1.34	2.04	0.04	9.02	6.18	−2.84
BHROT27	0.55	0.61	0.80	0.10	1.90	1.63	−0.27
PX13	−4.17	4.17	4.30	0.12	4.21	−1.96	−6.17
WCPT18	−2.14	2.44	3.02	0.07	7.64	1.99	−5.65
RG18	0.06	0.07	0.10	0.12	0.39	0.31	−0.08
ADIM6	−0.21	0.21	0.24	0.06	0.36	−0.08	−0.44
S22	0.19	0.38	0.55	0.05	2.51	1.73	−0.78
S66	0.10	0.30	0.43	0.05	2.25	1.74	−0.50
HEAVY28	0.29	0.31	0.39	0.25	0.96	0.80	−0.15
WATER27	2.59	3.05	3.79	0.04	17.32	11.05	−6.27
CARBHB12	1.14	1.14	1.38	0.19	2.26	2.61	0.36
PNICO23	0.90	0.92	1.23	0.22	3.65	3.53	−0.12
HAL59	0.43	0.62	0.98	0.14	3.84	3.25	−0.59
AHB21	−0.79	0.84	1.09	0.04	2.78	0.34	−2.44
CHB6	−1.28	1.48	1.73	0.06	3.70	0.59	−3.11
IL16	0.27	0.45	0.49	0.00	1.33	0.92	−0.41
IDISP	1.17	1.20	1.46	0.08	2.41	2.30	−0.10
ICONF	0.09	0.22	0.30	0.07	1.08	0.81	−0.27
ACONF	−0.09	0.10	0.10	0.05	0.17	0.01	−0.16
AMINO20x4	0.07	0.27	0.33	0.11	1.60	0.96	−0.64
PCONF21	−0.24	0.75	0.90	0.46	2.57	0.79	−1.77
MCONF	0.01	0.27	0.32	0.05	1.38	0.62	−0.76
SCONF	0.10	0.50	0.67	0.11	2.45	0.60	−1.85
UPU23	0.48	0.55	0.69	0.10	1.76	1.37	−0.40
BUT14DIOL	0.07	0.12	0.16	0.04	0.72	0.53	−0.19

[a] H_2^+ did not converge and was omitted from the statistics

Table S82: Statistical analysis for the revTPSS0-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−8.11	10.40	12.92	0.03	63.45	24.29	−39.16
G21EA	−2.59	3.75	4.69	0.11	12.66	3.53	−9.13
G21IP	−0.82	4.08	4.90	0.02	19.93	10.84	−9.09
DIPCS10	−2.42	4.23	5.45	0.01	16.81	4.52	−12.30
PA26	4.74	4.74	5.24	0.03	9.41	11.14	1.73
SIE4x4	13.04	13.04	15.22	0.39	27.84	31.24	3.40
ALKBDE10	−8.28	8.28	9.69	0.08	20.07	−0.24	−20.31
YBDE18	−3.27	3.60	4.61	0.07	10.65	1.48	−9.17
AL2X6	3.41	3.41	3.68	0.10	4.23	4.99	0.76
HEAVYSB11	0.21	1.23	1.52	0.02	5.22	2.34	−2.89
NBPRC	−1.54	2.20	2.42	0.08	6.97	3.17	−3.80
ALK8	5.99	5.99	8.20	0.10	16.45	17.33	0.88
RC21	3.58	4.18	4.80	0.12	14.15	10.96	−3.19
G2RC	0.93	7.33	8.68	0.14	32.06	13.69	−18.36
BH76RC	−0.29	4.34	5.31	0.20	21.76	12.17	−9.59
FH51	0.44	3.10	4.18	0.10	21.35	11.66	−9.69
TAUT15	0.21	0.77	0.97	0.25	3.25	1.95	−1.30
DC13	−2.30	8.83	10.79	0.16	37.76	22.21	−15.55
MB16-43	−20.04	24.05	27.81	0.06	105.42	49.35	−56.07
DARC	−3.01	3.01	3.54	0.09	5.66	−0.69	−6.35
RSE43	−0.74	0.77	0.97	0.10	2.82	0.24	−2.58
BSR36	−2.44	2.44	2.57	0.15	3.89	−0.67	−4.56
CDIE20	1.09	1.09	1.25	0.27	2.03	2.41	0.38
ISO34	−1.47	2.40	2.94	0.16	10.98	3.36	−7.62
ISOL24	−0.70	2.04	2.62	0.09	11.39	4.69	−6.71
C60ISO	1.85	2.82	2.93	0.03	6.67	4.08	−2.59
PArel	0.79	1.10	1.47	0.24	5.64	4.10	−1.54
BH76	−4.26	4.30	5.33	0.23	15.97	0.72	−15.24
BHPERI	−2.33	2.69	3.01	0.13	8.11	2.48	−5.63
BHDIV10	−2.63	2.84	3.10	0.06	5.54	1.01	−4.53
INV24	0.34	1.34	2.20	0.04	9.40	6.92	−2.48
BHROT27	0.52	0.59	0.74	0.09	1.91	1.62	−0.29
PX13	−1.89	1.89	2.15	0.06	2.93	−0.41	−3.34
WCPT18	−1.24	1.68	2.04	0.05	6.69	2.75	−3.94
RG18	0.00	0.07	0.11	0.12	0.55	0.21	−0.34
ADIM6	−0.36	0.36	0.38	0.11	0.33	−0.21	−0.54
S22	0.16	0.27	0.36	0.04	1.56	1.20	−0.36
S66	0.04	0.23	0.31	0.04	1.79	1.23	−0.56
HEAVY28	0.70	0.71	0.80	0.57	1.55	1.44	−0.11
WATER27	1.02	1.28	1.65	0.02	8.36	5.17	−3.19
CARBHB12	0.78	0.78	0.93	0.13	1.57	1.87	0.30
PNICO23	1.05	1.08	1.33	0.25	3.66	3.50	−0.16
HAL59	0.69	0.78	1.12	0.17	3.79	3.35	−0.44
AHB21	−0.41	0.50	0.65	0.02	1.81	0.37	−1.43
CHB6	−1.73	1.73	2.01	0.06	3.04	−0.59	−3.63
IL16	0.54	0.57	0.67	0.01	1.41	1.17	−0.24
IDISP	1.08	1.12	1.82	0.08	4.42	4.27	−0.15
ICONF	0.06	0.25	0.29	0.08	1.00	0.56	−0.45
ACONF	−0.02	0.03	0.04	0.02	0.12	0.03	−0.09
AMINO20x4	0.10	0.24	0.31	0.10	1.37	0.93	−0.44
PCONF21	−0.03	0.48	0.56	0.30	1.73	0.51	−1.22
MCONF	0.11	0.29	0.36	0.06	1.44	0.75	−0.69
SCONF	0.18	0.49	0.58	0.11	2.05	0.74	−1.31
UPU23	0.22	0.41	0.50	0.07	1.50	1.02	−0.48
BUT14DIOL	−0.07	0.12	0.14	0.04	0.53	0.27	−0.26

Table S83: Statistical analysis for the TPSS1KCIS-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	2.16	4.34	6.40	0.01	60.68	40.18	−20.50
G21EA	−1.24	2.31	2.62	0.07	8.01	3.66	−4.35
G21IP	−1.51	3.60	4.51	0.01	17.19	8.56	−8.62
DIPCS10	−5.00	5.00	6.20	0.01	11.17	−0.96	−12.13
PA26	4.23	4.23	4.74	0.02	8.69	10.61	1.92
SIE4x4	17.48	17.48	19.59	0.52	32.28	36.56	4.27
ALKBDE10	0.18	4.55	6.02	0.05	21.15	15.50	−5.65
YBDE18	−1.38	1.73	2.36	0.04	7.82	1.99	−5.83
AL2X6	7.77	7.77	8.20	0.22	8.52	11.05	2.53
HEAVYSB11	7.65	7.65	9.23	0.13	14.32	15.84	1.52
NBPRC	−1.17	2.23	2.76	0.08	7.09	1.83	−5.26
ALK8	15.78	16.47	21.73	0.26	42.12	39.40	−2.72
RC21	3.10	3.67	4.24	0.10	8.95	6.46	−2.49
G2RC	1.39	5.94	7.18	0.12	27.86	14.36	−13.49
BH76RC	0.44	2.41	3.30	0.11	16.53	9.75	−6.78
FH51	1.32	2.97	3.97	0.10	17.92	9.73	−8.19
TAUT15	0.10	1.26	1.47	0.41	4.74	3.01	−1.73
DC13	−1.55	8.45	11.94	0.15	48.56	17.42	−31.14
MB16-43	25.38	28.92	37.41	0.07	139.94	111.91	−28.03
DARC	2.48	3.13	3.35	0.10	7.12	4.91	−2.21
RSE43	−1.68	1.68	1.92	0.22	3.84	−0.63	−4.47
BSR36	−2.83	2.83	3.08	0.17	5.32	−0.86	−6.18
CDIE20	1.44	1.44	1.58	0.35	2.44	2.72	0.28
ISO34	−1.01	1.65	2.24	0.11	12.32	5.43	−6.89
ISOL24	−1.96	4.15	5.73	0.19	27.61	13.28	−14.32
C60ISO	−2.45	3.52	4.54	0.04	11.16	1.50	−9.66
PArel	0.33	1.17	1.66	0.25	7.86	5.06	−2.79
BH76	−6.04	6.10	6.70	0.33	17.28	1.94	−15.33
BHPERI	−3.81	3.81	4.13	0.18	6.92	−0.94	−7.87
BHDIV10	−5.09	5.51	5.88	0.12	11.19	2.10	−9.09
INV24	−0.63	1.09	1.53	0.03	7.38	3.23	−4.15
BHROT27	0.45	0.54	0.72	0.09	1.82	1.47	−0.36
PX13	−5.75	5.75	5.85	0.17	4.65	−3.60	−8.25
WCPT18	−3.93	3.93	4.42	0.11	7.42	−0.76	−8.18
RG18	0.28	0.28	0.32	0.48	0.54	0.62	0.07
ADIM6	−0.22	0.22	0.28	0.07	0.56	0.01	−0.55
S22	0.20	0.33	0.43	0.05	1.85	1.19	−0.66
S66	0.14	0.27	0.37	0.05	1.79	1.28	−0.51
HEAVY28	1.29	1.29	1.46	1.04	3.37	3.40	0.03
WATER27	2.61	3.17	4.19	0.04	20.31	12.85	−7.46
CARBHB12	1.46	1.46	1.75	0.24	2.87	3.42	0.55
PNICO23	1.84	1.85	2.45	0.43	7.28	7.27	−0.01
HAL59	1.62	1.62	2.16	0.35	5.69	5.58	−0.11
AHB21	−0.63	0.74	0.98	0.03	3.06	0.48	−2.58
CHB6	−3.61	3.61	3.96	0.13	4.16	−1.85	−6.01
IL16	0.11	0.33	0.40	0.00	1.43	0.82	−0.62
IDISP	2.20	2.45	3.31	0.17	7.83	7.08	−0.75
ICONF	−0.03	0.30	0.38	0.09	1.49	0.59	−0.90
ACONF	−0.07	0.07	0.09	0.04	0.19	0.04	−0.15
AMINO20x4	0.03	0.24	0.30	0.10	1.73	0.99	−0.75
PCONF21	−0.33	0.80	0.96	0.49	2.56	0.82	−1.75
MCONF	−0.06	0.30	0.36	0.06	1.44	0.60	−0.84
SCONF	0.04	0.48	0.71	0.10	2.77	0.60	−2.17
UPU23	0.37	0.48	0.61	0.08	1.75	1.31	−0.45
BUT14DIOL	0.15	0.17	0.23	0.06	0.91	0.66	−0.24

Table S84: Statistical analysis for the BMK-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	0.19	3.21	5.06	0.01	47.60	12.21	−35.39
G21EA	−0.72	1.92	2.28	0.06	9.50	5.64	−3.87
G21IP	0.29	3.42	4.53	0.01	23.54	11.96	−11.58
DIPCS10	−4.15	5.19	6.74	0.01	16.86	2.89	−13.97
PA26	1.90	2.24	2.79	0.01	8.56	7.03	−1.53
SIE4x4	10.36	10.36	11.77	0.31	21.51	23.54	2.03
ALKBDE10	−2.01	3.97	5.52	0.04	18.98	3.97	−15.01
YBDE18	−2.09	2.34	2.94	0.05	7.77	1.80	−5.97
AL2X6	3.15	3.15	3.23	0.09	1.89	4.27	2.38
HEAVYSB11	2.08	2.32	2.63	0.04	5.53	4.24	−1.29
NBPRC	−0.96	1.79	2.05	0.06	4.94	1.48	−3.46
ALK8	6.27	6.45	11.15	0.10	28.45	27.93	−0.52
RC21	3.05	3.28	3.85	0.09	9.77	8.32	−1.45
G2RC	−2.01	3.96	5.60	0.08	26.97	14.68	−12.29
BH76RC	−0.25	1.71	2.06	0.08	8.66	4.04	−4.62
FH51	−1.08	1.93	2.54	0.06	11.01	4.49	−6.52
TAUT15	−1.07	1.17	1.50	0.38	3.42	0.34	−3.08
DC13	−5.26	10.35	12.20	0.19	33.33	12.48	−20.85
MB16-43	31.46	32.21	35.73	0.08	96.47	80.39	−16.08
DARC	−4.07	4.07	4.29	0.13	3.62	−1.90	−5.52
RSE43	−0.98	1.03	1.27	0.14	3.58	0.33	−3.25
BSR36	−0.05	0.39	0.51	0.02	2.12	1.16	−0.96
CDIE20	0.32	0.41	0.49	0.10	1.54	1.01	−0.53
ISO34	−0.45	1.06	1.48	0.07	6.82	2.12	−4.70
ISOL24	1.11	3.23	4.82	0.15	22.22	16.25	−5.97
C60ISO	4.60	4.60	4.80	0.05	3.71	6.58	2.87
PArel	0.22	0.71	1.17	0.15	6.04	3.74	−2.29
BH76	−0.98	1.48	1.83	0.08	6.63	2.15	−4.48
BHPERI	0.10	1.33	1.90	0.06	9.44	5.06	−4.38
BHDIV10	−0.99	1.79	2.13	0.04	6.50	2.73	−3.76
INV24	0.58	1.54	2.55	0.05	11.47	7.98	−3.48
BHROT27	0.55	0.60	0.84	0.10	2.17	1.81	−0.35
PX13	−0.37	0.73	0.99	0.02	2.91	0.93	−1.98
WCPT18	−0.50	1.16	1.51	0.03	6.73	3.60	−3.13
RG18	−1.42	1.42	2.03	2.45	5.94	−0.38	−6.32
ADIM6	0.18	0.62	0.74	0.18	2.04	1.37	−0.68
S22	0.64	0.80	1.32	0.11	4.92	4.26	−0.67
S66	0.36	0.50	0.71	0.09	3.32	2.61	−0.71
HEAVY28	0.62	0.71	0.90	0.57	2.69	1.91	−0.78
WATER27	0.15	1.02	1.58	0.01	9.09	3.45	−5.64
CARBHB12	0.30	0.41	0.55	0.07	1.37	1.18	−0.19
PNICO23	0.45	0.52	0.68	0.12	2.25	1.93	−0.32
HAL59	0.54	0.76	0.96	0.17	3.52	2.42	−1.10
AHB21	−0.10	0.40	0.51	0.02	1.92	0.58	−1.34
CHB6	−0.34	0.43	0.58	0.02	1.56	0.26	−1.30
IL16	1.06	1.06	1.20	0.01	1.84	2.07	0.23
IDISP	0.51	3.49	4.29	0.25	13.38	8.01	−5.37
ICONF	−0.08	0.36	0.47	0.11	1.74	0.69	−1.06
ACONF	−0.46	0.46	0.53	0.25	0.87	−0.10	−0.96
AMINO20x4	0.05	0.38	0.50	0.16	2.82	1.56	−1.25
PCONF21	1.09	1.70	2.02	1.05	5.24	3.72	−1.52
MCONF	1.19	1.23	1.38	0.25	2.79	2.23	−0.56
SCONF	0.01	0.41	0.61	0.09	2.21	0.65	−1.55
UPU23	0.09	0.77	1.12	0.13	5.39	1.33	−4.07
BUT14DIOL	0.23	0.27	0.31	0.10	0.91	0.63	−0.28

Table S85: Statistical analysis for the τHCTHhyb-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	1.85	3.81	5.19	0.01	39.38	16.92	−22.46
G21EA	2.04	2.10	2.77	0.06	8.00	7.32	−0.68
G21IP	2.07	3.45	4.13	0.01	14.93	10.54	−4.39
DIPCS10	1.41	3.73	4.25	0.01	13.25	8.32	−4.94
PA26	4.09	4.09	4.67	0.02	9.54	10.33	0.80
SIE4x4	18.56	18.56	20.43	0.55	32.04	37.37	5.33
ALKBDE10	2.59	4.21	6.62	0.04	22.06	18.57	−3.50
YBDE18	−0.29	2.76	3.23	0.06	11.47	4.90	−6.57
AL2X6	4.48	4.48	4.89	0.12	6.57	7.32	0.75
HEAVYSB11	7.30	7.31	8.71	0.13	14.50	14.47	−0.04
NBPRC	−0.26	1.87	2.15	0.07	6.29	2.61	−3.67
ALK8	10.48	11.18	14.82	0.18	32.61	29.80	−2.81
RC21	4.11	4.50	5.33	0.13	12.00	9.22	−2.78
G2RC	0.09	5.07	6.11	0.10	26.37	11.33	−15.05
BH76RC	0.26	2.08	3.18	0.10	17.73	11.90	−5.83
FH51	0.52	2.36	3.28	0.08	17.11	9.83	−7.28
TAUT15	0.04	1.32	1.58	0.43	5.26	3.40	−1.86
DC13	−0.30	6.90	7.98	0.13	23.12	10.56	−12.56
MB16-43	20.25	22.53	27.83	0.05	99.95	81.48	−18.48
DARC	1.68	2.60	2.85	0.08	7.82	4.07	−3.74
RSE43	−2.48	2.48	2.70	0.33	4.36	−1.25	−5.61
BSR36	−2.83	2.83	3.16	0.17	5.33	−1.26	−6.58
CDIE20	1.12	1.12	1.21	0.28	1.68	1.85	0.18
ISO34	−0.29	1.10	1.69	0.08	10.16	6.32	−3.83
ISOL24	−0.84	3.64	5.02	0.17	22.30	12.81	−9.49
C60ISO	−2.77	3.53	4.68	0.04	10.98	1.19	−9.78
PArel	0.31	1.13	1.75	0.24	8.11	5.73	−2.38
BH76	−5.49	5.65	6.39	0.30	17.23	2.93	−14.30
BHPERI	−4.28	4.28	4.52	0.21	5.56	−1.73	−7.29
BHDIV10	−5.04	5.76	6.19	0.13	14.73	3.60	−11.13
INV24	−0.85	1.16	1.54	0.04	5.91	2.06	−3.85
BHROT27	0.40	0.45	0.62	0.07	1.54	1.35	−0.19
PX13	−7.23	7.23	7.39	0.22	6.20	−4.51	−10.70
WCPT18	−4.67	4.67	5.30	0.13	8.95	−0.99	−9.94
RG18	0.10	0.11	0.15	0.19	0.49	0.40	−0.10
ADIM6	−0.32	0.32	0.36	0.10	0.48	−0.11	−0.59
S22	0.26	0.35	0.50	0.05	2.03	1.60	−0.43
S66	0.15	0.31	0.43	0.06	2.30	1.73	−0.57
HEAVY28	1.19	1.20	1.36	0.97	3.31	3.23	−0.08
WATER27	3.62	4.23	5.24	0.05	22.42	14.15	−8.27
CARBHB12	1.42	1.42	1.75	0.24	3.02	3.52	0.49
PNICO23	1.67	1.68	2.17	0.39	6.18	6.11	−0.07
HAL59	1.50	1.52	2.03	0.33	5.31	5.01	−0.30
AHB21	−1.08	1.09	1.35	0.05	3.44	0.14	−3.30
CHB6	−2.48	2.48	2.76	0.09	3.03	−1.31	−4.35
IL16	−0.35	0.54	0.60	0.00	1.60	0.55	−1.05
IDISP	2.12	2.37	2.99	0.17	6.50	5.76	−0.75
ICONF	0.01	0.25	0.32	0.08	1.34	0.78	−0.56
ACONF	−0.02	0.05	0.06	0.03	0.25	0.14	−0.11
AMINO20x4	−0.01	0.29	0.35	0.12	1.92	0.93	−0.99
PCONF21	−0.30	0.79	0.97	0.49	2.81	1.00	−1.81
MCONF	−0.02	0.27	0.33	0.05	1.37	0.59	−0.78
SCONF	0.01	0.46	0.72	0.10	3.01	0.60	−2.42
UPU23	0.40	0.55	0.68	0.10	2.05	1.56	−0.50
BUT14DIOL	0.33	0.34	0.39	0.12	1.11	0.96	−0.15

Table S86: Statistical analysis for the M05-D3(0) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.65	2.99	4.45	0.01	39.35	20.93	−18.42
G21EA	−2.49	2.93	3.36	0.09	10.60	3.25	−7.35
G21IP	−1.81	3.27	4.17	0.01	18.72	7.14	−11.58
DIPCS10	−5.33	5.56	7.72	0.01	16.46	1.13	−15.33
PA26	2.84	2.92	4.00	0.02	10.50	9.80	−0.70
SIE4x4	14.88	14.88	17.20	0.44	32.17	35.42	3.25
ALKBDE10	−2.57	3.93	4.66	0.04	14.92	4.52	−10.40
YBDE18	−3.86	4.05	5.40	0.08	16.69	1.70	−14.99
AL2X6	−6.25	6.25	6.35	0.17	3.77	−4.68	−8.45
HEAVYSB11	−1.92	3.39	4.19	0.06	10.87	3.30	−7.57
NBPRC	3.12	3.71	4.94	0.13	13.71	12.33	−1.38
ALK8	1.87	3.02	3.97	0.05	8.87	6.77	−2.10
RC21	1.10	2.84	3.43	0.08	12.19	6.17	−6.01
G2RC	−0.41	4.05	5.82	0.08	27.17	15.47	−11.70
BH76RC	−0.47	2.22	3.55	0.10	21.98	13.86	−8.12
FH51	−0.76	3.03	4.05	0.10	21.84	7.55	−14.29
TAUT15	−1.16	1.59	1.79	0.52	4.41	1.35	−3.06
DC13	1.29	9.17	12.55	0.17	52.52	35.54	−16.98
MB16-43	−11.93	15.76	20.16	0.04	70.60	20.54	−50.06
DARC	3.66	3.67	4.08	0.11	6.20	6.15	−0.05
RSE43	−1.84	1.84	2.14	0.24	5.42	−0.59	−6.01
BSR36	−7.30	7.30	8.83	0.45	20.20	−2.14	−22.34
CDIE20	1.29	1.36	1.75	0.33	4.34	3.82	−0.52
ISO34	−1.46	2.14	3.16	0.15	10.63	2.95	−7.68
ISOL24	−4.59	6.26	9.00	0.29	39.42	10.28	−29.14
C60ISO	−1.34	2.41	3.01	0.02	8.30	1.93	−6.37
PArel	0.48	1.43	1.96	0.31	8.12	5.17	−2.95
BH76	−1.21	2.00	2.82	0.11	18.80	6.02	−12.78
BHPERI	3.28	3.67	4.07	0.18	10.90	6.27	−4.64
BHDIV10	−1.15	3.09	3.59	0.07	10.09	3.56	−6.53
INV24	−1.32	2.18	2.92	0.07	13.07	6.73	−6.34
BHROT27	0.48	0.51	0.69	0.08	1.73	1.54	−0.20
PX13	0.29	1.48	2.00	0.04	7.06	4.84	−2.22
WCPT18	−1.95	2.36	2.92	0.07	8.59	3.18	−5.41
RG18	0.30	0.30	0.38	0.52	1.04	1.12	0.08
ADIM6	0.75	0.75	0.78	0.22	0.61	1.07	0.46
S22	−0.26	0.52	0.72	0.07	2.83	0.62	−2.21
S66	0.18	0.35	0.42	0.06	1.65	0.74	−0.92
HEAVY28	0.20	0.25	0.35	0.20	1.35	1.01	−0.34
WATER27	3.35	3.35	4.80	0.04	11.44	11.60	0.16
CARBHB12	0.46	0.54	0.60	0.09	1.61	1.12	−0.50
PNICO23	−0.29	0.41	0.50	0.10	1.39	0.41	−0.98
HAL59	0.00	0.36	0.46	0.08	2.10	0.99	−1.12
AHB21	−0.51	0.52	0.78	0.02	2.13	0.11	−2.02
CHB6	−0.96	1.37	1.46	0.05	3.35	1.24	−2.10
IL16	1.37	1.37	1.44	0.01	1.25	2.01	0.75
IDISP	3.27	7.09	8.39	0.50	21.07	12.47	−8.60
ICONF	0.13	0.64	1.02	0.20	4.71	3.04	−1.67
ACONF	0.36	0.36	0.40	0.20	0.64	0.80	0.16
AMINO20x4	−0.16	0.41	0.53	0.17	2.23	0.99	−1.24
PCONF21	0.21	0.69	0.92	0.43	3.23	2.35	−0.88
MCONF	−0.39	0.47	0.57	0.09	1.65	0.41	−1.24
SCONF	−0.70	1.03	1.14	0.22	3.51	1.94	−1.57
UPU23	−0.18	0.52	0.65	0.09	2.63	1.03	−1.60
BUT14DIOL	−0.02	0.18	0.24	0.06	1.13	0.78	−0.36

Table S87: Statistical analysis for the M052X-D3(0) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−2.82	4.04	6.39	0.01	52.75	17.21	−35.54
G21EA	0.30	1.80	2.54	0.05	11.21	8.34	−2.86
G21IP	1.09	3.32	4.50	0.01	19.94	14.04	−5.90
DIPCS10	0.17	4.14	4.76	0.01	14.19	8.51	−5.68
PA26	0.08	1.13	1.50	0.01	6.24	3.67	−2.56
SIE4x4	8.71	8.71	10.14	0.26	19.24	22.33	3.09
ALKBDE10	−2.18	4.51	6.67	0.04	22.88	5.20	−17.68
YBDE18	0.38	0.93	1.08	0.02	3.15	2.15	−1.00
AL2X6	0.72	0.77	1.26	0.02	3.05	2.90	−0.15
HEAVYSB11	−3.20	3.20	4.24	0.06	8.57	−0.15	−8.71
NBPRC	0.83	1.53	1.97	0.06	5.96	4.60	−1.37
ALK8	0.73	2.18	3.11	0.03	9.10	6.51	−2.60
RC21	2.03	2.71	2.97	0.08	7.71	4.91	−2.80
G2RC	−3.28	4.02	4.85	0.08	12.56	3.01	−9.55
BH76RC	−0.73	1.37	1.98	0.06	9.53	2.67	−6.86
FH51	−1.42	1.76	2.22	0.06	8.64	3.27	−5.38
TAUT15	0.65	1.17	1.50	0.38	4.74	3.45	−1.28
DC13	−1.55	8.40	11.03	0.15	38.17	14.05	−24.12
MB16-43	25.84	26.32	32.14	0.06	90.56	80.29	−10.27
DARC	−0.06	0.96	1.26	0.03	4.32	1.41	−2.92
RSE43	−0.78	0.81	1.00	0.11	3.31	0.38	−2.93
BSR36	−1.03	1.04	1.31	0.06	3.74	0.16	−3.58
CDIE20	0.09	0.34	0.55	0.08	1.94	1.47	−0.47
ISO34	0.07	1.05	1.59	0.07	7.93	5.60	−2.34
ISOL24	0.31	2.54	4.08	0.12	22.38	6.79	−15.59
C60ISO	9.78	9.78	10.40	0.10	10.74	15.10	4.36
PArel	0.45	1.02	1.57	0.22	7.23	3.96	−3.27
BH76	−0.49	1.66	2.07	0.09	12.78	8.39	−4.39
BHPERI	−0.88	1.47	1.72	0.07	6.04	2.90	−3.14
BHDIV10	−0.39	1.51	1.81	0.03	5.97	3.34	−2.63
INV24	0.02	1.60	2.40	0.05	11.55	7.19	−4.36
BHROT27	0.44	0.46	0.63	0.07	1.43	1.32	−0.11
PX13	−7.43	7.43	8.61	0.22	14.22	−0.87	−15.09
WCPT18	−1.39	2.52	3.07	0.07	9.59	4.72	−4.87
RG18	0.06	0.16	0.22	0.28	1.07	0.62	−0.44
ADIM6	0.36	0.36	0.39	0.11	0.48	0.64	0.16
S22	0.12	0.35	0.47	0.05	2.05	1.29	−0.77
S66	0.28	0.31	0.40	0.06	1.59	1.35	−0.24
HEAVY28	−0.18	0.30	0.33	0.24	1.08	0.57	−0.50
WATER27	5.09	5.42	6.74	0.07	19.52	15.04	−4.48
CARBHB12	0.17	0.24	0.33	0.04	0.99	0.79	−0.20
PNICO23	0.30	0.40	0.50	0.09	1.58	1.07	−0.51
HAL59	−0.15	0.46	0.61	0.10	3.45	2.33	−1.12
AHB21	−1.07	1.14	1.71	0.05	5.72	0.62	−5.10
CHB6	−1.95	1.95	2.37	0.07	4.03	−0.60	−4.64
IL16	1.03	1.04	1.14	0.01	1.57	1.54	−0.03
IDISP	−0.19	1.37	1.61	0.10	4.87	1.87	−3.00
ICONF	0.12	0.27	0.36	0.08	1.28	0.75	−0.53
ACONF	−0.01	0.07	0.09	0.04	0.41	0.15	−0.25
AMINO20x4	0.13	0.28	0.36	0.11	1.56	0.98	−0.58
PCONF21	0.02	0.36	0.40	0.22	1.21	0.54	−0.68
MCONF	0.51	0.51	0.54	0.10	0.69	0.78	0.09
SCONF	0.15	0.27	0.33	0.06	1.10	0.59	−0.51
UPU23	0.25	0.48	0.62	0.08	2.70	1.51	−1.18
BUT14DIOL	−0.18	0.19	0.23	0.07	0.74	0.09	−0.66

Table S88: Statistical analysis for the M06-D3(0) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.15	3.15	5.10	0.01	51.53	18.57	−32.96
G21EA	−1.68	2.18	2.42	0.06	6.85	2.20	−4.66
G21IP	−1.48	3.09	3.81	0.01	15.41	6.58	−8.83
DIPCS10	−6.51	6.51	7.82	0.01	11.83	−1.15	−12.98
PA26	2.86	2.90	3.67	0.02	9.04	8.75	−0.29
SIE4x4	14.32	14.32	16.55	0.42	30.63	33.56	2.94
ALKBDE10	−0.14	3.44	4.40	0.03	15.44	5.45	−9.99
YBDE18	−4.52	4.54	5.27	0.09	9.24	0.25	−8.99
AL2X6	−2.45	2.46	2.80	0.07	4.36	0.02	−4.34
HEAVYSB11	−0.39	1.78	1.99	0.03	5.40	2.28	−3.12
NBPRC	1.84	2.82	3.41	0.10	9.68	6.82	−2.86
ALK8	−0.21	3.37	4.04	0.05	12.24	5.77	−6.48
RC21	0.81	1.69	2.21	0.05	8.18	4.81	−3.37
G2RC	−0.38	3.79	5.34	0.07	24.26	14.45	−9.81
BH76RC	−0.09	1.65	2.62	0.08	15.50	11.00	−4.50
FH51	−0.38	1.85	2.38	0.06	10.57	5.49	−5.08
TAUT15	−0.41	0.78	1.00	0.26	3.13	1.09	−2.04
DC13	−1.25	6.51	9.08	0.12	36.19	19.59	−16.60
MB16-43	−31.87	32.43	37.56	0.08	96.04	8.81	−87.23
DARC	3.83	3.83	4.09	0.12	4.88	5.57	0.69
RSE43	−1.54	1.54	1.87	0.20	5.68	−0.30	−5.98
BSR36	−1.19	1.29	1.82	0.08	7.03	0.64	−6.38
CDIE20	1.00	1.03	1.35	0.25	3.21	2.85	−0.36
ISO34	−0.67	1.43	1.91	0.10	9.40	4.47	−4.93
ISOL24	−2.51	3.52	5.51	0.16	26.05	5.32	−20.73
C60ISO	−0.83	2.10	2.65	0.02	7.59	1.82	−5.77
PArel	0.64	1.08	1.77	0.23	7.52	6.23	−1.29
BH76	−1.06	2.61	4.80	0.14	35.33	25.18	−10.15
BHPERI	1.42	1.90	2.32	0.09	7.44	4.71	−2.74
BHDIV10	−1.46	1.94	2.50	0.04	5.92	1.46	−4.46
INV24	−0.73	1.54	2.22	0.05	11.49	6.72	−4.76
BHROT27	0.63	0.67	0.87	0.11	2.28	2.06	−0.22
PX13	−0.10	1.45	1.60	0.04	4.74	2.62	−2.13
WCPT18	−1.80	2.01	2.55	0.06	6.49	1.20	−5.29
RG18	−0.20	0.32	0.38	0.55	1.15	0.40	−0.76
ADIM6	1.82	1.82	2.12	0.54	3.25	3.52	0.27
S22	−0.03	0.27	0.35	0.04	1.45	0.72	−0.73
S66	0.31	0.44	0.63	0.08	2.68	2.19	−0.49
HEAVY28	−0.04	0.31	0.39	0.25	1.48	1.00	−0.48
WATER27	0.75	1.52	2.39	0.02	13.17	6.95	−6.22
CARBHB12	0.18	0.31	0.38	0.05	1.40	0.75	−0.65
PNICO23	0.16	0.25	0.30	0.06	0.95	0.69	−0.25
HAL59	0.19	0.47	0.60	0.10	2.39	1.64	−0.75
AHB21	−0.04	0.31	0.38	0.01	1.46	0.71	−0.75
CHB6	1.19	1.28	1.60	0.05	2.83	2.58	−0.26
IL16	0.01	0.41	0.54	0.00	2.29	1.01	−1.28
IDISP	1.87	4.08	4.86	0.29	10.46	7.92	−2.54
ICONF	−0.06	0.36	0.45	0.11	1.71	1.05	−0.66
ACONF	−0.52	0.52	0.57	0.28	0.73	−0.19	−0.92
AMINO20x4	−0.03	0.41	0.51	0.17	2.49	1.36	−1.13
PCONF21	0.33	1.19	1.36	0.73	4.09	2.13	−1.96
MCONF	0.63	0.71	0.82	0.14	2.11	1.68	−0.43
SCONF	−0.28	0.32	0.45	0.07	1.09	0.16	−0.93
UPU23	−0.50	0.83	1.30	0.15	5.88	0.83	−5.06
BUT14DIOL	0.23	0.25	0.30	0.09	0.88	0.63	−0.25

Table S89: Statistical analysis for the M062X-D3(0) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−2.32	3.16	5.62	0.01	48.66	17.49	−31.17
G21EA	−0.61	1.76	2.08	0.05	7.49	4.15	−3.35
G21IP	0.12	2.64	3.67	0.01	17.85	11.55	−6.30
DIPCS10	−0.69	3.16	3.58	0.00	11.28	6.58	−4.70
PA26	−0.33	1.23	1.52	0.01	6.67	3.99	−2.68
SIE4x4	8.67	8.67	10.20	0.26	20.91	22.39	1.48
ALKBDE10	−4.04	4.79	7.02	0.05	19.46	1.77	−17.69
YBDE18	−2.40	2.40	2.78	0.05	5.80	−0.14	−5.94
AL2X6	0.72	0.90	1.49	0.03	4.01	3.50	−0.51
HEAVYSB11	−8.07	8.16	9.67	0.14	16.74	0.51	−16.23
NBPRC	−0.12	0.95	1.13	0.03	3.83	1.93	−1.91
ALK8	1.07	2.31	3.20	0.04	9.52	6.02	−3.50
RC21	0.98	1.63	1.96	0.05	7.35	4.95	−2.39
G2RC	−1.23	1.92	2.51	0.04	8.39	2.90	−5.49
BH76RC	−0.48	1.18	1.71	0.06	8.64	2.84	−5.80
FH51	−0.17	1.20	1.55	0.04	6.29	3.21	−3.07
TAUT15	0.36	0.78	0.94	0.26	3.13	1.93	−1.20
DC13	−3.14	7.51	10.38	0.14	39.27	15.24	−24.03
MB16-43	15.52	15.68	18.56	0.04	39.90	37.90	−1.99
DARC	2.06	2.16	2.40	0.07	4.02	3.54	−0.48
RSE43	−0.50	0.63	0.75	0.08	2.49	0.51	−1.98
BSR36	−2.48	2.48	3.26	0.15	9.15	−0.65	−9.80
CDIE20	0.34	0.54	0.83	0.13	2.63	2.09	−0.54
ISO34	−0.62	1.23	1.71	0.08	8.71	4.68	−4.03
ISOL24	−1.15	2.74	4.51	0.12	22.04	3.92	−18.12
C60ISO	6.88	6.88	7.39	0.07	8.17	10.82	2.65
PArel	0.37	0.97	1.49	0.21	6.53	3.90	−2.63
BH76	0.70	2.34	7.29	0.13	47.53	44.30	−3.23
BHPERI	0.68	1.35	1.78	0.06	7.44	4.40	−3.04
BHDIV10	−0.71	1.05	1.32	0.02	4.30	1.30	−3.00
INV24	−0.23	1.28	2.14	0.04	12.73	7.88	−4.85
BHROT27	0.34	0.36	0.52	0.06	1.29	1.17	−0.12
PX13	−5.32	5.32	5.85	0.16	7.87	−1.33	−9.20
WCPT18	−0.98	1.88	2.32	0.05	8.04	3.58	−4.46
RG18	0.00	0.23	0.32	0.40	1.45	0.87	−0.58
ADIM6	0.26	0.27	0.38	0.08	0.83	0.82	−0.01
S22	0.10	0.34	0.47	0.05	2.21	1.22	−0.99
S66	0.17	0.22	0.28	0.04	1.20	0.81	−0.39
HEAVY28	−0.13	0.33	0.40	0.27	1.52	0.99	−0.54
WATER27	3.44	3.70	4.34	0.05	13.40	9.98	−3.42
CARBHB12	0.20	0.25	0.34	0.04	0.99	0.88	−0.11
PNICO23	0.19	0.29	0.36	0.07	1.19	0.71	−0.47
HAL59	−0.15	0.35	0.46	0.08	2.72	1.07	−1.66
AHB21	−0.86	0.95	1.33	0.04	4.30	0.67	−3.63
CHB6	−1.42	1.42	1.66	0.05	2.60	−0.49	−3.08
IL16	0.38	0.47	0.53	0.00	1.35	0.85	−0.50
IDISP	1.31	2.07	2.73	0.15	5.80	4.82	−0.98
ICONF	−0.01	0.32	0.43	0.10	1.82	0.78	−1.04
ACONF	−0.27	0.27	0.31	0.15	0.48	−0.07	−0.54
AMINO20x4	−0.04	0.30	0.37	0.12	1.83	1.01	−0.82
PCONF21	0.47	1.09	1.26	0.67	3.84	2.04	−1.80
MCONF	0.54	0.55	0.63	0.11	1.36	1.15	−0.21
SCONF	−0.08	0.26	0.33	0.06	1.33	0.39	−0.95
UPU23	0.11	0.50	0.63	0.09	2.82	1.19	−1.63
BUT14DIOL	−0.06	0.13	0.19	0.05	0.88	0.22	−0.66

Table S90: Statistical analysis for the M08HX-D3(0) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−2.36	3.11	5.37	0.01	40.43	4.77	−35.66
G21EA	1.62	1.82	2.72	0.05	10.75	9.55	−1.20
G21IP	3.02	3.37	4.69	0.01	18.33	15.51	−2.81
DIPCS10	3.03	3.37	3.97	0.01	9.03	7.37	−1.66
PA26	0.23	1.00	1.26	0.01	5.60	2.66	−2.94
SIE4x4	8.64	8.64	9.96	0.26	19.12	21.78	2.66
ALKBDE10	−3.80	3.86	5.39	0.04	14.17	0.32	−13.85
YBDE18	−2.07	2.11	2.54	0.04	5.34	0.37	−4.97
AL2X6	2.38	2.38	2.44	0.07	1.56	3.17	1.61
HEAVYSB11	−2.14	2.95	4.14	0.05	12.95	1.92	−11.03
NBPRC	0.39	1.90	2.20	0.07	7.26	3.91	−3.35
ALK8	1.78	2.26	3.31	0.04	8.75	7.74	−1.02
RC21	0.65	1.52	1.89	0.04	6.19	4.08	−2.11
G2RC	−2.15	3.30	4.22	0.06	17.29	5.03	−12.26
BH76RC	−0.28	1.20	1.54	0.06	6.45	3.33	−3.12
FH51	−0.39	1.27	1.67	0.04	8.85	5.19	−3.67
TAUT15	0.09	0.65	0.90	0.21	3.20	1.44	−1.76
DC13	−1.36	7.36	9.88	0.13	37.57	15.84	−21.73
MB16-43	−10.69	15.87	20.30	0.04	82.50	25.44	−57.05
DARC	0.83	1.43	1.71	0.04	4.74	2.88	−1.85
RSE43	−0.30	0.56	0.70	0.07	2.30	0.83	−1.47
BSR36	−2.31	2.31	2.76	0.14	7.17	−0.22	−7.39
CDIE20	0.36	0.64	0.93	0.16	3.01	2.34	−0.68
ISO34	−0.15	0.95	1.31	0.07	6.12	3.06	−3.06
ISOL24	−0.10	2.29	3.70	0.10	19.52	5.45	−14.06
C60ISO	7.60	7.60	8.15	0.08	8.78	12.14	3.37
PArel	0.44	0.91	1.35	0.20	5.92	3.38	−2.54
BH76	−0.16	0.99	1.29	0.05	6.84	3.35	−3.49
BHPERI	0.18	1.64	1.97	0.08	7.75	4.91	−2.84
BHDIV10	−0.30	1.02	1.35	0.02	4.79	1.90	−2.89
INV24	0.21	1.91	3.09	0.06	15.11	10.42	−4.69
BHROT27	0.35	0.42	0.57	0.07	1.45	1.15	−0.30
PX13	0.32	2.62	3.00	0.08	9.55	5.12	−4.43
WCPT18	1.00	1.55	1.83	0.04	4.91	3.39	−1.52
RG18	−0.41	0.41	0.65	0.71	1.85	0.00	−1.85
ADIM6	0.10	0.18	0.29	0.05	0.85	0.68	−0.17
S22	0.10	0.38	0.49	0.05	1.92	0.75	−1.17
S66	0.22	0.27	0.34	0.05	1.14	0.73	−0.41
HEAVY28	0.19	0.31	0.53	0.25	2.03	1.76	−0.26
WATER27	1.56	1.57	1.83	0.02	4.03	3.99	−0.04
CARBHB12	0.25	0.49	0.53	0.08	1.68	0.90	−0.78
PNICO23	0.52	0.59	0.70	0.14	1.72	1.28	−0.44
HAL59	−0.14	0.45	0.62	0.10	3.70	1.77	−1.93
AHB21	−0.41	0.54	0.73	0.02	2.47	0.49	−1.98
CHB6	−2.50	2.50	2.91	0.09	4.48	−0.91	−5.39
IL16	1.04	1.04	1.13	0.01	1.58	1.59	0.01
IDISP	0.19	3.12	3.63	0.22	10.86	6.31	−4.55
ICONF	−0.08	0.50	0.60	0.15	1.84	0.70	−1.14
ACONF	−0.40	0.40	0.46	0.22	0.67	−0.04	−0.71
AMINO20x4	0.07	0.39	0.52	0.16	2.40	1.46	−0.94
PCONF21	0.52	1.04	1.20	0.64	3.85	2.01	−1.84
MCONF	0.72	0.73	0.85	0.15	1.83	1.58	−0.25
SCONF	0.08	0.32	0.46	0.07	1.93	0.69	−1.24
UPU23	0.21	0.60	0.73	0.10	2.50	1.59	−0.91
BUT14DIOL	−0.19	0.20	0.29	0.07	1.03	0.11	−0.91

Table S91: Statistical analysis for the M11-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.24	3.42	5.77	0.01	49.21	12.44	−36.77
G21EA	1.44	1.56	2.26	0.05	8.76	8.02	−0.74
G21IP	2.05	3.61	4.83	0.01	19.19	14.32	−4.87
DIPCS10	−2.26	3.26	3.99	0.00	10.68	3.42	−7.26
PA26	0.13	1.23	1.46	0.01	5.42	2.30	−3.12
SIE4x4	9.59	9.59	12.23	0.28	27.78	28.36	0.58
ALKBDE10	0.82	4.30	6.03	0.04	21.59	11.83	−9.76
YBDE18	−0.37	1.56	1.94	0.03	6.38	3.03	−3.35
AL2X6	2.39	2.39	2.53	0.07	2.46	4.17	1.71
HEAVYSB11	0.21	1.96	2.63	0.03	10.02	4.13	−5.89
NBPRC	1.00	2.76	3.22	0.10	10.40	5.69	−4.71
ALK8	0.82	3.74	4.57	0.06	14.61	7.62	−6.99
RC21	0.12	2.06	2.64	0.06	9.94	5.07	−4.87
G2RC	−2.11	2.81	3.86	0.05	13.27	2.91	−10.36
BH76RC	−0.50	1.44	1.83	0.07	7.60	4.16	−3.44
FH51	−0.63	1.47	1.86	0.05	7.46	3.14	−4.32
TAUT15	−0.27	1.09	1.31	0.36	4.77	2.40	−2.37
DC13	−0.38	9.11	13.31	0.17	57.59	23.66	−33.92
MB16-43	−11.16	18.01	22.91	0.04	86.68	24.28	−62.40
DARC	2.59	2.60	3.05	0.08	5.05	4.98	−0.07
RSE43	−1.40	1.41	1.68	0.19	4.06	0.24	−3.82
BSR36	−1.01	1.05	1.21	0.06	3.12	0.77	−2.35
CDIE20	−0.03	0.78	1.00	0.19	3.58	2.36	−1.22
ISO34	−0.36	1.32	1.96	0.09	8.60	4.28	−4.32
ISOL24	−0.43	3.40	5.81	0.16	31.57	8.55	−23.03
C60ISO	14.75	14.75	16.10	0.15	17.85	23.15	5.30
PArel	0.13	0.77	1.15	0.17	5.49	2.24	−3.25
BH76	−0.72	1.28	1.55	0.07	6.28	2.74	−3.54
BHPERI	1.25	1.89	2.47	0.09	9.89	5.78	−4.11
BHDIV10	−0.23	1.42	1.68	0.03	5.80	1.98	−3.81
INV24	−0.76	2.49	3.28	0.08	14.84	7.53	−7.31
BHROT27	0.54	0.66	0.97	0.11	2.70	2.33	−0.37
PX13	−3.47	3.47	4.35	0.10	7.71	−0.90	−8.61
WCPT18	−1.04	1.76	2.15	0.05	8.07	3.80	−4.27
RG18	−0.29	0.31	0.38	0.53	1.14	0.20	−0.95
ADIM6	0.58	0.58	0.76	0.17	1.38	1.42	0.04
S22	0.12	0.41	0.60	0.06	2.90	1.63	−1.27
S66	0.15	0.28	0.36	0.05	1.51	0.93	−0.59
HEAVY28	−0.02	0.27	0.35	0.22	1.70	1.07	−0.64
WATER27	0.12	1.34	1.85	0.02	7.46	2.99	−4.47
CARBHB12	−0.03	0.22	0.28	0.04	1.04	0.67	−0.36
PNICO23	−0.19	0.32	0.47	0.07	2.13	0.46	−1.68
HAL59	−0.56	0.65	0.82	0.14	3.06	0.69	−2.37
AHB21	−0.27	0.46	0.67	0.02	2.48	0.65	−1.83
CHB6	−2.75	2.75	3.24	0.10	5.18	−0.83	−6.01
IL16	1.53	1.53	1.58	0.01	1.36	2.03	0.67
IDISP	−0.43	3.65	4.40	0.26	14.00	7.96	−6.04
ICONF	0.01	0.53	0.62	0.16	2.00	1.00	−1.01
ACONF	−0.72	0.72	0.81	0.39	1.20	−0.21	−1.40
AMINO20x4	0.12	0.51	0.65	0.21	2.61	1.72	−0.89
PCONF21	0.53	1.34	1.59	0.83	5.65	2.75	−2.91
MCONF	1.24	1.24	1.38	0.25	2.42	2.42	0.00
SCONF	0.24	0.80	1.07	0.17	4.25	1.34	−2.90
UPU23	0.27	0.69	0.91	0.12	4.13	1.57	−2.56
BUT14DIOL	−0.05	0.26	0.38	0.09	1.74	0.55	−1.20

Table S92: Statistical analysis for the SOGGA11X-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−3.10	4.04	6.32	0.01	51.20	19.88	−31.32
G21EA	0.18	1.92	2.48	0.06	10.00	5.39	−4.61
G21IP	1.94	3.12	4.08	0.01	14.32	9.19	−5.13
DIPCS10	0.74	4.92	5.84	0.01	18.98	7.82	−11.17
PA26	3.83	3.83	4.46	0.02	9.32	9.76	0.43
SIE4x4	10.56	10.56	12.11	0.31	22.82	24.89	2.06
ALKBDE10	−7.32	7.32	8.57	0.07	16.50	−1.42	−17.92
YBDE18	1.34	2.61	3.11	0.05	10.26	5.29	−4.97
AL2X6	2.08	2.08	2.26	0.06	2.48	3.76	1.29
HEAVYSB11	2.52	2.55	2.98	0.04	5.31	5.22	−0.08
NBPRC	−0.52	2.39	2.86	0.09	9.85	5.29	−4.57
ALK8	8.79	8.79	11.58	0.14	22.04	22.45	0.40
RC21	3.90	4.44	5.24	0.12	14.13	11.81	−2.32
G2RC	−2.77	5.21	6.95	0.10	33.46	13.34	−20.12
BH76RC	0.12	2.24	2.49	0.10	8.43	4.17	−4.26
FH51	−1.40	2.18	2.95	0.07	11.95	5.02	−6.93
TAUT15	0.01	0.44	0.61	0.14	2.75	1.10	−1.65
DC13	−2.68	7.34	9.10	0.13	33.78	20.25	−13.53
MB16-43	2.39	12.15	16.87	0.03	88.42	58.09	−30.34
DARC	−4.17	4.17	4.45	0.13	5.88	−2.67	−8.55
RSE43	−1.32	1.32	1.47	0.17	2.57	−0.47	−3.05
BSR36	−2.76	2.76	3.21	0.17	6.69	−1.23	−7.92
CDIE20	0.80	0.84	1.10	0.21	2.67	2.50	−0.17
ISO34	−0.30	1.14	1.55	0.08	7.64	3.64	−4.00
ISOL24	0.34	1.60	2.03	0.07	8.32	3.99	−4.33
C60ISO	6.99	6.99	7.37	0.07	7.62	11.69	4.07
PArel	0.68	0.98	1.40	0.21	4.61	3.88	−0.74
BH76	−1.54	1.80	2.22	0.10	7.64	2.17	−5.48
BHPERI	0.10	1.25	1.64	0.06	7.62	5.26	−2.36
BHDIV10	−1.08	1.80	2.08	0.04	6.39	3.06	−3.34
INV24	0.71	1.43	2.47	0.04	12.85	9.66	−3.19
BHROT27	0.40	0.41	0.53	0.07	1.38	1.23	−0.15
PX13	0.55	0.64	0.80	0.02	1.85	1.45	−0.40
WCPT18	0.43	1.37	1.72	0.04	6.31	3.92	−2.39
RG18	−0.75	0.75	1.02	1.29	2.50	−0.09	−2.58
ADIM6	−0.28	0.37	0.41	0.11	0.89	0.26	−0.63
S22	0.54	0.62	0.85	0.08	2.52	1.90	−0.61
S66	0.32	0.37	0.54	0.07	2.11	1.73	−0.38
HEAVY28	0.73	0.78	0.94	0.63	2.59	2.14	−0.45
WATER27	1.82	1.82	2.28	0.02	6.58	6.65	0.07
CARBHB12	0.77	0.77	0.96	0.13	1.79	1.90	0.11
PNICO23	0.88	0.90	1.11	0.21	3.06	2.93	−0.13
HAL59	0.65	0.76	0.96	0.17	3.34	2.57	−0.77
AHB21	−0.66	0.69	0.94	0.03	2.60	0.23	−2.37
CHB6	−2.14	2.14	2.36	0.08	2.96	−0.87	−3.83
IL16	0.10	0.34	0.39	0.00	1.18	0.71	−0.48
IDISP	1.04	1.53	2.14	0.11	5.86	4.81	−1.05
ICONF	0.04	0.25	0.33	0.08	1.16	0.82	−0.34
ACONF	−0.29	0.29	0.33	0.16	0.56	−0.09	−0.65
AMINO20x4	−0.01	0.26	0.33	0.11	2.06	1.05	−1.01
PCONF21	0.55	0.76	1.02	0.47	2.68	2.16	−0.52
MCONF	0.49	0.56	0.63	0.11	1.61	1.11	−0.50
SCONF	−0.05	0.35	0.57	0.08	2.21	0.35	−1.86
UPU23	0.52	0.74	0.91	0.13	3.60	1.68	−1.92
BUT14DIOL	0.36	0.36	0.38	0.13	0.75	0.67	−0.09

Table S93: Statistical analysis for the N12SX-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.57	3.93	5.91	0.01	58.66	25.62	−33.04
G21EA	−2.38	2.87	3.44	0.09	10.75	4.28	−6.47
G21IP	−0.30	3.59	4.65	0.01	22.71	9.94	−12.77
DIPCS10	−4.81	5.76	7.00	0.01	14.87	3.20	−11.67
PA26	3.76	3.83	4.42	0.02	10.65	9.76	−0.89
SIE4x4	14.64	14.64	16.09	0.43	25.18	29.64	4.46
ALKBDE10	0.48	3.69	5.07	0.04	19.41	12.97	−6.44
YBDE18	0.88	1.95	2.42	0.04	8.84	3.79	−5.06
AL2X6	1.83	2.22	2.32	0.06	4.36	3.18	−1.18
HEAVYSB11	2.31	2.31	2.67	0.04	4.15	4.87	0.72
NBPRC	−1.31	3.38	3.76	0.12	11.21	5.79	−5.43
ALK8	7.69	7.69	10.72	0.12	19.75	19.96	0.22
RC21	5.49	6.05	7.21	0.17	17.28	15.20	−2.08
G2RC	−4.49	7.11	9.31	0.14	32.88	9.49	−23.39
BH76RC	−0.11	3.00	3.81	0.14	17.39	10.19	−7.20
FH51	−1.79	3.31	4.29	0.11	19.71	8.02	−11.69
TAUT15	0.10	1.60	2.15	0.52	7.06	4.43	−2.63
DC13	−4.22	10.34	12.26	0.19	44.29	19.61	−24.69
MB16-43	26.84	27.87	34.60	0.07	102.68	94.77	−7.92
DARC	−4.37	4.37	4.99	0.13	8.30	−1.79	−10.10
RSE43	−2.03	2.03	2.30	0.27	4.57	−0.78	−5.35
BSR36	−3.92	3.92	4.41	0.24	7.92	−1.49	−9.41
CDIE20	1.33	1.35	1.55	0.33	3.00	2.83	−0.18
ISO34	−0.18	1.62	2.03	0.11	7.10	3.33	−3.77
ISOL24	0.53	2.44	3.60	0.11	19.78	10.11	−9.66
C60ISO	0.35	2.49	2.85	0.03	8.13	2.96	−5.17
PArel	0.68	1.31	2.15	0.28	9.12	7.28	−1.84
BH76	−3.24	3.81	4.44	0.20	16.22	5.30	−10.92
BHPERI	−2.37	2.63	2.96	0.13	7.41	1.86	−5.55
BHDIV10	−4.20	4.51	5.11	0.10	9.21	1.52	−7.70
INV24	−1.46	2.10	3.02	0.07	12.37	5.32	−7.05
BHROT27	0.78	0.84	1.17	0.13	2.57	2.35	−0.23
PX13	−6.03	6.03	6.33	0.18	7.03	−3.38	−10.42
WCPT18	−3.69	3.70	4.55	0.11	9.17	0.10	−9.07
RG18	−0.28	0.33	0.47	0.57	1.61	0.22	−1.39
ADIM6	−0.02	0.16	0.18	0.05	0.46	0.21	−0.25
S22	0.55	0.58	0.92	0.08	3.01	2.71	−0.30
S66	0.44	0.45	0.73	0.08	2.90	2.82	−0.08
HEAVY28	0.36	0.36	0.43	0.29	0.93	0.88	−0.05
WATER27	7.58	7.99	10.56	0.10	30.90	25.37	−5.53
CARBHB12	1.45	1.45	1.72	0.24	2.85	3.19	0.34
PNICO23	0.83	0.83	1.32	0.19	5.10	5.08	−0.02
HAL59	0.58	0.65	0.98	0.14	3.34	3.07	−0.27
AHB21	−1.71	1.71	2.04	0.08	3.93	−0.17	−4.11
CHB6	−1.85	1.85	2.00	0.07	2.36	−0.52	−2.89
IL16	−0.19	0.39	0.47	0.00	1.35	0.39	−0.96
IDISP	1.42	2.33	2.81	0.16	7.71	5.00	−2.72
ICONF	0.17	0.44	0.61	0.13	2.32	1.49	−0.83
ACONF	−0.01	0.05	0.06	0.03	0.26	0.13	−0.13
AMINO20x4	0.16	0.34	0.47	0.14	2.33	1.38	−0.95
PCONF21	0.26	0.88	1.00	0.54	2.88	1.62	−1.26
MCONF	0.22	0.33	0.41	0.07	1.44	0.85	−0.59
SCONF	−0.09	0.27	0.47	0.06	2.00	0.30	−1.70
UPU23	0.34	0.65	0.80	0.11	3.24	1.48	−1.77
BUT14DIOL	0.41	0.42	0.43	0.15	0.83	0.79	−0.03

Table S94: Statistical analysis for the MN12SX-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−3.20	4.45	6.29	0.01	39.78	9.75	−30.03
G21EA	−0.81	2.39	3.06	0.07	10.51	3.71	−6.80
G21IP	−0.75	3.66	4.71	0.01	20.08	9.16	−10.91
DIPCS10	−8.15	8.15	10.37	0.01	18.14	−1.19	−19.33
PA26	0.94	1.62	2.01	0.01	5.94	4.23	−1.72
SIE4x4	8.92	9.03	10.72	0.27	20.53	19.63	−0.90
ALKBDE10	−0.46	3.84	5.30	0.04	18.85	5.65	−13.20
YBDE18	−2.64	3.35	3.99	0.07	9.82	1.77	−8.05
AL2X6	−1.35	1.35	1.57	0.04	2.36	−0.07	−2.43
HEAVYSB11	1.25	2.08	2.63	0.04	8.70	5.78	−2.92
NBPRC	0.48	2.29	2.52	0.08	7.98	3.63	−4.35
ALK8	−2.78	5.30	7.33	0.08	24.47	6.89	−17.58
RC21	0.63	1.54	1.96	0.04	7.92	4.85	−3.07
G2RC	0.13	2.78	3.56	0.05	15.90	9.63	−6.27
BH76RC	−0.08	1.56	2.33	0.07	12.27	4.26	−8.00
FH51	1.26	1.92	2.97	0.06	15.01	11.19	−3.82
TAUT15	0.77	1.57	1.88	0.51	5.77	3.49	−2.27
DC13	−1.53	7.87	10.01	0.14	35.11	14.48	−20.64
MB16-43	2.92	11.66	14.19	0.03	61.80	39.59	−22.21
DARC	3.47	3.48	3.95	0.11	5.80	5.71	−0.09
RSE43	−1.59	1.59	1.82	0.21	4.93	−0.13	−5.06
BSR36	−2.55	2.55	2.85	0.16	5.68	−0.91	−6.58
CDIE20	1.28	1.30	1.54	0.32	3.23	3.03	−0.20
ISO34	−0.28	1.12	1.50	0.08	7.47	4.14	−3.33
ISOL24	−1.27	3.29	4.31	0.15	19.62	12.24	−7.38
C60ISO	−0.08	2.31	2.84	0.02	8.34	2.74	−5.60
PArel	1.21	1.50	2.38	0.32	7.95	6.92	−1.03
BH76	−0.25	1.14	1.60	0.06	8.63	4.00	−4.63
BHPERI	1.77	2.10	2.56	0.10	8.26	4.85	−3.42
BHDIV10	0.05	1.57	1.71	0.03	4.78	2.08	−2.71
INV24	0.18	1.44	2.21	0.05	11.55	7.28	−4.26
BHROT27	0.58	0.59	0.86	0.09	2.48	2.39	−0.09
PX13	2.29	2.41	2.79	0.07	4.96	4.28	−0.68
WCPT18	0.58	1.11	1.28	0.03	4.28	2.30	−1.98
RG18	−0.60	0.60	0.88	1.03	2.50	−0.05	−2.55
ADIM6	0.34	0.41	0.54	0.12	1.29	1.08	−0.21
S22	−0.03	0.66	0.91	0.09	3.73	1.80	−1.94
S66	0.02	0.47	0.57	0.09	2.29	1.24	−1.05
HEAVY28	0.19	0.32	0.43	0.26	1.74	1.25	−0.48
WATER27	−5.30	5.53	8.23	0.07	25.23	3.11	−22.12
CARBHB12	−0.67	0.67	0.78	0.11	1.31	−0.20	−1.51
PNICO23	−0.02	0.28	0.34	0.07	1.24	0.54	−0.70
HAL59	−0.42	0.59	0.78	0.13	3.65	1.00	−2.65
AHB21	0.77	0.81	0.96	0.04	2.39	2.01	−0.38
CHB6	−0.55	0.55	0.66	0.02	1.09	−0.15	−1.24
IL16	1.28	1.28	1.31	0.01	1.25	1.66	0.41
IDISP	2.70	3.07	4.52	0.22	10.52	9.71	−0.81
ICONF	−0.05	0.29	0.39	0.09	1.52	0.57	−0.95
ACONF	−0.21	0.21	0.25	0.11	0.44	0.00	−0.44
AMINO20x4	0.00	0.51	0.64	0.21	3.01	1.50	−1.50
PCONF21	0.87	1.59	1.86	0.98	5.50	3.47	−2.03
MCONF	0.59	0.70	0.82	0.14	2.33	1.71	−0.62
SCONF	−0.37	0.49	0.58	0.11	1.86	0.94	−0.91
UPU23	−0.59	0.67	0.97	0.12	3.91	0.59	−3.32
BUT14DIOL	−0.54	0.54	0.55	0.19	0.70	−0.11	−0.81

Table S95: Statistical analysis for the MN15-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.03	2.72	4.23	0.01	40.01	12.04	−27.98
G21EA	0.82	1.37	1.76	0.04	7.19	4.53	−2.66
G21IP	0.30	2.75	3.70	0.01	17.36	8.97	−8.40
DIPCS10	−3.62	4.35	5.71	0.01	15.10	2.60	−12.50
PA26	0.84	1.64	1.94	0.01	6.61	4.59	−2.02
SIE4x4	10.97	11.30	13.47	0.34	32.21	29.56	−2.65
ALKBDE10	−1.13	2.88	4.31	0.03	14.65	4.01	−10.65
YBDE18	−1.62	3.37	3.91	0.07	11.44	3.62	−7.82
AL2X6	1.47	1.47	1.71	0.04	2.77	3.07	0.29
HEAVYSB11	−4.95	5.07	5.78	0.09	8.93	0.66	−8.27
NBPRC	−1.18	1.78	2.08	0.06	5.94	2.64	−3.29
ALK8	−0.79	3.72	4.82	0.06	16.10	9.67	−6.43
RC21	0.65	1.74	2.14	0.05	8.55	4.75	−3.80
G2RC	−1.02	2.63	3.13	0.05	11.63	6.98	−4.65
BH76RC	0.12	1.57	2.28	0.07	11.59	4.84	−6.75
FH51	0.27	1.61	2.17	0.05	10.79	5.52	−5.27
TAUT15	0.68	1.19	1.60	0.39	5.26	3.70	−1.56
DC13	−1.61	5.09	7.19	0.09	28.84	16.50	−12.34
MB16-43	16.72	20.23	23.72	0.05	89.97	57.26	−32.71
DARC	1.65	1.70	2.05	0.05	3.65	3.42	−0.23
RSE43	−1.35	1.35	1.54	0.18	3.35	−0.40	−3.75
BSR36	0.25	0.57	0.78	0.04	3.05	2.06	−0.99
CDIE20	0.55	0.64	0.89	0.16	2.61	2.20	−0.42
ISO34	−0.94	1.50	1.86	0.10	5.64	1.91	−3.73
ISOL24	−1.23	2.63	3.62	0.12	16.96	5.01	−11.94
C60ISO	1.96	1.96	2.24	0.02	3.41	3.46	0.05
PArel	0.80	1.34	2.03	0.29	8.35	6.38	−1.97
BH76	−1.07	1.50	2.00	0.08	9.20	2.56	−6.64
BHPERI	0.78	1.26	1.76	0.06	7.96	4.84	−3.13
BHDIV10	−1.70	1.70	2.01	0.04	3.41	−0.01	−3.43
INV24	−1.32	2.68	3.55	0.08	15.19	8.14	−7.04
BHROT27	0.46	0.48	0.67	0.08	1.48	1.37	−0.10
PX13	−1.91	2.03	2.17	0.06	4.28	0.73	−3.55
WCPT18	−1.28	1.50	1.72	0.04	5.89	1.98	−3.91
RG18	0.02	0.10	0.12	0.17	0.44	0.26	−0.18
ADIM6	1.32	1.32	1.47	0.39	1.78	2.24	0.46
S22	−0.14	0.56	0.81	0.08	2.92	0.71	−2.21
S66	0.17	0.44	0.56	0.08	2.95	1.64	−1.30
HEAVY28	0.21	0.34	0.41	0.27	1.31	0.85	−0.46
WATER27	1.13	1.23	1.48	0.02	4.39	3.48	−0.91
CARBHB12	−0.03	0.24	0.34	0.04	1.48	0.61	−0.87
PNICO23	0.28	0.30	0.36	0.07	0.84	0.69	−0.15
HAL59	0.18	0.54	0.69	0.12	3.31	1.97	−1.34
AHB21	−0.26	0.33	0.43	0.01	1.26	0.24	−1.01
CHB6	−0.18	0.32	0.41	0.01	1.20	0.40	−0.80
IL16	0.94	1.02	1.11	0.01	2.63	1.95	−0.68
IDISP	0.75	3.60	4.33	0.25	11.96	6.37	−5.59
ICONF	0.13	0.51	0.61	0.16	2.00	1.15	−0.85
ACONF	−0.50	0.50	0.57	0.27	0.87	−0.14	−1.01
AMINO20x4	0.08	0.52	0.68	0.21	3.38	1.99	−1.40
PCONF21	0.51	1.10	1.29	0.68	4.14	1.99	−2.15
MCONF	0.51	0.57	0.70	0.11	1.85	1.49	−0.36
SCONF	0.11	0.50	0.68	0.11	2.96	1.23	−1.73
UPU23	0.14	0.53	0.69	0.09	3.18	1.43	−1.74
BUT14DIOL	−0.36	0.36	0.45	0.13	1.26	0.11	−1.14

Table S96: Statistical analysis for the LC-ωhPBE-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−2.05	3.98	6.70	0.01	48.04	7.35	−40.69
G21EA	0.07	2.83	3.22	0.08	10.90	5.08	−5.82
G21IP	2.77	4.60	5.64	0.02	18.54	11.73	−6.81
DIPCS10	3.02	3.16	4.11	0.00	7.26	6.89	−0.37
PA26	2.87	2.96	3.32	0.02	6.66	5.44	−1.22
SIE4x4	9.61	9.61	12.38	0.28	25.31	28.53	3.22
ALKBDE10	−0.69	5.42	6.94	0.05	24.25	12.64	−11.61
YBDE18	−0.05	2.75	3.14	0.06	11.52	4.97	−6.55
AL2X6	2.39	2.92	3.15	0.08	6.49	4.91	−1.58
HEAVYSB11	−3.00	3.11	3.48	0.05	6.12	0.58	−5.54
NBPRC	−1.71	3.73	4.30	0.13	11.90	5.20	−6.70
ALK8	5.83	5.83	7.69	0.09	12.67	13.73	1.06
RC21	4.11	4.81	6.01	0.13	18.39	13.93	−4.46
G2RC	−3.90	6.10	7.80	0.12	30.17	12.36	−17.80
BH76RC	−0.64	2.37	2.96	0.11	11.89	5.43	−6.46
FH51	−2.63	3.52	4.74	0.11	25.01	8.21	−16.80
TAUT15	−0.33	0.94	1.11	0.31	3.47	1.74	−1.73
DC13	−5.05	11.08	14.49	0.20	56.73	26.41	−30.32
MB16-43	−0.06	18.09	24.28	0.04	124.34	82.53	−41.81
DARC	−10.90	10.90	10.99	0.34	4.64	−8.85	−13.49
RSE43	−0.44	0.59	0.76	0.08	2.48	0.60	−1.88
BSR36	−0.76	0.84	0.92	0.05	2.59	0.84	−1.75
CDIE20	−0.01	0.87	1.20	0.21	4.36	2.74	−1.62
ISO34	−0.55	1.83	2.82	0.13	12.81	5.88	−6.93
ISOL24	2.17	5.78	8.35	0.26	39.02	15.75	−23.28
C60ISO	17.64	17.64	19.31	0.18	22.08	28.18	6.10
PArel	0.38	0.96	1.23	0.21	5.25	1.80	−3.45
BH76	−0.11	1.62	2.16	0.09	11.08	5.86	−5.22
BHPERI	1.72	2.18	3.87	0.10	17.30	15.56	−1.74
BHDIV10	−0.71	1.74	2.08	0.04	5.88	2.17	−3.71
INV24	0.61	2.27	3.91	0.07	22.01	13.03	−8.98
BHROT27	0.43	0.58	0.84	0.09	2.83	1.95	−0.88
PX13	−4.92	4.92	5.21	0.15	6.07	−1.39	−7.46
WCPT18	−1.23	2.57	3.17	0.07	12.86	8.06	−4.80
RG18	−0.12	0.12	0.19	0.21	0.66	0.02	−0.64
ADIM6	−0.20	0.20	0.21	0.06	0.09	−0.15	−0.24
S22	0.06	0.28	0.36	0.04	1.43	0.82	−0.61
S66	0.01	0.18	0.24	0.03	1.32	0.93	−0.39
HEAVY28	0.30	0.33	0.39	0.27	0.91	0.74	−0.17
WATER27	0.11	1.37	1.84	0.02	7.61	2.39	−5.23
CARBHB12	0.65	0.65	0.81	0.11	1.45	1.54	0.09
PNICO23	0.44	0.50	0.62	0.12	2.04	1.60	−0.43
HAL59	0.00	0.47	0.61	0.10	3.23	1.58	−1.65
AHB21	−0.48	0.66	0.92	0.03	2.94	0.55	−2.39
CHB6	−1.87	1.87	2.31	0.07	3.95	−0.51	−4.46
IL16	0.84	0.84	0.96	0.01	1.52	1.57	0.05
IDISP	−2.79	3.70	7.93	0.26	20.31	0.95	−19.36
ICONF	0.19	0.38	0.54	0.12	1.76	1.32	−0.44
ACONF	−0.08	0.08	0.10	0.04	0.21	−0.01	−0.22
AMINO20x4	0.04	0.33	0.41	0.14	2.02	1.06	−0.97
PCONF21	0.09	0.52	0.63	0.32	2.20	0.79	−1.41
MCONF	0.35	0.41	0.48	0.08	1.39	1.05	−0.34
SCONF	−0.01	0.18	0.28	0.04	1.16	0.39	−0.77
UPU23	0.82	0.86	1.00	0.15	1.99	1.72	−0.28
BUT14DIOL	−0.08	0.12	0.14	0.04	0.51	0.20	−0.30

Table S97: Statistical analysis for the ωB97X-D3(0) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−2.39	2.86	5.12	0.01	40.15	4.13	−36.02
G21EA	−0.14	1.53	1.92	0.05	8.13	4.46	−3.67
G21IP	−0.38	2.87	3.72	0.01	17.69	6.91	−10.78
DIPCS10	−4.71	5.45	7.24	0.01	16.78	1.98	−14.79
PA26	3.66	3.66	4.06	0.02	6.70	7.77	1.07
SIE4x4	12.35	12.35	14.33	0.37	26.97	30.87	3.90
ALKBDE10	−2.40	4.43	5.80	0.04	19.97	7.54	−12.43
YBDE18	−2.32	2.41	2.87	0.05	6.48	0.51	−5.97
AL2X6	−3.02	3.02	3.13	0.08	2.46	−1.93	−4.40
HEAVYSB11	−1.61	2.37	2.59	0.04	6.84	2.50	−4.34
NBPRC	1.10	1.89	2.57	0.07	8.48	6.34	−2.14
ALK8	−3.57	3.58	4.80	0.06	8.87	0.04	−8.83
RC21	2.63	2.98	3.42	0.08	7.78	6.10	−1.68
G2RC	−1.72	3.88	4.77	0.08	20.13	10.99	−9.14
BH76RC	−0.18	1.59	2.01	0.07	8.54	4.06	−4.48
FH51	−0.79	1.88	2.42	0.06	10.47	4.10	−6.37
TAUT15	−0.33	0.74	0.91	0.24	3.18	1.28	−1.90
DC13	−1.01	6.40	8.25	0.12	31.53	16.49	−15.04
MB16-43	−36.17	36.50	41.78	0.09	100.60	6.89	−93.71
DARC	0.06	1.32	1.74	0.04	6.25	1.80	−4.45
RSE43	−1.39	1.39	1.53	0.18	2.64	−0.61	−3.26
BSR36	−4.13	4.13	4.90	0.25	10.92	−1.36	−12.28
CDIE20	0.24	0.63	0.92	0.16	3.24	2.12	−1.12
ISO34	−0.51	1.03	1.41	0.07	6.84	3.29	−3.55
ISOL24	−0.94	2.64	3.44	0.12	15.00	6.86	−8.14
C60ISO	13.56	13.56	14.71	0.14	15.84	20.82	4.98
PArel	0.25	0.58	0.88	0.13	3.39	2.45	−0.93
BH76	−0.98	1.88	2.18	0.10	9.29	4.12	−5.17
BHPERI	2.94	3.06	3.41	0.15	7.84	6.27	−1.56
BHDIV10	0.22	1.00	1.27	0.02	4.16	2.63	−1.53
INV24	−0.16	1.48	2.41	0.05	12.24	7.12	−5.12
BHROT27	0.25	0.39	0.54	0.06	1.82	1.33	−0.49
PX13	−1.81	1.81	2.04	0.05	3.17	−0.30	−3.47
WCPT18	−0.25	1.41	1.87	0.04	8.45	5.33	−3.12
RG18	−0.21	0.21	0.31	0.36	0.83	0.03	−0.80
ADIM6	0.34	0.34	0.42	0.10	0.64	0.66	0.03
S22	0.07	0.21	0.29	0.03	1.46	0.93	−0.53
S66	0.23	0.24	0.30	0.04	1.42	1.10	−0.32
HEAVY28	−0.12	0.19	0.22	0.15	0.82	0.37	−0.45
WATER27	2.21	2.33	3.13	0.03	8.98	7.41	−1.57
CARBHB12	0.57	0.57	0.67	0.09	1.29	1.38	0.09
PNICO23	−0.20	0.24	0.30	0.06	0.90	0.18	−0.72
HAL59	−0.36	0.42	0.50	0.09	1.85	0.31	−1.54
AHB21	−0.19	0.30	0.40	0.01	1.26	0.41	−0.85
CHB6	1.26	1.26	1.43	0.05	1.76	2.19	0.44
IL16	1.05	1.06	1.27	0.01	2.52	2.45	−0.07
IDISP	0.57	2.68	3.49	0.19	11.08	5.52	−5.56
ICONF	0.15	0.42	0.58	0.13	2.35	1.31	−1.03
ACONF	0.01	0.07	0.08	0.04	0.28	0.17	−0.11
AMINO20x4	−0.06	0.24	0.32	0.10	1.64	0.76	−0.88
PCONF21	0.08	0.31	0.37	0.19	1.27	0.68	−0.59
MCONF	0.29	0.30	0.33	0.06	0.66	0.59	−0.07
SCONF	−0.23	0.27	0.35	0.06	1.26	0.23	−1.03
UPU23	0.65	0.77	0.90	0.13	2.78	1.72	−1.06
BUT14DIOL	0.07	0.11	0.14	0.04	0.62	0.43	−0.19

Table S98: Statistical analysis for the ωB97X-V DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.79	2.78	5.09	0.01	49.05	12.28	−36.77
G21EA	−0.54	1.84	2.21	0.05	9.54	5.53	−4.01
G21IP	−0.20	2.96	3.52	0.01	14.16	7.17	−6.99
DIPCS10	−3.38	4.10	5.18	0.01	12.19	1.84	−10.35
PA26	2.65	2.65	3.21	0.01	6.59	6.86	0.27
SIE4x4	11.49	11.49	13.85	0.34	28.22	30.80	2.58
ALKBDE10	−2.36	4.07	5.66	0.04	19.78	7.17	−12.61
YBDE18	−0.65	2.03	2.22	0.04	6.93	2.94	−3.99
AL2X6	−1.21	1.21	1.24	0.03	0.85	−0.83	−1.68
HEAVYSB11	−1.10	1.39	1.55	0.02	4.04	1.10	−2.94
NBPRC	0.26	1.43	1.92	0.05	6.90	4.17	−2.74
ALK8	−0.55	0.95	1.30	0.02	3.78	0.88	−2.90
RC21	3.12	3.53	4.03	0.10	9.46	7.35	−2.11
G2RC	−1.52	3.92	4.72	0.08	20.49	9.54	−10.94
BH76RC	−0.02	1.81	2.10	0.08	7.72	3.62	−4.11
FH51	−0.91	2.30	2.92	0.07	13.41	5.26	−8.15
TAUT15	−0.13	0.72	0.84	0.24	2.95	1.51	−1.43
DC13	−2.85	6.52	8.27	0.12	31.07	17.35	−13.72
MB16-43	−31.38	32.51	38.12	0.08	115.23	19.49	−95.75
DARC	−4.31	4.31	4.38	0.13	3.09	−3.46	−6.56
RSE43	−0.98	0.98	1.11	0.13	2.17	−0.31	−2.48
BSR36	−2.11	2.11	2.31	0.13	3.61	−1.00	−4.60
CDIE20	−0.10	0.63	0.82	0.16	2.74	1.80	−0.94
ISO34	−0.66	1.17	1.56	0.08	6.13	2.69	−3.44
ISOL24	0.21	2.98	4.20	0.14	20.53	6.98	−13.56
C60ISO	13.74	13.74	15.02	0.14	17.22	21.90	4.68
PArel	0.32	0.63	0.95	0.14	3.42	2.40	−1.02
BH76	−1.22	1.83	2.16	0.10	8.61	3.07	−5.54
BHPERI	1.98	2.07	2.74	0.10	10.48	9.37	−1.11
BHDIV10	−0.11	0.85	1.16	0.02	4.54	2.37	−2.16
INV24	−0.08	1.22	1.97	0.04	11.98	6.70	−5.28
BHROT27	0.16	0.31	0.42	0.05	1.51	0.97	−0.55
PX13	−2.56	2.56	2.86	0.08	4.22	−0.19	−4.41
WCPT18	−0.18	1.71	2.30	0.05	10.19	6.98	−3.21
RG18	0.09	0.10	0.15	0.17	0.57	0.48	−0.09
ADIM6	0.15	0.16	0.21	0.05	0.40	0.35	−0.05
S22	−0.10	0.22	0.29	0.03	1.26	0.61	−0.64
S66	0.04	0.12	0.16	0.02	1.09	0.80	−0.30
HEAVY28	−0.09	0.18	0.21	0.15	0.69	0.38	−0.31
WATER27	1.14	1.30	1.53	0.02	6.02	3.84	−2.18
CARBHB12	0.32	0.33	0.42	0.05	1.03	0.96	−0.07
PNICO23	−0.08	0.19	0.24	0.04	0.95	0.36	−0.59
HAL59	−0.19	0.30	0.41	0.07	2.30	0.66	−1.65
AHB21	−0.17	0.34	0.46	0.02	1.42	0.52	−0.90
CHB6	−0.79	0.87	1.08	0.03	2.40	0.26	−2.14
IL16	1.02	1.02	1.09	0.01	1.25	1.46	0.21
IDISP	−1.07	2.59	3.88	0.18	11.07	2.23	−8.83
ICONF	0.09	0.26	0.37	0.08	1.19	0.83	−0.36
ACONF	0.02	0.03	0.03	0.02	0.11	0.09	−0.02
AMINO20x4	−0.05	0.19	0.24	0.08	1.09	0.32	−0.77
PCONF21	0.07	0.30	0.35	0.19	1.16	0.65	−0.51
MCONF	0.20	0.24	0.27	0.05	0.68	0.50	−0.19
SCONF	−0.14	0.15	0.21	0.03	0.70	0.06	−0.64
UPU23	0.44	0.59	0.72	0.10	2.69	1.35	−1.34
BUT14DIOL	0.01	0.04	0.05	0.01	0.29	0.17	−0.13

Table S99: Statistical analysis for the APFD DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−1.08	3.17	4.77	0.01	33.30	7.17	−26.12
G21EA	−0.05	2.43	2.75	0.07	8.34	4.49	−3.85
G21IP	0.52	3.65	4.33	0.01	17.37	9.61	−7.76
DIPCS10	−0.71	3.01	3.48	0.00	9.88	3.39	−6.49
PA26	3.13	3.15	3.72	0.02	8.88	8.63	−0.25
SIE4x4	15.24	15.24	17.14	0.45	29.79	33.25	3.46
ALKBDE10	−2.37	4.45	5.72	0.04	19.93	7.82	−12.10
YBDE18	−1.99	2.11	2.71	0.04	7.84	0.99	−6.85
AL2X6	−1.34	1.34	1.61	0.04	2.88	−0.15	−3.03
HEAVYSB11	−2.13	2.13	2.47	0.04	3.60	−0.24	−3.84
NBPRC	−0.19	2.17	2.57	0.08	8.31	4.60	−3.71
ALK8	1.00	1.51	1.95	0.02	5.27	3.51	−1.75
RC21	4.18	4.76	5.43	0.13	11.75	9.31	−2.44
G2RC	−2.28	5.53	6.94	0.11	29.16	12.66	−16.50
BH76RC	−0.23	2.22	3.08	0.10	16.39	9.68	−6.72
FH51	−0.99	2.36	3.28	0.08	16.92	7.88	−9.04
TAUT15	0.17	1.21	1.55	0.40	5.36	3.59	−1.77
DC13	−2.15	8.65	13.22	0.16	59.04	20.49	−38.56
MB16-43	−6.40	14.82	18.62	0.04	87.77	46.09	−41.68
DARC	−1.96	1.97	2.60	0.06	6.21	0.06	−6.15
RSE43	−1.41	1.41	1.62	0.19	3.40	−0.50	−3.90
BSR36	−3.91	3.91	4.45	0.24	8.93	−1.48	−10.40
CDIE20	1.17	1.18	1.38	0.29	2.71	2.69	−0.02
ISO34	−0.43	1.29	1.75	0.09	7.98	3.65	−4.34
ISOL24	−0.56	1.97	2.70	0.09	13.37	5.80	−7.57
C60ISO	−0.76	2.37	2.97	0.02	8.44	2.20	−6.23
PArel	0.61	1.15	1.74	0.25	7.46	5.80	−1.66
BH76	−4.26	4.45	4.92	0.24	15.96	2.38	−13.58
BHPERI	−2.44	2.53	2.84	0.12	6.24	1.14	−5.10
BHDIV10	−4.00	4.47	4.90	0.10	9.67	2.36	−7.32
INV24	−0.69	1.12	1.62	0.04	7.66	3.58	−4.08
BHROT27	0.53	0.54	0.71	0.09	1.63	1.56	−0.07
PX13	−6.59	6.59	6.82	0.20	6.79	−3.56	−10.35
WCPT18	−4.30	4.30	5.05	0.12	9.39	−0.35	−9.75
RG18	0.05	0.07	0.10	0.12	0.30	0.23	−0.07
ADIM6	0.66	0.66	0.77	0.20	1.09	1.24	0.15
S22	0.93	0.93	1.19	0.13	2.73	2.73	0.00
S66	0.75	0.75	0.91	0.14	3.01	2.90	−0.11
HEAVY28	0.12	0.20	0.25	0.16	0.91	0.65	−0.26
WATER27	6.35	6.84	8.96	0.08	27.95	21.39	−6.56
CARBHB12	1.21	1.21	1.54	0.20	3.03	3.07	0.04
PNICO23	0.47	0.49	0.79	0.11	3.13	3.05	−0.08
HAL59	0.42	0.49	0.76	0.11	3.39	2.82	−0.57
AHB21	−1.11	1.12	1.35	0.05	3.00	0.16	−2.83
CHB6	−3.08	3.08	3.34	0.11	3.77	−1.69	−5.45
IL16	−0.63	0.69	0.87	0.01	1.97	0.36	−1.61
IDISP	1.66	1.92	2.33	0.14	4.71	3.93	−0.78
ICONF	0.22	0.35	0.51	0.11	1.95	1.31	−0.64
ACONF	0.02	0.06	0.07	0.03	0.23	0.10	−0.13
AMINO20x4	0.14	0.30	0.41	0.12	1.93	1.37	−0.57
PCONF21	0.07	0.65	0.86	0.40	2.80	1.97	−0.83
MCONF	0.75	0.84	0.95	0.17	2.15	1.60	−0.55
SCONF	0.37	1.28	1.61	0.28	5.65	1.45	−4.20
UPU23	0.14	0.67	0.92	0.12	4.16	1.36	−2.80
BUT14DIOL	0.56	0.58	0.65	0.21	1.54	1.22	−0.33

SI.7.4 Results for dispersion-corrected double-hybrid functionals

Table S100: Statistical analysis for the B2PLYP-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.43	1.98	2.72	0.01	20.85	9.11	−11.75
G21EA	−0.53	1.29	1.65	0.04	7.02	4.17	−2.85
G21IP	−0.91	2.28	2.78	0.01	13.01	5.78	−7.23
DIPCS10	−3.11	3.96	4.55	0.01	13.38	4.23	−9.14
PA26	1.20	1.30	2.00	0.01	7.01	6.20	−0.81
SIE4x4	10.08	10.08	11.39	0.30	19.47	21.41	1.94
ALKBDE10	0.25	3.17	3.80	0.03	12.05	6.53	−5.53
YBDE18	−1.37	2.12	2.59	0.04	8.76	3.74	−5.02
AL2X6	−2.21	2.21	2.26	0.06	1.22	−1.75	−2.97
HEAVYSB11	−1.37	1.70	1.88	0.03	3.72	0.92	−2.80
NBPRC	0.99	1.36	2.12	0.05	6.54	5.66	−0.88
ALK8	0.48	1.07	1.30	0.02	3.20	2.12	−1.08
RC21	−0.34	1.16	1.43	0.03	5.08	1.75	−3.32
G2RC	0.48	1.44	1.94	0.03	10.14	6.19	−3.94
BH76RC	−0.22	1.13	1.54	0.05	7.85	4.89	−2.96
FH51	0.70	1.50	2.04	0.05	11.87	6.62	−5.25
TAUT15	−0.02	0.72	0.85	0.24	2.90	1.69	−1.21
DC13	2.68	6.77	7.94	0.12	25.63	12.60	−13.02
MB16-43	−16.02	16.62	20.90	0.04	88.41	9.35	−79.06
DARC	5.03	5.03	5.16	0.15	4.00	6.52	2.52
RSE43	−0.51	0.57	0.73	0.07	3.31	1.22	−2.09
BSR36	−2.42	2.42	2.68	0.15	4.37	−1.18	−5.55
CDIE20	0.75	0.75	0.80	0.18	1.03	1.33	0.31
ISO34	0.12	1.13	1.74	0.08	9.52	7.33	−2.19
ISOL24	−1.27	3.83	5.41	0.17	26.68	14.13	−12.55
C60ISO	−6.75	6.76	9.14	0.07	17.89	0.07	−17.83
PArel	0.06	0.74	1.16	0.16	5.88	3.02	−2.86
BH76	−2.52	2.59	2.93	0.14	7.12	1.00	−6.13
BHPERI	−1.63	1.67	1.90	0.08	5.37	0.52	−4.85
BHDIV10	−1.11	2.13	2.60	0.05	8.47	4.06	−4.41
INV24	−0.22	0.69	0.97	0.02	4.82	2.27	−2.55
BHROT27	0.24	0.26	0.37	0.04	1.16	1.01	−0.15
PX13	−2.74	2.74	2.83	0.08	2.77	−1.38	−4.15
WCPT18	−1.71	1.71	2.09	0.05	4.03	−0.08	−4.11
RG18	−0.07	0.15	0.18	0.26	0.73	0.30	−0.44
ADIM6	−0.25	0.25	0.28	0.07	0.36	−0.11	−0.47
S22	0.11	0.15	0.20	0.02	0.66	0.53	−0.13
S66	0.05	0.18	0.23	0.03	1.02	0.71	−0.31
HEAVY28	0.15	0.17	0.20	0.14	0.64	0.40	−0.24
WATER27	1.78	2.03	2.84	0.03	11.57	8.17	−3.41
CARBHB12	0.56	0.56	0.70	0.09	1.33	1.43	0.10
PNICO23	0.18	0.19	0.26	0.04	0.81	0.71	−0.10
HAL59	0.35	0.41	0.59	0.09	2.38	2.12	−0.27
AHB21	−0.18	0.25	0.35	0.01	1.14	0.26	−0.88
CHB6	−1.16	1.18	1.32	0.04	1.80	0.08	−1.73
IL16	0.61	0.61	0.68	0.01	1.10	1.13	0.03
IDISP	1.96	1.96	2.91	0.14	6.03	6.64	0.61
ICONF	0.01	0.20	0.27	0.06	1.20	0.52	−0.68
ACONF	−0.12	0.13	0.14	0.07	0.28	0.02	−0.25
AMINO20x4	−0.03	0.15	0.20	0.06	1.32	0.85	−0.47
PCONF21	0.02	0.34	0.38	0.21	1.24	0.57	−0.67
MCONF	0.13	0.23	0.26	0.05	0.87	0.49	−0.38
SCONF	−0.04	0.12	0.24	0.03	1.12	0.19	−0.93
UPU23	0.34	0.48	0.58	0.08	1.87	1.25	−0.62
BUT14DIOL	0.13	0.13	0.15	0.05	0.41	0.34	−0.07

Table S101: Statistical analysis for the B2GPPLYP-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−2.46	2.77	3.88	0.01	19.27	2.87	−16.40
G21EA	−1.14	1.71	1.92	0.05	6.58	3.22	−3.36
G21IP	−0.81	2.01	2.52	0.01	12.84	5.08	−7.76
DIPCS10	−2.94	3.40	4.20	0.01	11.44	2.27	−9.17
PA26	0.96	1.13	1.73	0.01	6.58	5.47	−1.11
SIE4x4	6.69	6.69	7.58	0.20	13.10	14.52	1.41
ALKBDE10	−0.85	2.91	3.23	0.03	9.54	4.29	−5.25
YBDE18	−0.25	0.93	1.29	0.02	5.81	3.20	−2.61
AL2X6	−0.58	0.63	0.71	0.02	1.36	0.17	−1.19
HEAVYSB11	0.35	1.91	2.14	0.03	6.06	3.23	−2.83
NBPRC	0.61	0.93	1.40	0.03	4.44	3.68	−0.77
ALK8	2.40	2.60	3.76	0.04	9.37	8.56	−0.81
RC21	−0.68	1.39	1.62	0.04	5.64	2.35	−3.29
G2RC	−0.57	1.36	1.76	0.03	7.99	3.91	−4.08
BH76RC	−0.38	0.96	1.34	0.04	6.53	3.24	−3.29
FH51	−0.10	1.05	1.55	0.03	8.31	4.10	−4.21
TAUT15	0.11	0.54	0.68	0.18	2.53	1.39	−1.14
DC13	1.74	4.13	5.24	0.08	18.28	9.90	−8.38
MB16-43	−6.35	9.44	16.06	0.02	102.20	17.59	−84.61
DARC	2.58	2.58	2.80	0.08	3.53	4.09	0.56
RSE43	0.11	0.41	0.76	0.05	4.45	3.26	−1.19
BSR36	−2.08	2.08	2.26	0.13	3.26	−1.03	−4.28
CDIE20	0.64	0.64	0.70	0.16	1.04	1.20	0.16
ISO34	0.28	0.74	1.34	0.05	7.31	6.26	−1.06
ISOL24	−0.46	2.66	3.73	0.12	17.85	10.17	−7.68
C60ISO	−5.79	6.04	8.23	0.06	17.27	0.74	−16.52
PArel	0.20	0.55	0.89	0.12	3.75	2.37	−1.38
BH76	−0.86	1.38	1.81	0.07	11.65	6.89	−4.76
BHPERI	−1.45	1.47	1.64	0.07	3.64	0.29	−3.35
BHDIV10	−0.35	1.45	1.86	0.03	6.61	3.84	−2.77
INV24	0.19	0.79	1.12	0.02	4.59	3.13	−1.46
BHROT27	0.32	0.33	0.48	0.05	1.74	1.65	−0.09
PX13	−1.68	1.68	1.80	0.05	2.29	−0.40	−2.69
WCPT18	−0.84	1.15	1.43	0.03	4.19	1.53	−2.66
RG18	−0.07	0.16	0.20	0.28	0.82	0.44	−0.39
ADIM6	−0.44	0.44	0.49	0.13	0.60	−0.17	−0.78
S22	0.09	0.14	0.20	0.02	0.84	0.68	−0.16
S66	0.00	0.23	0.28	0.04	1.31	0.83	−0.48
HEAVY28	0.17	0.20	0.26	0.16	1.03	0.74	−0.28
WATER27	1.67	1.87	2.49	0.02	10.04	7.39	−2.65
CARBHB12	0.51	0.51	0.65	0.08	1.32	1.36	0.04
PNICO23	0.22	0.23	0.33	0.05	1.01	0.89	−0.12
HAL59	0.38	0.44	0.62	0.10	2.23	1.98	−0.25
AHB21	−0.39	0.42	0.56	0.02	1.62	0.19	−1.43
CHB6	−1.81	1.81	1.90	0.07	1.83	−0.99	−2.82
IL16	0.53	0.53	0.58	0.00	1.01	0.99	−0.02
IDISP	1.16	1.16	1.62	0.08	3.19	3.59	0.41
ICONF	0.03	0.20	0.26	0.06	0.99	0.54	−0.45
ACONF	−0.14	0.14	0.16	0.08	0.33	0.03	−0.31
AMINO20x4	−0.02	0.13	0.18	0.05	1.14	0.67	−0.47
PCONF21	0.09	0.28	0.32	0.17	1.03	0.59	−0.44
MCONF	0.15	0.21	0.24	0.04	0.77	0.47	−0.30
SCONF	−0.03	0.07	0.13	0.02	0.61	0.10	−0.51
UPU23	0.38	0.47	0.58	0.08	1.52	1.19	−0.33
BUT14DIOL	0.09	0.09	0.11	0.03	0.29	0.27	−0.02

Table S102: Statistical analysis for the MPW2PLYP-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−2.04	2.66	3.71	0.01	21.81	4.87	−16.94
G21EA	−0.71	1.48	1.81	0.04	7.44	4.55	−2.90
G21IP	−0.66	2.34	2.82	0.01	12.84	6.10	−6.73
DIPCS10	−2.38	3.49	4.50	0.01	15.13	5.57	−9.56
PA26	1.00	1.19	1.90	0.01	7.20	6.03	−1.18
SIE4x4	9.22	9.22	10.47	0.27	18.42	20.08	1.66
ALKBDE10	−1.19	3.23	3.60	0.03	11.10	4.00	−7.11
YBDE18	−1.68	2.10	2.50	0.04	7.43	2.21	−5.22
AL2X6	−2.66	2.66	2.77	0.07	2.05	−1.90	−3.95
HEAVYSB11	−2.44	2.44	2.62	0.04	2.94	−0.90	−3.84
NBPRC	0.99	1.71	2.26	0.06	7.05	5.24	−1.82
ALK8	−0.57	1.40	1.95	0.02	5.96	1.94	−4.02
RC21	0.05	1.05	1.35	0.03	4.68	2.01	−2.66
G2RC	−0.54	1.59	1.91	0.03	7.90	4.42	−3.48
BH76RC	−0.40	1.26	1.58	0.06	6.80	2.99	−3.81
FH51	0.20	1.18	1.70	0.04	10.50	5.07	−5.43
TAUT15	0.02	0.65	0.83	0.21	2.99	1.65	−1.34
DC13	2.07	6.42	8.11	0.12	28.10	13.30	−14.80
MB16-43	−21.28	22.08	26.72	0.05	80.68	9.56	−71.11
DARC	4.64	4.64	4.82	0.14	4.53	6.08	1.54
RSE43	−0.43	0.49	0.64	0.06	2.96	1.09	−1.87
BSR36	−3.76	3.76	4.38	0.23	8.89	−1.51	−10.41
CDIE20	0.70	0.70	0.77	0.17	1.19	1.40	0.21
ISO34	0.16	1.08	1.70	0.07	9.78	7.56	−2.22
ISOL24	−1.29	3.78	5.42	0.17	27.55	13.70	−13.85
C60ISO	−4.18	4.65	6.42	0.05	14.36	1.13	−13.22
PArel	0.15	0.68	1.06	0.15	4.98	3.21	−1.76
BH76	−2.19	2.32	2.64	0.12	7.35	1.49	−5.86
BHPERI	−0.61	0.85	1.08	0.04	5.00	1.53	−3.47
BHDIV10	−0.38	1.73	2.14	0.04	7.62	4.34	−3.28
INV24	0.01	0.71	0.96	0.02	4.03	2.22	−1.81
BHROT27	0.30	0.32	0.44	0.05	1.25	1.10	−0.15
PX13	−2.15	2.15	2.27	0.06	2.59	−0.81	−3.40
WCPT18	−1.10	1.45	1.81	0.04	4.67	1.31	−3.36
RG18	0.26	0.27	0.40	0.47	1.12	1.08	−0.05
ADIM6	0.04	0.10	0.12	0.03	0.34	0.16	−0.18
S22	0.23	0.31	0.41	0.04	1.58	1.13	−0.45
S66	0.26	0.29	0.43	0.05	1.53	1.29	−0.24
HEAVY28	0.06	0.12	0.16	0.10	0.56	0.38	−0.18
WATER27	4.79	4.99	6.97	0.06	20.89	18.10	−2.79
CARBHB12	0.75	0.75	0.85	0.12	1.32	1.61	0.28
PNICO23	0.19	0.22	0.25	0.05	0.50	0.43	−0.08
HAL59	0.31	0.34	0.53	0.07	2.28	2.07	−0.22
AHB21	−0.63	0.63	0.72	0.03	1.11	−0.10	−1.21
CHB6	−1.47	1.55	1.71	0.06	2.56	0.24	−2.31
IL16	0.47	0.50	0.59	0.00	1.45	1.19	−0.26
IDISP	1.91	2.78	3.81	0.20	10.67	8.05	−2.61
ICONF	0.05	0.25	0.35	0.08	1.44	0.60	−0.84
ACONF	−0.05	0.08	0.10	0.04	0.33	0.10	−0.23
AMINO20x4	−0.01	0.14	0.21	0.06	1.28	0.78	−0.50
PCONF21	0.01	0.39	0.46	0.24	1.67	0.88	−0.79
MCONF	0.03	0.10	0.13	0.02	0.54	0.30	−0.24
SCONF	−0.09	0.12	0.18	0.03	0.75	0.18	−0.57
UPU23	0.39	0.50	0.62	0.09	1.66	1.27	−0.39
BUT14DIOL	0.15	0.15	0.17	0.05	0.37	0.38	0.01

Table S103: Statistical analysis for the PWPB95-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.15	1.86	2.96	0.01	28.70	15.22	−13.49
G21EA	−1.64	1.71	1.84	0.05	3.36	0.63	−2.73
G21IP	−1.29	1.94	2.37	0.01	10.15	3.61	−6.54
DIPCS10	−4.04	4.09	4.62	0.01	8.88	0.21	−8.66
PA26	1.88	1.90	2.30	0.01	6.27	6.02	−0.25
SIE4x4	10.02	10.02	11.44	0.30	20.87	22.65	1.78
ALKBDE10	−2.27	3.13	3.52	0.03	8.70	3.54	−5.16
YBDE18	−0.65	1.91	2.22	0.04	6.55	2.62	−3.93
AL2X6	0.65	0.91	0.92	0.03	2.03	1.24	−0.78
HEAVYSB11	0.52	0.73	1.00	0.01	2.75	2.17	−0.58
NBPRC	0.11	0.85	1.01	0.03	3.41	2.02	−1.39
ALK8	3.96	4.23	6.65	0.07	16.40	15.84	−0.56
RC21	0.66	1.32	1.53	0.04	5.65	3.09	−2.55
G2RC	0.26	2.17	2.80	0.04	10.14	6.11	−4.03
BH76RC	0.14	1.14	1.61	0.05	9.02	5.15	−3.86
FH51	0.48	1.16	1.49	0.04	6.22	3.23	−2.99
TAUT15	−0.08	0.62	0.73	0.20	2.34	1.30	−1.04
DC13	−0.18	3.71	4.96	0.07	19.87	10.47	−9.40
MB16-43	−0.08	6.71	10.59	0.02	69.35	20.19	−49.16
DARC	1.69	1.72	2.05	0.05	3.41	3.29	−0.12
RSE43	−0.97	0.97	1.14	0.13	2.57	−0.29	−2.86
BSR36	−2.42	2.42	2.56	0.15	4.01	−0.59	−4.60
CDIE20	0.68	0.70	0.84	0.17	1.78	1.67	−0.11
ISO34	−0.53	0.79	0.96	0.05	3.30	1.19	−2.11
ISOL24	−1.09	2.09	2.67	0.10	11.03	5.35	−5.68
C60ISO	−3.05	3.48	4.81	0.04	10.95	1.02	−9.93
PArel	0.36	0.68	1.07	0.15	5.01	3.64	−1.37
BH76	−1.68	1.76	2.07	0.09	5.84	0.97	−4.87
BHPERI	0.07	0.80	0.90	0.04	3.41	1.63	−1.78
BHDIV10	−1.58	1.59	1.79	0.04	2.95	0.05	−2.90
INV24	−0.30	0.78	1.02	0.02	4.70	2.37	−2.33
BHROT27	0.27	0.32	0.42	0.05	1.04	0.80	−0.24
PX13	−1.23	1.25	1.37	0.04	2.24	0.09	−2.15
WCPT18	−1.10	1.10	1.32	0.03	2.70	−0.10	−2.80
RG18	0.08	0.19	0.31	0.33	1.24	0.92	−0.32
ADIM6	0.03	0.18	0.20	0.05	0.50	0.33	−0.16
S22	−0.35	0.41	0.63	0.06	1.80	0.21	−1.59
S66	−0.24	0.26	0.36	0.05	1.31	0.18	−1.14
HEAVY28	0.09	0.17	0.21	0.14	0.80	0.57	−0.24
WATER27	−3.54	3.59	5.67	0.04	15.63	0.45	−15.18
CARBHB12	0.05	0.22	0.28	0.04	1.09	0.63	−0.45
PNICO23	0.03	0.14	0.22	0.03	1.06	0.86	−0.20
HAL59	−0.01	0.30	0.40	0.07	1.94	1.09	−0.85
AHB21	0.27	0.31	0.37	0.01	1.01	0.82	−0.19
CHB6	−1.53	1.53	1.83	0.06	2.73	−0.29	−3.02
IL16	1.25	1.25	1.28	0.01	0.95	1.87	0.91
IDISP	1.13	1.38	1.81	0.10	4.28	3.51	−0.77
ICONF	−0.04	0.18	0.29	0.06	1.29	0.49	−0.80
ACONF	−0.25	0.25	0.28	0.14	0.47	0.01	−0.46
AMINO20x4	−0.01	0.23	0.31	0.09	1.56	0.95	−0.61
PCONF21	0.27	0.45	0.55	0.28	1.68	1.07	−0.60
MCONF	0.25	0.34	0.43	0.07	1.35	0.91	−0.44
SCONF	−0.07	0.18	0.28	0.04	1.26	0.35	−0.91
UPU23	0.43	0.53	0.65	0.09	1.46	1.21	−0.25
BUT14DIOL	−0.36	0.36	0.37	0.13	0.55	−0.10	−0.64

Table S104: Statistical analysis for the DSD-BLYP-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−1.95	2.51	3.48	0.01	21.80	4.53	−17.26
G21EA	−1.27	1.76	1.99	0.05	7.36	3.85	−3.52
G21IP	−1.12	2.02	2.52	0.01	12.60	4.75	−7.85
DIPCS10	−3.81	3.99	4.61	0.01	10.01	0.91	−9.10
PA26	0.87	1.02	1.59	0.01	6.15	4.96	−1.19
SIE4x4	5.88	5.88	6.65	0.17	11.22	12.48	1.26
ALKBDE10	−0.17	2.78	3.17	0.03	9.62	5.21	−4.41
YBDE18	0.39	0.95	1.48	0.02	6.12	4.55	−1.57
AL2X6	−0.37	0.54	0.56	0.02	1.27	0.50	−0.77
HEAVYSB11	1.01	2.10	2.45	0.04	6.50	4.13	−2.37
NBPRC	0.59	0.88	1.30	0.03	4.03	3.45	−0.59
ALK8	2.49	2.71	4.06	0.04	10.12	9.23	−0.88
RC21	−1.48	1.84	2.24	0.05	5.02	1.19	−3.83
G2RC	−0.05	1.03	1.46	0.02	7.22	4.23	−2.99
BH76RC	−0.21	0.81	1.21	0.04	6.96	4.09	−2.87
FH51	0.07	1.11	1.56	0.04	8.95	4.52	−4.43
TAUT15	0.04	0.46	0.54	0.15	1.96	0.98	−0.98
DC13	1.87	3.94	4.76	0.07	16.63	8.85	−7.77
MB16-43	−4.99	7.92	16.81	0.02	116.54	17.08	−99.46
DARC	2.38	2.38	2.54	0.07	2.67	3.77	1.10
RSE43	0.48	0.59	1.22	0.08	5.72	4.98	−0.74
BSR36	−1.49	1.49	1.57	0.09	1.77	−0.79	−2.55
CDIE20	0.56	0.56	0.60	0.14	0.84	0.98	0.15
ISO34	0.25	0.69	1.19	0.05	6.32	5.36	−0.96
ISOL24	−0.37	2.38	3.34	0.11	15.66	9.33	−6.33
C60ISO	−7.63	7.63	10.12	0.08	19.56	−0.06	−19.62
PArel	0.11	0.53	0.83	0.11	4.06	2.10	−1.96
BH76	−0.38	1.22	1.94	0.07	13.68	8.96	−4.72
BHPERI	−1.88	1.88	2.06	0.09	3.52	−0.32	−3.84
BHDIV10	−0.42	1.35	1.78	0.03	6.13	3.30	−2.83
INV24	0.19	0.80	1.15	0.03	5.69	2.90	−2.79
BHROT27	0.22	0.23	0.32	0.04	0.90	0.83	−0.07
PX13	−1.58	1.58	1.67	0.05	2.03	−0.43	−2.45
WCPT18	−0.90	1.04	1.30	0.03	3.46	0.91	−2.55
RG18	−0.08	0.16	0.21	0.28	0.90	0.47	−0.43
ADIM6	−0.37	0.37	0.41	0.11	0.51	−0.14	−0.66
S22	0.11	0.17	0.23	0.02	0.81	0.54	−0.26
S66	0.01	0.17	0.21	0.03	0.88	0.47	−0.41
HEAVY28	0.15	0.19	0.24	0.15	0.99	0.68	−0.31
WATER27	0.68	0.94	1.29	0.01	6.64	4.15	−2.49
CARBHB12	0.42	0.42	0.55	0.07	1.18	1.18	−0.01
PNICO23	0.20	0.21	0.31	0.05	1.02	0.89	−0.12
HAL59	0.37	0.43	0.59	0.09	2.29	2.00	−0.30
AHB21	−0.20	0.26	0.36	0.01	1.43	0.25	−1.18
CHB6	−1.70	1.70	1.80	0.06	1.93	−0.94	−2.86
IL16	0.56	0.56	0.61	0.01	0.88	0.99	0.11
IDISP	1.02	1.02	1.31	0.07	2.24	2.23	0.00
ICONF	0.00	0.18	0.24	0.06	0.99	0.41	−0.58
ACONF	−0.19	0.19	0.21	0.10	0.35	0.01	−0.34
AMINO20x4	−0.04	0.13	0.18	0.05	1.09	0.60	−0.49
PCONF21	0.09	0.23	0.29	0.14	0.94	0.63	−0.30
MCONF	0.23	0.30	0.33	0.06	0.93	0.59	−0.34
SCONF	−0.03	0.06	0.12	0.01	0.55	0.08	−0.47
UPU23	0.32	0.43	0.53	0.08	1.56	1.10	−0.46
BUT14DIOL	0.04	0.06	0.08	0.02	0.29	0.22	−0.07

Table S105: Statistical analysis for the DSD-PBEP86-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−2.54	2.72	3.76	0.01	21.77	2.41	−19.36
G21EA	−1.02	1.51	1.79	0.04	7.69	4.72	−2.97
G21IP	−1.06	2.10	2.62	0.01	13.63	6.57	−7.05
DIPCS10	−3.90	3.90	4.35	0.01	6.72	−0.96	−7.68
PA26	1.03	1.10	1.49	0.01	5.06	4.41	−0.65
SIE4x4	5.04	5.04	5.78	0.15	10.35	11.45	1.10
ALKBDE10	−2.01	3.01	3.44	0.03	8.23	2.32	−5.91
YBDE18	1.18	1.53	2.00	0.03	6.51	5.26	−1.25
AL2X6	−0.03	0.31	0.46	0.01	1.36	0.36	−1.01
HEAVYSB11	−0.04	0.92	1.09	0.02	3.45	1.79	−1.66
NBPRC	−0.18	0.88	0.99	0.03	2.83	1.44	−1.39
ALK8	2.13	2.28	3.50	0.04	8.99	8.42	−0.57
RC21	−0.72	1.77	2.05	0.05	6.31	2.96	−3.35
G2RC	−0.63	1.83	2.45	0.04	11.43	5.12	−6.31
BH76RC	−0.21	0.86	1.39	0.04	8.25	5.08	−3.18
FH51	−0.55	0.87	1.20	0.03	5.91	2.58	−3.33
TAUT15	0.02	0.46	0.51	0.15	1.47	0.84	−0.63
DC13	0.57	2.55	3.65	0.05	14.87	5.17	−9.70
MB16-43	−3.43	6.46	16.04	0.02	113.19	15.30	−97.90
DARC	−1.30	1.32	1.56	0.04	2.53	0.08	−2.46
RSE43	0.90	0.90	1.72	0.12	7.21	7.21	0.00
BSR36	−1.36	1.36	1.50	0.08	2.47	−0.59	−3.06
CDIE20	0.47	0.47	0.54	0.12	0.96	0.99	0.03
ISO34	0.08	0.41	0.65	0.03	3.13	2.16	−0.97
ISOL24	0.30	1.12	1.53	0.05	6.13	3.96	−2.17
C60ISO	−7.56	7.56	9.82	0.08	18.58	−0.32	−18.90
PArel	0.21	0.50	0.76	0.11	3.31	1.72	−1.59
BH76	−0.25	1.28	2.08	0.07	14.20	9.80	−4.41
BHPERI	−2.41	2.45	2.61	0.12	4.69	0.53	−4.16
BHDIV10	−1.18	1.71	1.88	0.04	5.24	1.85	−3.38
INV24	0.25	0.75	1.12	0.02	5.91	3.68	−2.23
BHROT27	0.20	0.21	0.27	0.03	0.68	0.63	−0.06
PX13	−2.51	2.51	2.59	0.08	2.57	−1.27	−3.84
WCPT18	−1.76	1.77	2.08	0.05	4.04	0.09	−3.94
RG18	−0.03	0.15	0.21	0.26	1.01	0.64	−0.37
ADIM6	−0.02	0.06	0.07	0.02	0.21	0.08	−0.13
S22	0.29	0.31	0.37	0.04	0.90	0.76	−0.14
S66	0.20	0.21	0.25	0.04	0.76	0.64	−0.12
HEAVY28	0.15	0.18	0.22	0.15	0.69	0.48	−0.22
WATER27	2.04	2.26	2.95	0.03	11.03	8.11	−2.93
CARBHB12	0.61	0.61	0.73	0.10	1.25	1.46	0.21
PNICO23	0.40	0.40	0.52	0.09	1.54	1.55	0.00
HAL59	0.41	0.44	0.61	0.10	2.14	1.98	−0.16
AHB21	−0.43	0.43	0.53	0.02	1.56	−0.02	−1.58
CHB6	−1.12	1.12	1.22	0.04	1.45	−0.56	−2.01
IL16	0.13	0.23	0.28	0.00	1.09	0.49	−0.60
IDISP	0.34	1.43	1.57	0.10	4.26	2.54	−1.72
ICONF	0.04	0.14	0.18	0.04	0.79	0.37	−0.42
ACONF	−0.25	0.25	0.27	0.14	0.36	−0.01	−0.37
AMINO20x4	−0.03	0.13	0.16	0.05	0.75	0.39	−0.37
PCONF21	0.03	0.27	0.34	0.17	1.22	0.72	−0.50
MCONF	0.34	0.38	0.43	0.08	0.99	0.74	−0.26
SCONF	0.03	0.13	0.17	0.03	0.73	0.17	−0.56
UPU23	0.25	0.38	0.48	0.07	1.66	1.05	−0.61
BUT14DIOL	0.03	0.05	0.07	0.02	0.28	0.21	−0.07

Table S106: Statistical analysis for the DSD-PBEB95-D3(BJ) DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−1.57	2.38	3.52	0.01	30.84	13.55	−17.29
G21EA	−2.76	2.89	2.97	0.09	5.92	1.59	−4.34
G21IP	−2.18	2.58	2.89	0.01	10.89	3.21	−7.68
DIPCS10	−6.03	6.03	6.33	0.01	7.77	−2.50	−10.27
PA26	1.50	1.51	1.85	0.01	5.01	4.87	−0.15
SIE4x4	5.97	5.97	6.82	0.18	12.47	13.62	1.16
ALKBDE10	−2.85	2.97	3.58	0.03	6.61	0.48	−6.13
YBDE18	1.19	1.23	1.40	0.02	2.71	2.37	−0.34
AL2X6	0.85	0.97	1.09	0.03	2.21	1.84	−0.37
HEAVYSB11	0.97	1.07	1.31	0.02	2.78	2.22	−0.57
NBPRC	−0.27	0.73	0.81	0.03	2.37	0.96	−1.41
ALK8	3.82	3.92	5.99	0.06	14.00	13.58	−0.42
RC21	−0.19	1.17	1.43	0.03	6.51	3.00	−3.51
G2RC	−0.24	1.70	2.33	0.03	9.36	4.59	−4.77
BH76RC	0.14	1.13	1.52	0.05	8.31	4.82	−3.49
FH51	−0.26	0.69	0.98	0.02	4.49	1.82	−2.67
TAUT15	−0.16	0.41	0.49	0.13	1.44	0.51	−0.93
DC13	−0.40	3.41	4.64	0.06	17.17	8.86	−8.32
MB16-43	1.85	6.52	13.71	0.02	98.39	21.37	−77.02
DARC	−0.98	1.09	1.24	0.03	2.14	0.37	−1.78
RSE43	0.04	0.45	0.73	0.06	3.93	2.62	−1.31
BSR36	−1.20	1.20	1.26	0.07	1.81	−0.45	−2.26
CDIE20	0.49	0.51	0.64	0.13	1.41	1.32	−0.09
ISO34	−0.29	0.56	0.77	0.04	3.16	1.25	−1.90
ISOL24	−0.18	0.96	1.33	0.04	6.17	2.78	−3.39
C60ISO	−4.50	4.76	6.40	0.05	13.68	0.77	−12.91
PArel	0.31	0.55	0.78	0.12	3.35	2.32	−1.03
BH76	0.11	1.03	1.65	0.06	11.10	7.55	−3.55
BHPERI	−0.46	0.95	1.16	0.05	3.90	1.60	−2.29
BHDIV10	−0.74	0.83	1.02	0.02	1.91	0.30	−1.61
INV24	0.30	0.79	1.20	0.02	6.12	4.55	−1.57
BHROT27	0.24	0.25	0.33	0.04	0.72	0.68	−0.04
PX13	−0.16	0.43	0.51	0.01	1.66	0.81	−0.85
WCPT18	−0.46	0.58	0.76	0.02	2.39	0.69	−1.70
RG18	0.10	0.17	0.28	0.29	1.13	0.83	−0.30
ADIM6	0.49	0.49	0.58	0.15	0.85	1.00	0.15
S22	0.17	0.51	0.63	0.07	2.50	1.50	−1.00
S66	0.18	0.29	0.37	0.05	1.55	0.88	−0.67
HEAVY28	0.07	0.14	0.18	0.11	0.64	0.39	−0.25
WATER27	−1.84	1.88	2.97	0.02	8.31	0.28	−8.03
CARBHB12	0.17	0.22	0.28	0.04	0.91	0.68	−0.23
PNICO23	0.17	0.17	0.25	0.04	0.85	0.82	−0.03
HAL59	0.15	0.30	0.40	0.07	1.67	1.06	−0.60
AHB21	0.09	0.20	0.24	0.01	1.00	0.45	−0.55
CHB6	−1.58	1.58	1.83	0.06	2.40	−0.51	−2.90
IL16	0.77	0.77	0.81	0.01	0.92	1.35	0.43
IDISP	0.43	2.12	2.28	0.15	5.96	3.56	−2.39
ICONF	−0.02	0.19	0.29	0.06	1.32	0.44	−0.88
ACONF	−0.37	0.37	0.39	0.20	0.53	−0.04	−0.56
AMINO20x4	−0.03	0.22	0.29	0.09	1.49	0.98	−0.51
PCONF21	0.31	0.68	0.83	0.42	2.33	1.52	−0.81
MCONF	0.51	0.57	0.65	0.11	1.52	1.19	−0.33
SCONF	−0.08	0.15	0.21	0.03	0.81	0.15	−0.66
UPU23	0.20	0.45	0.56	0.08	2.34	1.10	−1.23
BUT14DIOL	−0.28	0.28	0.29	0.10	0.43	−0.06	−0.49

SI.7.5 Results for dispersion-uncorrected GGA/NGA functionals

Table S107: Statistical analysis for the PBE DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	13.35	14.96	18.50	0.05	71.84	53.52	−18.32
G21EA	2.96	3.43	4.11	0.10	10.49	7.72	−2.77
G21IP	−0.12	3.85	4.83	0.01	19.31	10.17	−9.14
DIPCS10	−2.55	4.51	6.00	0.01	19.98	7.11	−12.86
PA26	1.43	1.97	2.67	0.01	9.16	6.97	−2.19
SIE4x4	23.44	23.44	26.19	0.70	42.31	46.56	4.25
ALKBDE10	5.69	6.21	10.19	0.06	28.30	27.17	−1.13
YBDE18	−2.31	5.91	7.03	0.12	22.75	9.97	−12.78
AL2X6	−4.24	4.26	4.90	0.12	7.52	0.07	−7.45
HEAVYSB11	−1.63	4.58	5.14	0.08	15.11	5.94	−9.17
NBPRC	1.01	2.82	3.48	0.10	11.26	5.78	−5.48
ALK8	0.41	2.78	3.55	0.04	11.52	7.25	−4.28
RC21	4.53	5.48	6.40	0.15	16.86	13.00	−3.85
G2RC	1.02	6.29	7.75	0.12	30.86	19.43	−11.42
BH76RC	0.83	4.09	6.04	0.19	30.00	22.52	−7.49
FH51	1.82	3.40	4.68	0.11	22.85	12.69	−10.16
TAUT15	0.31	1.81	2.33	0.59	7.46	5.10	−2.37
DC13	1.85	10.14	13.31	0.18	48.96	18.04	−30.92
MB16-43	−10.23	22.78	30.20	0.05	135.71	50.64	−85.07
DARC	6.78	6.94	7.83	0.21	11.56	10.45	−1.11
RSE43	−3.10	3.10	3.41	0.41	6.68	−0.95	−7.63
BSR36	−7.67	7.67	8.85	0.47	18.51	−1.84	−20.35
CDIE20	1.81	1.81	1.99	0.45	3.25	3.26	0.01
ISO34	−0.92	1.80	2.52	0.12	12.12	5.25	−6.87
ISOL24	−3.48	6.83	10.43	0.31	56.52	22.85	−33.68
C60ISO	−11.06	11.06	13.04	0.11	20.40	−1.98	−22.39
PArel	0.29	1.81	2.54	0.39	12.80	6.87	−5.92
BH76	−9.11	9.15	10.39	0.49	31.67	1.62	−30.06
BHPERI	−3.95	3.95	4.41	0.19	7.34	−1.09	−8.43
BHDIV10	−7.77	8.23	9.19	0.18	16.27	2.29	−13.99
INV24	−2.48	2.67	3.16	0.08	10.58	2.31	−8.27
BHROT27	0.34	0.47	0.64	0.07	2.05	1.63	−0.41
PX13	−11.54	11.54	11.73	0.35	8.24	−8.63	−16.87
WCPT18	−8.61	8.61	9.00	0.25	10.46	−4.95	−15.41
RG18	−0.19	0.28	0.41	0.48	1.15	0.17	−0.98
ADIM6	−3.38	3.38	3.75	1.01	4.71	−1.16	−5.87
S22	−2.52	2.55	3.58	0.35	10.45	0.39	−10.06
S66	−2.07	2.11	2.65	0.39	7.49	0.45	−7.04
HEAVY28	−0.42	0.47	0.57	0.38	1.46	0.21	−1.25
WATER27	1.88	2.83	3.88	0.03	22.62	10.69	−11.93
CARBHB12	1.07	1.09	1.56	0.18	3.74	3.62	−0.12
PNICO23	0.02	0.82	1.30	0.19	7.22	4.98	−2.24
HAL59	−0.15	1.30	1.85	0.28	11.79	5.85	−5.94
AHB21	−0.37	0.83	1.04	0.04	4.01	1.93	−2.08
CHB6	0.12	0.79	1.04	0.03	3.15	2.19	−0.96
IL16	1.49	1.49	1.63	0.01	2.82	3.05	0.23
IDISP	3.20	10.78	12.55	0.76	34.81	23.39	−11.42
ICONF	0.16	0.43	0.68	0.13	2.92	2.29	−0.63
ACONF	0.61	0.61	0.68	0.33	1.06	1.27	0.22
AMINO20x4	−0.01	0.51	0.64	0.21	3.13	1.78	−1.35
PCONF21	−0.79	3.48	3.77	2.15	10.58	5.60	−4.98
MCONF	−1.70	1.80	2.05	0.36	4.41	0.88	−3.53
SCONF	0.16	0.35	0.47	0.08	2.02	0.92	−1.10
UPU23	1.41	1.99	2.83	0.35	9.28	7.51	−1.76
BUT14DIOL	0.15	0.26	0.35	0.09	1.46	1.10	−0.35

Table S108: Statistical analysis for the PBEhPBE DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	12.13	13.67	17.11	0.04	68.52	51.45	−17.08
G21EA	2.75	3.22	3.94	0.10	10.09	7.40	−2.69
G21IP	−0.01	3.89	4.92	0.02	20.13	11.05	−9.08
DIPCS10	−2.35	4.39	5.84	0.01	19.73	7.38	−12.35
PA26	1.29	1.88	2.59	0.01	9.11	6.86	−2.25
SIE4x4	23.35	23.35	26.11	0.69	42.37	46.45	4.08
ALKBDE10	5.64	6.29	10.04	0.06	28.01	26.67	−1.34
YBDE18	−2.85	6.05	7.22	0.12	23.29	10.01	−13.28
AL2X6	−4.56	4.56	5.14	0.13	6.88	−0.30	−7.18
HEAVYSB11	−1.42	4.26	4.84	0.07	14.03	5.27	−8.76
NBPRC	1.26	2.92	3.68	0.11	11.48	6.64	−4.84
ALK8	0.23	2.76	3.52	0.04	11.98	6.95	−5.03
RC21	4.01	4.99	5.90	0.14	16.10	12.18	−3.92
G2RC	1.27	5.95	7.38	0.12	30.48	19.42	−11.06
BH76RC	0.90	3.95	5.91	0.18	29.26	22.10	−7.16
FH51	1.97	3.49	4.75	0.11	22.46	12.62	−9.85
TAUT15	0.21	1.89	2.36	0.62	7.56	5.05	−2.51
DC13	2.40	11.28	13.74	0.21	47.56	17.21	−30.36
MB16-43	−14.16	23.37	30.43	0.06	128.12	44.45	−83.66
DARC	8.16	8.16	9.03	0.25	11.60	11.73	0.13
RSE43	−3.04	3.04	3.35	0.40	6.62	−0.93	−7.55
BSR36	−7.68	7.68	8.87	0.47	17.63	−2.12	−19.75
CDIE20	1.78	1.78	1.95	0.44	3.11	3.15	0.04
ISO34	−0.90	1.87	2.61	0.13	13.48	6.48	−7.00
ISOL24	−3.77	7.28	11.14	0.33	60.03	24.68	−35.36
C60ISO	−10.46	10.46	12.49	0.11	20.30	−1.42	−21.72
PArel	0.22	1.75	2.53	0.38	13.16	6.86	−6.30
BH76	−9.26	9.30	10.50	0.50	31.02	1.49	−29.53
BHPERI	−3.59	3.59	4.09	0.17	7.02	−0.90	−7.93
BHDIV10	−7.39	7.95	8.91	0.18	16.65	2.82	−13.84
INV24	−2.78	2.96	3.63	0.09	11.34	2.22	−9.12
BHROT27	0.36	0.49	0.67	0.08	2.18	1.71	−0.47
PX13	−10.95	10.95	11.09	0.33	7.24	−8.35	−15.59
WCPT18	−8.31	8.31	8.71	0.24	10.36	−4.54	−14.91
RG18	−0.17	0.29	0.40	0.50	1.17	0.22	−0.94
ADIM6	−3.37	3.37	3.73	1.00	4.67	−1.16	−5.84
S22	−2.38	2.43	3.47	0.33	10.30	0.53	−9.77
S66	−1.97	2.04	2.59	0.37	7.53	0.63	−6.90
HEAVY28	−0.37	0.44	0.54	0.35	1.45	0.23	−1.22
WATER27	3.37	4.22	5.34	0.05	27.54	16.05	−11.49
CARBHB12	1.15	1.15	1.61	0.19	3.71	3.71	−0.01
PNICO23	0.10	0.77	1.24	0.18	6.85	4.72	−2.13
HAL59	−0.01	1.31	1.87	0.29	11.90	6.10	−5.80
AHB21	−0.57	0.93	1.10	0.04	3.84	1.83	−2.01
CHB6	0.12	0.76	1.00	0.03	2.84	2.13	−0.72
IL16	1.27	1.27	1.43	0.01	2.71	2.74	0.03
IDISP	3.44	10.78	12.82	0.76	35.78	24.82	−10.95
ICONF	0.16	0.43	0.66	0.13	2.90	2.21	−0.69
ACONF	0.58	0.58	0.65	0.32	1.04	1.26	0.22
AMINO20x4	0.01	0.50	0.64	0.20	3.17	1.77	−1.40
PCONF21	−0.80	3.41	3.69	2.10	10.33	5.34	−4.99
MCONF	−1.64	1.74	1.98	0.35	4.36	0.92	−3.44
SCONF	0.24	0.46	0.62	0.10	2.70	1.09	−1.61
UPU23	1.40	1.95	2.79	0.34	9.06	7.39	−1.67
BUT14DIOL	0.28	0.31	0.41	0.11	1.45	1.23	−0.22

Table S109: Statistical analysis for the revPBE DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	0.71	7.52	10.06	0.02	63.64	32.41	−31.23
G21EA	1.66	2.76	3.29	0.08	10.49	6.14	−4.35
G21IP	−1.23	4.19	5.08	0.02	18.80	9.09	−9.72
DIPCS10	−3.94	4.84	6.42	0.01	16.80	4.14	−12.65
PA26	3.66	3.66	4.48	0.02	9.81	10.01	0.19
SIE4x4	22.77	22.77	25.76	0.68	42.98	48.03	5.05
ALKBDE10	0.52	5.21	7.79	0.05	27.97	21.65	−6.32
YBDE18	−8.34	8.73	10.51	0.18	23.22	2.76	−20.46
AL2X6	−9.34	9.34	9.85	0.26	8.83	−3.93	−12.76
HEAVYSB11	−6.75	6.85	8.33	0.12	14.55	0.54	−14.01
NBPRC	4.48	5.24	7.07	0.19	19.05	17.06	−1.99
ALK8	−3.69	4.01	6.00	0.06	15.78	0.86	−14.92
RC21	0.52	2.84	3.63	0.08	13.75	6.62	−7.12
G2RC	3.84	5.12	7.15	0.10	28.94	18.86	−10.08
BH76RC	0.91	2.78	4.59	0.13	23.62	17.53	−6.09
FH51	4.04	4.96	6.48	0.16	29.34	17.82	−11.52
TAUT15	−0.12	1.44	1.63	0.47	5.10	2.61	−2.48
DC13	5.63	14.71	16.71	0.27	54.93	27.08	−27.85
MB16-43	−45.40	48.58	56.30	0.12	173.18	45.15	−128.03
DARC	14.24	14.24	14.83	0.44	11.79	17.88	6.09
RSE43	−2.69	2.69	2.96	0.35	6.16	−0.93	−7.10
BSR36	−10.96	10.96	12.34	0.68	26.09	−1.57	−27.67
CDIE20	1.92	1.93	2.15	0.48	3.89	3.79	−0.10
ISO34	−1.24	2.28	3.31	0.16	17.82	6.53	−11.29
ISOL24	−5.80	9.73	15.48	0.44	83.88	28.22	−55.66
C60ISO	−10.68	10.68	12.77	0.11	20.53	−1.39	−21.92
PArel	0.10	1.49	2.40	0.32	13.48	6.18	−7.30
BH76	−7.08	7.11	8.11	0.38	24.77	1.33	−23.43
BHPERI	0.13	2.96	3.44	0.14	12.32	5.65	−6.67
BHDIV10	−5.72	6.11	7.10	0.13	12.74	1.93	−10.80
INV24	−2.97	3.24	3.81	0.10	11.68	3.24	−8.44
BHROT27	0.13	0.34	0.45	0.05	1.61	1.12	−0.49
PX13	−7.36	7.36	7.46	0.22	4.99	−5.44	−10.43
WCPT18	−5.34	5.34	5.87	0.15	8.41	−1.45	−9.86
RG18	−0.79	0.79	1.01	1.36	2.22	−0.08	−2.30
ADIM6	−6.25	6.25	6.86	1.86	8.21	−2.40	−10.61
S22	−5.20	5.20	6.39	0.71	15.30	−0.98	−16.28
S66	−4.44	4.44	4.96	0.81	10.67	−1.00	−11.67
HEAVY28	−1.46	1.46	1.55	1.18	2.09	−0.43	−2.52
WATER27	−16.85	16.87	25.45	0.21	67.09	0.33	−66.77
CARBHB12	−0.67	1.03	1.16	0.17	3.36	1.33	−2.03
PNICO23	−1.93	2.05	2.18	0.48	5.34	1.34	−4.00
HAL59	−2.11	2.26	2.77	0.49	12.30	2.84	−9.46
AHB21	2.15	2.15	2.47	0.10	4.64	5.23	0.59
CHB6	1.82	1.82	2.28	0.07	3.92	4.64	0.71
IL16	5.17	5.17	5.27	0.05	4.10	7.70	3.60
IDISP	4.50	17.69	20.04	1.24	56.05	34.46	−21.59
ICONF	0.07	0.67	0.99	0.20	4.51	2.91	−1.60
ACONF	1.24	1.24	1.37	0.68	1.89	2.37	0.48
AMINO20x4	−0.25	0.81	0.99	0.33	4.49	2.39	−2.10
PCONF21	−0.97	5.01	5.57	3.09	16.37	8.95	−7.42
MCONF	−3.03	3.09	3.47	0.62	6.05	0.74	−5.31
SCONF	−0.50	1.03	1.26	0.22	4.65	2.49	−2.16
UPU23	2.18	3.05	4.39	0.53	15.10	12.35	−2.75
BUT14DIOL	−0.73	0.86	0.95	0.31	2.71	0.97	−1.74

Table S110: Statistical analysis for the RPBE DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.86	7.44	9.99	0.02	64.41	29.81	−34.60
G21EA	2.10	2.96	3.55	0.09	10.39	6.37	−4.01
G21IP	−0.94	4.17	5.05	0.02	18.72	9.28	−9.44
DIPCS10	−2.99	5.20	6.35	0.01	18.50	6.73	−11.77
PA26	3.68	3.68	4.54	0.02	9.91	10.17	0.27
SIE4x4	22.83	22.83	25.86	0.68	43.29	48.29	5.00
ALKBDE10	−0.15	5.06	7.36	0.05	26.65	19.96	−6.69
YBDE18	−8.78	9.05	10.87	0.18	23.34	2.19	−21.16
AL2X6	−9.56	9.56	10.06	0.27	8.80	−4.22	−13.02
HEAVYSB11	−7.28	7.28	8.69	0.13	14.43	−0.22	−14.65
NBPRC	4.70	5.44	7.38	0.20	20.08	17.96	−2.12
ALK8	−3.28	3.99	5.67	0.06	15.78	1.82	−13.96
RC21	0.21	2.89	3.75	0.08	15.32	7.08	−8.25
G2RC	4.15	5.27	7.25	0.10	28.28	18.59	−9.69
BH76RC	0.93	2.76	4.43	0.13	22.69	16.63	−6.06
FH51	4.21	5.09	6.65	0.16	30.39	18.09	−12.31
TAUT15	−0.25	1.33	1.51	0.44	4.66	2.16	−2.50
DC13	5.90	15.36	17.29	0.28	56.32	27.48	−28.84
MB16-43	−49.17	51.78	59.38	0.12	172.95	41.46	−131.49
DARC	14.99	14.99	15.52	0.46	11.56	18.62	7.06
RSE43	−2.59	2.59	2.85	0.34	6.02	−0.93	−6.95
BSR36	−11.38	11.38	12.90	0.70	27.10	−1.87	−28.97
CDIE20	1.89	1.90	2.11	0.47	3.78	3.76	−0.02
ISO34	−1.27	2.35	3.43	0.16	18.33	6.86	−11.48
ISOL24	−6.22	10.21	16.13	0.47	86.99	28.77	−58.22
C60ISO	−10.86	10.86	12.95	0.11	20.64	−1.48	−22.11
PArel	0.03	1.46	2.40	0.32	13.67	6.02	−7.65
BH76	−7.05	7.08	8.06	0.38	23.86	1.27	−22.60
BHPERI	0.36	3.07	3.51	0.15	12.93	5.99	−6.94
BHDIV10	−5.36	5.75	6.78	0.13	12.60	1.95	−10.65
INV24	−2.91	3.21	3.78	0.10	11.90	3.61	−8.30
BHROT27	0.08	0.33	0.44	0.05	1.51	1.01	−0.50
PX13	−6.37	6.37	6.45	0.19	4.11	−4.85	−8.96
WCPT18	−4.92	4.92	5.53	0.14	8.38	−0.88	−9.26
RG18	−0.31	0.42	0.59	0.72	1.84	0.37	−1.47
ADIM6	−5.42	5.42	6.02	1.61	7.62	−1.88	−9.51
S22	−4.88	4.88	6.07	0.67	14.99	−0.64	−15.63
S66	−4.03	4.03	4.53	0.74	10.25	−0.73	−10.98
HEAVY28	−1.20	1.20	1.31	0.97	1.99	−0.20	−2.19
WATER27	−15.82	15.84	23.79	0.20	62.83	0.18	−62.64
CARBHB12	−0.53	0.88	1.05	0.15	3.20	1.34	−1.87
PNICO23	−1.74	1.84	2.00	0.43	4.95	1.22	−3.72
HAL59	−1.89	2.03	2.53	0.44	11.59	2.80	−8.79
AHB21	2.14	2.14	2.49	0.10	4.93	5.57	0.64
CHB6	1.40	1.40	1.98	0.05	4.11	4.32	0.21
IL16	5.15	5.15	5.24	0.05	3.93	7.59	3.65
IDISP	4.79	18.03	20.45	1.27	56.71	35.35	−21.36
ICONF	0.04	0.70	1.05	0.21	4.78	3.04	−1.73
ACONF	1.25	1.25	1.38	0.68	1.93	2.41	0.48
AMINO20x4	−0.28	0.84	1.02	0.34	4.62	2.44	−2.18
PCONF21	−0.97	4.79	5.34	2.96	15.98	8.70	−7.28
MCONF	−2.98	3.02	3.40	0.61	5.71	0.56	−5.15
SCONF	−0.68	1.32	1.55	0.29	5.45	2.95	−2.51
UPU23	1.99	2.89	4.10	0.51	14.18	11.50	−2.68
BUT14DIOL	−0.82	0.95	1.04	0.34	2.84	0.99	−1.85

Table S111: Statistical analysis for the PW91 DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	14.28	15.22	18.68	0.05	65.82	53.74	−12.08
G21EA	3.64	3.84	4.56	0.11	9.56	8.22	−1.33
G21IP	1.17	3.90	4.97	0.02	19.55	11.96	−7.59
DIPCS10	0.21	4.19	5.06	0.01	18.25	8.86	−9.39
PA26	1.46	1.92	2.67	0.01	9.11	7.13	−1.98
SIE4x4	23.57	23.57	26.34	0.70	42.56	46.66	4.10
ALKBDE10	7.06	7.08	11.17	0.07	29.22	29.16	−0.07
YBDE18	−2.22	5.86	6.95	0.12	22.87	10.46	−12.41
AL2X6	−3.74	3.87	4.42	0.11	7.05	0.40	−6.65
HEAVYSB11	−1.27	4.48	4.97	0.08	14.65	6.04	−8.62
NBPRC	0.80	2.87	3.41	0.10	10.99	5.61	−5.38
ALK8	0.64	2.50	3.29	0.04	10.59	6.83	−3.75
RC21	4.66	5.49	6.49	0.15	17.15	13.28	−3.87
G2RC	0.75	6.14	7.52	0.12	30.05	18.74	−11.31
BH76RC	0.71	4.08	5.95	0.19	29.65	21.77	−7.89
FH51	1.71	3.39	4.68	0.11	23.10	12.68	−10.41
TAUT15	0.32	1.87	2.42	0.61	7.79	5.31	−2.48
DC13	1.51	10.29	13.29	0.19	47.03	16.26	−30.77
MB16-43	−8.76	20.49	26.97	0.05	116.35	40.29	−76.06
DARC	7.00	7.13	8.00	0.22	11.46	10.56	−0.91
RSE43	−3.08	3.08	3.39	0.41	6.58	−0.97	−7.55
BSR36	−7.76	7.76	8.99	0.48	17.78	−2.18	−19.97
CDIE20	1.75	1.75	1.90	0.43	2.93	3.04	0.10
ISO34	−0.82	1.71	2.47	0.12	12.81	5.99	−6.82
ISOL24	−3.41	6.89	10.59	0.31	57.58	24.23	−33.36
C60ISO	−10.31	10.31	12.34	0.10	20.20	−1.34	−21.55
PArel	0.24	1.83	2.57	0.40	12.83	6.96	−5.87
BH76	−9.55	9.60	10.78	0.52	31.46	1.76	−29.70
BHPERI	−4.23	4.23	4.63	0.20	6.63	−1.57	−8.20
BHDIV10	−7.68	8.22	9.17	0.18	16.94	2.67	−14.26
INV24	−2.77	2.96	3.61	0.09	11.34	2.21	−9.12
BHROT27	0.36	0.49	0.68	0.08	2.16	1.71	−0.45
PX13	−11.94	11.94	12.15	0.36	8.84	−8.73	−17.57
WCPT18	−8.73	8.73	9.16	0.25	10.98	−4.70	−15.67
RG18	0.23	0.39	0.59	0.67	2.60	1.90	−0.70
ADIM6	−3.01	3.01	3.39	0.90	4.51	−0.89	−5.40
S22	−2.10	2.22	3.27	0.30	10.19	0.73	−9.45
S66	−1.68	1.83	2.36	0.33	7.37	0.85	−6.52
HEAVY28	−0.20	0.36	0.44	0.29	1.45	0.42	−1.03
WATER27	4.83	5.76	7.18	0.07	33.73	21.12	−12.61
CARBHB12	1.40	1.40	1.83	0.23	3.80	4.02	0.22
PNICO23	0.33	0.74	1.33	0.17	7.08	5.18	−1.90
HAL59	0.17	1.26	1.87	0.27	11.74	6.38	−5.37
AHB21	−0.95	1.17	1.35	0.05	3.59	0.91	−2.67
CHB6	−0.42	0.99	1.15	0.04	3.25	1.71	−1.54
IL16	0.93	0.99	1.17	0.01	2.97	2.51	−0.46
IDISP	3.23	10.62	12.46	0.75	34.45	23.51	−10.94
ICONF	0.16	0.42	0.65	0.13	2.84	2.19	−0.65
ACONF	0.58	0.58	0.65	0.32	1.05	1.27	0.22
AMINO20x4	0.01	0.50	0.63	0.20	3.14	1.74	−1.39
PCONF21	−0.84	3.41	3.68	2.10	10.36	5.28	−5.08
MCONF	−1.61	1.70	1.94	0.34	4.22	0.87	−3.35
SCONF	0.21	0.42	0.59	0.09	2.58	1.04	−1.54
UPU23	1.35	1.88	2.70	0.33	8.70	7.16	−1.54
BUT14DIOL	0.27	0.30	0.40	0.11	1.44	1.22	−0.22

Table S112: Statistical analysis for the BLYP DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	4.14	7.50	10.58	0.02	60.97	37.70	−23.27
G21EA	1.75	3.28	3.94	0.10	11.89	8.53	−3.37
G21IP	−1.86	4.67	5.56	0.02	23.01	12.28	−10.74
DIPCS10	−5.91	7.90	9.07	0.01	23.53	9.92	−13.61
PA26	1.69	2.44	3.33	0.01	10.48	8.47	−2.00
SIE4x4	24.73	24.73	28.02	0.73	47.97	52.18	4.21
ALKBDE10	4.23	5.73	8.48	0.06	27.42	21.29	−6.13
YBDE18	−10.16	11.13	13.76	0.23	32.46	7.96	−24.50
AL2X6	−12.02	12.02	12.50	0.34	10.82	−6.58	−17.40
HEAVYSB11	−8.03	8.03	9.29	0.14	13.89	−1.95	−15.84
NBPRC	5.74	7.29	9.96	0.26	29.38	24.97	−4.41
ALK8	−8.58	8.58	11.29	0.14	19.82	−1.09	−20.91
RC21	−0.94	4.19	5.85	0.12	25.75	9.00	−16.75
G2RC	5.12	5.99	7.49	0.12	23.00	15.08	−7.92
BH76RC	0.54	3.21	4.36	0.15	18.86	12.00	−6.86
FH51	5.43	6.49	8.39	0.21	45.93	25.40	−20.53
TAUT15	−0.23	1.60	1.86	0.52	5.82	3.19	−2.63
DC13	7.81	21.87	26.01	0.40	81.71	38.12	−43.59
MB16-43	−67.87	67.87	73.16	0.16	122.96	−5.00	−127.96
DARC	23.22	23.22	23.55	0.72	12.28	27.14	14.86
RSE43	−3.12	3.12	3.43	0.41	6.51	−1.03	−7.55
BSR36	−11.59	11.59	13.20	0.72	27.56	−2.60	−30.16
CDIE20	1.61	1.61	1.75	0.40	2.61	2.84	0.24
ISO34	−0.90	3.29	4.63	0.23	23.68	13.06	−10.62
ISOL24	−7.38	13.44	20.50	0.61	110.14	41.89	−68.25
C60ISO	−10.18	10.18	11.96	0.10	18.60	−1.81	−20.41
PArel	−0.43	1.75	2.76	0.38	14.92	6.54	−8.38
BH76	−8.32	8.32	9.44	0.45	23.98	0.35	−23.64
BHPERI	1.97	4.56	5.29	0.22	20.21	8.69	−11.52
BHDIV10	−3.73	5.31	6.19	0.12	15.61	4.98	−10.63
INV24	−2.74	3.07	3.57	0.10	10.46	3.42	−7.03
BHROT27	0.08	0.41	0.53	0.07	1.74	1.26	−0.48
PX13	−6.93	6.93	7.02	0.21	4.62	−5.02	−9.64
WCPT18	−4.07	4.07	4.46	0.12	6.48	−1.18	−7.67
RG18	−1.04	1.04	1.32	1.79	2.80	−0.14	−2.94
ADIM6	−6.07	6.07	6.61	1.81	7.59	−2.47	−10.06
S22	−4.75	4.75	5.94	0.65	14.77	−0.49	−15.26
S66	−4.07	4.07	4.66	0.74	10.33	−0.53	−10.86
HEAVY28	−1.55	1.55	1.65	1.25	2.22	−0.54	−2.76
WATER27	−8.89	9.00	13.80	0.11	38.37	1.12	−37.25
CARBHB12	−0.65	0.90	1.05	0.15	3.05	1.16	−1.88
PNICO23	−2.13	2.13	2.26	0.50	3.17	−1.12	−4.29
HAL59	−1.84	2.03	2.62	0.44	12.83	3.60	−9.23
AHB21	1.81	1.81	2.09	0.08	4.75	5.00	0.25
CHB6	1.44	1.69	2.27	0.06	5.25	4.68	−0.58
IL16	4.86	4.86	4.93	0.04	3.31	6.78	3.47
IDISP	6.12	19.19	22.98	1.35	64.31	44.88	−19.43
ICONF	−0.06	0.69	1.01	0.21	4.88	2.64	−2.24
ACONF	1.08	1.08	1.20	0.59	1.79	2.19	0.40
AMINO20x4	−0.19	0.77	0.97	0.32	4.86	2.51	−2.35
PCONF21	−0.74	4.56	5.09	2.81	14.93	8.13	−6.80
MCONF	−2.92	2.97	3.36	0.60	5.60	0.47	−5.13
SCONF	−0.31	0.61	0.78	0.13	3.12	1.67	−1.45
UPU23	2.21	2.90	4.21	0.51	13.58	11.41	−2.18
BUT14DIOL	−0.18	0.44	0.51	0.16	1.97	1.07	−0.90

Table S113: Statistical analysis for the BP86 DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	12.12	13.14	15.74	0.04	67.67	45.45	−22.22
G21EA	5.04	5.08	5.78	0.15	9.99	9.57	−0.42
G21IP	1.69	4.10	5.04	0.02	19.13	12.00	−7.13
DIPCS10	0.75	4.02	4.60	0.01	14.63	6.95	−7.69
PA26	2.10	2.32	3.14	0.01	9.33	7.90	−1.43
SIE4x4	24.21	24.21	27.50	0.72	47.87	52.14	4.26
ALKBDE10	4.91	5.89	9.41	0.06	28.95	25.88	−3.07
YBDE18	−5.40	6.74	8.49	0.14	22.65	7.01	−15.63
AL2X6	−6.80	6.80	7.29	0.19	7.62	−1.98	−9.60
HEAVYSB11	−4.35	5.35	6.56	0.09	14.44	3.17	−11.27
NBPRC	2.50	3.33	4.68	0.12	13.16	10.63	−2.53
ALK8	−4.33	4.33	5.73	0.07	12.16	−0.71	−12.87
RC21	2.98	3.93	4.83	0.11	14.36	10.58	−3.78
G2RC	2.12	5.06	6.58	0.10	28.27	18.23	−10.04
BH76RC	−0.04	3.50	5.02	0.16	26.65	16.29	−10.36
FH51	2.87	4.07	5.29	0.13	20.77	12.99	−7.78
TAUT15	0.38	1.82	2.37	0.60	7.46	5.15	−2.32
DC13	3.88	12.56	14.19	0.23	45.98	21.71	−24.27
MB16-43	−27.82	31.78	38.88	0.08	133.77	38.22	−95.56
DARC	10.95	10.95	11.67	0.34	11.79	14.45	2.66
RSE43	−2.94	2.94	3.23	0.39	6.34	−1.00	−7.35
BSR36	−8.45	8.45	9.51	0.52	20.24	−1.55	−21.79
CDIE20	1.78	1.78	1.95	0.44	3.13	3.11	−0.02
ISO34	−0.91	1.90	2.76	0.13	14.92	6.97	−7.95
ISOL24	−4.14	8.07	12.63	0.37	69.13	27.82	−41.31
C60ISO	−10.69	10.69	12.61	0.11	19.87	−1.87	−21.74
PArel	0.17	1.81	2.56	0.39	13.01	6.86	−6.15
BH76	−9.10	9.15	10.19	0.49	28.53	1.91	−26.63
BHPERI	−2.42	2.66	3.58	0.13	9.37	1.60	−7.77
BHDIV10	−7.08	7.64	8.56	0.17	16.15	2.82	−13.32
INV24	−2.65	2.87	3.32	0.09	10.59	2.59	−8.00
BHROT27	0.27	0.42	0.59	0.07	1.89	1.46	−0.43
PX13	−11.64	11.64	11.83	0.35	8.71	−8.28	−16.98
WCPT18	−7.67	7.67	8.00	0.22	9.09	−4.50	−13.58
RG18	−1.45	1.45	1.83	2.50	4.13	−0.42	−4.55
ADIM6	−5.73	5.73	6.18	1.71	6.68	−2.52	−9.20
S22	−3.99	3.99	5.06	0.55	12.68	−0.47	−13.15
S66	−3.59	3.59	4.15	0.66	9.25	−0.43	−9.67
HEAVY28	−1.27	1.27	1.35	1.02	1.77	−0.53	−2.30
WATER27	−5.34	5.97	9.39	0.07	28.63	2.43	−26.20
CARBHB12	0.08	0.76	1.11	0.13	3.86	2.59	−1.27
PNICO23	−1.13	1.39	1.58	0.33	6.43	2.87	−3.56
HAL59	−1.22	1.79	2.34	0.39	13.22	4.84	−8.38
AHB21	0.65	0.88	1.13	0.04	3.48	2.71	−0.76
CHB6	2.03	2.03	2.29	0.08	2.97	3.96	0.99
IL16	2.90	2.90	3.00	0.03	3.06	4.78	1.71
IDISP	3.70	13.19	15.45	0.93	44.02	29.03	−14.99
ICONF	0.13	0.48	0.71	0.15	3.23	2.26	−0.97
ACONF	0.77	0.77	0.86	0.42	1.28	1.55	0.28
AMINO20x4	−0.06	0.60	0.77	0.25	3.83	2.06	−1.78
PCONF21	−0.83	4.24	4.64	2.62	12.73	6.98	−5.75
MCONF	−2.26	2.35	2.66	0.47	5.33	0.97	−4.37
SCONF	0.22	0.40	0.56	0.09	2.37	1.12	−1.25
UPU23	1.97	2.60	3.80	0.45	12.45	10.28	−2.17
BUT14DIOL	0.10	0.28	0.37	0.10	1.60	1.12	−0.48

Table S114: Statistical analysis for the BPBE DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	6.24	9.31	12.22	0.03	62.27	41.27	−20.99
G21EA	1.72	2.71	3.28	0.08	10.50	6.72	−3.78
G21IP	−0.71	4.04	4.95	0.02	19.03	9.65	−9.38
DIPCS10	−3.70	4.32	5.70	0.01	13.91	1.69	−12.22
PA26	3.31	3.33	4.08	0.02	9.45	9.26	−0.19
SIE4x4	22.69	22.69	25.50	0.67	41.91	46.90	4.99
ALKBDE10	3.37	5.77	9.48	0.06	31.08	26.99	−4.09
YBDE18	−6.29	7.21	8.94	0.15	22.68	5.38	−17.30
AL2X6	−7.60	7.60	8.16	0.21	8.46	−2.36	−10.82
HEAVYSB11	−4.50	5.50	6.80	0.09	14.66	3.08	−11.57
NBPRC	3.23	3.96	5.46	0.14	15.04	12.53	−2.52
ALK8	−3.42	3.61	5.53	0.06	14.33	0.64	−13.69
RC21	1.99	3.35	4.07	0.09	12.94	9.35	−3.59
G2RC	2.49	5.17	6.82	0.10	29.61	18.91	−10.70
BH76RC	0.79	3.22	5.15	0.15	26.35	19.77	−6.58
FH51	3.19	4.31	5.61	0.14	23.08	14.76	−8.32
TAUT15	0.25	1.77	2.18	0.58	6.80	4.41	−2.39
DC13	4.12	12.55	14.75	0.23	48.83	23.90	−24.92
MB16-43	−29.67	34.57	42.53	0.08	156.26	48.63	−107.63
DARC	11.27	11.27	12.04	0.35	12.31	15.04	2.73
RSE43	−2.92	2.92	3.22	0.38	6.47	−0.95	−7.42
BSR36	−9.46	9.46	10.54	0.58	22.44	−1.14	−23.58
CDIE20	1.93	1.95	2.15	0.48	3.80	3.60	−0.20
ISO34	−1.04	2.00	2.91	0.14	15.79	5.91	−9.88
ISOL24	−4.38	8.18	13.12	0.37	72.01	26.61	−45.39
C60ISO	−10.11	10.11	12.20	0.10	20.14	−1.14	−21.28
PArel	0.25	1.76	2.51	0.38	12.94	6.72	−6.21
BH76	−7.66	7.70	8.77	0.41	27.55	1.56	−26.00
BHPERI	−1.37	2.40	3.26	0.11	10.97	3.31	−7.65
BHDIV10	−6.89	7.32	8.24	0.16	14.10	2.14	−11.96
INV24	−3.06	3.25	3.83	0.10	10.93	2.29	−8.64
BHROT27	0.27	0.42	0.57	0.07	1.89	1.47	−0.42
PX13	−10.51	10.51	10.68	0.32	7.97	−7.33	−15.31
WCPT18	−6.87	6.87	7.19	0.20	8.26	−4.00	−12.25
RG18	−1.62	1.62	2.01	2.79	4.22	−0.42	−4.64
ADIM6	−7.13	7.13	7.71	2.12	8.47	−3.10	−11.56
S22	−5.18	5.18	6.34	0.71	14.89	−1.18	−16.07
S66	−4.68	4.68	5.24	0.86	10.72	−1.17	−11.89
HEAVY28	−1.73	1.73	1.81	1.40	2.09	−0.79	−2.88
WATER27	−13.98	14.12	21.72	0.17	59.22	1.44	−57.78
CARBHB12	−0.54	1.10	1.21	0.18	3.92	1.88	−2.04
PNICO23	−1.86	2.06	2.19	0.48	6.69	2.35	−4.33
HAL59	−2.08	2.34	2.90	0.51	13.62	3.68	−9.95
AHB21	1.48	1.53	1.85	0.07	4.25	3.89	−0.36
CHB6	2.24	2.24	2.55	0.08	3.54	4.68	1.14
IL16	4.25	4.25	4.37	0.04	4.13	6.74	2.61
IDISP	3.67	15.42	17.50	1.08	49.79	30.33	−19.46
ICONF	0.15	0.56	0.81	0.17	3.58	2.45	−1.13
ACONF	1.07	1.07	1.18	0.58	1.61	2.02	0.41
AMINO20x4	−0.12	0.70	0.88	0.29	4.16	2.28	−1.88
PCONF21	−0.96	5.08	5.60	3.14	15.56	8.59	−6.97
MCONF	−2.81	2.90	3.27	0.58	6.27	1.08	−5.20
SCONF	0.00	0.43	0.51	0.09	2.04	1.01	−1.02
UPU23	2.36	3.11	4.57	0.54	15.39	12.79	−2.59
BUT14DIOL	−0.32	0.51	0.59	0.18	2.14	0.96	−1.18

Table S115: Statistical analysis for the OPBE DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	5.19	8.40	10.92	0.03	60.19	33.97	−26.22
G21EA	−0.78	3.10	3.81	0.09	15.81	6.48	−9.32
G21IP	−1.61	4.51	5.31	0.02	16.91	6.80	−10.11
DIPCS10	−3.54	4.99	6.19	0.01	18.00	4.31	−13.69
PA26	6.19	6.21	6.74	0.03	12.45	12.11	−0.34
SIE4x4	22.29	22.29	25.30	0.66	42.04	48.48	6.45
ALKBDE10	−0.67	6.23	9.93	0.06	36.38	27.20	−9.17
YBDE18	−5.81	6.26	7.98	0.13	23.21	3.05	−20.16
AL2X6	−9.91	9.91	10.70	0.28	12.69	−3.78	−16.46
HEAVYSB11	−6.67	8.27	9.61	0.14	19.78	5.34	−14.44
NBPRC	4.39	5.12	6.86	0.18	17.28	12.88	−4.40
ALK8	−3.30	5.55	7.68	0.09	22.69	4.28	−18.41
RC21	3.15	4.29	5.06	0.12	17.01	10.79	−6.23
G2RC	1.46	7.39	9.76	0.14	37.51	23.16	−14.35
BH76RC	0.26	3.17	5.51	0.15	32.20	24.11	−8.09
FH51	2.23	4.01	5.67	0.13	24.92	17.33	−7.60
TAUT15	0.20	1.44	1.69	0.47	5.10	2.85	−2.26
DC13	4.89	18.10	20.90	0.33	66.97	40.50	−26.47
MB16-43	−24.71	42.42	54.04	0.10	230.83	92.60	−138.24
DARC	5.43	6.56	7.45	0.20	14.34	10.46	−3.88
RSE43	−2.98	2.98	3.29	0.39	6.87	−0.87	−7.75
BSR36	−11.51	11.54	12.92	0.71	27.40	0.39	−27.01
CDIE20	2.55	2.62	2.99	0.65	6.33	5.64	−0.70
ISO34	−1.56	3.16	4.51	0.22	21.79	6.15	−15.64
ISOL24	−4.36	8.16	13.23	0.37	66.88	16.32	−50.56
C60ISO	−10.44	10.44	12.74	0.11	21.44	−1.00	−22.44
PArel	0.93	2.05	2.62	0.44	11.12	6.50	−4.62
BH76	−5.07	5.32	6.66	0.29	31.61	3.68	−27.94
BHPERI	1.09	3.66	4.31	0.18	15.74	7.29	−8.45
BHDIV10	−6.84	6.84	8.00	0.15	11.79	−1.16	−12.95
INV24	−2.96	3.07	3.95	0.10	11.97	1.18	−10.79
BHROT27	0.33	0.49	0.64	0.08	2.30	1.52	−0.78
PX13	−8.18	8.18	8.39	0.25	7.51	−5.04	−12.55
WCPT18	−5.74	5.87	6.69	0.17	11.68	1.23	−10.44
RG18	−1.33	1.33	1.61	2.29	3.20	−0.20	−3.40
ADIM6	−9.35	9.35	10.22	2.78	11.97	−3.67	−15.64
S22	−7.72	7.72	9.23	1.06	21.30	−1.55	−22.85
S66	−6.80	6.80	7.40	1.24	14.56	−1.80	−16.37
HEAVY28	−2.60	2.60	2.73	2.10	2.94	−1.13	−4.08
WATER27	−34.99	34.99	52.53	0.43	133.95	−0.93	−134.88
CARBHB12	−1.87	1.97	2.26	0.33	4.40	0.40	−4.01
PNICO23	−3.52	3.70	3.85	0.87	8.34	2.17	−6.17
HAL59	−4.13	4.14	4.63	0.90	13.26	0.18	−13.08
AHB21	3.39	3.48	3.83	0.15	7.88	6.98	−0.91
CHB6	2.56	2.65	3.18	0.10	6.30	6.02	−0.27
IL16	7.45	7.45	7.66	0.07	7.20	11.46	4.25
IDISP	2.74	21.33	23.25	1.50	62.23	29.05	−33.18
ICONF	0.35	0.97	1.42	0.30	6.26	4.36	−1.90
ACONF	2.00	2.00	2.21	1.09	2.82	3.57	0.75
AMINO20x4	−0.33	1.24	1.48	0.51	6.63	3.47	−3.15
PCONF21	−1.28	7.23	8.17	4.46	24.54	13.55	−10.99
MCONF	−4.23	4.31	4.85	0.87	8.39	1.23	−7.16
SCONF	−0.93	2.21	2.66	0.48	9.34	5.44	−3.90
UPU23	2.60	4.02	5.76	0.70	20.84	16.94	−3.90
BUT14DIOL	−1.59	1.72	1.88	0.61	4.41	1.18	−3.23

Table S116: Statistical analysis for the OLYP DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	2.91	5.56	8.06	0.02	55.73	29.87	−25.85
G21EA	−0.96	2.44	3.02	0.07	10.04	3.80	−6.24
G21IP	−3.03	4.32	5.29	0.02	16.65	5.50	−11.15
DIPCS10	−6.16	7.06	8.65	0.01	18.66	3.26	−15.39
PA26	4.58	4.58	5.25	0.02	9.74	11.28	1.54
SIE4x4	24.31	24.31	27.81	0.72	47.94	53.76	5.82
ALKBDE10	0.50	4.75	7.76	0.05	28.35	22.27	−6.07
YBDE18	−9.71	9.99	12.33	0.20	28.06	1.45	−26.61
AL2X6	−14.40	14.40	14.84	0.40	10.43	−8.24	−18.67
HEAVYSB11	−10.16	10.19	11.79	0.18	18.65	0.16	−18.49
NBPRC	6.95	8.12	10.34	0.29	28.70	24.94	−3.76
ALK8	−8.85	8.85	12.05	0.14	23.08	−0.07	−23.15
RC21	−0.21	2.83	3.83	0.08	17.64	7.77	−9.87
G2RC	4.19	5.37	7.21	0.10	29.53	19.22	−10.31
BH76RC	0.03	3.01	4.37	0.14	24.45	16.16	−8.29
FH51	4.52	5.79	7.74	0.19	40.55	23.99	−16.56
TAUT15	−0.29	1.30	1.46	0.43	4.50	1.97	−2.52
DC13	8.73	15.92	18.98	0.29	62.81	35.22	−27.58
MB16-43	−63.90	65.88	73.22	0.16	176.05	37.58	−138.47
DARC	17.86	17.86	18.46	0.55	13.40	22.04	8.64
RSE43	−3.15	3.15	3.45	0.41	6.67	−1.18	−7.85
BSR36	−13.43	13.43	15.10	0.83	31.87	−1.11	−32.98
CDIE20	2.22	2.25	2.53	0.55	5.07	4.81	−0.26
ISO34	−1.39	2.59	4.01	0.18	23.25	7.11	−16.14
ISOL24	−7.33	11.74	19.21	0.54	102.85	29.71	−73.14
C60ISO	−9.86	9.86	11.95	0.10	19.88	−0.99	−20.87
PArel	0.25	1.42	2.33	0.31	13.09	6.32	−6.76
BH76	−5.84	5.92	7.05	0.32	25.06	2.36	−22.70
BHPERI	4.45	6.32	6.80	0.30	17.30	12.50	−4.80
BHDIV10	−3.59	4.60	5.54	0.10	12.32	1.90	−10.42
INV24	−3.03	3.22	3.89	0.10	11.57	2.27	−9.30
BHROT27	0.16	0.40	0.53	0.06	2.01	1.34	−0.67
PX13	−4.58	4.58	4.69	0.14	4.02	−2.74	−6.76
WCPT18	−2.87	3.77	4.31	0.11	10.19	2.73	−7.46
RG18	−0.86	0.86	1.17	1.48	2.67	0.01	−2.66
ADIM6	−8.52	8.52	9.36	2.54	11.32	−3.18	−14.50
S22	−7.32	7.32	8.83	1.00	20.64	−1.28	−21.93
S66	−6.26	6.26	6.88	1.14	13.93	−1.50	−15.42
HEAVY28	−2.46	2.46	2.60	1.98	3.08	−0.94	−4.01
WATER27	−30.19	30.19	44.91	0.37	113.76	−1.26	−115.03
CARBHB12	−1.99	1.99	2.27	0.33	3.58	−0.34	−3.92
PNICO23	−3.78	3.78	3.97	0.89	4.85	−1.74	−6.58
HAL59	−3.90	3.91	4.40	0.85	12.61	0.18	−12.44
AHB21	3.71	3.71	3.94	0.16	4.46	6.46	2.00
CHB6	1.77	1.83	2.74	0.07	6.18	6.01	−0.17
IL16	8.02	8.02	8.15	0.07	5.66	11.41	5.74
IDISP	5.31	24.73	27.38	1.74	74.83	42.55	−32.28
ICONF	0.14	1.00	1.49	0.31	6.93	4.34	−2.58
ACONF	1.98	1.98	2.19	1.08	2.87	3.63	0.75
AMINO20x4	−0.39	1.27	1.55	0.52	7.24	3.77	−3.47
PCONF21	−1.03	6.66	7.62	4.11	23.59	12.92	−10.67
MCONF	−4.30	4.34	4.90	0.87	7.72	0.66	−7.06
SCONF	−1.16	2.49	2.89	0.54	9.88	5.75	−4.13
UPU23	2.58	3.86	5.53	0.67	19.49	16.01	−3.48
BUT14DIOL	−1.40	1.56	1.71	0.56	4.25	1.34	−2.91

Table S117: Statistical analysis for the XLYP DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	3.06	7.04	9.85	0.02	59.57	35.10	−24.48
G21EA	2.63	3.62	4.52	0.11	12.48	9.68	−2.81
G21IP	−1.04	4.51	5.53	0.02	23.97	14.09	−9.88
DIPCS10	−3.73	7.15	8.24	0.01	24.78	13.24	−11.54
PA26	1.83	2.60	3.53	0.01	10.91	8.82	−2.09
SIE4x4	24.78	24.78	28.10	0.73	48.13	52.29	4.16
ALKBDE10	4.23	5.93	8.40	0.06	27.32	20.86	−6.47
YBDE18	−10.71	11.58	14.20	0.23	32.93	7.69	−25.24
AL2X6	−12.18	12.18	12.67	0.34	10.88	−6.79	−17.67
HEAVYSB11	−8.51	8.51	9.64	0.15	13.67	−2.65	−16.32
NBPRC	5.96	7.65	10.42	0.28	30.80	26.13	−4.68
ALK8	−8.40	8.40	11.23	0.13	19.93	−1.39	−21.31
RC21	−1.81	4.01	5.99	0.11	26.39	7.96	−18.43
G2RC	5.42	6.37	7.85	0.12	22.03	14.52	−7.51
BH76RC	0.56	3.25	4.31	0.15	17.52	10.75	−6.78
FH51	5.65	6.74	8.68	0.22	47.68	25.86	−21.82
TAUT15	−0.37	1.53	1.77	0.50	5.40	2.69	−2.70
DC13	8.07	23.38	27.84	0.43	90.00	41.92	−48.08
MB16-43	−72.17	72.17	77.26	0.17	118.75	−13.28	−132.04
DARC	24.45	24.45	24.75	0.75	12.17	28.40	16.23
RSE43	−3.02	3.02	3.33	0.40	6.43	−0.95	−7.38
BSR36	−12.14	12.14	13.92	0.75	28.73	−3.05	−31.78
CDIE20	1.56	1.56	1.69	0.38	2.40	2.74	0.33
ISO34	−0.91	3.53	4.96	0.24	24.79	13.93	−10.87
ISOL24	−7.81	14.12	21.45	0.64	114.71	43.47	−71.24
C60ISO	−9.74	9.74	11.63	0.10	18.69	−1.22	−19.91
PArel	−0.53	1.83	2.83	0.40	15.17	6.39	−8.78
BH76	−8.46	8.46	9.58	0.45	23.77	0.28	−23.49
BHPERI	2.25	4.71	5.55	0.23	21.11	9.06	−12.05
BHDIV10	−3.25	5.08	5.98	0.11	15.72	5.28	−10.44
INV24	−3.07	3.38	3.99	0.11	12.55	3.73	−8.82
BHROT27	0.04	0.41	0.52	0.07	1.79	1.19	−0.61
PX13	−5.93	5.93	6.01	0.18	3.78	−4.37	−8.16
WCPT18	−3.55	3.55	3.99	0.10	6.34	−0.62	−6.96
RG18	−0.56	0.57	0.83	0.98	2.14	0.10	−2.04
ADIM6	−5.31	5.31	5.84	1.58	7.13	−1.99	−9.12
S22	−4.38	4.38	5.57	0.60	14.33	−0.22	−14.55
S66	−3.62	3.62	4.21	0.66	9.88	−0.28	−10.17
HEAVY28	−1.28	1.28	1.39	1.03	2.14	−0.30	−2.44
WATER27	−7.44	7.54	11.47	0.09	32.46	1.08	−31.37
CARBHB12	−0.45	0.71	0.92	0.12	3.08	1.24	−1.84
PNICO23	−1.89	1.89	2.04	0.44	3.14	−0.76	−3.90
HAL59	−1.56	1.77	2.37	0.39	12.26	3.72	−8.54
AHB21	1.67	1.67	1.99	0.07	4.94	5.08	0.14
CHB6	0.98	1.58	2.05	0.06	5.42	4.35	−1.07
IL16	4.71	4.71	4.77	0.04	3.22	6.55	3.34
IDISP	6.55	19.50	23.49	1.37	64.88	46.32	−18.57
ICONF	−0.10	0.70	1.05	0.21	5.08	2.68	−2.40
ACONF	1.09	1.09	1.21	0.60	1.80	2.22	0.42
AMINO20x4	−0.21	0.76	0.98	0.31	4.94	2.50	−2.44
PCONF21	−0.73	4.34	4.85	2.68	14.37	7.77	−6.60
MCONF	−2.86	2.90	3.27	0.58	5.25	0.30	−4.96
SCONF	−0.45	0.77	0.95	0.17	3.61	1.90	−1.71
UPU23	2.14	2.79	4.01	0.49	12.88	10.86	−2.02
BUT14DIOL	−0.23	0.47	0.54	0.17	2.08	1.09	−0.98

Table S118: Statistical analysis for the mPWLYP DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	8.03	9.42	12.65	0.03	62.81	43.65	−19.17
G21EA	2.72	3.60	4.51	0.11	12.47	9.80	−2.68
G21IP	−1.17	4.53	5.49	0.02	23.47	13.40	−10.07
DIPCS10	−4.22	7.41	8.59	0.01	25.94	13.44	−12.50
PA26	0.83	2.25	2.90	0.01	10.22	7.44	−2.78
SIE4x4	25.12	25.12	28.36	0.74	48.09	51.91	3.82
ALKBDE10	6.07	7.11	9.66	0.07	27.89	23.18	−4.71
YBDE18	−8.19	9.73	12.43	0.20	33.06	10.24	−22.82
AL2X6	−10.13	10.13	10.60	0.28	9.67	−5.21	−14.87
HEAVYSB11	−6.40	6.40	7.86	0.11	13.93	−0.42	−14.35
NBPRC	4.57	6.05	8.43	0.22	24.20	21.04	−3.17
ALK8	−6.72	6.72	9.25	0.11	17.33	−1.32	−18.65
RC21	0.11	4.00	5.21	0.11	21.72	7.13	−14.59
G2RC	4.28	5.36	6.75	0.10	23.07	15.12	−7.95
BH76RC	0.52	3.19	4.52	0.15	20.65	13.16	−7.49
FH51	4.72	5.81	7.47	0.19	39.19	21.21	−17.98
TAUT15	−0.19	1.65	1.94	0.54	6.24	3.60	−2.65
DC13	6.52	20.65	24.39	0.38	79.41	37.64	−41.77
MB16-43	−57.30	57.30	62.74	0.14	109.81	−4.49	−114.30
DARC	20.99	20.99	21.31	0.65	11.76	24.68	12.91
RSE43	−3.18	3.18	3.50	0.42	6.53	−1.06	−7.60
BSR36	−10.92	10.92	12.68	0.67	25.86	−3.11	−28.97
CDIE20	1.54	1.54	1.65	0.38	2.26	2.62	0.36
ISO34	−0.83	3.18	4.47	0.22	22.96	12.93	−10.04
ISOL24	−6.87	12.72	19.24	0.58	103.24	40.52	−62.72
C60ISO	−9.80	9.80	11.73	0.10	18.94	−1.20	−20.14
PArel	−0.41	1.74	2.75	0.38	14.80	6.63	−8.17
BH76	−9.35	9.36	10.48	0.50	25.76	0.41	−25.34
BHPERI	0.54	3.63	4.33	0.17	17.92	6.34	−11.59
BHDIV10	−4.19	5.69	6.52	0.13	15.77	5.13	−10.64
INV24	−3.00	3.28	3.89	0.10	12.46	3.38	−9.08
BHROT27	0.12	0.42	0.56	0.07	1.80	1.36	−0.44
PX13	−7.72	7.72	7.82	0.23	5.21	−5.74	−10.95
WCPT18	−5.03	5.03	5.41	0.14	7.65	−1.83	−9.48
RG18	−0.06	0.46	0.59	0.79	2.39	1.22	−1.18
ADIM6	−4.13	4.13	4.60	1.23	5.93	−1.38	−7.31
S22	−3.32	3.36	4.51	0.46	12.73	0.45	−12.28
S66	−2.65	2.68	3.29	0.49	8.78	0.37	−8.41
HEAVY28	−0.81	0.81	0.94	0.65	1.90	0.00	−1.90
WATER27	−0.49	2.31	3.16	0.03	13.54	4.77	−8.77
CARBHB12	0.29	0.61	0.85	0.10	2.97	2.20	−0.77
PNICO23	−1.07	1.07	1.28	0.25	3.13	0.01	−3.12
HAL59	−0.77	1.30	1.92	0.28	11.98	4.88	−7.10
AHB21	0.67	0.79	1.18	0.04	4.62	3.79	−0.83
CHB6	0.07	1.27	1.68	0.05	5.13	3.28	−1.85
IL16	3.34	3.34	3.40	0.03	2.77	4.86	2.10
IDISP	5.96	17.00	20.71	1.20	56.74	41.48	−15.26
ICONF	−0.05	0.61	0.91	0.19	4.51	2.51	−2.00
ACONF	0.91	0.91	1.01	0.50	1.54	1.90	0.35
AMINO20x4	−0.13	0.67	0.84	0.27	4.22	2.21	−2.01
PCONF21	−0.72	3.86	4.26	2.38	12.25	6.65	−5.60
MCONF	−2.40	2.45	2.77	0.49	4.74	0.41	−4.32
SCONF	−0.23	0.45	0.57	0.10	2.30	1.20	−1.09
UPU23	1.84	2.41	3.45	0.42	10.85	9.20	−1.65
BUT14DIOL	0.07	0.29	0.40	0.10	1.58	1.04	−0.54

Table S119: Statistical analysis for the PW91P86 DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	20.61	20.72	24.14	0.07	62.69	59.14	−3.56
G21EA	7.00	7.00	7.55	0.21	10.21	11.78	1.58
G21IP	3.02	4.67	5.64	0.02	19.87	13.91	−5.96
DIPCS10	3.65	5.45	6.53	0.01	20.21	13.93	−6.28
PA26	0.10	1.60	2.19	0.01	8.99	5.48	−3.51
SIE4x4	24.94	24.94	28.09	0.74	47.78	51.23	3.45
ALKBDE10	8.63	8.63	11.81	0.09	28.98	29.13	0.15
YBDE18	−0.96	5.82	6.85	0.12	24.19	12.20	−12.00
AL2X6	−2.69	3.03	3.35	0.08	5.77	1.02	−4.75
HEAVYSB11	−0.59	4.28	4.75	0.07	14.58	6.67	−7.91
NBPRC	−0.10	2.77	3.27	0.10	10.90	5.13	−5.77
ALK8	−0.13	1.98	2.33	0.03	6.37	4.00	−2.37
RC21	5.76	6.42	7.44	0.18	18.99	15.00	−4.00
G2RC	0.29	6.51	7.84	0.13	31.63	18.37	−13.26
BH76RC	−0.04	3.88	5.73	0.18	30.65	19.13	−11.52
FH51	1.27	3.35	4.72	0.11	24.31	12.85	−11.47
TAUT15	0.49	1.92	2.67	0.63	8.81	6.14	−2.66
DC13	1.05	9.46	12.35	0.17	43.33	14.09	−29.23
MB16-43	−4.25	18.99	25.12	0.05	114.38	47.90	−66.48
DARC	5.82	6.07	6.85	0.19	10.92	9.13	−1.79
RSE43	−3.12	3.12	3.42	0.41	6.50	−1.01	−7.52
BSR36	−6.61	6.61	7.99	0.41	18.03	−1.97	−19.99
CDIE20	1.61	1.61	1.73	0.40	2.38	2.62	0.25
ISO34	−0.74	1.61	2.36	0.11	13.45	6.48	−6.97
ISOL24	−2.93	6.53	9.75	0.30	52.38	24.29	−28.09
C60ISO	−10.35	10.35	12.48	0.11	20.44	−1.20	−21.63
PArel	0.22	1.92	2.64	0.41	12.73	7.09	−5.64
BH76	−11.17	11.22	12.34	0.60	32.99	2.02	−30.97
BHPERI	−5.61	5.61	5.89	0.27	6.68	−3.11	−9.79
BHDIV10	−8.20	8.82	9.81	0.19	19.11	3.07	−16.04
INV24	−2.69	2.89	3.59	0.09	11.88	2.48	−9.40
BHROT27	0.36	0.48	0.68	0.08	2.20	1.67	−0.53
PX13	−13.52	13.52	13.75	0.41	10.06	−9.98	−20.04
WCPT18	−9.85	9.85	10.42	0.28	12.45	−5.12	−17.57
RG18	0.41	0.45	0.65	0.78	2.41	2.09	−0.33
ADIM6	−1.55	1.55	1.83	0.46	2.84	−0.28	−3.13
S22	−0.95	1.54	2.28	0.21	8.64	2.04	−6.61
S66	−0.61	1.29	1.56	0.24	6.50	2.14	−4.36
HEAVY28	0.25	0.34	0.45	0.27	1.49	1.01	−0.48
WATER27	12.82	13.77	18.44	0.17	59.57	46.75	−12.82
CARBHB12	2.01	2.01	2.38	0.33	4.11	4.73	0.63
PNICO23	1.08	1.20	1.72	0.28	7.09	5.96	−1.13
HAL59	1.01	1.47	2.19	0.32	11.40	7.53	−3.87
AHB21	−1.70	1.72	1.88	0.08	3.32	0.28	−3.04
CHB6	−0.64	1.00	1.05	0.04	2.41	1.07	−1.34
IL16	−0.36	0.48	0.56	0.00	1.84	0.59	−1.25
IDISP	3.21	8.13	10.21	0.57	28.33	21.18	−7.15
ICONF	0.17	0.36	0.57	0.11	2.36	1.95	−0.41
ACONF	0.36	0.36	0.41	0.20	0.73	0.86	0.14
AMINO20x4	0.08	0.48	0.61	0.20	2.74	1.42	−1.32
PCONF21	−0.77	2.66	2.88	1.64	8.31	3.73	−4.58
MCONF	−1.08	1.21	1.39	0.24	3.51	0.94	−2.57
SCONF	0.42	0.83	0.98	0.18	3.83	1.35	−2.48
UPU23	1.09	1.45	2.06	0.25	6.20	5.14	−1.06
BUT14DIOL	0.65	0.65	0.69	0.23	1.53	1.46	−0.07

Table S120: Statistical analysis for the mPWPW91 DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	9.86	11.50	14.60	0.04	62.28	46.38	−15.90
G21EA	3.07	3.43	4.13	0.10	9.88	7.69	−2.19
G21IP	0.53	3.92	4.89	0.02	19.23	11.18	−8.05
DIPCS10	−1.10	3.76	4.69	0.01	15.38	5.50	−9.88
PA26	2.55	2.64	3.44	0.01	9.28	8.44	−0.84
SIE4x4	23.21	23.21	26.02	0.69	42.50	47.08	4.58
ALKBDE10	5.37	6.20	10.27	0.06	29.92	28.31	−1.62
YBDE18	−4.63	6.39	7.99	0.13	23.08	7.75	−15.33
AL2X6	−5.92	5.92	6.50	0.16	7.64	−1.19	−8.83
HEAVYSB11	−3.16	4.85	5.83	0.08	14.52	4.14	−10.38
NBPRC	2.21	3.23	4.40	0.12	13.10	9.53	−3.57
ALK8	−1.61	2.87	3.83	0.05	12.38	3.31	−9.07
RC21	3.04	4.14	4.94	0.12	14.65	10.89	−3.76
G2RC	1.80	5.42	6.82	0.11	29.18	18.58	−10.59
BH76RC	0.72	3.47	5.38	0.16	27.37	20.11	−7.27
FH51	2.62	3.89	5.12	0.13	21.01	12.62	−8.38
TAUT15	0.24	1.81	2.26	0.59	7.15	4.72	−2.43
DC13	3.00	12.03	14.18	0.22	47.11	20.81	−26.31
MB16-43	−21.25	27.07	34.41	0.07	133.93	41.80	−92.12
DARC	9.93	9.93	10.72	0.31	11.88	13.55	1.67
RSE43	−2.97	2.97	3.27	0.39	6.46	−0.97	−7.43
BSR36	−8.92	8.92	10.09	0.55	21.12	−1.78	−22.90
CDIE20	1.83	1.84	2.02	0.45	3.36	3.32	−0.04
ISO34	−0.94	1.90	2.75	0.13	14.94	6.41	−8.53
ISOL24	−4.09	7.80	12.32	0.36	67.44	26.31	−41.14
C60ISO	−10.04	10.04	12.14	0.10	20.03	−1.12	−21.15
PArel	0.21	1.75	2.52	0.38	13.00	6.82	−6.19
BH76	−8.54	8.58	9.68	0.46	28.94	1.70	−27.24
BHPERI	−2.54	2.68	3.52	0.13	8.94	1.30	−7.64
BHDIV10	−7.05	7.56	8.48	0.17	15.35	2.57	−12.78
INV24	−2.92	3.11	3.71	0.10	11.09	2.25	−8.84
BHROT27	0.30	0.44	0.61	0.07	1.94	1.58	−0.36
PX13	−10.83	10.83	11.01	0.32	8.10	−7.73	−15.82
WCPT18	−7.50	7.50	7.84	0.21	9.22	−4.30	−13.52
RG18	−0.64	0.64	0.85	1.10	1.98	−0.04	−2.03
ADIM6	−5.08	5.08	5.56	1.51	6.57	−1.98	−8.55
S22	−3.67	3.67	4.79	0.50	12.63	−0.21	−12.84
S66	−3.19	3.19	3.77	0.58	9.10	−0.16	−9.26
HEAVY28	−0.95	0.95	1.05	0.77	1.72	−0.23	−1.95
WATER27	−4.97	5.62	8.99	0.07	28.38	2.51	−25.87
CARBHB12	0.41	0.74	1.16	0.12	3.77	2.87	−0.91
PNICO23	−0.79	1.16	1.40	0.27	6.64	3.53	−3.12
HAL59	−0.96	1.59	2.14	0.35	12.64	4.96	−7.67
AHB21	0.34	0.80	1.07	0.04	3.76	2.43	−1.33
CHB6	0.90	0.95	1.48	0.04	3.44	3.28	−0.16
IL16	2.70	2.70	2.83	0.02	3.54	4.74	1.20
IDISP	3.64	13.35	15.35	0.94	43.06	27.87	−15.20
ICONF	0.14	0.48	0.72	0.15	3.28	2.30	−0.98
ACONF	0.85	0.85	0.94	0.46	1.33	1.66	0.33
AMINO20x4	−0.06	0.60	0.76	0.25	3.63	1.98	−1.65
PCONF21	−0.90	4.27	4.66	2.64	12.75	7.00	−5.76
MCONF	−2.25	2.33	2.64	0.47	5.23	0.91	−4.32
SCONF	0.07	0.38	0.44	0.08	1.61	0.82	−0.79
UPU23	1.94	2.54	3.70	0.44	12.21	10.20	−2.01
BUT14DIOL	−0.05	0.32	0.40	0.11	1.78	1.04	−0.73

Table S121: Statistical analysis for the rPW86PBE DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	4.89	8.85	11.89	0.03	61.29	37.44	−23.85
G21EA	5.40	5.40	6.28	0.16	11.47	11.65	0.18
G21IP	2.57	4.53	6.09	0.02	25.86	19.40	−6.46
DIPCS10	3.46	4.59	6.23	0.01	18.77	14.91	−3.86
PA26	2.65	2.74	3.69	0.01	9.57	9.09	−0.49
SIE4x4	23.05	23.05	25.88	0.68	42.30	46.57	4.27
ALKBDE10	4.40	6.57	9.19	0.07	28.25	23.10	−5.15
YBDE18	−7.04	8.18	10.20	0.17	27.31	8.18	−19.13
AL2X6	−7.37	7.37	7.85	0.21	8.31	−2.64	−10.95
HEAVYSB11	−4.79	4.89	6.34	0.08	12.32	0.54	−11.78
NBPRC	3.41	4.54	6.60	0.16	18.52	16.55	−1.97
ALK8	−2.11	2.75	3.74	0.04	11.61	2.56	−9.05
RC21	0.49	3.38	4.26	0.09	16.80	6.51	−10.29
G2RC	3.54	4.70	6.36	0.09	27.01	17.07	−9.95
BH76RC	1.10	3.05	4.78	0.14	21.89	16.12	−5.77
FH51	3.89	4.98	6.43	0.16	30.27	16.67	−13.59
TAUT15	−0.26	1.71	1.97	0.56	6.26	3.41	−2.85
DC13	5.07	18.82	20.95	0.34	61.04	28.10	−32.94
MB16-43	−42.04	43.06	48.16	0.10	113.67	17.08	−96.59
DARC	16.88	16.88	17.29	0.52	11.53	20.28	8.75
RSE43	−2.73	2.73	3.03	0.36	6.03	−1.03	−7.05
BSR36	−9.93	9.93	11.50	0.61	23.36	−3.08	−26.45
CDIE20	1.68	1.68	1.82	0.41	2.72	2.92	0.20
ISO34	−0.90	2.66	3.78	0.18	20.58	11.33	−9.26
ISOL24	−5.99	10.98	16.35	0.50	86.47	34.39	−52.08
C60ISO	−9.69	9.69	11.65	0.10	18.98	−1.15	−20.13
PArel	−0.25	1.56	2.59	0.34	14.65	6.40	−8.25
BH76	−8.38	8.40	9.53	0.45	24.80	0.94	−23.86
BHPERI	−0.83	2.57	3.15	0.12	11.66	3.58	−8.08
BHDIV10	−4.96	5.93	6.94	0.13	15.18	4.64	−10.54
INV24	−2.76	3.02	3.63	0.09	11.76	3.08	−8.67
BHROT27	0.21	0.42	0.58	0.07	1.95	1.45	−0.50
PX13	−7.01	7.01	7.07	0.21	3.78	−5.43	−9.21
WCPT18	−5.20	5.20	5.62	0.15	8.02	−2.01	−10.03
RG18	−0.48	0.50	0.67	0.86	1.71	0.10	−1.61
ADIM6	−3.53	3.53	3.88	1.05	4.73	−1.36	−6.08
S22	−2.79	2.81	3.76	0.38	10.53	0.27	−10.26
S66	−2.26	2.28	2.79	0.42	7.53	0.26	−7.27
HEAVY28	−0.51	0.51	0.62	0.41	1.42	0.10	−1.32
WATER27	0.01	1.67	2.29	0.02	11.45	4.21	−7.24
CARBHB12	0.65	0.70	1.07	0.12	3.05	2.71	−0.33
PNICO23	−0.45	0.70	0.90	0.16	4.31	1.89	−2.42
HAL59	−0.31	1.22	1.74	0.27	11.49	5.31	−6.18
AHB21	0.26	0.66	1.02	0.03	4.59	3.57	−1.02
CHB6	0.95	1.13	1.52	0.04	3.41	3.11	−0.30
IL16	2.27	2.27	2.35	0.02	2.48	3.69	1.22
IDISP	5.31	13.58	16.98	0.95	46.24	35.10	−11.14
ICONF	−0.03	0.51	0.76	0.16	3.63	2.12	−1.51
ACONF	0.60	0.60	0.68	0.33	1.11	1.35	0.24
AMINO20x4	−0.09	0.52	0.65	0.21	3.06	1.65	−1.41
PCONF21	−0.62	3.20	3.48	1.98	9.64	5.32	−4.32
MCONF	−1.83	1.90	2.15	0.38	4.21	0.61	−3.60
SCONF	−0.09	0.30	0.39	0.07	1.62	0.56	−1.06
UPU23	1.71	2.13	3.06	0.37	9.45	7.87	−1.58
BUT14DIOL	0.09	0.23	0.32	0.08	1.41	0.97	−0.44

Table S122: Statistical analysis for the B97-D DFA (no dispersion correction) for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	0.08	4.24	6.71	0.01	59.99	24.60	−35.39
G21EA	0.89	2.35	2.98	0.07	12.56	8.73	−3.83
G21IP	−1.25	3.47	4.48	0.01	17.34	8.49	−8.85
DIPCS10	−4.65	5.04	6.30	0.01	11.91	1.30	−10.62
PA26	4.90	4.90	5.56	0.03	9.72	11.48	1.76
SIE4x4	23.78	23.78	26.71	0.71	43.69	50.71	7.02
ALKBDE10	2.50	5.05	7.77	0.05	28.12	20.65	−7.46
YBDE18	−10.24	10.48	12.42	0.21	25.79	2.12	−23.68
AL2X6	−12.52	12.52	12.98	0.35	10.82	−6.89	−17.70
HEAVYSB11	−9.06	9.06	10.05	0.16	14.14	−3.23	−17.37
NBPRC	6.49	7.82	10.38	0.28	30.51	26.06	−4.45
ALK8	−8.93	8.93	11.70	0.14	22.39	−0.37	−22.76
RC21	−1.49	3.24	4.87	0.09	21.14	5.79	−15.35
G2RC	4.57	5.57	6.95	0.11	26.45	17.34	−9.12
BH76RC	−0.15	3.05	4.12	0.14	20.66	13.35	−7.30
FH51	4.80	6.03	7.98	0.19	46.17	26.07	−20.10
TAUT15	−0.10	1.47	1.68	0.48	5.36	2.99	−2.37
DC13	10.00	20.74	23.81	0.38	76.73	41.13	−35.59
MB16-43	−73.21	73.22	78.71	0.18	135.97	0.14	−135.82
DARC	22.18	22.18	22.60	0.68	13.26	26.23	12.97
RSE43	−3.35	3.35	3.62	0.44	6.04	−1.70	−7.74
BSR36	−12.32	12.32	13.91	0.76	28.86	−2.45	−31.31
CDIE20	1.96	1.96	2.18	0.48	3.89	3.84	−0.05
ISO34	−1.05	2.95	4.25	0.20	24.48	12.34	−12.14
ISOL24	−7.78	13.07	20.42	0.60	109.07	38.05	−71.03
C60ISO	−9.60	9.60	11.41	0.10	18.40	−1.46	−19.85
PArel	−0.04	1.48	2.47	0.32	14.05	6.69	−7.36
BH76	−5.83	6.04	6.95	0.32	21.19	3.62	−17.57
BHPERI	2.93	5.00	5.45	0.24	16.80	9.45	−7.35
BHDIV10	−3.14	4.87	5.66	0.11	14.66	3.98	−10.68
INV24	−2.74	2.94	3.39	0.09	10.56	2.50	−8.06
BHROT27	0.19	0.34	0.52	0.05	1.78	1.33	−0.45
PX13	−6.17	6.17	6.31	0.18	5.36	−3.74	−9.10
WCPT18	−3.28	3.29	3.82	0.09	6.53	0.05	−6.48
RG18	−0.87	0.87	1.08	1.50	2.14	−0.13	−2.27
ADIM6	−6.35	6.35	6.96	1.89	8.28	−2.45	−10.73
S22	−5.23	5.23	6.43	0.72	15.56	−1.00	−16.56
S66	−4.51	4.51	5.03	0.82	10.67	−1.10	−11.78
HEAVY28	−1.40	1.40	1.48	1.13	1.99	−0.32	−2.32
WATER27	−17.22	17.23	26.18	0.21	68.83	0.23	−68.60
CARBHB12	−0.85	1.06	1.24	0.18	3.20	0.94	−2.26
PNICO23	−2.20	2.20	2.33	0.52	2.91	−1.26	−4.17
HAL59	−2.21	2.31	2.79	0.50	11.71	2.19	−9.52
AHB21	2.06	2.06	2.26	0.09	3.11	4.02	0.91
CHB6	2.79	2.79	3.16	0.10	4.14	5.40	1.26
IL16	5.45	5.45	5.54	0.05	4.03	8.10	4.07
IDISP	6.05	20.51	23.86	1.44	66.61	43.94	−22.67
ICONF	0.04	0.75	1.14	0.23	5.47	3.04	−2.43
ACONF	1.30	1.30	1.45	0.71	2.03	2.50	0.48
AMINO20x4	−0.29	0.90	1.11	0.37	5.22	2.69	−2.52
PCONF21	−0.89	5.08	5.70	3.14	17.01	9.40	−7.61
MCONF	−3.15	3.18	3.59	0.64	5.90	0.57	−5.33
SCONF	−0.68	1.30	1.53	0.28	5.53	3.05	−2.48
UPU23	2.24	3.06	4.42	0.53	14.64	12.14	−2.50
BUT14DIOL	−0.72	0.88	0.97	0.31	2.86	1.14	−1.72

Table S123: Statistical analysis for the HCTH/407 DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	0.80	5.52	7.53	0.02	49.45	30.05	−19.40
G21EA	4.51	4.82	5.82	0.14	12.16	10.64	−1.51
G21IP	3.26	4.81	5.91	0.02	19.06	13.99	−5.07
DIPCS10	5.78	6.38	7.52	0.01	16.42	13.42	−3.00
PA26	4.40	4.40	4.91	0.02	8.57	10.35	1.78
SIE4x4	23.51	23.51	26.43	0.70	42.73	49.34	6.61
ALKBDE10	3.12	4.85	7.87	0.05	29.06	21.57	−7.50
YBDE18	−8.17	8.28	10.07	0.17	23.73	1.06	−22.68
AL2X6	−11.97	11.97	12.38	0.33	9.23	−6.63	−15.86
HEAVYSB11	−8.85	8.85	10.18	0.15	15.48	−0.17	−15.65
NBPRC	5.59	6.28	8.68	0.23	24.26	21.87	−2.39
ALK8	−4.72	5.14	7.45	0.08	19.36	1.66	−17.69
RC21	0.60	2.64	3.58	0.07	16.29	8.64	−7.65
G2RC	2.37	4.39	6.35	0.09	32.58	20.64	−11.94
BH76RC	−0.01	2.66	4.71	0.12	27.65	20.90	−6.75
FH51	2.97	4.84	6.50	0.16	33.92	19.05	−14.88
TAUT15	−0.35	1.49	1.71	0.49	5.22	2.47	−2.76
DC13	8.93	16.83	19.03	0.31	54.49	33.56	−20.93
MB16-43	−52.35	54.32	60.55	0.13	144.33	29.62	−114.71
DARC	16.53	16.53	17.17	0.51	14.02	20.77	6.75
RSE43	−3.32	3.32	3.59	0.44	6.58	−1.51	−8.10
BSR36	−12.13	12.13	13.91	0.75	27.74	−2.47	−30.20
CDIE20	2.33	2.35	2.65	0.58	5.29	5.03	−0.26
ISO34	−1.24	2.80	4.02	0.19	23.38	9.75	−13.63
ISOL24	−7.63	11.81	18.67	0.54	97.05	28.24	−68.81
C60ISO	−9.06	9.06	11.05	0.09	18.83	−0.85	−19.68
PArel	0.34	1.42	2.42	0.31	13.47	6.89	−6.58
BH76	−5.30	5.45	6.63	0.29	27.75	3.97	−23.77
BHPERI	3.88	5.16	5.70	0.25	15.19	9.93	−5.26
BHDIV10	−2.69	4.35	5.08	0.10	12.40	3.22	−9.18
INV24	−2.76	2.81	3.72	0.09	10.67	0.70	−9.97
BHROT27	0.42	0.51	0.74	0.08	2.47	1.99	−0.49
PX13	−4.12	4.12	4.28	0.12	3.96	−2.07	−6.03
WCPT18	−3.23	3.39	3.99	0.10	7.87	0.61	−7.26
RG18	0.54	0.61	0.92	1.05	3.67	3.06	−0.61
ADIM6	−3.84	3.84	4.45	1.14	6.66	−0.84	−7.50
S22	−4.20	4.21	5.50	0.58	15.03	0.04	−14.99
S66	−3.19	3.19	3.71	0.58	9.54	−0.24	−9.78
HEAVY28	−0.74	0.77	0.90	0.62	1.95	0.28	−1.67
WATER27	−13.57	13.60	20.37	0.17	55.07	0.35	−54.72
CARBHB12	−0.18	0.69	0.90	0.11	3.18	1.53	−1.65
PNICO23	−1.70	1.70	1.96	0.40	3.99	−0.05	−4.04
HAL59	−1.72	1.79	2.25	0.39	9.64	1.94	−7.70
AHB21	1.45	1.49	1.79	0.07	4.05	3.70	−0.35
CHB6	1.33	1.33	1.91	0.05	4.01	4.13	0.12
IL16	4.92	4.92	5.03	0.05	4.07	7.47	3.40
IDISP	5.75	20.93	23.49	1.47	62.10	38.86	−23.23
ICONF	0.18	0.95	1.46	0.29	6.99	4.37	−2.62
ACONF	1.53	1.53	1.69	0.84	2.31	2.89	0.57
AMINO20x4	−0.29	1.05	1.29	0.43	6.04	3.23	−2.81
PCONF21	−0.81	4.94	5.60	3.05	17.55	9.88	−7.67
MCONF	−2.96	2.99	3.40	0.60	5.55	0.53	−5.01
SCONF	−1.23	2.45	2.79	0.53	9.33	5.53	−3.79
UPU23	1.50	2.58	3.51	0.45	12.00	9.69	−2.32
BUT14DIOL	−1.02	1.19	1.30	0.42	3.57	1.38	−2.19

Table S124: Statistical analysis for the N12 DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	0.27	7.42	9.71	0.02	61.04	37.40	−23.63
G21EA	−2.83	3.53	4.13	0.10	12.56	5.07	−7.49
G21IP	−2.92	4.87	6.19	0.02	26.80	9.81	−17.00
DIPCS10	−7.73	7.73	9.27	0.01	14.13	−1.25	−15.38
PA26	3.32	3.40	4.21	0.02	10.92	10.24	−0.68
SIE4x4	21.10	21.10	23.78	0.63	40.16	43.33	3.17
ALKBDE10	0.14	6.85	8.96	0.07	32.31	20.96	−11.35
YBDE18	−3.42	5.59	7.01	0.11	24.04	8.61	−15.43
AL2X6	−5.72	5.72	6.25	0.16	7.45	−1.18	−8.63
HEAVYSB11	2.27	5.06	5.89	0.09	17.44	10.30	−7.13
NBPRC	1.99	2.95	4.07	0.11	12.81	9.31	−3.50
ALK8	−0.33	3.89	4.92	0.06	16.90	7.57	−9.33
RC21	4.42	5.19	6.23	0.15	15.68	12.20	−3.48
G2RC	−1.24	5.67	7.05	0.11	29.39	15.12	−14.28
BH76RC	0.63	3.65	5.02	0.17	26.96	17.86	−9.10
FH51	0.74	2.80	4.16	0.09	22.53	12.62	−9.91
TAUT15	−0.01	2.30	3.00	0.75	9.93	5.99	−3.93
DC13	1.18	8.80	11.36	0.16	39.31	17.78	−21.53
MB16-43	5.34	17.74	22.34	0.04	93.84	56.05	−37.78
DARC	6.36	6.70	7.65	0.21	13.04	10.65	−2.39
RSE43	−3.06	3.06	3.47	0.40	6.96	−0.83	−7.78
BSR36	−8.11	8.11	9.09	0.50	18.63	−1.18	−19.82
CDIE20	1.84	1.84	1.98	0.45	2.77	2.89	0.12
ISO34	−0.62	1.74	2.49	0.12	14.47	5.67	−8.79
ISOL24	−2.58	6.92	10.43	0.32	55.42	22.78	−32.64
C60ISO	−8.74	8.74	10.73	0.09	18.90	−0.56	−19.47
PArel	0.46	1.79	2.65	0.39	12.13	8.51	−3.63
BH76	−7.10	7.23	8.33	0.39	27.43	3.12	−24.31
BHPERI	−1.47	2.29	3.09	0.11	9.34	1.91	−7.43
BHDIV10	−6.61	7.09	7.84	0.16	14.84	2.44	−12.40
INV24	−3.55	3.55	4.31	0.11	9.33	−0.70	−10.03
BHROT27	0.71	0.86	1.17	0.14	3.20	2.74	−0.45
PX13	−8.51	8.51	8.64	0.26	6.32	−5.71	−12.03
WCPT18	−5.93	5.93	6.29	0.17	8.50	−2.45	−10.95
RG18	−1.07	1.07	1.39	1.84	3.21	−0.10	−3.32
ADIM6	−6.41	6.41	6.92	1.91	7.51	−2.82	−10.32
S22	−3.88	3.94	5.25	0.54	14.43	0.65	−13.78
S66	−3.60	3.62	4.39	0.66	10.49	0.58	−9.91
HEAVY28	−1.66	1.66	1.75	1.34	2.13	−0.83	−2.96
WATER27	−3.83	5.13	8.01	0.06	27.19	3.85	−23.34
CARBHB12	0.26	0.89	1.22	0.15	4.17	2.83	−1.34
PNICO23	−1.41	1.74	1.96	0.41	8.15	3.89	−4.26
HAL59	−1.51	1.94	2.51	0.42	12.85	4.47	−8.38
AHB21	−0.72	1.40	1.72	0.06	6.36	2.66	−3.70
CHB6	−0.56	1.42	1.69	0.05	4.76	2.56	−2.20
IL16	2.40	2.40	2.62	0.02	4.29	4.69	0.40
IDISP	3.14	13.65	15.39	0.96	42.77	26.37	−16.40
ICONF	0.25	0.61	0.87	0.19	3.98	2.56	−1.43
ACONF	0.88	0.88	0.98	0.48	1.42	1.73	0.30
AMINO20x4	0.08	0.69	0.88	0.28	4.19	2.59	−1.60
PCONF21	−0.66	4.64	5.13	2.86	14.03	7.88	−6.15
MCONF	−2.46	2.56	2.90	0.52	5.75	0.98	−4.77
SCONF	0.16	0.38	0.53	0.08	2.33	1.09	−1.24
UPU23	2.05	2.65	3.96	0.46	12.08	10.60	−1.49
BUT14DIOL	0.29	0.33	0.44	0.12	1.52	1.24	−0.28

SI.7.6 Results for dispersion-uncorrected meta-GGA/meta-NGA functionals

Table S125: Statistical analysis for the PKZB DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	0.16	5.60	8.20	0.02	62.54	23.10	−39.44
G21EA	−1.40	2.25	2.92	0.07	8.70	1.93	−6.78
G21IP	−3.93	4.39	5.71	0.02	15.52	3.91	−11.61
DIPCS10	−9.75	9.75	11.37	0.01	16.90	−1.53	−18.43
PA26	4.10	4.10	5.00	0.02	10.29	11.05	0.75
SIE4x4	22.25	22.25	25.77	0.66	46.59	50.81	4.22
ALKBDE10	−4.18	7.37	8.21	0.07	27.52	15.96	−11.56
YBDE18	−7.82	7.93	9.72	0.16	18.76	0.64	−18.12
AL2X6	−6.57	6.57	6.86	0.18	5.97	−3.53	−9.49
HEAVYSB11	−6.22	6.31	7.65	0.11	15.25	0.50	−14.75
NBPRC	4.47	5.81	7.20	0.21	21.89	17.57	−4.32
ALK8	−2.29	3.40	4.64	0.05	12.66	2.83	−9.84
RC21	0.23	3.28	4.02	0.09	17.32	9.00	−8.31
G2RC	6.68	7.89	10.67	0.15	36.84	26.05	−10.79
BH76RC	0.81	3.67	4.71	0.17	18.89	11.89	−7.00
FH51	4.35	4.99	6.61	0.16	32.13	23.18	−8.95
TAUT15	−0.35	1.03	1.26	0.34	4.54	2.77	−1.77
DC13	6.97	12.09	13.84	0.22	41.96	24.36	−17.60
MB16-43	−49.04	54.78	64.31	0.13	208.57	73.90	−134.67
DARC	11.16	11.16	11.49	0.34	7.97	13.64	5.67
RSE43	−2.56	2.56	2.82	0.34	6.11	−1.18	−7.29
BSR36	−1.13	2.39	2.90	0.15	12.25	5.48	−6.76
CDIE20	1.61	1.61	1.72	0.40	2.31	2.85	0.54
ISO34	−1.64	2.29	3.09	0.16	14.49	3.92	−10.57
ISOL24	−4.96	7.77	10.80	0.35	56.08	20.47	−35.61
C60ISO	−12.28	12.28	14.46	0.12	22.57	−2.02	−24.59
PArel	0.51	1.70	2.43	0.37	12.55	5.55	−7.00
BH76	−5.53	5.63	6.67	0.30	19.76	1.55	−18.21
BHPERI	0.49	2.86	3.28	0.14	11.08	5.06	−6.02
BHDIV10	−4.05	4.36	5.27	0.10	10.24	1.58	−8.65
INV24	−1.83	2.33	2.95	0.07	13.08	5.00	−8.08
BHROT27	0.24	0.46	0.60	0.07	2.24	1.48	−0.76
PX13	−2.04	2.16	2.53	0.06	6.00	0.76	−5.25
WCPT18	−3.11	4.50	4.96	0.13	12.07	3.53	−8.54
RG18	−0.36	0.45	0.60	0.78	1.70	0.42	−1.28
ADIM6	−3.74	3.74	4.11	1.11	4.94	−1.37	−6.31
S22	−4.95	4.95	5.78	0.68	9.98	−0.56	−10.54
S66	−4.00	4.00	4.30	0.73	6.94	−1.22	−8.16
HEAVY28	−1.75	1.75	1.83	1.41	2.01	−0.57	−2.57
WATER27	−31.23	31.23	46.12	0.38	109.45	−1.94	−111.39
CARBHB12	−2.40	2.40	2.58	0.40	3.03	−1.05	−4.09
PNICO23	−2.57	2.57	2.75	0.60	4.06	−0.50	−4.56
HAL59	−2.75	2.75	2.96	0.60	6.45	−0.07	−6.51
AHB21	4.43	4.43	4.64	0.20	5.75	8.57	2.83
CHB6	1.47	1.85	2.09	0.07	4.86	3.72	−1.14
IL16	6.24	6.24	6.27	0.06	2.02	7.42	5.40
IDISP	3.19	10.30	13.41	0.72	41.76	27.26	−14.49
ICONF	−0.01	0.47	0.72	0.14	3.50	1.65	−1.85
ACONF	0.75	0.75	0.82	0.41	1.18	1.50	0.32
AMINO20x4	−0.31	0.86	1.07	0.35	4.87	1.81	−3.06
PCONF21	−0.35	1.88	2.45	1.16	8.57	4.00	−4.57
MCONF	−1.79	1.84	2.06	0.37	4.22	0.94	−3.27
SCONF	−0.84	1.81	2.10	0.39	6.82	4.31	−2.51
UPU23	0.71	2.00	2.63	0.35	10.59	7.03	−3.56
BUT14DIOL	−1.81	1.81	1.88	0.65	2.24	−0.20	−2.44

Table S126: Statistical analysis for the TPSS DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	3.27	5.11	6.65	0.02	43.30	24.96	−18.33
G21EA	0.43	2.21	2.66	0.07	9.67	5.84	−3.83
G21IP	−0.96	3.95	4.83	0.02	19.85	11.95	−7.90
DIPCS10	−3.58	3.69	4.99	0.01	10.11	0.57	−9.54
PA26	4.38	4.38	5.01	0.02	10.12	11.28	1.16
SIE4x4	21.56	21.56	24.42	0.64	40.77	45.65	4.88
ALKBDE10	1.49	4.26	7.38	0.04	26.08	22.07	−4.01
YBDE18	−7.28	7.29	8.41	0.15	14.28	0.03	−14.26
AL2X6	−3.83	3.96	4.56	0.11	6.83	0.36	−6.46
HEAVYSB11	−3.70	4.44	5.61	0.08	12.77	2.28	−10.49
NBPRC	1.48	2.78	3.92	0.10	12.35	8.74	−3.62
ALK8	−0.76	1.61	2.28	0.03	7.56	2.09	−5.47
RC21	1.66	3.14	3.87	0.09	14.90	6.88	−8.02
G2RC	3.81	6.57	8.87	0.13	33.09	20.44	−12.66
BH76RC	0.45	3.63	4.94	0.17	21.86	12.72	−9.14
FH51	3.74	5.09	6.44	0.16	25.69	15.90	−9.79
TAUT15	0.19	1.61	1.88	0.53	5.83	3.52	−2.31
DC13	2.53	12.56	15.31	0.23	53.39	20.84	−32.55
MB16-43	−47.14	47.14	51.90	0.11	99.64	−4.69	−104.33
DARC	11.39	11.39	11.98	0.35	9.84	14.48	4.64
RSE43	−2.17	2.17	2.43	0.29	5.17	−0.87	−6.04
BSR36	−10.21	10.21	11.47	0.63	23.84	−2.08	−25.92
CDIE20	1.86	1.86	2.00	0.46	2.83	3.23	0.40
ISO34	−1.87	2.64	3.63	0.18	18.41	5.76	−12.65
ISOL24	−5.18	8.87	13.48	0.40	73.75	28.23	−45.52
C60ISO	−8.80	8.80	10.84	0.09	18.58	−0.69	−19.27
PArel	0.18	1.54	2.21	0.33	11.66	5.66	−6.00
BH76	−8.61	8.63	9.58	0.46	22.93	0.67	−22.26
BHPERI	−2.02	2.26	2.90	0.11	7.84	1.26	−6.58
BHDIV10	−5.81	6.09	6.73	0.13	11.61	1.40	−10.22
INV24	−2.49	2.72	3.13	0.09	9.56	2.79	−6.77
BHROT27	0.32	0.54	0.69	0.09	2.26	1.52	−0.74
PX13	−8.35	8.35	8.46	0.25	6.11	−5.45	−11.55
WCPT18	−5.45	5.45	5.72	0.16	6.64	−2.58	−9.22
RG18	−0.48	0.48	0.68	0.83	1.64	0.00	−1.63
ADIM6	−4.70	4.70	5.16	1.40	6.20	−1.78	−7.97
S22	−3.44	3.44	4.57	0.47	12.18	−0.12	−12.30
S66	−2.99	2.99	3.56	0.55	8.81	−0.09	−8.90
HEAVY28	−0.86	0.86	0.97	0.69	1.57	−0.20	−1.77
WATER27	−3.99	4.65	7.57	0.06	24.61	2.01	−22.60
CARBHB12	0.33	0.63	0.97	0.10	3.35	2.48	−0.87
PNICO23	−0.64	0.94	1.16	0.22	5.61	2.60	−3.01
HAL59	−0.87	1.55	2.08	0.34	12.33	4.98	−7.35
AHB21	0.44	0.71	0.96	0.03	3.16	2.35	−0.82
CHB6	0.49	1.02	1.38	0.04	3.82	3.02	−0.80
IL16	2.92	2.92	2.99	0.03	2.79	4.60	1.81
IDISP	3.88	12.85	15.30	0.90	43.93	29.61	−14.31
ICONF	0.05	0.37	0.54	0.11	2.50	1.68	−0.82
ACONF	0.75	0.75	0.84	0.41	1.19	1.48	0.29
AMINO20x4	−0.02	0.53	0.68	0.22	3.30	1.84	−1.46
PCONF21	−0.90	3.99	4.33	2.46	11.62	6.14	−5.48
MCONF	−2.16	2.23	2.51	0.45	4.95	0.84	−4.11
SCONF	0.17	0.42	0.53	0.09	2.13	0.93	−1.20
UPU23	1.76	2.36	3.47	0.41	11.56	9.76	−1.81
BUT14DIOL	−0.13	0.30	0.35	0.11	1.49	0.76	−0.72

Table S127: Statistical analysis for the revTPSS DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	2.23	5.19	6.92	0.02	45.88	25.77	−20.12
G21EA	−0.60	2.32	2.54	0.07	7.79	3.90	−3.89
G21IP	−1.59	3.99	4.90	0.02	20.05	11.49	−8.56
DIPCS10	−4.47	4.47	5.66	0.01	10.62	−0.57	−11.19
PA26	4.20	4.20	4.96	0.02	10.61	11.33	0.72
SIE4x4	21.02	21.02	23.85	0.62	39.76	44.29	4.54
ALKBDE10	−0.69	4.40	6.57	0.04	23.29	17.99	−5.30
YBDE18	−6.22	6.25	7.16	0.13	12.60	0.30	−12.30
AL2X6	−2.62	2.77	3.16	0.08	5.09	0.45	−4.63
HEAVYSB11	−2.11	3.79	4.56	0.07	12.22	3.73	−8.49
NBPRC	0.62	2.43	3.29	0.09	10.69	7.29	−3.39
ALK8	−1.32	1.85	2.33	0.03	5.91	1.26	−4.65
RC21	2.36	3.81	4.66	0.11	16.17	9.14	−7.03
G2RC	6.06	9.98	13.09	0.19	46.86	30.18	−16.68
BH76RC	0.96	4.76	6.09	0.22	22.97	14.42	−8.55
FH51	4.08	5.77	7.37	0.19	29.00	19.93	−9.07
TAUT15	0.15	1.29	1.61	0.42	5.20	3.15	−2.05
DC13	1.48	10.39	14.11	0.19	55.45	19.30	−36.15
MB16-43	−54.63	54.64	60.99	0.13	115.55	0.10	−115.45
DARC	7.72	7.72	8.40	0.24	9.53	10.66	1.13
RSE43	−1.90	1.90	2.18	0.25	5.05	−0.59	−5.63
BSR36	−7.49	7.49	8.33	0.46	16.85	−1.07	−17.92
CDIE20	1.67	1.67	1.74	0.41	2.11	2.80	0.69
ISO34	−2.48	3.11	4.32	0.21	19.45	3.51	−15.94
ISOL24	−4.64	7.77	11.01	0.35	59.81	23.88	−35.94
C60ISO	−9.88	9.88	11.94	0.10	19.99	−1.15	−21.13
PArel	0.41	1.50	2.05	0.32	10.43	4.97	−5.46
BH76	−8.34	8.34	9.53	0.45	24.33	−0.41	−24.74
BHPERI	−3.00	3.00	3.42	0.14	7.22	−0.10	−7.32
BHDIV10	−5.45	5.49	6.15	0.12	10.15	0.20	−9.95
INV24	−1.92	2.32	2.70	0.07	9.28	3.28	−6.00
BHROT27	0.32	0.51	0.67	0.08	2.08	1.48	−0.60
PX13	−5.73	5.73	5.91	0.17	5.23	−3.63	−8.86
WCPT18	−4.69	4.69	5.01	0.13	5.95	−1.75	−7.70
RG18	−0.50	0.50	0.68	0.86	1.64	−0.02	−1.66
ADIM6	−4.20	4.20	4.60	1.25	5.40	−1.61	−7.02
S22	−3.05	3.05	3.96	0.42	10.25	−0.08	−10.33
S66	−2.66	2.66	3.12	0.49	7.47	−0.16	−7.63
HEAVY28	−0.72	0.73	0.82	0.59	1.51	0.03	−1.48
WATER27	−3.94	4.15	6.87	0.05	21.01	0.94	−20.08
CARBHB12	0.02	0.50	0.68	0.08	2.52	1.67	−0.85
PNICO23	−0.39	0.79	1.01	0.19	5.34	2.70	−2.64
HAL59	−0.62	1.42	1.89	0.31	11.46	4.99	−6.47
AHB21	0.75	0.78	1.04	0.03	3.22	2.95	−0.27
CHB6	0.41	0.90	1.19	0.03	3.56	2.49	−1.07
IL16	2.75	2.75	2.81	0.03	2.30	3.83	1.54
IDISP	3.56	8.92	11.69	0.63	35.69	24.16	−11.53
ICONF	0.06	0.33	0.43	0.10	1.90	1.22	−0.68
ACONF	0.57	0.57	0.64	0.31	0.94	1.14	0.20
AMINO20x4	0.03	0.44	0.53	0.18	2.50	1.53	−0.97
PCONF21	−0.65	3.06	3.34	1.89	9.12	4.79	−4.32
MCONF	−1.35	1.78	1.99	0.36	4.46	1.00	−3.46
SCONF	0.39	0.62	0.71	0.13	2.23	1.15	−1.07
UPU23	1.32	2.05	2.96	0.36	10.49	8.29	−2.20
BUT14DIOL	−0.27	0.33	0.38	0.12	1.23	0.47	−0.75

Table S128: Statistical analysis for the SCAN DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.17	4.01	5.72	0.01	41.95	13.50	−28.45
G21EA	0.27	3.64	4.20	0.11	13.53	8.05	−5.48
G21IP	0.01	4.69	5.68	0.02	24.45	12.51	−11.94
DIPCS10	−2.82	4.92	5.99	0.01	16.69	4.67	−12.02
PA26	3.00	3.09	3.94	0.02	11.04	10.28	−0.76
SIE4x4	17.91	17.91	20.45	0.53	35.83	39.28	3.45
ALKBDE10	19.21	19.21	21.00	0.19	31.17	39.21	8.04
YBDE18	−3.16	3.61	4.01	0.07	9.65	2.49	−7.15
AL2X6	1.17	1.44	1.59	0.04	3.69	2.87	−0.81
HEAVYSB11	2.69	7.17	8.87	0.12	22.99	16.79	−6.20
NBPRC	−1.17	2.04	2.63	0.07	8.78	2.94	−5.84
ALK8	2.07	2.92	3.94	0.05	9.61	7.53	−2.08
RC21	5.70	6.29	8.10	0.18	28.64	25.62	−3.01
G2RC	−1.19	6.24	7.64	0.12	31.56	13.14	−18.42
BH76RC	−0.26	3.38	4.40	0.16	18.58	9.40	−9.19
FH51	−0.55	2.58	3.90	0.08	21.66	10.87	−10.79
TAUT15	0.45	1.74	2.35	0.57	7.93	5.47	−2.45
DC13	0.19	7.19	10.82	0.13	43.31	12.02	−31.29
MB16-43	9.66	15.68	19.98	0.04	95.87	67.98	−27.89
DARC	0.30	2.53	2.79	0.08	8.79	3.18	−5.62
RSE43	−1.33	1.33	1.82	0.17	5.47	0.00	−5.47
BSR36	−2.81	2.81	3.35	0.17	7.38	−0.80	−8.17
CDIE20	1.49	1.49	1.62	0.37	2.31	2.33	0.02
ISO34	−0.29	1.35	1.91	0.09	10.69	6.22	−4.47
ISOL24	−0.88	3.89	5.66	0.18	28.04	16.90	−11.14
C60ISO	−6.05	6.12	8.07	0.06	15.81	0.28	−15.53
PArel	0.71	1.50	2.25	0.32	10.07	7.69	−2.38
BH76	−7.36	7.66	8.37	0.41	23.73	6.06	−17.68
BHPERI	−4.77	4.77	5.05	0.23	7.44	−0.51	−7.96
BHDIV10	−5.57	6.50	7.02	0.14	15.73	4.66	−11.08
INV24	−0.73	1.20	1.73	0.04	8.03	1.75	−6.28
BHROT27	0.82	0.84	1.16	0.13	2.49	2.36	−0.13
PX13	−8.25	8.25	8.43	0.25	6.82	−5.39	−12.21
WCPT18	−6.04	6.04	6.74	0.17	10.02	−2.32	−12.34
RG18	−0.04	0.22	0.27	0.38	1.08	0.53	−0.56
ADIM6	−1.70	1.70	1.87	0.51	2.24	−0.58	−2.82
S22	−0.60	0.93	1.24	0.13	5.08	2.18	−2.90
S66	−0.57	0.88	1.06	0.16	4.20	2.22	−1.97
HEAVY28	−0.35	0.40	0.46	0.32	1.27	0.46	−0.81
WATER27	7.39	7.99	10.03	0.10	30.18	22.04	−8.14
CARBHB12	1.10	1.11	1.66	0.18	3.71	3.66	−0.05
PNICO23	0.67	0.87	1.37	0.20	6.16	5.21	−0.95
HAL59	0.56	1.06	1.62	0.23	8.22	5.99	−2.23
AHB21	−1.50	1.50	1.80	0.07	4.02	−0.08	−4.10
CHB6	−0.04	0.43	0.55	0.02	1.79	0.98	−0.81
IL16	−0.31	0.52	0.61	0.00	1.83	0.96	−0.88
IDISP	1.83	4.84	6.35	0.34	17.66	13.72	−3.94
ICONF	0.28	0.32	0.46	0.10	1.66	1.47	−0.19
ACONF	0.32	0.32	0.35	0.17	0.50	0.62	0.12
AMINO20x4	0.10	0.26	0.34	0.11	1.58	0.94	−0.64
PCONF21	−0.10	0.88	0.97	0.54	2.52	1.29	−1.23
MCONF	−0.28	0.51	0.62	0.10	2.18	0.87	−1.30
SCONF	0.35	0.54	0.59	0.12	1.84	0.74	−1.10
UPU23	0.32	0.81	1.07	0.14	3.73	2.71	−1.02
BUT14DIOL	0.31	0.32	0.34	0.11	0.73	0.59	−0.14

Table S129: Statistical analysis for the τHCTH DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	0.89	4.27	6.06	0.01	43.11	27.45	−15.66
G21EA	2.71	3.08	3.97	0.09	11.85	9.92	−1.93
G21IP	2.10	4.04	5.07	0.02	17.27	11.71	−5.56
DIPCS10	2.90	4.24	5.27	0.01	12.02	9.41	−2.60
PA26	5.02	5.02	5.59	0.03	9.74	11.45	1.71
SIE4x4	22.94	22.94	25.43	0.68	39.59	46.86	7.27
ALKBDE10	4.27	5.70	9.48	0.06	30.63	26.08	−4.56
YBDE18	−6.75	7.17	8.81	0.15	21.72	2.27	−19.45
AL2X6	−9.84	9.84	10.27	0.27	9.26	−4.98	−14.24
HEAVYSB11	−6.80	6.86	8.24	0.12	14.88	0.31	−14.57
NBPRC	4.44	5.20	7.19	0.19	19.44	17.64	−1.81
ALK8	−5.95	5.95	8.18	0.10	16.16	−0.37	−16.54
RC21	1.24	2.85	3.76	0.08	17.02	9.70	−7.32
G2RC	2.13	4.36	6.22	0.09	30.93	19.88	−11.05
BH76RC	−0.01	2.64	4.53	0.12	26.76	19.01	−7.75
FH51	3.05	4.46	5.82	0.14	29.54	16.81	−12.73
TAUT15	0.26	1.66	2.05	0.54	6.39	4.16	−2.23
DC13	7.35	15.67	17.46	0.29	50.78	29.88	−20.90
MB16-43	−56.18	56.18	62.08	0.14	114.80	−4.08	−118.88
DARC	15.00	15.00	15.72	0.46	14.23	19.12	4.88
RSE43	−3.30	3.30	3.57	0.43	6.38	−1.79	−8.17
BSR36	−13.45	13.45	15.28	0.83	30.25	−3.58	−33.83
CDIE20	2.17	2.18	2.44	0.54	4.63	4.44	−0.19
ISO34	−1.18	2.48	3.60	0.17	22.30	9.95	−12.35
ISOL24	−6.42	10.69	17.06	0.49	91.51	30.79	−60.72
C60ISO	−8.83	8.83	10.76	0.09	18.35	−0.88	−19.23
PArel	0.29	1.56	2.41	0.34	12.91	7.14	−5.77
BH76	−6.36	6.56	7.56	0.35	26.43	4.37	−22.05
BHPERI	0.51	2.80	3.20	0.13	11.14	5.99	−5.15
BHDIV10	−4.72	5.58	6.52	0.12	13.89	3.03	−10.86
INV24	−3.09	3.16	3.82	0.10	10.26	0.85	−9.41
BHROT27	0.33	0.46	0.64	0.07	2.19	1.64	−0.55
PX13	−8.95	8.95	9.17	0.27	8.30	−5.08	−13.39
WCPT18	−5.22	5.22	5.54	0.15	7.42	−2.35	−9.76
RG18	−0.21	0.32	0.46	0.55	1.70	0.43	−1.27
ADIM6	−5.19	5.19	5.78	1.54	7.43	−1.74	−9.17
S22	−3.99	3.99	5.42	0.55	15.08	−0.28	−15.36
S66	−3.37	3.37	4.05	0.62	10.39	−0.15	−10.54
HEAVY28	−0.73	0.74	0.86	0.60	1.72	0.08	−1.64
WATER27	−6.51	7.18	11.41	0.09	36.15	2.39	−33.76
CARBHB12	0.37	0.69	1.06	0.11	3.60	2.64	−0.97
PNICO23	−1.09	1.17	1.31	0.27	3.91	0.88	−3.03
HAL59	−1.28	1.62	2.19	0.35	12.10	3.76	−8.33
AHB21	0.05	0.81	1.12	0.04	4.84	2.84	−2.00
CHB6	1.35	1.38	1.91	0.05	4.12	4.02	−0.10
IL16	3.20	3.20	3.38	0.03	4.56	6.00	1.44
IDISP	5.21	18.56	20.97	1.31	56.81	35.80	−21.01
ICONF	0.17	0.73	1.12	0.22	5.51	3.29	−2.22
ACONF	1.26	1.26	1.40	0.69	2.02	2.49	0.47
AMINO20x4	−0.17	0.83	1.04	0.34	4.84	2.59	−2.24
PCONF21	−1.12	5.30	5.85	3.27	16.59	9.32	−7.28
MCONF	−2.94	2.97	3.35	0.60	5.66	0.59	−5.07
SCONF	−0.48	0.86	1.11	0.19	4.41	2.42	−1.99
UPU23	1.92	2.73	3.92	0.48	12.78	10.81	−1.97
BUT14DIOL	−0.27	0.58	0.68	0.21	2.64	1.37	−1.27

Table S130: Statistical analysis for the M06L DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.22	4.46	6.09	0.01	47.60	18.28	−29.32
G21EA	−3.39	3.80	4.64	0.11	14.32	4.07	−10.25
G21IP	−2.77	4.46	5.49	0.02	23.24	8.35	−14.89
DIPCS10	−8.12	8.42	10.87	0.01	23.19	1.51	−21.67
PA26	5.08	5.09	5.81	0.03	12.48	12.33	−0.15
SIE4x4	17.94	17.94	20.11	0.53	31.54	36.44	4.89
ALKBDE10	1.38	5.59	7.02	0.06	23.97	16.20	−7.77
YBDE18	−4.60	4.90	6.15	0.10	14.07	1.53	−12.55
AL2X6	−0.69	0.80	1.10	0.02	2.67	0.29	−2.38
HEAVYSB11	−1.93	2.71	3.51	0.05	10.82	2.58	−8.24
NBPRC	1.39	4.04	4.95	0.15	17.39	11.26	−6.14
ALK8	2.05	3.76	6.21	0.06	18.64	16.42	−2.22
RC21	2.30	3.04	3.66	0.09	11.20	8.28	−2.92
G2RC	0.06	5.89	7.56	0.11	32.52	18.31	−14.21
BH76RC	1.44	2.92	4.22	0.14	22.70	17.14	−5.56
FH51	0.66	2.67	3.55	0.09	16.11	8.56	−7.56
TAUT15	−0.50	1.45	1.77	0.48	5.88	3.23	−2.65
DC13	2.16	10.47	13.27	0.19	55.13	24.61	−30.52
MB16-43[a]	−63.92	63.92	68.76	0.15	108.47	−14.26	−122.72
DARC	8.30	8.30	8.87	0.26	9.69	11.72	2.03
RSE43	−2.68	2.68	3.06	0.35	7.84	−0.98	−8.82
BSR36	−5.64	5.64	6.47	0.35	12.80	−2.27	−15.07
CDIE20	2.19	2.22	2.47	0.55	4.17	3.89	−0.28
ISO34	−1.09	2.31	2.99	0.16	14.70	8.57	−6.14
ISOL24	−4.39	6.71	9.11	0.31	38.96	16.31	−22.65
C60ISO	−7.20	7.20	8.81	0.07	14.89	−1.26	−16.16
PArel	0.80	1.63	2.31	0.35	11.66	6.65	−5.00
BH76	−3.29	3.92	4.92	0.21	23.52	8.03	−15.49
BHPERI	1.10	1.91	2.19	0.09	7.99	4.42	−3.57
BHDIV10	−2.09	3.09	3.67	0.07	9.85	2.74	−7.11
INV24	−0.69	1.47	2.16	0.05	11.07	3.94	−7.12
BHROT27	0.90	0.98	1.32	0.16	3.98	3.13	−0.86
PX13	0.55	0.92	1.15	0.03	3.77	2.57	−1.20
WCPT18	−1.85	2.09	2.55	0.06	5.28	0.79	−4.49
RG18	−0.18	0.32	0.39	0.55	1.37	0.66	−0.71
ADIM6	0.15	0.17	0.23	0.05	0.53	0.46	−0.07
S22	−0.77	0.81	0.92	0.11	2.04	0.35	−1.69
S66	−0.57	0.59	0.68	0.11	1.98	0.57	−1.41
HEAVY28	−0.49	0.56	0.61	0.45	1.40	0.41	−0.99
WATER27	−1.54	1.95	3.17	0.02	13.97	2.79	−11.18
CARBHB12	0.13	0.46	0.67	0.08	2.02	1.57	−0.45
PNICO23	−0.33	0.40	0.46	0.09	1.28	0.38	−0.90
HAL59	−0.16	0.56	0.72	0.12	4.11	2.81	−1.31
AHB21	0.18	0.49	0.62	0.02	2.89	0.99	−1.90
CHB6	1.90	1.90	2.22	0.07	2.81	3.41	0.59
IL16	−0.24	0.62	0.71	0.01	2.32	1.02	−1.30
IDISP	3.01	6.37	9.87	0.45	31.58	21.51	−10.08
ICONF	−0.04	0.30	0.35	0.09	1.16	0.56	−0.60
ACONF	−0.46	0.46	0.51	0.25	0.70	−0.14	−0.85
AMINO20x4	0.01	0.35	0.43	0.14	2.01	1.05	−0.96
PCONF21	0.30	1.02	1.23	0.63	4.19	1.83	−2.36
MCONF	0.40	0.81	0.98	0.16	2.80	1.89	−0.91
SCONF	−0.06	0.41	0.66	0.09	2.63	0.66	−1.97
UPU23	−0.37	0.50	0.68	0.09	2.56	0.61	−1.95
BUT14DIOL	0.09	0.21	0.25	0.07	0.98	0.59	−0.40

[a] Systems **6** and **16** did not converge and were omitted from the statistics

Table S131: Statistical analysis for the M11L DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−3.66	6.57	8.43	0.02	45.58	19.70	−25.88
G21EA	2.71	5.66	6.55	0.17	26.45	12.65	−13.80
G21IP	−1.01	3.86	5.07	0.01	23.32	10.25	−13.08
DIPCS10	−4.27	7.37	8.62	0.01	20.77	4.70	−16.07
PA26	3.71	4.06	4.94	0.02	14.02	11.58	−2.45
SIE4x4	11.33	11.34	13.47	0.34	25.75	25.67	−0.08
ALKBDE10	−10.80	10.80	12.59	0.11	19.80	−2.97	−22.77
YBDE18	−2.18	5.45	6.38	0.11	21.42	6.98	−14.44
AL2X6	−8.06	8.06	8.45	0.22	7.24	−2.75	−9.99
HEAVYSB11	−1.23	3.33	4.14	0.06	13.35	5.36	−7.99
NBPRC	3.92	4.84	6.19	0.17	17.52	14.73	−2.79
ALK8	−3.96	10.64	14.10	0.17	46.98	26.13	−20.85
RC21	0.43	2.16	2.58	0.06	9.51	5.25	−4.26
G2RC	1.54	5.63	7.66	0.11	37.41	23.89	−13.52
BH76RC	0.24	3.24	4.67	0.15	23.71	7.77	−15.94
FH51	1.09	2.59	3.47	0.08	16.53	12.19	−4.34
TAUT15	1.14	1.49	1.85	0.49	5.26	3.42	−1.84
DC13	5.40	9.12	12.27	0.17	42.29	31.44	−10.85
MB16-43	−51.73	51.73	57.26	0.12	105.21	−4.23	−109.44
DARC	4.81	4.81	5.46	0.15	7.11	7.45	0.34
RSE43	−2.47	2.47	2.87	0.33	8.28	−0.21	−8.49
BSR36	−2.73	2.73	3.08	0.17	5.89	−0.19	−6.08
CDIE20	1.74	1.75	2.02	0.43	3.74	3.62	−0.12
ISO34	0.48	1.31	1.78	0.09	7.05	3.63	−3.42
ISOL24	−1.96	4.92	6.88	0.22	35.02	20.72	−14.30
C60ISO	−6.49	6.55	8.52	0.07	16.56	0.26	−16.30
PArel	1.87	2.34	3.12	0.51	9.08	7.40	−1.69
BH76	−1.00	2.16	3.01	0.12	17.24	8.23	−9.01
BHPERI	1.61	2.80	3.21	0.13	10.60	5.58	−5.02
BHDIV10	−0.14	3.33	3.89	0.07	12.80	6.76	−6.04
INV24	−0.60	2.20	3.50	0.07	18.68	6.84	−11.84
BHROT27	0.48	0.63	0.91	0.10	3.31	2.80	−0.51
PX13	1.70	1.91	2.26	0.06	5.66	4.29	−1.37
WCPT18	−0.99	2.25	2.69	0.06	8.69	3.34	−5.36
RG18	−1.64	1.64	2.27	2.83	6.14	−0.58	−6.71
ADIM6	−0.75	0.75	0.76	0.22	0.33	−0.60	−0.93
S22	−1.36	1.36	1.59	0.19	2.65	−0.43	−3.08
S66	−1.14	1.14	1.23	0.21	2.25	−0.19	−2.44
HEAVY28	−0.50	0.53	0.59	0.43	1.09	0.20	−0.89
WATER27	−10.26	10.66	15.32	0.13	46.00	5.43	−40.57
CARBHB12	−1.53	1.53	1.74	0.25	2.65	−0.62	−3.28
PNICO23	−0.66	0.66	0.85	0.15	2.03	−0.05	−2.08
HAL59	−1.41	1.43	1.66	0.31	6.16	0.38	−5.77
AHB21	1.28	1.48	1.88	0.07	5.99	5.04	−0.95
CHB6	1.20	1.20	1.27	0.04	1.05	1.71	0.67
IL16	0.70	0.78	0.92	0.01	1.78	1.51	−0.27
IDISP	2.96	4.02	7.38	0.28	18.97	17.84	−1.13
ICONF	0.16	0.36	0.59	0.11	2.69	2.05	−0.63
ACONF	0.22	0.22	0.24	0.12	0.42	0.49	0.07
AMINO20x4	−0.09	0.56	0.73	0.23	3.40	1.38	−2.02
PCONF21	0.59	0.63	0.80	0.39	1.77	1.60	−0.17
MCONF	−0.33	0.54	0.67	0.11	2.31	0.90	−1.41
SCONF	−0.26	0.67	0.85	0.15	3.31	1.83	−1.48
UPU23	−0.67	0.85	1.03	0.15	3.23	0.74	−2.49
BUT14DIOL	−0.52	0.52	0.56	0.19	0.96	0.09	−0.87

Table S132: Statistical analysis for the MN12L DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.74	4.16	5.56	0.01	40.63	15.45	−25.18
G21EA	−1.63	3.41	4.58	0.10	17.74	5.35	−12.39
G21IP	−2.64	4.65	5.74	0.02	22.22	10.30	−11.92
DIPCS10	−14.64	14.64	16.40	0.02	22.12	−1.14	−23.26
PA26	2.25	3.11	3.78	0.02	10.88	6.94	−3.94
SIE4x4	7.45	9.22	11.47	0.27	30.58	24.19	−6.39
ALKBDE10	−7.74	7.74	10.51	0.08	19.71	−0.78	−20.49
YBDE18	−0.53	6.78	7.26	0.14	21.13	11.71	−9.42
AL2X6	1.51	1.52	1.88	0.04	3.24	3.21	−0.03
HEAVYSB11	−8.57	8.61	9.91	0.15	13.87	0.18	−13.69
NBPRC	−0.07	2.64	3.25	0.10	10.81	5.18	−5.63
ALK8	−3.19	8.67	14.82	0.14	51.18	12.31	−38.86
RC21	0.93	2.11	2.65	0.06	9.54	5.61	−3.94
G2RC	1.72	6.55	13.41	0.13	70.25	59.47	−10.79
BH76RC	0.59	2.34	3.46	0.11	17.10	6.07	−11.03
FH51	1.22	2.38	3.51	0.08	16.83	11.19	−5.64
TAUT15	1.01	2.14	2.81	0.70	9.05	6.00	−3.05
DC13	−0.52	8.09	10.58	0.15	40.47	11.52	−28.95
MB16-43	7.16	16.54	20.46	0.04	80.21	45.86	−34.35
DARC	5.83	5.83	6.57	0.18	8.50	9.24	0.75
RSE43	−2.35	2.35	2.81	0.31	8.32	−0.36	−8.69
BSR36	−0.75	1.14	1.37	0.07	5.83	2.50	−3.34
CDIE20	1.84	1.84	2.07	0.45	3.37	3.50	0.14
ISO34	0.02	1.39	1.99	0.10	9.43	5.24	−4.19
ISOL24	−1.26	4.41	6.24	0.20	30.27	20.95	−9.33
C60ISO	−2.12	3.39	4.65	0.03	12.13	1.93	−10.20
PArel	1.70	2.01	3.15	0.43	10.89	9.25	−1.64
BH76	−0.80	1.75	2.41	0.09	13.60	5.01	−8.58
BHPERI	1.96	2.70	3.04	0.13	9.73	5.61	−4.12
BHDIV10	−0.37	2.10	2.21	0.05	5.67	2.81	−2.86
INV24	0.26	2.07	3.62	0.06	19.13	12.05	−7.08
BHROT27	1.14	1.16	1.58	0.19	3.85	3.58	−0.27
PX13	4.39	4.57	5.36	0.14	10.16	9.53	−0.63
WCPT18	0.14	1.51	1.85	0.04	6.75	3.04	−3.70
RG18	−1.08	1.08	1.42	1.86	3.21	−0.28	−3.49
ADIM6	−0.50	0.57	0.63	0.17	1.12	0.22	−0.90
S22	−0.97	1.10	1.40	0.15	4.26	0.72	−3.53
S66	−0.86	0.87	1.02	0.16	2.16	0.04	−2.12
HEAVY28	−0.64	0.65	0.74	0.52	1.45	0.13	−1.32
WATER27	−10.82	11.15	16.65	0.14	45.75	4.46	−41.29
CARBHB12	−1.04	1.04	1.12	0.17	1.64	−0.28	−1.92
PNICO23	−0.49	0.52	0.60	0.12	1.80	0.42	−1.38
HAL59	−0.93	0.95	1.09	0.21	2.86	0.32	−2.54
AHB21	1.44	1.47	1.61	0.07	3.43	3.13	−0.29
CHB6	−0.06	0.59	0.69	0.02	2.12	0.92	−1.19
IL16	1.87	1.87	1.99	0.02	2.32	2.94	0.61
IDISP	2.62	6.78	9.24	0.48	26.80	19.40	−7.40
ICONF	0.02	0.49	0.62	0.15	2.34	1.27	−1.07
ACONF	−0.63	0.63	0.73	0.34	1.17	−0.15	−1.32
AMINO20x4	0.13	0.75	0.98	0.31	4.70	2.63	−2.07
PCONF21	1.35	2.47	2.87	1.52	8.94	5.23	−3.71
MCONF	0.89	1.05	1.28	0.21	3.27	2.60	−0.67
SCONF	0.17	0.57	0.83	0.12	3.80	1.67	−2.12
UPU23	−0.18	0.83	1.05	0.15	4.01	1.94	−2.07
BUT14DIOL	−0.68	0.68	0.75	0.24	1.30	−0.23	−1.53

Table S133: Statistical analysis for the MN15L DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	0.05	3.41	4.67	0.01	33.14	11.22	−21.92
G21EA	0.97	2.40	2.88	0.07	11.74	6.23	−5.51
G21IP	−1.89	3.46	4.51	0.01	20.87	8.64	−12.24
DIPCS10	−10.18	10.46	12.05	0.02	20.95	1.40	−19.55
PA26	0.92	2.25	2.91	0.01	12.29	7.37	−4.92
SIE4x4	10.81	10.99	13.42	0.33	26.10	24.92	−1.18
ALKBDE10	−4.48	4.48	5.13	0.04	9.80	−0.06	−9.86
YBDE18	−4.11	4.20	5.04	0.09	9.63	0.81	−8.82
AL2X6	1.03	1.35	1.46	0.04	2.92	1.97	−0.95
HEAVYSB11	−5.72	6.47	7.54	0.11	17.18	2.87	−14.31
NBPRC	−0.47	1.93	2.98	0.07	11.76	2.92	−8.85
ALK8	−1.12	3.23	4.29	0.05	14.95	7.84	−7.10
RC21	0.75	2.00	2.55	0.06	8.51	5.92	−2.58
G2RC	2.29	6.73	8.33	0.13	28.84	18.58	−10.26
BH76RC	0.98	2.43	3.44	0.11	19.58	10.35	−9.23
FH51	0.82	2.55	3.67	0.08	19.78	13.91	−5.87
TAUT15	0.46	0.70	0.96	0.23	3.20	2.03	−1.17
DC13	3.18	7.83	10.28	0.14	32.39	25.31	−7.08
MB16-43	−9.44	20.42	25.52	0.05	103.56	44.64	−58.92
DARC	2.39	2.78	3.12	0.09	6.11	4.62	−1.49
RSE43	−0.99	1.23	1.53	0.16	7.24	1.92	−5.32
BSR36	3.55	3.55	4.40	0.22	10.87	11.29	0.42
CDIE20	1.78	1.78	1.94	0.44	2.91	3.34	0.43
ISO34	−0.82	1.88	2.34	0.13	9.49	4.80	−4.69
ISOL24	−2.29	3.54	4.70	0.16	20.31	10.32	−10.00
C60ISO	−5.79	5.94	7.92	0.06	16.54	0.67	−15.87
PArel	1.66	2.19	2.93	0.47	10.13	7.04	−3.10
BH76	−1.10	1.81	2.64	0.10	13.59	3.53	−10.06
BHPERI	0.85	1.78	2.12	0.09	8.41	4.20	−4.21
BHDIV10	−0.03	2.08	2.49	0.05	8.96	4.82	−4.15
INV24	1.26	2.02	3.74	0.06	19.15	13.52	−5.63
BHROT27	0.82	0.87	1.17	0.14	3.39	2.85	−0.54
PX13	6.38	6.38	6.87	0.19	9.00	11.11	2.10
WCPT18	1.08	1.81	2.41	0.05	6.84	4.70	−2.14
RG18	0.10	0.17	0.29	0.29	1.02	0.77	−0.25
ADIM6	3.88	3.88	4.35	1.15	5.38	6.61	1.23
S22	0.03	1.82	2.40	0.25	9.46	5.26	−4.20
S66	0.60	1.66	1.97	0.30	8.03	4.72	−3.31
HEAVY28	0.06	0.58	0.71	0.47	2.66	1.21	−1.45
WATER27	−11.26	12.01	16.74	0.15	56.07	10.09	−45.98
CARBHB12	−1.20	1.20	1.42	0.20	2.63	−0.19	−2.82
PNICO23	−0.18	0.40	0.48	0.09	1.80	0.55	−1.25
HAL59	−0.18	0.59	0.78	0.13	3.96	2.06	−1.90
AHB21	2.28	2.29	2.46	0.10	4.33	4.20	−0.12
CHB6	0.64	0.64	0.75	0.02	0.91	1.03	0.12
IL16	2.40	2.40	2.62	0.02	3.32	4.17	0.86
IDISP	2.99	7.55	8.62	0.53	22.53	14.07	−8.46
ICONF	0.11	0.53	0.65	0.16	2.50	1.43	−1.07
ACONF	−0.69	0.69	0.81	0.38	1.35	−0.15	−1.51
AMINO20x4	−0.04	0.92	1.18	0.38	6.10	3.19	−2.91
PCONF21	1.28	4.10	4.60	2.53	13.44	7.42	−6.01
MCONF	1.52	1.61	1.81	0.32	4.08	3.28	−0.80
SCONF	−0.37	0.92	1.14	0.20	3.86	1.87	−1.99
UPU23	−1.48	1.68	2.44	0.29	8.95	0.87	−8.07
BUT14DIOL	−1.10	1.10	1.16	0.39	1.76	−0.36	−2.12

SI.7.7 Results for dispersion-uncorrected hybrid functionals

Table S134: Statistical analysis for the B3LYP DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−2.95	4.22	6.44	0.01	39.87	8.01	−31.86
G21EA	0.55	1.91	2.49	0.06	10.10	7.55	−2.56
G21IP	−0.14	3.55	4.37	0.01	16.77	9.59	−7.17
DIPCS10	−2.21	4.75	5.96	0.01	19.98	9.22	−10.76
PA26	2.16	2.28	3.12	0.01	9.57	8.50	−1.07
SIE4x4	17.63	17.63	20.30	0.52	37.03	40.20	3.17
ALKBDE10	−2.08	4.57	5.37	0.05	16.24	6.39	−9.85
YBDE18	−8.38	8.47	9.92	0.17	18.80	0.82	−17.98
AL2X6	−9.05	9.05	9.52	0.25	8.81	−5.02	−13.84
HEAVYSB11	−7.91	7.91	8.43	0.14	8.73	−4.39	−13.12
NBPRC	4.37	5.19	7.27	0.19	20.33	18.01	−2.32
ALK8	−6.07	6.07	8.84	0.10	17.44	−0.30	−17.75
RC21	−0.78	2.30	3.20	0.06	13.91	3.23	−10.68
G2RC	1.25	2.56	3.24	0.05	12.32	7.44	−4.88
BH76RC	−0.38	2.38	2.87	0.11	11.37	4.36	−7.00
FH51	2.81	3.97	5.21	0.13	29.91	13.93	−15.98
TAUT15	−0.03	1.13	1.38	0.37	4.12	2.40	−1.72
DC13	4.75	15.14	19.45	0.28	66.93	31.89	−35.04
MB16-43	−57.89	57.89	61.82	0.14	105.47	−14.48	−119.95
DARC	15.75	15.75	16.13	0.49	11.30	18.98	7.68
RSE43	−1.96	1.96	2.19	0.26	3.90	−0.82	−4.71
BSR36	−10.70	10.70	12.19	0.66	24.67	−2.98	−27.65
CDIE20	1.24	1.26	1.44	0.31	2.83	2.72	−0.11
ISO34	−0.46	2.31	3.39	0.16	21.03	11.53	−9.50
ISOL24	−4.94	9.53	14.91	0.43	80.73	29.63	−51.10
C60ISO	−0.58	2.01	2.57	0.02	6.60	1.44	−5.16
PArel	0.02	1.17	1.79	0.25	8.93	5.71	−3.22
BH76	−4.02	4.94	5.90	0.27	27.38	16.59	−10.79
BHPERI	3.74	4.42	5.19	0.21	14.02	9.43	−4.59
BHDIV10	−0.92	2.76	3.40	0.06	11.14	5.33	−5.82
INV24	−1.63	1.87	2.12	0.06	5.60	1.17	−4.44
BHROT27	0.30	0.40	0.59	0.06	1.57	1.30	−0.27
PX13	−3.54	3.54	3.68	0.11	3.52	−1.75	−5.27
WCPT18	−0.94	1.11	1.45	0.03	4.53	1.12	−3.41
RG18	−0.80	0.80	1.02	1.38	2.22	−0.09	−2.31
ADIM6	−5.06	5.06	5.53	1.51	6.44	−2.00	−8.44
S22	−3.78	3.78	4.92	0.52	12.66	−0.25	−12.92
S66	−3.24	3.24	3.82	0.59	8.80	−0.20	−8.99
HEAVY28	−1.30	1.30	1.37	1.05	1.75	−0.55	−2.30
WATER27	−5.55	5.79	9.26	0.07	27.14	1.23	−25.91
CARBHB12	−0.46	0.62	0.79	0.10	2.31	0.79	−1.52
PNICO23	−1.78	1.78	1.88	0.42	2.77	−0.96	−3.72
HAL59	−1.72	1.78	2.24	0.39	9.56	1.73	−7.82
AHB21	0.83	0.86	1.03	0.04	2.78	2.43	−0.35
CHB6	0.37	1.21	1.60	0.05	4.79	3.38	−1.42
IL16	4.02	4.02	4.09	0.04	2.82	5.85	3.03
IDISP	4.29	16.42	18.96	1.15	51.07	34.73	−16.34
ICONF	0.04	0.58	0.85	0.18	4.26	2.30	−1.97
ACONF	0.96	0.96	1.07	0.52	1.50	1.85	0.35
AMINO20x4	−0.10	0.66	0.84	0.27	4.27	2.43	−1.84
PCONF21	−0.41	3.81	4.35	2.35	12.82	7.08	−5.74
MCONF	−2.43	2.49	2.82	0.50	4.71	0.38	−4.32
SCONF	−0.38	0.73	0.88	0.16	3.38	1.97	−1.41
UPU23	2.03	2.49	3.64	0.44	10.85	9.50	−1.35
BUT14DIOL	−0.19	0.38	0.44	0.14	1.61	0.82	−0.78

Table S135: Statistical analysis for the B3PW91 DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−1.21	2.99	4.69	0.01	32.87	7.33	−25.55
G21EA	1.03	2.14	2.71	0.06	7.93	5.74	−2.19
G21IP	1.08	3.63	4.37	0.01	17.95	10.56	−7.38
DIPCS10	0.45	3.14	3.39	0.00	10.09	5.06	−5.03
PA26	3.49	3.49	4.01	0.02	8.09	9.17	1.08
SIE4x4	16.02	16.02	18.25	0.48	32.32	36.11	3.79
ALKBDE10	−2.40	5.37	6.29	0.05	21.58	11.31	−10.27
YBDE18	−5.49	5.49	6.36	0.11	12.47	−0.44	−12.91
AL2X6	−5.94	5.94	6.34	0.17	6.71	−1.97	−8.68
HEAVYSB11	−5.34	5.34	6.24	0.09	9.23	−0.85	−10.07
NBPRC	2.57	2.96	4.07	0.11	10.45	8.88	−1.57
ALK8	−2.28	2.90	3.86	0.05	11.16	2.08	−9.08
RC21	1.68	2.30	2.83	0.06	7.79	5.59	−2.20
G2RC	−0.76	4.07	5.04	0.08	20.09	10.25	−9.84
BH76RC	−0.23	1.97	2.87	0.09	15.74	8.88	−6.86
FH51	1.14	2.60	3.47	0.08	16.66	9.78	−6.88
TAUT15	0.30	1.23	1.64	0.40	5.01	3.36	−1.65
DC13	1.95	8.90	11.59	0.16	36.94	18.51	−18.43
MB16-43	−29.45	29.94	34.24	0.07	76.88	7.79	−69.09
DARC	6.85	7.04	7.79	0.22	11.54	10.21	−1.34
RSE43	−1.80	1.80	2.02	0.24	3.99	−0.63	−4.62
BSR36	−9.56	9.56	10.67	0.59	21.71	−2.12	−23.83
CDIE20	1.48	1.53	1.77	0.38	3.77	3.32	−0.45
ISO34	−0.56	1.51	2.39	0.10	15.04	6.12	−8.92
ISOL24	−2.70	5.87	9.55	0.27	52.15	18.01	−34.14
C60ISO	−0.59	2.34	2.88	0.02	7.80	1.96	−5.84
PArel	0.51	1.20	1.77	0.26	7.82	5.82	−2.00
BH76	−3.98	4.11	4.64	0.22	15.62	2.57	−13.05
BHPERI	1.23	2.28	2.56	0.11	8.88	5.33	−3.54
BHDIV10	−3.27	3.91	4.37	0.09	9.38	3.20	−6.18
INV24	−1.67	1.87	2.17	0.06	8.01	2.39	−5.63
BHROT27	0.45	0.52	0.70	0.08	1.70	1.43	−0.27
PX13	−6.03	6.03	6.19	0.18	5.78	−3.39	−9.18
WCPT18	−2.95	2.95	3.27	0.08	5.77	−0.97	−6.74
RG18	−1.23	1.23	1.51	2.12	3.04	−0.30	−3.34
ADIM6	−5.91	5.91	6.41	1.76	7.19	−2.48	−9.67
S22	−4.15	4.15	5.25	0.57	12.75	−0.82	−13.57
S66	−3.74	3.74	4.28	0.68	9.09	−0.75	−9.84
HEAVY28	−1.45	1.45	1.52	1.17	1.65	−0.74	−2.40
WATER27	−9.89	10.09	15.95	0.12	44.66	1.38	−43.29
CARBHB12	−0.39	0.78	0.89	0.13	2.99	1.36	−1.63
PNICO23	−1.62	1.68	1.78	0.39	4.54	0.74	−3.80
HAL59	−1.94	2.04	2.47	0.44	10.11	1.72	−8.39
AHB21	0.62	0.88	1.14	0.04	4.12	2.96	−1.17
CHB6	1.04	1.13	1.61	0.04	3.60	3.42	−0.18
IL16	3.65	3.65	3.75	0.03	3.63	5.95	2.31
IDISP	2.49	13.52	14.93	0.95	40.00	23.88	−16.12
ICONF	0.19	0.48	0.70	0.15	3.20	2.03	−1.17
ACONF	0.89	0.89	1.00	0.49	1.37	1.65	0.28
AMINO20x4	−0.06	0.61	0.77	0.25	3.56	2.15	−1.42
PCONF21	−0.57	4.22	4.74	2.60	13.36	7.49	−5.87
MCONF	−2.36	2.45	2.77	0.49	5.20	0.81	−4.39
SCONF	−0.18	0.47	0.63	0.10	2.66	1.51	−1.15
UPU23	2.19	2.70	3.97	0.47	12.38	10.70	−1.68
BUT14DIOL	−0.33	0.46	0.52	0.16	1.65	0.67	−0.98

Table S136: Statistical analysis for the B3P86 DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	3.87	5.88	7.50	0.02	45.12	19.99	−25.13
G21EA	3.37	3.37	4.14	0.10	7.97	8.06	0.09
G21IP	2.54	3.85	4.81	0.01	16.33	11.91	−4.42
DIPCS10	3.19	3.89	4.73	0.01	9.92	7.94	−1.98
PA26	2.41	2.41	3.08	0.01	7.68	7.89	0.21
SIE4x4	17.16	17.16	19.80	0.51	36.57	39.82	3.25
ALKBDE10	−1.27	4.42	5.57	0.04	20.22	10.85	−9.37
YBDE18	−4.48	4.55	5.52	0.09	11.65	0.48	−11.17
AL2X6	−5.07	5.07	5.46	0.14	6.27	−1.47	−7.74
HEAVYSB11	−4.85	4.85	5.77	0.08	9.07	−0.35	−9.42
NBPRC	1.85	2.75	3.42	0.10	8.51	6.60	−1.91
ALK8	−2.90	3.36	4.25	0.05	10.06	1.84	−8.22
RC21	2.56	2.91	3.64	0.08	9.10	6.78	−2.31
G2RC	−1.12	4.41	5.35	0.09	21.38	10.01	−11.36
BH76RC	−0.82	2.59	3.50	0.12	16.56	6.82	−9.74
FH51	0.79	2.46	3.25	0.08	15.21	8.60	−6.61
TAUT15	0.44	1.27	1.85	0.42	5.73	3.92	−1.81
DC13	1.65	8.80	10.70	0.16	33.09	16.10	−17.00
MB16-43	−26.42	27.83	32.13	0.07	74.72	13.70	−61.02
DARC	5.95	6.24	6.93	0.19	11.15	9.12	−2.02
RSE43	−1.84	1.84	2.06	0.24	3.96	−0.67	−4.63
BSR36	−8.58	8.58	9.66	0.53	19.40	−2.34	−21.75
CDIE20	1.37	1.40	1.61	0.34	3.26	2.94	−0.32
ISO34	−0.48	1.40	2.19	0.10	13.98	6.54	−7.45
ISOL24	−2.33	5.58	8.77	0.25	48.03	18.23	−29.79
C60ISO	−0.76	2.35	2.96	0.02	7.89	1.79	−6.10
PArel	0.50	1.28	1.84	0.28	8.03	5.92	−2.11
BH76	−5.28	5.42	6.04	0.29	16.92	2.85	−14.07
BHPERI	0.14	1.60	1.87	0.08	7.56	3.62	−3.94
BHDIV10	−3.68	4.39	4.86	0.10	10.49	3.55	−6.94
INV24	−1.62	1.77	2.03	0.06	7.16	1.91	−5.25
BHROT27	0.45	0.52	0.70	0.08	1.68	1.43	−0.24
PX13	−7.37	7.37	7.56	0.22	6.77	−4.46	−11.23
WCPT18	−3.90	3.90	4.30	0.11	6.95	−1.33	−8.28
RG18	−1.13	1.13	1.41	1.95	3.05	−0.31	−3.36
ADIM6	−4.83	4.83	5.24	1.44	5.87	−2.05	−7.91
S22	−3.24	3.24	4.30	0.44	11.13	−0.20	−11.33
S66	−2.91	2.91	3.47	0.53	7.95	−0.20	−8.15
HEAVY28	−1.11	1.11	1.17	0.90	1.41	−0.56	−1.97
WATER27	−3.49	4.25	6.82	0.05	21.90	2.22	−19.69
CARBHB12	0.09	0.59	0.83	0.10	3.00	1.94	−1.06
PNICO23	−1.03	1.15	1.27	0.27	4.58	1.38	−3.20
HAL59	−1.29	1.53	1.98	0.33	9.88	2.66	−7.22
AHB21	−0.04	0.73	0.86	0.03	3.56	2.00	−1.57
CHB6	0.86	0.92	1.34	0.03	3.01	2.85	−0.16
IL16	2.58	2.58	2.67	0.02	2.83	4.41	1.58
IDISP	2.43	11.56	12.98	0.81	34.58	22.15	−12.42
ICONF	0.19	0.42	0.62	0.13	2.82	1.87	−0.95
ACONF	0.68	0.68	0.77	0.37	1.12	1.32	0.20
AMINO20x4	−0.01	0.53	0.67	0.22	3.21	1.94	−1.27
PCONF21	−0.51	3.60	4.02	2.22	11.00	6.22	−4.78
MCONF	−1.93	2.02	2.29	0.41	4.50	0.75	−3.75
SCONF	0.01	0.25	0.33	0.05	1.33	0.79	−0.54
UPU23	1.91	2.34	3.41	0.41	10.30	8.92	−1.38
BUT14DIOL	−0.01	0.24	0.30	0.09	1.27	0.78	−0.49

Table S137: Statistical analysis for the BHLYP DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−21.46	21.50	25.52	0.07	65.23	2.46	−62.76
G21EA	−4.33	5.35	6.09	0.16	17.54	5.54	−12.00
G21IP	−1.53	4.53	5.53	0.02	22.39	11.35	−11.04
DIPCS10	−3.77	7.12	8.81	0.01	26.63	8.17	−18.47
PA26	3.19	3.30	4.08	0.02	10.98	9.54	−1.44
SIE4x4	7.13	7.14	9.61	0.21	22.19	22.13	−0.06
ALKBDE10	−13.74	13.74	15.52	0.14	26.82	−4.60	−31.43
YBDE18	−8.80	8.80	9.05	0.18	7.54	−5.71	−13.25
AL2X6	−6.53	6.53	7.24	0.18	9.59	−1.59	−11.18
HEAVYSB11	−10.01	10.01	10.17	0.17	6.91	−5.85	−12.76
NBPRC	3.43	4.61	5.68	0.17	16.89	12.68	−4.20
ALK8	−4.39	5.77	8.77	0.09	21.60	3.41	−18.19
RC21	−0.44	2.47	3.15	0.07	12.85	5.55	−7.30
G2RC	−2.88	3.94	4.84	0.08	19.35	6.83	−12.52
BH76RC	−1.23	3.94	4.97	0.18	22.34	9.35	−12.99
FH51	−0.05	2.08	3.20	0.07	22.68	9.56	−13.12
TAUT15	−0.01	0.60	0.84	0.20	3.57	1.26	−2.30
DC13	1.38	13.45	16.67	0.24	64.40	32.99	−31.41
MB16-43	−57.78	58.30	67.57	0.14	179.80	11.11	−168.69
DARC	8.34	8.34	8.78	0.26	9.94	10.89	0.95
RSE43	−0.47	0.58	0.73	0.08	2.46	0.73	−1.73
BSR36	−10.29	10.29	11.75	0.64	22.54	−3.73	−26.27
CDIE20	0.69	0.83	1.05	0.20	2.98	2.37	−0.61
ISO34	0.06	1.62	2.63	0.11	18.74	10.18	−8.55
ISOL24	−2.51	6.33	9.49	0.29	50.16	16.03	−34.13
C60ISO	12.59	12.59	13.63	0.13	16.35	21.63	5.28
PArel	0.53	1.23	1.71	0.27	6.52	4.82	−1.70
BH76	1.85	3.50	8.52	0.19	60.64	51.41	−9.22
BHPERI	7.69	7.69	8.18	0.37	11.42	12.62	1.20
BHDIV10	3.63	3.63	4.35	0.08	6.68	7.00	0.32
INV24	0.10	2.12	3.46	0.07	19.75	13.20	−6.55
BHROT27	0.54	0.57	0.85	0.09	2.11	1.95	−0.16
PX13	2.65	2.65	2.94	0.08	3.55	4.09	0.54
WCPT18	4.43	4.43	4.68	0.13	6.48	8.92	2.44
RG18	−0.55	0.55	0.73	0.95	1.71	−0.01	−1.72
ADIM6	−4.06	4.06	4.45	1.21	5.31	−1.52	−6.83
S22	−2.83	2.87	3.99	0.39	10.88	0.35	−10.52
S66	−2.42	2.44	3.04	0.45	7.40	0.33	−7.07
HEAVY28	−1.12	1.12	1.19	0.90	1.47	−0.46	−1.93
WATER27	−2.86	3.20	5.57	0.04	17.27	1.19	−16.08
CARBHB12	−0.43	0.59	0.77	0.10	2.32	0.50	−1.82
PNICO23	−1.54	1.54	1.74	0.36	3.10	−0.49	−3.59
HAL59	−1.69	1.69	2.02	0.37	6.14	−0.32	−6.45
AHB21	−0.02	0.94	1.26	0.04	5.40	1.66	−3.75
CHB6	−1.12	1.75	1.98	0.07	4.78	1.89	−2.89
IL16	3.48	3.48	3.59	0.03	3.20	5.19	1.99
IDISP	2.25	14.05	15.64	0.99	43.47	24.52	−18.94
ICONF	0.13	0.67	0.85	0.20	3.78	1.95	−1.82
ACONF	0.88	0.88	0.98	0.48	1.26	1.57	0.31
AMINO20x4	−0.02	0.61	0.78	0.25	3.90	2.43	−1.47
PCONF21	0.01	2.88	3.46	1.78	10.56	5.85	−4.71
MCONF	−1.97	2.04	2.33	0.41	4.18	0.59	−3.58
SCONF	−0.54	1.06	1.21	0.23	4.09	2.53	−1.56
UPU23	1.91	2.14	3.12	0.37	8.53	7.57	−0.96
BUT14DIOL	−0.25	0.37	0.42	0.13	1.50	0.61	−0.89

Table S138: Statistical analysis for the B1P86 DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.94	4.79	6.69	0.02	45.21	14.51	−30.70
G21EA	1.97	2.75	3.54	0.08	9.82	7.20	−2.62
G21IP	1.65	3.77	4.58	0.01	16.51	11.24	−5.26
DIPCS10	1.92	3.67	4.13	0.01	11.16	7.04	−4.12
PA26	2.64	2.64	3.27	0.01	8.07	8.06	−0.01
SIE4x4	15.09	15.09	17.61	0.45	33.23	36.39	3.16
ALKBDE10	−4.29	5.48	6.68	0.05	19.81	5.47	−14.34
YBDE18	−4.55	4.55	5.02	0.09	8.70	−0.98	−9.67
AL2X6	−4.41	4.41	4.78	0.12	5.75	−1.09	−6.84
HEAVYSB11	−5.45	5.45	6.06	0.09	7.82	−1.81	−9.63
NBPRC	1.56	2.56	3.04	0.09	7.66	5.58	−2.08
ALK8	−2.58	3.27	4.03	0.05	10.26	2.78	−7.48
RC21	2.64	3.06	3.75	0.09	10.01	8.17	−1.83
G2RC	−1.90	4.89	5.94	0.10	23.90	9.91	−13.99
BH76RC	−0.94	2.70	3.50	0.13	14.08	4.44	−9.64
FH51	0.22	2.20	2.95	0.07	14.22	7.77	−6.45
TAUT15	0.50	1.15	1.73	0.38	5.36	3.72	−1.65
DC13	0.98	7.98	10.10	0.15	32.15	17.68	−14.47
MB16-43	−25.20	26.90	31.18	0.06	79.97	19.45	−60.52
DARC	3.74	4.38	5.06	0.13	10.80	6.79	−4.01
RSE43	−1.46	1.46	1.65	0.19	3.33	−0.54	−3.87
BSR36	−8.36	8.36	9.39	0.52	18.69	−2.36	−21.05
CDIE20	1.27	1.31	1.54	0.32	3.27	2.89	−0.38
ISO34	−0.41	1.45	2.10	0.10	12.71	5.64	−7.07
ISOL24	−1.65	4.65	7.29	0.21	39.44	14.61	−24.83
C60ISO	1.26	2.45	2.58	0.02	6.69	3.91	−2.77
PArel	0.62	1.17	1.76	0.25	7.68	5.65	−2.03
BH76	−4.32	4.53	5.09	0.24	13.83	2.91	−10.92
BHPERI	0.38	1.40	1.70	0.07	6.86	3.53	−3.33
BHDIV10	−3.23	3.90	4.27	0.09	9.48	3.35	−6.13
INV24	−1.67	1.87	2.17	0.06	8.01	2.39	−5.63
BHROT27	0.48	0.53	0.71	0.08	1.58	1.36	−0.22
PX13	−6.56	6.56	6.75	0.20	6.34	−3.76	−10.10
WCPT18	−3.20	3.20	3.68	0.09	6.76	−0.57	−7.32
RG18	−1.19	1.19	1.49	2.05	3.29	−0.34	−3.63
ADIM6	−4.84	4.84	5.23	1.44	5.79	−2.07	−7.86
S22	−3.17	3.17	4.21	0.43	10.95	−0.07	−11.02
S66	−2.89	2.89	3.43	0.53	7.86	−0.10	−7.97
HEAVY28	−1.13	1.13	1.19	0.91	1.38	−0.58	−1.96
WATER27	−3.94	4.62	7.46	0.06	23.41	2.05	−21.36
CARBHB12	0.04	0.58	0.80	0.10	2.96	1.87	−1.09
PNICO23	−1.01	1.13	1.25	0.26	4.51	1.33	−3.18
HAL59	−1.36	1.55	1.97	0.34	9.27	2.15	−7.11
AHB21	−0.10	0.81	0.96	0.04	3.79	1.97	−1.82
CHB6	0.77	0.86	1.24	0.03	2.79	2.65	−0.14
IL16	2.52	2.52	2.62	0.02	2.78	4.35	1.57
IDISP	1.87	10.73	11.88	0.75	31.13	19.22	−11.91
ICONF	0.21	0.41	0.59	0.13	2.55	1.73	−0.82
ACONF	0.64	0.64	0.72	0.35	1.06	1.22	0.16
AMINO20x4	0.00	0.51	0.64	0.21	3.11	1.88	−1.22
PCONF21	−0.45	3.45	3.87	2.13	10.61	6.01	−4.60
MCONF	−1.86	1.94	2.21	0.39	4.35	0.73	−3.62
SCONF	0.01	0.23	0.31	0.05	1.31	0.79	−0.51
UPU23	1.92	2.32	3.37	0.41	10.07	8.77	−1.30
BUT14DIOL	−0.04	0.23	0.29	0.08	1.19	0.70	−0.49

Table S139: Statistical analysis for the B1LYP DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−9.02	9.15	11.17	0.03	37.78	3.30	−34.49
G21EA	−1.52	2.61	3.08	0.08	11.27	6.65	−4.62
G21IP	−1.93	4.22	4.95	0.02	17.22	7.88	−9.34
DIPCS10	−4.80	6.28	7.86	0.01	22.35	7.30	−15.05
PA26	2.33	2.46	3.30	0.01	10.13	8.80	−1.33
SIE4x4	15.68	15.68	18.20	0.47	33.80	36.86	3.06
ALKBDE10	−5.16	5.29	7.00	0.05	14.75	0.57	−14.18
YBDE18	−9.36	9.36	10.39	0.19	16.01	−2.13	−18.14
AL2X6	−9.30	9.30	9.80	0.26	8.83	−5.46	−14.30
HEAVYSB11	−9.13	9.13	9.46	0.16	7.68	−6.36	−14.04
NBPRC	4.67	5.50	7.65	0.20	21.34	18.80	−2.55
ALK8	−6.50	6.50	9.76	0.10	19.59	−0.05	−19.64
RC21	−1.49	2.37	3.51	0.07	15.21	3.68	−11.53
G2RC	1.04	2.39	2.98	0.05	9.52	5.88	−3.64
BH76RC	−0.37	2.39	2.87	0.11	11.49	5.28	−6.21
FH51	2.70	3.87	5.15	0.12	30.36	13.33	−17.03
TAUT15	−0.11	0.95	1.14	0.31	3.60	1.71	−1.89
DC13	4.87	15.23	20.37	0.28	73.60	36.07	−37.53
MB16-43	−64.03	64.03	68.24	0.15	118.16	−19.16	−137.32
DARC	15.91	15.91	16.25	0.49	11.07	19.09	8.02
RSE43	−1.53	1.53	1.75	0.20	3.35	−0.52	−3.87
BSR36	−11.44	11.44	13.02	0.71	25.92	−3.46	−29.37
CDIE20	1.11	1.12	1.31	0.28	2.73	2.60	−0.13
ISO34	−0.39	2.35	3.44	0.16	21.53	11.90	−9.63
ISOL24	−4.88	9.50	14.83	0.43	80.12	28.73	−51.38
C60ISO	1.82	2.51	2.73	0.03	6.91	5.10	−1.81
PArel	0.03	1.13	1.66	0.24	7.77	5.38	−2.39
BH76	−3.51	3.62	4.30	0.19	11.79	1.31	−10.49
BHPERI	4.89	5.33	6.13	0.26	14.25	10.74	−3.51
BHDIV10	0.20	2.30	3.05	0.05	10.16	5.58	−4.58
INV24	−1.37	1.80	2.03	0.06	6.51	2.95	−3.55
BHROT27	0.30	0.37	0.56	0.06	1.37	1.17	−0.20
PX13	−1.85	1.85	2.06	0.06	2.95	−0.43	−3.38
WCPT18	0.45	0.84	1.01	0.02	3.54	2.22	−1.32
RG18	−0.77	0.77	0.98	1.33	2.01	−0.05	−2.06
ADIM6	−5.05	5.05	5.53	1.50	6.56	−1.96	−8.52
S22	−3.85	3.85	4.98	0.53	12.64	−0.33	−12.96
S66	−3.27	3.27	3.84	0.60	8.76	−0.23	−8.99
HEAVY28	−1.39	1.39	1.46	1.12	1.76	−0.63	−2.38
WATER27	−6.61	6.71	10.58	0.08	29.80	0.84	−28.97
CARBHB12	−0.65	0.73	0.93	0.12	2.50	0.46	−2.04
PNICO23	−1.93	1.93	2.05	0.45	2.84	−0.99	−3.83
HAL59	−1.89	1.93	2.34	0.42	8.91	1.03	−7.88
AHB21	0.96	0.98	1.15	0.04	2.65	2.49	−0.16
CHB6	0.16	1.30	1.64	0.05	5.03	3.33	−1.70
IL16	4.28	4.28	4.36	0.04	2.95	6.12	3.17
IDISP	4.30	16.59	19.18	1.17	52.29	35.02	−17.28
ICONF	0.03	0.58	0.85	0.18	4.21	2.17	−2.05
ACONF	0.92	0.92	1.04	0.50	1.53	1.81	0.28
AMINO20x4	−0.12	0.67	0.85	0.27	4.36	2.48	−1.88
PCONF21	−0.35	3.69	4.27	2.28	12.74	6.98	−5.75
MCONF	−2.47	2.52	2.86	0.51	4.77	0.44	−4.32
SCONF	−0.49	0.91	1.06	0.20	3.83	2.21	−1.62
UPU23	2.12	2.55	3.70	0.45	10.92	9.65	−1.27
BUT14DIOL	−0.29	0.45	0.50	0.16	1.65	0.80	−0.84

Table S140: Statistical analysis for the B1B95 DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	0.33	2.90	4.27	0.01	38.15	15.62	−22.53
G21EA	−1.72	2.01	2.34	0.06	6.76	1.30	−5.46
G21IP	−1.74	2.91	3.61	0.01	14.22	4.57	−9.65
DIPCS10	−5.38	5.38	6.09	0.01	7.96	−2.14	−10.10
PA26	2.31	2.33	2.92	0.01	7.56	7.36	−0.20
SIE4x4	16.01	16.01	18.24	0.47	32.82	35.88	3.06
ALKBDE10	−2.58	4.65	5.56	0.05	18.83	8.85	−9.98
YBDE18	−3.83	4.46	5.66	0.09	13.70	2.76	−10.95
AL2X6	−3.40	3.40	3.71	0.09	4.25	−0.53	−4.79
HEAVYSB11	−3.05	3.72	4.53	0.06	10.48	2.20	−8.28
NBPRC	1.55	2.13	3.19	0.08	9.13	7.16	−1.97
ALK8	−0.24	2.67	2.98	0.04	7.77	3.39	−4.38
RC21	1.61	2.37	2.95	0.07	9.62	6.71	−2.91
G2RC	0.06	3.29	4.19	0.06	16.13	9.67	−6.46
BH76RC	0.20	1.58	2.39	0.07	13.45	9.09	−4.36
FH51	1.30	2.36	3.13	0.08	15.71	9.42	−6.30
TAUT15	0.37	0.98	1.42	0.32	4.42	3.10	−1.33
DC13	1.29	8.65	10.81	0.16	38.41	22.46	−15.95
MB16-43	−10.44	15.74	19.29	0.04	66.29	26.23	−40.06
DARC	5.90	5.90	6.62	0.18	8.56	8.97	0.41
RSE43	−2.45	2.45	2.73	0.32	5.00	−0.86	−5.86
BSR36	−6.28	6.28	6.87	0.39	14.07	−0.38	−14.45
CDIE20	1.37	1.42	1.66	0.35	3.45	3.04	−0.42
ISO34	−0.90	1.59	2.09	0.11	8.87	3.13	−5.75
ISOL24	−2.59	5.17	7.44	0.24	38.06	13.49	−24.57
C60ISO	−0.45	2.34	2.82	0.02	8.11	2.60	−5.52
PArel	0.66	1.14	1.72	0.25	6.88	5.54	−1.34
BH76	−3.24	3.29	3.81	0.18	12.96	1.48	−11.48
BHPERI	1.33	2.32	2.53	0.11	7.99	3.81	−4.18
BHDIV10	−3.08	3.15	3.51	0.07	6.36	0.35	−6.01
INV24	−1.49	1.70	2.07	0.05	7.65	2.38	−5.27
BHROT27	0.48	0.58	0.76	0.09	2.04	1.54	−0.51
PX13	−2.87	2.87	2.95	0.09	2.75	−1.18	−3.93
WCPT18	−1.96	1.99	2.36	0.06	4.79	0.29	−4.51
RG18	−1.00	1.00	1.19	1.72	2.19	−0.24	−2.43
ADIM6	−4.03	4.03	4.27	1.20	4.07	−1.97	−6.04
S22	−3.44	3.44	4.07	0.47	8.23	−0.79	−9.02
S66	−3.02	3.02	3.28	0.55	6.43	−0.86	−7.29
HEAVY28	−1.37	1.37	1.40	1.10	1.31	−0.67	−1.98
WATER27	−12.73	12.74	19.77	0.16	50.81	0.11	−50.70
CARBHB12	−0.89	0.93	1.06	0.15	2.05	0.27	−1.78
PNICO23	−1.59	1.60	1.70	0.37	3.61	0.13	−3.48
HAL59	−1.85	1.88	2.15	0.41	6.97	0.72	−6.25
AHB21	1.19	1.19	1.35	0.05	2.47	2.66	0.19
CHB6	0.31	0.98	1.33	0.04	4.22	2.41	−1.81
IL16	3.72	3.72	3.75	0.03	2.21	4.96	2.75
IDISP	2.16	8.33	9.99	0.59	27.89	19.50	−8.39
ICONF	0.11	0.27	0.39	0.08	1.35	0.88	−0.48
ACONF	0.37	0.37	0.40	0.20	0.56	0.68	0.12
AMINO20x4	−0.01	0.44	0.55	0.18	2.67	1.50	−1.16
PCONF21	0.07	2.37	2.74	1.46	7.80	4.70	−3.10
MCONF	−1.45	1.54	1.78	0.31	3.99	0.85	−3.13
SCONF	−0.08	0.25	0.31	0.05	1.08	0.56	−0.52
UPU23	1.73	2.09	3.00	0.37	8.94	7.82	−1.12
BUT14DIOL	−0.65	0.65	0.68	0.23	0.85	−0.12	−0.97

Table S141: Statistical analysis for the MPW1B95 DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.18	2.56	4.14	0.01	42.08	15.97	−26.11
G21EA	−1.74	2.10	2.51	0.06	7.11	1.57	−5.54
G21IP	−1.16	2.80	3.39	0.01	14.71	5.98	−8.73
DIPCS10	−3.91	3.91	4.94	0.01	9.35	−0.28	−9.63
PA26	1.87	1.95	2.56	0.01	7.10	6.71	−0.40
SIE4x4	14.16	14.16	16.13	0.42	29.53	32.06	2.53
ALKBDE10	−3.52	4.74	5.75	0.05	17.92	5.08	−12.84
YBDE18	−2.24	3.17	3.90	0.06	10.92	3.06	−7.86
AL2X6	−1.46	1.70	1.84	0.05	3.50	0.71	−2.79
HEAVYSB11	−2.13	2.94	3.48	0.05	8.62	2.13	−6.49
NBPRC	0.44	2.00	2.31	0.07	7.77	4.83	−2.94
ALK8	1.56	2.54	3.35	0.04	8.02	5.22	−2.80
RC21	2.62	3.13	3.80	0.09	11.03	8.03	−2.99
G2RC	−1.50	3.98	4.87	0.08	20.71	10.21	−10.50
BH76RC	−0.03	1.72	2.35	0.08	11.89	7.18	−4.70
FH51	0.14	1.64	2.28	0.05	11.47	6.43	−5.05
TAUT15	0.43	0.95	1.42	0.31	4.43	3.12	−1.32
DC13	−0.39	8.70	10.33	0.16	36.98	23.05	−13.93
MB16-43	−1.85	10.30	12.68	0.02	55.43	25.46	−29.96
DARC	2.52	3.26	3.72	0.10	8.06	5.43	−2.63
RSE43	−2.13	2.13	2.40	0.28	4.55	−0.75	−5.30
BSR36	−5.69	5.69	6.24	0.35	12.38	−0.91	−13.29
CDIE20	1.21	1.26	1.50	0.31	3.29	2.89	−0.40
ISO34	−0.72	1.52	1.96	0.10	7.72	3.22	−4.50
ISOL24	−1.63	3.87	5.43	0.18	25.65	9.31	−16.33
C60ISO	2.08	2.68	2.90	0.03	5.84	4.48	−1.36
PArel	0.77	1.08	1.69	0.23	6.89	5.40	−1.49
BH76	−2.78	2.91	3.32	0.16	10.94	1.69	−9.25
BHPERI	0.96	1.71	1.97	0.08	7.39	3.48	−3.91
BHDIV10	−2.55	2.66	2.97	0.06	5.55	0.54	−5.01
INV24	−0.97	1.51	2.00	0.05	8.90	4.58	−4.32
BHROT27	0.56	0.64	0.85	0.10	2.18	1.75	−0.43
PX13	−2.30	2.30	2.39	0.07	2.38	−0.76	−3.14
WCPT18	−1.64	1.67	1.97	0.05	4.58	0.22	−4.36
RG18	−0.28	0.41	0.55	0.71	1.88	0.72	−1.15
ADIM6	−2.42	2.42	2.57	0.72	2.56	−1.09	−3.65
S22	−2.19	2.19	2.76	0.30	6.07	−0.24	−6.31
S66	−1.83	1.83	2.08	0.33	4.88	−0.21	−5.09
HEAVY28	−0.80	0.80	0.84	0.65	0.97	−0.32	−1.29
WATER27	−6.00	6.13	10.08	0.08	27.93	0.86	−27.07
CARBHB12	−0.21	0.43	0.54	0.07	1.84	0.93	−0.92
PNICO23	−0.78	0.85	0.97	0.20	3.41	0.86	−2.55
HAL59	−1.08	1.16	1.40	0.25	5.49	1.10	−4.39
AHB21	0.20	0.63	0.74	0.03	2.73	1.50	−1.23
CHB6	−0.93	1.38	1.70	0.05	4.50	1.07	−3.43
IL16	2.48	2.48	2.52	0.02	1.72	3.41	1.68
IDISP	1.53	6.07	7.45	0.43	22.48	14.56	−7.92
ICONF	0.14	0.27	0.38	0.08	1.33	0.99	−0.35
ACONF	0.18	0.18	0.20	0.10	0.34	0.36	0.02
AMINO20x4	0.05	0.41	0.52	0.17	2.37	1.26	−1.10
PCONF21	0.18	1.67	1.95	1.03	5.49	3.54	−1.96
MCONF	−0.96	1.06	1.25	0.21	3.08	0.73	−2.35
SCONF	−0.05	0.18	0.23	0.04	0.93	0.54	−0.38
UPU23	1.40	1.63	2.31	0.28	6.42	5.64	−0.78
BUT14DIOL	−0.48	0.48	0.50	0.17	0.61	−0.10	−0.72

Table S142: Statistical analysis for the PW6B95 DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.82	2.43	4.75	0.01	45.77	11.35	−34.42
G21EA	0.29	1.27	1.67	0.04	6.75	4.60	−2.15
G21IP	0.97	2.77	3.47	0.01	14.45	8.06	−6.39
DIPCS10	0.26	2.74	3.35	0.00	11.27	5.09	−6.18
PA26	2.31	2.35	2.93	0.01	8.23	7.66	−0.57
SIE4x4	15.23	15.23	17.37	0.45	31.58	34.27	2.69
ALKBDE10	−2.50	4.06	5.02	0.04	16.84	5.97	−10.87
YBDE18	−3.71	4.12	5.26	0.08	11.97	2.15	−9.82
AL2X6	−2.39	2.39	2.68	0.07	3.50	−0.11	−3.61
HEAVYSB11	−3.11	3.24	4.04	0.06	8.39	0.70	−7.69
NBPRC	1.09	2.19	2.92	0.08	8.64	6.23	−2.40
ALK8	1.36	2.08	2.72	0.03	6.98	4.94	−2.04
RC21	1.60	2.36	2.83	0.07	8.86	6.06	−2.79
G2RC	−0.43	2.89	3.50	0.06	13.62	7.97	−5.64
BH76RC	−0.01	1.45	2.05	0.07	10.44	5.66	−4.78
FH51	0.99	2.04	2.69	0.07	13.75	6.99	−6.76
TAUT15	0.22	0.90	1.23	0.30	4.25	2.69	−1.56
DC13	0.51	8.30	10.18	0.15	35.06	17.58	−17.48
MB16-43	−10.68	12.21	14.95	0.03	46.06	10.32	−35.75
DARC	6.10	6.10	6.67	0.19	7.85	8.78	0.93
RSE43	−2.23	2.23	2.48	0.29	4.40	−0.94	−5.33
BSR36	−6.08	6.08	6.78	0.38	14.39	−1.07	−15.47
CDIE20	1.19	1.21	1.42	0.30	2.82	2.59	−0.23
ISO34	−0.73	1.43	1.83	0.10	8.75	4.09	−4.66
ISOL24	−2.72	5.13	7.34	0.23	37.61	14.36	−23.25
C60ISO	−0.57	1.58	2.13	0.02	5.77	1.31	−4.46
PArel	0.56	0.98	1.58	0.21	6.47	5.43	−1.05
BH76	−2.46	3.81	5.39	0.20	33.05	24.62	−8.43
BHPERI	1.35	1.92	2.15	0.09	6.61	3.46	−3.15
BHDIV10	−2.06	2.30	2.52	0.05	5.53	1.20	−4.33
INV24	−1.18	1.50	1.88	0.05	7.54	3.29	−4.25
BHROT27	0.48	0.57	0.76	0.09	1.85	1.54	−0.32
PX13	−1.29	1.35	1.52	0.04	3.05	0.35	−2.70
WCPT18	−1.04	1.10	1.45	0.03	3.64	0.27	−3.37
RG18	−0.09	0.24	0.31	0.41	1.26	0.49	−0.77
ADIM6	−2.04	2.04	2.28	0.61	2.97	−0.68	−3.65
S22	−1.96	1.96	2.50	0.27	5.61	−0.17	−5.78
S66	−1.60	1.60	1.83	0.29	4.51	−0.07	−4.58
HEAVY28	−0.61	0.61	0.65	0.49	0.87	−0.14	−1.00
WATER27	−5.09	5.20	8.76	0.06	24.62	0.67	−23.95
CARBHB12	−0.13	0.35	0.47	0.06	1.78	0.83	−0.94
PNICO23	−0.70	0.73	0.85	0.17	2.66	0.31	−2.35
HAL59	−0.87	0.96	1.20	0.21	5.21	1.37	−3.84
AHB21	0.25	0.51	0.60	0.02	1.83	1.27	−0.57
CHB6	−0.89	1.17	1.47	0.04	3.79	0.84	−2.95
IL16	2.50	2.50	2.54	0.02	1.59	3.42	1.83
IDISP	2.32	7.13	8.99	0.50	26.96	18.30	−8.66
ICONF	0.05	0.26	0.35	0.08	1.17	0.83	−0.35
ACONF	0.21	0.21	0.22	0.11	0.24	0.33	0.09
AMINO20x4	0.02	0.38	0.49	0.16	2.21	1.14	−1.08
PCONF21	0.25	1.38	1.66	0.85	4.64	3.03	−1.61
MCONF	−0.91	1.00	1.17	0.20	2.84	0.62	−2.22
SCONF	−0.12	0.25	0.29	0.05	1.06	0.52	−0.54
UPU23	1.20	1.47	2.04	0.26	5.47	4.73	−0.74
BUT14DIOL	−0.50	0.50	0.51	0.18	0.59	−0.07	−0.66

Table S143: Statistical analysis for the MPWB1K DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−6.98	7.26	9.68	0.02	46.71	9.51	−37.21
G21EA	−3.24	3.57	4.36	0.11	10.47	1.87	−8.61
G21IP	−1.18	3.10	3.84	0.01	17.53	8.55	−8.97
DIPCS10	−3.47	4.21	5.29	0.01	15.14	3.67	−11.46
PA26	2.35	2.41	3.03	0.01	7.42	7.04	−0.38
SIE4x4	9.58	9.58	11.27	0.28	22.30	24.33	2.02
ALKBDE10	−8.09	8.09	9.60	0.08	20.41	−1.61	−22.01
YBDE18	−2.08	2.26	2.91	0.05	7.05	0.90	−6.15
AL2X6	−0.41	0.80	0.96	0.02	2.80	1.15	−1.66
HEAVYSB11	−2.75	2.80	3.32	0.05	5.38	0.28	−5.10
NBPRC	−0.02	2.12	2.42	0.08	7.06	4.30	−2.76
ALK8	2.29	2.88	3.71	0.05	8.64	6.73	−1.91
RC21	2.85	3.43	4.29	0.10	15.53	12.45	−3.08
G2RC	−3.48	5.10	6.27	0.10	26.57	11.84	−14.73
BH76RC	−0.47	2.40	2.76	0.11	9.36	3.19	−6.17
FH51	−1.20	2.00	2.46	0.06	10.27	4.02	−6.25
TAUT15	0.47	0.93	1.28	0.30	4.03	2.53	−1.50
DC13	−1.99	9.62	11.69	0.17	42.03	25.29	−16.74
MB16-43	−0.14	9.99	13.00	0.02	59.02	30.75	−28.27
DARC	−1.14	2.03	2.70	0.06	7.56	1.51	−6.05
RSE43	−1.43	1.43	1.65	0.19	3.44	−0.46	−3.90
BSR36	−5.68	5.68	6.20	0.35	11.77	−1.26	−13.04
CDIE20	1.00	1.11	1.38	0.27	3.51	2.96	−0.55
ISO34	−0.50	1.70	2.18	0.12	8.22	3.52	−4.70
ISOL24	−0.45	3.04	3.90	0.14	16.99	8.62	−8.37
C60ISO	7.48	7.48	7.97	0.08	9.59	13.05	3.45
PArel	1.01	1.23	1.80	0.27	6.30	5.02	−1.28
BH76	−0.49	1.31	1.68	0.07	8.30	3.71	−4.59
BHPERI	2.55	2.79	3.21	0.13	9.97	6.91	−3.06
BHDIV10	−0.74	1.54	1.73	0.03	4.66	1.53	−3.13
INV24	−0.06	1.89	3.00	0.06	16.06	9.81	−6.25
BHROT27	0.68	0.74	0.99	0.12	2.42	2.11	−0.30
PX13	0.15	0.69	0.80	0.02	2.78	1.86	−0.92
WCPT18	0.55	0.86	1.20	0.02	5.21	3.99	−1.22
RG18	−0.27	0.40	0.52	0.69	1.78	0.68	−1.10
ADIM6	−2.19	2.19	2.32	0.65	2.26	−0.99	−3.25
S22	−1.89	1.89	2.45	0.26	5.35	−0.16	−5.51
S66	−1.60	1.60	1.84	0.29	4.37	−0.11	−4.48
HEAVY28	−0.79	0.79	0.82	0.64	0.81	−0.43	−1.24
WATER27	−5.44	5.56	9.43	0.07	25.92	0.64	−25.28
CARBHB12	−0.24	0.42	0.54	0.07	1.90	0.83	−1.07
PNICO23	−0.74	0.76	0.90	0.18	2.69	0.24	−2.46
HAL59	−1.14	1.16	1.37	0.25	4.54	0.60	−3.94
AHB21	−0.15	0.85	1.10	0.04	4.55	1.26	−3.29
CHB6	−1.42	1.61	2.12	0.06	4.80	0.49	−4.30
IL16	2.32	2.32	2.37	0.02	1.66	3.28	1.61
IDISP	0.55	4.93	5.90	0.35	18.50	9.61	−8.88
ICONF	0.18	0.35	0.48	0.11	1.73	1.20	−0.54
ACONF	0.11	0.12	0.14	0.07	0.35	0.29	−0.06
AMINO20x4	0.08	0.43	0.58	0.18	2.52	1.23	−1.28
PCONF21	0.34	1.39	1.72	0.86	5.00	3.43	−1.58
MCONF	−0.80	0.90	1.08	0.18	2.71	0.66	−2.05
SCONF	−0.11	0.26	0.30	0.06	1.19	0.72	−0.46
UPU23	1.39	1.58	2.19	0.28	5.78	5.08	−0.70
BUT14DIOL	−0.52	0.52	0.53	0.19	0.62	−0.11	−0.73

Table S144: Statistical analysis for the mPW1LYP DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−6.27	6.61	8.51	0.02	36.66	3.84	−32.82
G21EA	−0.81	2.23	2.77	0.07	11.22	7.16	−4.06
G21IP	−1.34	4.08	4.78	0.02	17.03	8.46	−8.57
DIPCS10	−3.55	5.97	7.43	0.01	23.70	9.96	−13.74
PA26	1.69	1.96	2.84	0.01	9.85	8.05	−1.81
SIE4x4	16.00	16.00	18.42	0.47	33.92	36.69	2.77
ALKBDE10	−3.90	4.63	6.15	0.05	14.27	1.58	−12.70
YBDE18	−7.87	7.87	9.08	0.16	15.92	−0.39	−16.31
AL2X6	−7.86	7.86	8.37	0.22	7.98	−4.42	−12.40
HEAVYSB11	−7.90	7.90	8.24	0.14	7.16	−5.27	−12.43
NBPRC	3.78	4.76	6.57	0.17	18.98	15.82	−3.16
ALK8	−5.05	5.54	8.39	0.09	19.46	1.53	−17.93
RC21	−0.50	2.21	2.97	0.06	13.54	3.63	−9.91
G2RC	0.42	2.50	2.88	0.05	8.99	5.34	−3.65
BH76RC	−0.38	2.21	2.71	0.10	11.08	4.41	−6.67
FH51	2.16	3.38	4.52	0.11	25.31	10.19	−15.12
TAUT15	−0.07	1.01	1.22	0.33	3.92	2.06	−1.86
DC13	3.91	14.45	19.11	0.26	67.96	31.73	−36.23
MB16-43	−56.02	56.02	61.12	0.14	120.41	−12.17	−132.58
DARC	14.23	14.23	14.58	0.44	10.68	17.24	6.57
RSE43	−1.57	1.57	1.80	0.21	3.41	−0.52	−3.92
BSR36	−10.90	10.90	12.62	0.67	24.61	−3.83	−28.44
CDIE20	1.05	1.06	1.23	0.26	2.50	2.43	−0.07
ISO34	−0.32	2.26	3.31	0.16	20.41	11.81	−8.61
ISOL24	−4.49	8.99	13.85	0.41	74.77	27.72	−47.06
C60ISO	1.78	2.50	2.71	0.03	6.84	4.99	−1.86
PArel	0.04	1.12	1.67	0.24	7.82	5.46	−2.36
BH76	−4.19	4.27	4.90	0.23	11.93	1.35	−10.58
BHPERI	3.79	4.26	4.97	0.20	12.58	8.95	−3.63
BHDIV10	−0.15	2.24	3.04	0.05	10.29	5.72	−4.57
INV24	−1.27	1.66	1.88	0.05	6.15	2.77	−3.38
BHROT27	0.33	0.40	0.59	0.06	1.49	1.24	−0.25
PX13	−2.46	2.46	2.63	0.07	3.02	−0.99	−4.00
WCPT18	−0.29	1.14	1.36	0.03	4.73	2.04	−2.68
RG18	−0.04	0.38	0.50	0.66	2.18	1.14	−1.04
ADIM6	−3.59	3.59	4.01	1.07	5.25	−1.15	−6.39
S22	−2.76	2.79	3.93	0.38	11.07	0.36	−10.70
S66	−2.21	2.25	2.84	0.41	7.58	0.45	−7.13
HEAVY28	−0.82	0.82	0.92	0.66	1.54	−0.18	−1.72
WATER27	−0.10	1.77	2.29	0.02	9.47	3.34	−6.12
CARBHB12	0.05	0.47	0.60	0.08	2.30	1.21	−1.10
PNICO23	−1.14	1.14	1.29	0.27	2.76	−0.19	−2.95
HAL59	−1.08	1.19	1.66	0.26	8.27	2.00	−6.27
AHB21	0.12	0.51	0.62	0.02	2.42	1.45	−0.97
CHB6	−0.86	1.61	1.82	0.06	4.90	2.26	−2.64
IL16	3.12	3.12	3.20	0.03	2.61	4.64	2.03
IDISP	4.12	14.92	17.46	1.05	48.82	32.41	−16.41
ICONF	0.04	0.54	0.79	0.17	3.93	2.07	−1.87
ACONF	0.77	0.77	0.87	0.42	1.34	1.55	0.22
AMINO20x4	−0.08	0.59	0.75	0.24	3.92	2.29	−1.63
PCONF21	−0.33	3.15	3.62	1.94	10.70	5.87	−4.83
MCONF	−2.06	2.12	2.41	0.43	4.17	0.46	−3.71
SCONF	−0.41	0.73	0.86	0.16	3.15	1.84	−1.31
UPU23	1.80	2.15	3.09	0.38	8.77	7.83	−0.94
BUT14DIOL	−0.09	0.29	0.34	0.10	1.32	0.79	−0.53

Table S145: Statistical analysis for the MPW1PW91 DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−4.45	4.71	6.39	0.02	33.53	3.97	−29.56
G21EA	−0.17	2.66	2.99	0.08	9.60	4.86	−4.74
G21IP	0.44	3.72	4.42	0.01	17.90	10.01	−7.89
DIPCS10	−0.19	3.02	3.51	0.00	10.91	4.37	−6.55
PA26	3.31	3.31	3.86	0.02	8.64	8.85	0.21
SIE4x4	13.98	13.98	15.87	0.41	28.08	31.61	3.53
ALKBDE10	−4.40	6.12	7.01	0.06	20.92	7.02	−13.90
YBDE18	−4.29	4.29	4.82	0.09	9.23	−0.74	−9.97
AL2X6	−4.02	4.02	4.42	0.11	5.43	−0.64	−6.06
HEAVYSB11	−4.79	4.79	5.47	0.08	7.49	−1.29	−8.78
NBPRC	1.53	2.57	3.10	0.09	8.37	5.59	−2.78
ALK8	−0.29	1.92	2.56	0.03	9.42	4.67	−4.75
RC21	2.56	3.03	3.74	0.08	10.66	8.89	−1.77
G2RC	−2.11	5.14	6.33	0.10	25.30	10.52	−14.78
BH76RC	−0.23	2.04	2.78	0.10	14.38	7.83	−6.55
FH51	0.09	2.19	3.02	0.07	15.32	8.60	−6.72
TAUT15	0.36	1.12	1.55	0.37	4.85	3.27	−1.57
DC13	0.36	8.52	10.64	0.15	37.35	19.72	−17.63
MB16-43	−20.73	22.95	27.07	0.06	80.27	24.57	−55.70
DARC	3.11	4.13	4.67	0.13	10.99	6.33	−4.66
RSE43	−1.44	1.44	1.64	0.19	3.38	−0.48	−3.86
BSR36	−8.99	8.99	10.11	0.55	20.13	−2.45	−22.58
CDIE20	1.35	1.39	1.64	0.34	3.61	3.17	−0.44
ISO34	−0.45	1.56	2.23	0.11	12.83	5.01	−7.82
ISOL24	−1.71	4.53	7.28	0.21	38.88	13.23	−25.65
C60ISO	1.42	2.53	2.66	0.03	6.73	4.17	−2.56
PArel	0.65	1.13	1.71	0.24	7.51	5.60	−1.91
BH76	−3.40	3.61	4.01	0.19	13.71	2.58	−11.13
BHPERI	0.60	1.53	1.80	0.07	7.16	3.80	−3.37
BHDIV10	−3.07	3.68	4.06	0.08	9.19	3.05	−6.15
INV24	−1.22	1.66	2.04	0.05	9.17	4.28	−4.89
BHROT27	0.50	0.56	0.75	0.09	1.67	1.43	−0.24
PX13	−5.50	5.50	5.67	0.16	5.55	−2.99	−8.54
WCPT18	−2.77	2.77	3.24	0.08	6.31	−0.48	−6.79
RG18	−0.61	0.61	0.77	1.05	1.51	−0.06	−1.58
ADIM6	−4.66	4.66	5.11	1.39	6.05	−1.78	−7.83
S22	−3.18	3.18	4.27	0.44	11.13	−0.32	−11.45
S66	−2.82	2.82	3.38	0.52	7.92	−0.22	−8.14
HEAVY28	−0.99	0.99	1.06	0.80	1.38	−0.43	−1.81
WATER27	−5.23	5.80	9.42	0.07	29.00	1.88	−27.12
CARBHB12	0.15	0.55	0.79	0.09	2.88	1.91	−0.97
PNICO23	−0.93	1.07	1.20	0.25	4.66	1.63	−3.03
HAL59	−1.34	1.50	1.92	0.33	8.87	1.97	−6.90
AHB21	−0.14	0.87	1.06	0.04	4.25	2.09	−2.16
CHB6	−0.02	1.00	1.26	0.04	4.03	2.28	−1.75
IL16	2.66	2.66	2.78	0.02	3.33	4.74	1.41
IDISP	1.75	11.40	12.44	0.80	31.97	18.63	−13.34
ICONF	0.21	0.44	0.63	0.13	2.72	1.82	−0.90
ACONF	0.73	0.73	0.83	0.40	1.16	1.36	0.20
AMINO20x4	−0.02	0.54	0.68	0.22	3.22	1.92	−1.31
PCONF21	−0.51	3.65	4.10	2.25	11.41	6.41	−4.99
MCONF	−1.97	2.06	2.33	0.41	4.48	0.71	−3.77
SCONF	−0.15	0.39	0.53	0.08	2.26	1.31	−0.95
UPU23	1.93	2.34	3.42	0.41	10.34	9.07	−1.28
BUT14DIOL	−0.24	0.36	0.42	0.13	1.36	0.58	−0.78

Table S146: Statistical analysis for the PW1PW DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−1.03	3.23	4.76	0.01	33.57	6.22	−27.35
G21EA	0.49	2.45	2.88	0.07	9.07	5.29	−3.78
G21IP	0.91	3.68	4.40	0.01	17.25	10.20	−7.05
DIPCS10	0.74	3.14	3.56	0.00	10.17	4.78	−5.39
PA26	2.53	2.59	3.18	0.01	8.66	7.89	−0.77
SIE4x4	14.29	14.29	16.10	0.42	28.14	31.37	3.23
ALKBDE10	−3.04	5.25	6.16	0.05	20.24	8.04	−12.19
YBDE18	−2.43	2.55	3.21	0.05	8.72	1.03	−7.69
AL2X6	−2.33	2.53	2.81	0.07	4.40	0.60	−3.80
HEAVYSB11	−3.30	3.33	4.16	0.06	6.95	0.17	−6.78
NBPRC	0.45	2.58	3.01	0.09	9.59	5.43	−4.15
ALK8	1.45	1.77	2.85	0.03	7.51	6.70	−0.81
RC21	3.77	4.18	5.06	0.12	13.11	11.26	−1.86
G2RC	−2.89	6.07	7.48	0.12	28.61	10.45	−18.17
BH76RC	−0.25	2.32	3.13	0.11	16.11	9.05	−7.06
FH51	−0.58	2.50	3.32	0.08	15.86	7.59	−8.27
TAUT15	0.43	1.17	1.71	0.38	5.35	3.63	−1.72
DC13	−0.78	8.18	10.37	0.15	40.89	19.84	−21.05
MB16-43	−10.74	17.33	21.46	0.04	86.67	39.63	−47.03
DARC	0.90	3.11	3.47	0.10	10.70	4.08	−6.62
RSE43	−1.50	1.50	1.71	0.20	3.45	−0.47	−3.93
BSR36	−8.17	8.17	9.35	0.50	18.16	−2.77	−20.93
CDIE20	1.29	1.33	1.56	0.33	3.32	2.98	−0.35
ISO34	−0.37	1.53	2.10	0.11	11.25	4.73	−6.52
ISOL24	−1.16	3.99	6.04	0.18	31.38	11.61	−19.77
C60ISO	1.32	2.49	2.63	0.03	6.70	3.96	−2.74
PArel	0.68	1.19	1.79	0.26	7.75	5.72	−2.03
BH76	−4.15	4.37	4.80	0.23	15.64	2.64	−13.00
BHPERI	−0.71	1.24	1.55	0.06	5.22	1.62	−3.60
BHDIV10	−3.57	4.20	4.62	0.09	10.07	3.15	−6.92
INV24	−1.10	1.50	1.91	0.05	8.82	4.07	−4.74
BHROT27	0.54	0.60	0.80	0.10	1.71	1.51	−0.20
PX13	−6.37	6.37	6.55	0.19	6.17	−3.75	−9.92
WCPT18	−3.69	3.69	4.31	0.11	7.71	−0.72	−8.44
RG18	0.01	0.29	0.40	0.50	1.89	1.06	−0.83
ADIM6	−3.07	3.07	3.43	0.91	4.49	−0.96	−5.45
S22	−2.01	2.12	3.14	0.29	9.77	0.92	−8.85
S66	−1.69	1.78	2.31	0.33	6.93	0.88	−6.05
HEAVY28	−0.43	0.45	0.55	0.36	1.27	0.16	−1.12
WATER27	1.96	2.67	3.38	0.03	17.51	9.44	−8.06
CARBHB12	0.87	0.90	1.20	0.15	2.84	2.71	−0.13
PNICO23	−0.09	0.55	0.84	0.13	4.99	2.88	−2.11
HAL59	−0.49	0.98	1.38	0.21	8.19	3.01	−5.18
AHB21	−1.05	1.16	1.47	0.05	4.04	0.96	−3.08
CHB6	−0.99	1.38	1.60	0.05	4.07	1.16	−2.91
IL16	1.35	1.35	1.51	0.01	2.81	3.05	0.24
IDISP	1.49	9.26	10.15	0.65	26.63	15.27	−11.36
ICONF	0.23	0.38	0.57	0.12	2.34	1.70	−0.65
ACONF	0.54	0.54	0.62	0.30	0.93	1.05	0.12
AMINO20x4	0.04	0.46	0.58	0.19	2.88	1.68	−1.19
PCONF21	−0.47	3.00	3.34	1.85	9.03	5.10	−3.93
MCONF	−1.49	1.57	1.79	0.32	3.69	0.64	−3.05
SCONF	−0.05	0.23	0.32	0.05	1.40	0.85	−0.56
UPU23	1.55	1.88	2.70	0.33	7.76	6.90	−0.86
BUT14DIOL	−0.01	0.20	0.25	0.07	1.09	0.69	−0.40

Table S147: Statistical analysis for the MPW1KCIS DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	6.97	8.54	10.05	0.03	41.44	24.09	−17.35
G21EA	0.61	1.77	2.16	0.05	7.45	4.25	−3.21
G21IP	−0.76	3.33	4.13	0.01	15.82	7.51	−8.32
DIPCS10	−3.15	4.23	5.18	0.01	14.14	3.64	−10.50
PA26	1.75	2.11	2.76	0.01	8.98	7.11	−1.87
SIE4x4	18.91	18.91	21.49	0.56	38.13	41.27	3.13
ALKBDE10	0.93	4.43	5.88	0.04	19.65	14.62	−5.03
YBDE18	−4.20	5.52	6.94	0.11	19.60	4.31	−15.29
AL2X6	−6.76	6.76	7.21	0.19	7.17	−2.25	−9.42
HEAVYSB11	−4.44	4.78	5.91	0.08	11.95	1.69	−10.26
NBPRC	3.08	3.66	5.07	0.13	13.65	10.65	−3.00
ALK8	−0.95	3.72	4.74	0.06	16.27	6.31	−9.96
RC21	2.19	2.74	3.47	0.08	11.13	8.15	−2.98
G2RC	−0.99	4.36	5.40	0.09	22.00	10.61	−11.39
BH76RC	−0.18	2.53	3.57	0.12	19.44	11.70	−7.74
FH51	1.23	2.75	3.74	0.09	17.41	10.27	−7.15
TAUT15	0.22	1.30	1.74	0.43	5.36	3.52	−1.84
DC13	2.70	10.29	12.73	0.19	44.65	20.32	−24.33
MB16-43	−20.61	24.74	30.09	0.06	89.00	19.14	−69.87
DARC	8.53	8.53	9.36	0.26	11.92	11.99	0.07
RSE43	−2.62	2.62	2.89	0.34	5.49	−0.76	−6.25
BSR36	−8.92	8.92	10.11	0.55	20.35	−1.94	−22.29
CDIE20	1.63	1.67	1.92	0.41	4.05	3.57	−0.48
ISO34	−0.40	1.83	2.63	0.13	16.00	6.85	−9.15
ISOL24	−3.54	6.91	11.00	0.32	59.25	20.14	−39.10
C60ISO	−3.65	3.86	5.32	0.04	11.43	0.70	−10.73
PArel	0.40	1.31	2.00	0.28	9.88	6.36	−3.52
BH76	−5.63	5.71	6.45	0.31	20.16	2.54	−17.61
BHPERI	0.79	2.36	2.69	0.11	10.18	5.20	−4.98
BHDIV10	−4.33	4.97	5.73	0.11	11.54	3.18	−8.36
INV24	−2.17	2.17	2.59	0.07	6.60	−0.42	−7.02
BHROT27	0.37	0.44	0.61	0.07	1.71	1.39	−0.32
PX13	−6.46	6.46	6.58	0.19	5.23	−4.39	−9.62
WCPT18	−4.29	4.29	4.63	0.12	6.90	−2.17	−9.07
RG18	−0.52	0.52	0.72	0.90	1.70	−0.02	−1.72
ADIM6	−4.84	4.84	5.32	1.44	6.40	−1.80	−8.19
S22	−3.65	3.65	4.77	0.50	12.45	−0.35	−12.80
S66	−3.12	3.12	3.66	0.57	8.69	−0.31	−9.00
HEAVY28	−1.01	1.01	1.09	0.81	1.62	−0.30	−1.92
WATER27	−7.17	7.44	11.81	0.09	34.62	1.67	−32.96
CARBHB12	0.06	0.57	0.82	0.09	2.94	1.84	−1.11
PNICO23	−1.20	1.35	1.46	0.32	4.88	1.70	−3.18
HAL59	−1.45	1.61	2.06	0.35	9.89	2.40	−7.49
AHB21	0.45	0.74	0.97	0.03	3.78	2.48	−1.29
CHB6	0.67	0.96	1.39	0.04	3.54	3.10	−0.44
IL16	3.23	3.23	3.35	0.03	3.59	5.41	1.81
IDISP	2.80	14.56	16.13	1.02	42.34	26.08	−16.26
ICONF	0.17	0.57	0.86	0.17	4.06	2.67	−1.39
ACONF	0.96	0.96	1.06	0.52	1.48	1.84	0.36
AMINO20x4	−0.10	0.65	0.80	0.27	3.80	2.21	−1.60
PCONF21	−0.61	4.08	4.57	2.52	13.16	7.42	−5.74
MCONF	−2.31	2.38	2.70	0.48	5.00	0.72	−4.28
SCONF	−0.34	0.72	0.92	0.16	3.65	2.17	−1.48
UPU23	1.86	2.44	3.55	0.43	11.26	9.52	−1.74
BUT14DIOL	−0.30	0.47	0.53	0.17	1.83	0.83	−1.01

Table S148: Statistical analysis for the MPWKCIS1K DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−7.08	8.17	11.00	0.03	46.10	8.40	−37.70
G21EA	−2.51	3.40	4.18	0.10	11.28	2.76	−8.52
G21IP	−0.85	3.44	4.28	0.01	17.40	8.56	−8.84
DIPCS10	−2.27	3.68	4.84	0.01	14.89	4.67	−10.21
PA26	2.66	2.89	3.47	0.02	9.81	7.74	−2.07
SIE4x4	9.58	9.58	11.52	0.28	23.43	25.52	2.09
ALKBDE10	−8.57	8.57	10.16	0.09	21.32	−1.47	−22.79
YBDE18	−3.89	3.89	4.60	0.08	9.32	−0.87	−10.19
AL2X6	−4.68	4.68	5.05	0.13	5.61	−1.53	−7.14
HEAVYSB11	−5.85	5.85	6.16	0.10	5.55	−2.79	−8.34
NBPRC	2.29	2.99	3.97	0.11	11.63	9.20	−2.43
ALK8	0.64	2.68	3.81	0.04	13.01	8.07	−4.94
RC21	2.36	3.16	4.01	0.09	15.39	11.36	−4.03
G2RC	−4.99	6.54	8.46	0.13	29.34	11.03	−18.31
BH76RC	−1.12	2.37	3.30	0.11	12.54	2.92	−9.63
FH51	−1.44	2.65	3.37	0.09	16.75	9.41	−7.34
TAUT15	0.33	0.90	1.27	0.30	4.36	2.72	−1.65
DC13	−0.41	8.93	10.98	0.16	39.40	23.32	−16.08
MB16-43	−17.21	20.85	25.41	0.05	79.08	21.29	−57.78
DARC	1.16	3.09	3.50	0.10	10.86	4.12	−6.74
RSE43	−1.27	1.27	1.44	0.17	2.96	−0.37	−3.32
BSR36	−8.48	8.48	9.55	0.52	18.48	−2.37	−20.85
CDIE20	1.19	1.32	1.63	0.33	4.23	3.41	−0.82
ISO34	0.08	1.93	2.64	0.13	13.53	5.07	−8.47
ISOL24	−1.09	4.16	6.27	0.19	31.08	8.55	−22.53
C60ISO	7.88	7.88	8.41	0.08	9.64	13.83	4.19
PArel	0.88	1.11	1.75	0.24	6.98	5.45	−1.53
BH76	−0.71	1.87	2.31	0.10	10.18	5.30	−4.88
BHPERI	3.97	4.23	4.59	0.20	10.77	7.67	−3.11
BHDIV10	−0.47	1.90	2.30	0.04	8.17	3.47	−4.70
INV24	−0.40	1.92	2.95	0.06	15.83	9.74	−6.09
BHROT27	0.59	0.63	0.87	0.10	2.14	1.91	−0.22
PX13	−1.27	1.31	1.55	0.04	2.77	0.23	−2.54
WCPT18	0.27	1.06	1.32	0.03	5.46	2.83	−2.63
RG18	−0.52	0.52	0.69	0.90	1.58	−0.04	−1.62
ADIM6	−4.36	4.36	4.78	1.30	5.74	−1.60	−7.35
S22	−3.07	3.07	4.16	0.42	10.87	−0.34	−11.21
S66	−2.66	2.66	3.19	0.49	7.60	−0.15	−7.75
HEAVY28	−0.98	0.98	1.05	0.79	1.31	−0.41	−1.73
WATER27	−6.44	6.68	10.98	0.08	31.68	1.15	−30.53
CARBHB12	−0.06	0.50	0.65	0.08	2.48	1.41	−1.07
PNICO23	−1.22	1.23	1.33	0.29	3.13	0.12	−3.01
HAL59	−1.67	1.67	2.00	0.36	6.61	−0.03	−6.64
AHB21	−0.17	0.99	1.27	0.04	5.26	2.01	−3.25
CHB6	−0.30	1.06	1.35	0.04	4.22	2.03	−2.19
IL16	3.00	3.00	3.13	0.03	3.29	5.18	1.89
IDISP	0.77	12.45	13.41	0.88	33.46	16.01	−17.45
ICONF	0.26	0.58	0.83	0.18	3.57	2.31	−1.26
ACONF	0.91	0.91	1.01	0.50	1.32	1.66	0.33
AMINO20x4	−0.04	0.62	0.78	0.25	3.83	2.21	−1.62
PCONF21	−0.25	3.42	3.98	2.11	11.72	6.67	−5.05
MCONF	−1.98	2.06	2.34	0.41	4.23	0.56	−3.67
SCONF	−0.49	1.06	1.24	0.23	4.45	2.77	−1.67
UPU23	1.85	2.21	3.23	0.39	9.24	8.28	−0.96
BUT14DIOL	−0.41	0.51	0.57	0.18	1.62	0.57	−1.05

Table S149: Statistical analysis for the PBE0 DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−1.75	3.62	5.73	0.01	38.04	7.01	−31.02
G21EA	−0.40	2.62	2.91	0.08	8.81	4.03	−4.77
G21IP	−0.02	3.68	4.35	0.01	17.03	9.00	−8.03
DIPCS10	−1.51	2.99	3.77	0.00	10.39	3.06	−7.33
PA26	2.46	2.56	3.14	0.01	9.09	7.71	−1.38
SIE4x4	14.15	14.15	15.95	0.42	27.86	31.18	3.32
ALKBDE10	−4.26	5.83	6.72	0.06	19.30	6.00	−13.30
YBDE18	−2.40	2.55	3.21	0.05	9.13	1.32	−7.81
AL2X6	−2.63	2.76	3.08	0.08	4.42	0.39	−4.03
HEAVYSB11	−3.54	3.58	4.40	0.06	7.25	0.21	−7.04
NBPRC	0.57	2.55	2.99	0.09	9.76	5.43	−4.33
ALK8	1.33	1.87	2.94	0.03	8.17	6.70	−1.47
RC21	3.75	4.22	5.10	0.12	13.51	11.47	−2.04
G2RC	−2.73	6.21	7.69	0.12	30.46	11.91	−18.55
BH76RC	−0.14	2.37	3.20	0.11	16.64	9.94	−6.70
FH51	−0.54	2.47	3.27	0.08	15.74	7.57	−8.18
TAUT15	0.44	1.15	1.66	0.38	5.19	3.55	−1.64
DC13	−0.59	8.87	10.85	0.16	43.37	22.23	−21.14
MB16-43	−11.90	17.55	22.35	0.04	90.01	39.35	−50.66
DARC	0.45	3.10	3.43	0.10	10.78	3.73	−7.05
RSE43	−1.59	1.59	1.78	0.21	3.53	−0.53	−4.06
BSR36	−7.59	7.59	8.64	0.47	17.32	−2.19	−19.52
CDIE20	1.34	1.38	1.63	0.34	3.53	3.13	−0.39
ISO34	−0.45	1.64	2.22	0.11	10.59	3.93	−6.66
ISOL24	−1.17	3.96	5.87	0.18	29.72	10.35	−19.38
C60ISO	0.69	2.16	2.38	0.02	6.60	3.05	−3.56
PArel	0.72	1.22	1.80	0.26	7.72	5.64	−2.08
BH76	−3.17	4.62	5.90	0.25	38.51	24.98	−13.53
BHPERI	−0.59	1.30	1.64	0.06	5.86	1.86	−4.00
BHDIV10	−3.71	4.27	4.70	0.09	9.80	2.77	−7.03
INV24	−1.20	1.54	1.94	0.05	9.08	4.06	−5.01
BHROT27	0.53	0.59	0.78	0.09	1.76	1.53	−0.24
PX13	−6.18	6.18	6.35	0.19	5.82	−3.76	−9.58
WCPT18	−3.72	3.72	4.24	0.11	7.28	−1.10	−8.38
RG18	−0.34	0.34	0.49	0.59	1.17	0.04	−1.13
ADIM6	−3.44	3.44	3.80	1.02	4.65	−1.23	−5.87
S22	−2.33	2.37	3.38	0.32	9.76	0.38	−9.38
S66	−2.00	2.03	2.56	0.37	6.88	0.38	−6.50
HEAVY28	−0.58	0.58	0.68	0.47	1.30	0.01	−1.29
WATER27	−0.13	2.21	3.13	0.03	11.52	3.11	−8.41
CARBHB12	0.65	0.72	1.04	0.12	2.82	2.43	−0.39
PNICO23	−0.33	0.65	0.92	0.15	5.15	2.79	−2.37
HAL59	−0.75	1.09	1.49	0.24	8.24	2.61	−5.63
AHB21	−0.69	0.94	1.20	0.04	4.06	1.26	−2.81
CHB6	−0.60	1.08	1.35	0.04	3.98	1.44	−2.53
IL16	1.73	1.73	1.86	0.02	2.77	3.45	0.68
IDISP	1.31	9.51	10.30	0.67	26.05	14.80	−11.25
ICONF	0.23	0.40	0.61	0.12	2.53	1.91	−0.62
ACONF	0.63	0.63	0.70	0.34	0.94	1.16	0.22
AMINO20x4	0.03	0.48	0.60	0.20	3.02	1.79	−1.23
PCONF21	−0.43	3.06	3.43	1.89	9.41	5.38	−4.02
MCONF	−1.57	1.65	1.88	0.33	3.87	0.70	−3.17
SCONF	−0.06	0.28	0.39	0.06	1.74	1.08	−0.65
UPU23	1.51	1.90	2.74	0.33	8.11	7.00	−1.11
BUT14DIOL	−0.07	0.23	0.28	0.08	1.16	0.63	−0.52

Table S150: Statistical analysis for the PBEh1PBE DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−2.67	3.77	5.45	0.01	32.93	5.49	−27.44
G21EA	−0.54	2.68	2.98	0.08	8.94	4.12	−4.82
G21IP	0.06	3.71	4.39	0.01	17.19	9.25	−7.94
DIPCS10	−1.37	3.01	3.74	0.00	10.57	3.24	−7.32
PA26	2.36	2.44	3.05	0.01	8.69	7.65	−1.04
SIE4x4	14.07	14.07	15.88	0.42	27.90	31.08	3.18
ALKBDE10	−4.36	5.83	6.70	0.06	18.82	5.52	−13.30
YBDE18	−2.83	2.91	3.52	0.06	8.69	0.68	−8.01
AL2X6	−2.87	2.91	3.28	0.08	4.61	0.11	−4.51
HEAVYSB11	−3.39	3.39	4.17	0.06	7.20	−0.31	−7.51
NBPRC	0.77	2.48	2.97	0.09	9.78	5.93	−3.85
ALK8	1.23	1.84	2.86	0.03	7.73	6.53	−1.20
RC21	3.36	3.82	4.65	0.11	12.28	10.41	−1.87
G2RC	−2.54	5.84	7.21	0.11	27.77	10.67	−17.10
BH76RC	−0.09	2.29	3.08	0.11	16.08	9.61	−6.46
FH51	−0.44	2.36	3.16	0.08	15.43	7.50	−7.92
TAUT15	0.36	1.18	1.65	0.39	5.09	3.44	−1.65
DC13	−0.18	8.08	10.47	0.15	41.98	21.29	−20.69
MB16-43	−14.94	19.07	23.60	0.05	85.10	33.24	−51.86
DARC	1.46	3.33	3.68	0.10	10.79	4.66	−6.13
RSE43	−1.56	1.56	1.75	0.21	3.51	−0.52	−4.03
BSR36	−7.60	7.60	8.66	0.47	16.64	−2.43	−19.07
CDIE20	1.32	1.35	1.60	0.33	3.41	3.04	−0.36
ISO34	−0.43	1.54	2.14	0.11	11.29	4.84	−6.46
ISOL24	−1.39	4.14	6.28	0.19	32.33	11.71	−20.62
C60ISO	1.18	2.43	2.54	0.02	6.53	3.52	−3.01
PArel	0.67	1.16	1.74	0.25	7.52	5.62	−1.90
BH76	−3.94	4.14	4.60	0.22	15.50	2.39	−13.11
BHPERI	−0.29	1.20	1.50	0.06	5.79	2.02	−3.77
BHDIV10	−3.42	4.05	4.48	0.09	9.84	3.17	−6.67
INV24	−1.13	1.52	1.92	0.05	8.93	4.02	−4.91
BHROT27	0.55	0.60	0.80	0.10	1.79	1.56	−0.22
PX13	−5.74	5.74	5.88	0.17	5.11	−3.54	−8.65
WCPT18	−3.49	3.49	4.04	0.10	7.20	−0.79	−7.99
RG18	−0.32	0.33	0.48	0.57	1.21	0.05	−1.16
ADIM6	−3.44	3.44	3.79	1.02	4.63	−1.22	−5.85
S22	−2.22	2.30	3.30	0.32	9.84	0.68	−9.16
S66	−1.92	1.97	2.52	0.36	7.09	0.68	−6.40
HEAVY28	−0.55	0.55	0.65	0.44	1.27	0.01	−1.26
WATER27	0.97	2.11	2.72	0.03	13.10	5.76	−7.35
CARBHB12	0.71	0.76	1.08	0.13	2.82	2.51	−0.31
PNICO23	−0.27	0.61	0.86	0.14	4.88	2.59	−2.29
HAL59	−0.64	1.06	1.46	0.23	8.31	2.80	−5.51
AHB21	−0.82	1.00	1.25	0.04	3.87	1.13	−2.74
CHB6	−0.60	1.07	1.30	0.04	3.76	1.40	−2.36
IL16	1.58	1.58	1.71	0.01	2.68	3.24	0.56
IDISP	1.48	9.52	10.41	0.67	27.03	15.88	−11.16
ICONF	0.23	0.40	0.60	0.12	2.53	1.86	−0.66
ACONF	0.61	0.61	0.68	0.33	0.92	1.15	0.23
AMINO20x4	0.04	0.47	0.59	0.19	2.98	1.78	−1.20
PCONF21	−0.44	3.02	3.37	1.86	9.11	5.19	−3.92
MCONF	−1.52	1.60	1.83	0.32	3.83	0.73	−3.10
SCONF	0.00	0.22	0.29	0.05	1.25	0.79	−0.45
UPU23	1.50	1.88	2.72	0.33	7.96	6.92	−1.04
BUT14DIOL	0.02	0.20	0.25	0.07	1.13	0.72	−0.41

Table S151: Statistical analysis for the PBE1KCIS DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	6.02	7.74	9.27	0.03	39.15	20.81	−18.34
G21EA	−0.14	1.68	2.04	0.05	7.30	3.44	−3.87
G21IP	−0.83	3.33	3.98	0.01	14.39	6.24	−8.15
DIPCS10	−3.32	4.33	5.30	0.01	14.52	4.77	−9.76
PA26	1.20	1.77	2.37	0.01	9.30	6.26	−3.03
SIE4x4	16.66	16.66	18.97	0.49	34.40	36.98	2.58
ALKBDE10	−1.25	4.40	5.08	0.04	16.53	8.21	−8.32
YBDE18	−2.52	4.15	5.12	0.08	16.35	4.18	−12.17
AL2X6	−5.06	5.06	5.47	0.14	5.91	−1.26	−7.17
HEAVYSB11	−3.87	4.14	5.05	0.07	10.12	1.33	−8.78
NBPRC	2.10	3.20	4.17	0.12	13.52	9.57	−3.96
ALK8	0.94	3.17	4.48	0.05	13.75	8.73	−5.02
RC21	3.04	3.53	4.20	0.10	11.30	8.76	−2.55
G2RC	−2.55	5.34	6.73	0.10	23.42	8.98	−14.44
BH76RC	−0.39	2.42	3.31	0.11	17.45	9.66	−7.78
FH51	0.02	2.27	3.13	0.07	15.23	8.88	−6.36
TAUT15	0.26	1.15	1.62	0.38	5.03	3.33	−1.69
DC13	1.20	8.22	11.36	0.15	46.49	21.18	−25.31
MB16-43	−13.29	19.03	24.04	0.05	80.54	24.09	−56.45
DARC	4.86	5.32	6.03	0.16	11.39	8.18	−3.21
RSE43	−2.29	2.29	2.54	0.30	4.77	−0.62	−5.40
BSR36	−8.05	8.05	9.26	0.50	18.17	−2.25	−20.42
CDIE20	1.47	1.53	1.79	0.38	3.96	3.44	−0.51
ISO34	−0.25	1.70	2.44	0.12	13.94	6.06	−7.88
ISOL24	−2.56	5.45	8.57	0.25	44.92	14.64	−30.28
C60ISO	−0.71	2.22	2.84	0.02	7.84	1.89	−5.95
PArel	0.55	1.13	1.83	0.24	7.93	6.07	−1.86
BH76	−4.74	4.91	5.53	0.26	17.71	2.79	−14.92
BHPERI	0.80	1.90	2.21	0.09	9.00	4.36	−4.64
BHDIV10	−3.56	4.30	4.91	0.09	11.03	3.32	−7.71
INV24	−1.58	1.73	2.10	0.05	7.93	1.82	−6.11
BHROT27	0.45	0.50	0.68	0.08	1.64	1.40	−0.24
PX13	−5.20	5.20	5.31	0.16	4.37	−3.53	−7.90
WCPT18	−3.62	3.62	4.01	0.10	6.97	−1.37	−8.34
RG18	−0.18	0.25	0.37	0.43	1.04	0.14	−0.89
ADIM6	−3.30	3.30	3.67	0.98	4.71	−1.08	−5.79
S22	−2.57	2.58	3.63	0.35	10.25	0.14	−10.11
S66	−2.08	2.09	2.62	0.38	7.07	0.20	−6.86
HEAVY28	−0.57	0.57	0.67	0.46	1.26	−0.05	−1.31
WATER27	−1.65	2.55	4.04	0.03	14.31	2.02	−12.30
CARBHB12	0.52	0.61	0.91	0.10	2.65	2.17	−0.48
PNICO23	−0.61	0.80	0.97	0.19	4.55	2.12	−2.43
HAL59	−0.89	1.08	1.50	0.24	8.16	2.28	−5.88
AHB21	−0.27	0.64	0.82	0.03	3.50	1.45	−2.05
CHB6	−0.18	0.90	1.15	0.03	3.50	2.01	−1.49
IL16	2.24	2.24	2.36	0.02	2.92	4.02	1.10
IDISP	2.15	12.21	13.46	0.86	35.67	20.84	−14.82
ICONF	0.20	0.52	0.80	0.16	3.70	2.55	−1.16
ACONF	0.78	0.78	0.87	0.43	1.21	1.50	0.30
AMINO20x4	−0.05	0.56	0.69	0.23	3.42	1.95	−1.47
PCONF21	−0.41	3.25	3.66	2.01	10.56	6.06	−4.50
MCONF	−1.79	1.87	2.13	0.38	4.08	0.60	−3.48
SCONF	−0.35	0.73	0.89	0.16	3.43	2.12	−1.31
UPU23	1.49	1.95	2.79	0.34	8.38	7.13	−1.25
BUT14DIOL	−0.18	0.34	0.40	0.12	1.47	0.74	−0.74

Table S152: Statistical analysis for the X3LYP DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−2.34	3.74	5.55	0.01	36.86	8.04	−28.82
G21EA	0.11	1.88	2.43	0.06	10.17	7.16	−3.01
G21IP	−0.73	3.72	4.48	0.01	16.41	8.88	−7.53
DIPCS10	−2.85	5.17	6.47	0.01	21.16	9.50	−11.66
PA26	1.68	1.90	2.75	0.01	9.31	7.88	−1.43
SIE4x4	17.14	17.14	19.68	0.51	35.91	38.84	2.93
ALKBDE10	−2.12	4.52	5.33	0.04	15.53	5.68	−9.84
YBDE18	−7.37	7.51	8.92	0.15	17.61	1.22	−16.39
AL2X6	−8.02	8.02	8.49	0.22	8.10	−4.34	−12.44
HEAVYSB11	−7.23	7.23	7.71	0.12	8.07	−3.94	−12.01
NBPRC	3.73	4.56	6.41	0.16	18.20	15.60	−2.60
ALK8	−5.19	5.42	8.07	0.09	17.82	0.90	−16.93
RC21	−0.15	2.23	2.85	0.06	12.23	3.07	−9.16
G2RC	0.59	2.49	3.01	0.05	11.35	6.79	−4.56
BH76RC	−0.40	2.21	2.73	0.10	10.90	3.80	−7.10
FH51	2.27	3.50	4.61	0.11	25.65	11.17	−14.48
TAUT15	0.01	1.12	1.40	0.37	4.27	2.57	−1.70
DC13	4.01	14.16	18.13	0.26	62.61	29.47	−33.14
MB16-43	−52.45	52.45	56.96	0.13	108.80	−9.36	−118.16
DARC	14.10	14.10	14.48	0.43	10.95	17.16	6.21
RSE43	−1.83	1.83	2.07	0.24	3.76	−0.74	−4.50
BSR36	−10.59	10.59	12.17	0.65	24.05	−3.43	−27.48
CDIE20	1.16	1.17	1.35	0.29	2.66	2.58	−0.09
ISO34	−0.38	2.17	3.20	0.15	20.05	11.31	−8.74
ISOL24	−4.46	8.87	13.80	0.40	74.83	27.91	−46.93
C60ISO	0.40	2.17	2.38	0.02	6.54	2.81	−3.73
PArel	0.07	1.12	1.73	0.24	8.35	5.69	−2.66
BH76	−4.72	4.78	5.43	0.26	12.04	1.56	−10.48
BHPERI	3.24	3.85	4.55	0.18	12.40	8.39	−4.01
BHDIV10	−0.96	2.72	3.30	0.06	10.86	5.42	−5.44
INV24	−1.54	1.74	1.97	0.05	5.80	1.72	−4.08
BHROT27	0.34	0.41	0.61	0.07	1.60	1.34	−0.26
PX13	−3.76	3.76	3.89	0.11	3.72	−1.94	−5.66
WCPT18	−1.18	1.38	1.78	0.04	5.10	1.15	−3.95
RG18	−0.43	0.44	0.63	0.76	1.46	0.11	−1.35
ADIM6	−4.18	4.18	4.61	1.24	5.68	−1.52	−7.19
S22	−3.12	3.14	4.27	0.43	11.56	0.12	−11.45
S66	−2.60	2.61	3.21	0.48	8.00	0.19	−7.81
HEAVY28	−1.02	1.02	1.11	0.82	1.58	−0.38	−1.96
WATER27	−1.73	2.54	3.98	0.03	14.07	2.02	−12.05
CARBHB12	−0.09	0.48	0.63	0.08	2.28	1.20	−1.08
PNICO23	−1.33	1.33	1.45	0.31	2.74	−0.51	−3.25
HAL59	−1.29	1.40	1.87	0.31	9.03	2.15	−6.88
AHB21	0.30	0.53	0.68	0.02	2.64	1.79	−0.85
CHB6	−0.28	1.28	1.56	0.05	4.71	2.70	−2.00
IL16	3.30	3.30	3.37	0.03	2.60	4.92	2.32
IDISP	4.10	15.00	17.49	1.05	48.19	32.43	−15.76
ICONF	0.06	0.53	0.78	0.16	3.90	2.11	−1.79
ACONF	0.80	0.80	0.90	0.44	1.36	1.61	0.24
AMINO20x4	−0.07	0.60	0.76	0.25	3.86	2.26	−1.60
PCONF21	−0.38	3.42	3.90	2.11	11.36	6.28	−5.08
MCONF	−2.15	2.21	2.52	0.44	4.32	0.40	−3.91
SCONF	−0.34	0.61	0.75	0.13	2.91	1.70	−1.21
UPU23	1.89	2.28	3.30	0.40	9.56	8.48	−1.08
BUT14DIOL	−0.08	0.29	0.35	0.10	1.33	0.78	−0.56

Table S153: Statistical analysis for the O3LYP DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	17.75	17.96	20.83	0.06	53.57	42.10	−11.47
G21EA	0.66	1.91	2.42	0.06	9.32	4.72	−4.61
G21IP	−0.22	3.12	3.94	0.01	14.76	7.37	−7.39
DIPCS10	−1.91	3.92	4.89	0.01	15.79	5.79	−10.00
PA26	1.44	1.74	2.40	0.01	8.18	6.60	−1.58
SIE4x4	21.07	21.07	23.72	0.62	40.66	44.57	3.91
ALKBDE10	5.29	5.86	8.99	0.06	25.64	23.72	−1.92
YBDE18	−0.25	5.01	5.71	0.10	19.87	8.24	−11.63
AL2X6	−5.37	5.37	5.76	0.15	5.97	−1.49	−7.46
HEAVYSB11	−2.27	5.10	5.54	0.09	15.30	6.47	−8.83
NBPRC	1.17	2.70	3.34	0.10	11.11	6.53	−4.58
ALK8	−2.10	3.47	4.51	0.06	14.94	5.49	−9.45
RC21	5.39	5.99	6.98	0.17	16.71	13.84	−2.87
G2RC	−2.10	6.22	7.95	0.12	32.61	15.05	−17.56
BH76RC	−0.65	3.28	4.86	0.15	28.09	17.76	−10.33
FH51	−0.03	2.60	3.80	0.08	20.78	10.31	−10.46
TAUT15	0.57	1.67	2.49	0.55	7.91	5.34	−2.57
DC13	1.48	9.10	11.67	0.17	46.43	24.64	−21.79
MB16-43	−7.87	18.02	23.12	0.04	89.58	35.08	−54.49
DARC	3.41	4.79	5.36	0.15	12.97	7.59	−5.38
RSE43	−3.02	3.02	3.35	0.40	6.28	−0.94	−7.22
BSR36	−8.28	8.28	9.39	0.51	18.97	−1.79	−20.76
CDIE20	1.78	1.82	2.06	0.45	4.13	3.80	−0.34
ISO34	−0.62	1.90	2.64	0.13	13.94	4.89	−9.05
ISOL24	−2.30	5.78	8.93	0.26	47.50	16.59	−30.91
C60ISO	−3.89	4.22	5.83	0.04	12.66	0.93	−11.73
PArel	0.74	1.75	2.36	0.38	10.13	6.91	−3.22
BH76	−6.90	7.05	8.10	0.38	28.76	3.41	−25.34
BHPERI	−0.74	1.71	2.30	0.08	8.91	2.88	−6.04
BHDIV10	−5.19	5.78	6.50	0.13	12.78	2.91	−9.87
INV24	−2.07	2.07	2.67	0.06	7.13	−0.28	−7.41
BHROT27	0.61	0.68	0.91	0.11	2.54	2.14	−0.40
PX13	−9.78	9.78	10.03	0.29	9.06	−6.15	−15.21
WCPT18	−6.16	6.16	6.50	0.18	8.22	−3.40	−11.62
RG18	−0.23	0.41	0.56	0.71	1.96	0.65	−1.32
ADIM6	−4.58	4.58	5.07	1.36	6.35	−1.59	−7.94
S22	−3.21	3.22	4.51	0.44	12.50	0.10	−12.40
S66	−2.76	2.77	3.44	0.51	8.63	0.16	−8.48
HEAVY28	−1.04	1.04	1.16	0.84	1.81	−0.31	−2.11
WATER27	−1.67	3.44	5.23	0.04	18.83	3.68	−15.15
CARBHB12	0.49	0.74	1.12	0.12	3.48	2.62	−0.86
PNICO23	−0.95	1.20	1.41	0.28	6.22	2.93	−3.29
HAL59	−1.18	1.50	2.02	0.33	10.85	3.57	−7.28
AHB21	−0.49	1.03	1.27	0.05	4.99	2.05	−2.94
CHB6	−0.84	1.56	1.83	0.06	5.14	2.16	−2.98
IL16	2.28	2.28	2.45	0.02	3.38	4.29	0.91
IDISP	2.31	13.03	14.21	0.92	36.99	21.26	−15.73
ICONF	0.33	0.57	0.87	0.17	3.81	2.84	−0.97
ACONF	1.01	1.01	1.12	0.55	1.49	1.84	0.36
AMINO20x4	0.03	0.66	0.83	0.27	3.91	2.38	−1.53
PCONF21	−0.68	4.35	4.84	2.69	13.55	7.67	−5.88
MCONF	−2.21	2.31	2.62	0.46	5.18	0.91	−4.27
SCONF	−0.07	0.47	0.68	0.10	3.01	2.00	−1.01
UPU23	1.69	2.29	3.37	0.40	10.81	9.28	−1.53
BUT14DIOL	−0.04	0.33	0.41	0.12	1.67	0.95	−0.72

Table S154: Statistical analysis for the B97-1 DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.37	3.46	4.75	0.01	35.25	10.26	−24.99
G21EA	−0.39	1.45	1.77	0.04	7.07	4.29	−2.78
G21IP	−0.36	2.86	3.52	0.01	13.69	6.81	−6.88
DIPCS10	−3.73	4.56	5.71	0.01	14.24	2.56	−11.68
PA26	3.51	3.51	4.15	0.02	9.37	9.74	0.37
SIE4x4	16.59	16.59	18.43	0.49	29.90	34.24	4.33
ALKBDE10	−1.07	3.57	4.63	0.04	17.08	9.19	−7.88
YBDE18	−3.79	4.95	6.23	0.10	15.64	3.11	−12.53
AL2X6	−4.93	4.93	5.29	0.14	5.75	−1.53	−7.29
HEAVYSB11	−2.92	3.11	3.96	0.05	8.19	1.07	−7.12
NBPRC	2.23	2.89	3.77	0.10	9.51	7.91	−1.59
ALK8	−0.91	1.87	2.56	0.03	9.01	3.85	−5.16
RC21	2.23	3.04	3.53	0.09	9.44	6.66	−2.79
G2RC	−0.42	3.87	4.70	0.08	18.49	9.91	−8.58
BH76RC	0.33	2.11	2.74	0.10	13.00	8.35	−4.65
FH51	1.17	2.57	3.35	0.08	15.50	8.61	−6.89
TAUT15	−0.10	0.96	1.15	0.31	3.76	2.00	−1.76
DC13	0.86	8.64	10.86	0.16	40.93	15.47	−25.46
MB16-43	−32.84	33.11	37.54	0.08	71.32	5.81	−65.51
DARC	7.07	7.07	7.74	0.22	9.72	9.78	0.06
RSE43	−2.29	2.29	2.50	0.30	4.08	−1.05	−5.13
BSR36	−9.62	9.62	11.10	0.59	21.95	−2.95	−24.90
CDIE20	1.10	1.11	1.25	0.27	2.16	2.14	−0.03
ISO34	−0.42	1.37	2.14	0.09	13.87	6.42	−7.45
ISOL24	−2.74	6.01	9.47	0.27	51.43	19.18	−32.25
C60ISO	−1.14	2.19	2.98	0.02	7.66	1.36	−6.30
PArel	0.25	0.97	1.56	0.21	7.55	5.30	−2.25
BH76	−4.04	4.21	4.83	0.23	12.51	2.44	−10.07
BHPERI	0.35	1.74	2.11	0.08	10.01	3.96	−6.05
BHDIV10	−2.70	3.50	3.81	0.08	9.09	3.60	−5.48
INV24	−1.42	1.69	1.95	0.05	6.41	2.14	−4.27
BHROT27	0.30	0.38	0.53	0.06	1.46	1.20	−0.26
PX13	−3.72	3.72	3.81	0.11	3.19	−2.53	−5.72
WCPT18	−2.45	2.45	2.93	0.07	6.16	0.02	−6.13
RG18	−0.13	0.22	0.31	0.38	0.90	0.15	−0.75
ADIM6	−2.82	2.82	3.14	0.84	4.12	−0.89	−5.01
S22	−2.34	2.35	3.31	0.32	9.46	0.17	−9.29
S66	−1.83	1.85	2.32	0.34	6.49	0.23	−6.26
HEAVY28	−0.39	0.40	0.49	0.32	1.07	0.06	−1.01
WATER27	−1.28	2.04	3.30	0.03	11.78	1.63	−10.15
CARBHB12	0.48	0.57	0.81	0.09	2.39	1.97	−0.42
PNICO23	−0.47	0.58	0.73	0.14	3.40	1.26	−2.14
HAL59	−0.72	0.94	1.35	0.20	7.93	2.52	−5.41
AHB21	−0.17	0.52	0.65	0.02	2.65	1.25	−1.40
CHB6	−0.07	0.82	1.04	0.03	3.12	1.96	−1.16
IL16	2.34	2.34	2.43	0.02	2.70	4.05	1.34
IDISP	2.98	11.82	13.39	0.83	36.11	23.25	−12.86
ICONF	0.07	0.39	0.63	0.12	3.13	1.95	−1.18
ACONF	0.62	0.62	0.69	0.34	1.07	1.30	0.22
AMINO20x4	−0.09	0.48	0.60	0.20	3.06	1.71	−1.35
PCONF21	−0.40	2.76	3.10	1.70	9.03	5.11	−3.92
MCONF	−1.66	1.71	1.94	0.34	3.51	0.40	−3.10
SCONF	−0.40	0.63	0.74	0.14	2.60	1.39	−1.22
UPU23	1.41	1.83	2.58	0.32	7.44	6.29	−1.15
BUT14DIOL	−0.21	0.34	0.38	0.12	1.37	0.66	−0.71

Table S155: Statistical analysis for the B97-2 DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.60	3.18	4.48	0.01	36.19	13.49	−22.70
G21EA	−1.66	2.13	2.52	0.06	9.52	3.39	−6.13
G21IP	−0.81	2.62	3.32	0.01	13.26	6.27	−6.99
DIPCS10	−4.41	4.73	6.02	0.01	13.13	1.26	−11.87
PA26	4.87	4.87	5.31	0.03	9.05	10.95	1.90
SIE4x4	16.07	16.07	17.88	0.48	28.77	33.92	5.15
ALKBDE10	−1.86	4.32	5.43	0.04	20.46	10.57	−9.89
YBDE18	−3.68	4.80	6.13	0.10	18.28	3.78	−14.51
AL2X6	−7.20	7.20	7.56	0.20	7.18	−3.20	−10.38
HEAVYSB11	−3.50	3.62	4.63	0.06	8.85	0.64	−8.21
NBPRC	3.55	3.66	5.21	0.13	12.57	12.30	−0.28
ALK8	−2.50	3.43	4.55	0.05	14.09	3.23	−10.86
RC21	1.52	2.48	2.93	0.07	8.78	6.07	−2.71
G2RC	−0.50	3.65	4.58	0.07	18.03	10.05	−7.98
BH76RC	0.25	1.87	2.79	0.09	15.27	10.84	−4.43
FH51	1.23	2.63	3.60	0.08	20.08	11.07	−9.01
TAUT15	0.09	0.99	1.20	0.32	3.56	2.10	−1.46
DC13	3.02	9.41	11.91	0.17	36.98	20.43	−16.55
MB16-43	−41.64	41.64	44.98	0.10	66.08	−7.73	−73.82
DARC	8.44	8.44	9.22	0.26	11.48	11.64	0.16
RSE43	−2.61	2.61	2.84	0.34	4.57	−1.26	−5.83
BSR36	−10.42	10.42	11.71	0.64	23.29	−2.47	−25.76
CDIE20	1.55	1.59	1.85	0.39	3.99	3.61	−0.38
ISO34	−0.68	1.67	2.65	0.11	16.95	7.03	−9.92
ISOL24	−3.71	6.75	10.98	0.31	58.71	18.12	−40.59
C60ISO	−0.05	2.18	2.60	0.02	7.20	2.25	−4.95
PArel	0.54	0.97	1.63	0.21	7.37	5.58	−1.79
BH76	−2.52	2.93	3.54	0.16	13.67	3.60	−10.08
BHPERI	2.81	3.40	3.78	0.16	10.31	7.21	−3.10
BHDIV10	−1.83	2.70	3.09	0.06	8.39	3.20	−5.19
INV24	−1.51	1.83	2.18	0.06	9.46	3.72	−5.73
BHROT27	0.43	0.49	0.65	0.08	1.62	1.30	−0.32
PX13	−3.14	3.14	3.29	0.09	3.80	−1.16	−4.96
WCPT18	−1.21	1.31	1.68	0.04	4.47	0.47	−4.00
RG18	−0.69	0.69	0.87	1.19	1.86	−0.10	−1.96
ADIM6	−5.16	5.16	5.65	1.54	6.73	−1.96	−8.69
S22	−3.97	3.97	5.06	0.54	12.60	−0.72	−13.32
S66	−3.43	3.43	3.92	0.63	8.78	−0.61	−9.39
HEAVY28	−1.14	1.14	1.21	0.92	1.50	−0.43	−1.92
WATER27	−11.70	11.75	18.40	0.14	49.73	0.63	−49.10
CARBHB12	−0.39	0.68	0.82	0.11	2.66	1.14	−1.51
PNICO23	−1.57	1.57	1.69	0.37	3.20	−0.14	−3.35
HAL59	−1.91	1.94	2.32	0.42	8.63	0.84	−7.79
AHB21	0.74	0.96	1.22	0.04	4.15	2.91	−1.23
CHB6	1.00	1.06	1.55	0.04	3.50	3.36	−0.14
IL16	3.95	3.95	4.06	0.04	3.75	6.36	2.61
IDISP	3.04	15.13	16.66	1.06	43.66	26.26	−17.41
ICONF	0.17	0.60	0.87	0.18	4.16	2.57	−1.60
ACONF	1.04	1.04	1.15	0.57	1.53	1.92	0.39
AMINO20x4	−0.14	0.69	0.86	0.28	3.94	2.34	−1.60
PCONF21	−0.52	4.04	4.60	2.49	13.66	7.66	−5.99
MCONF	−2.42	2.48	2.81	0.50	4.88	0.60	−4.28
SCONF	−0.56	1.11	1.30	0.24	4.65	2.67	−1.98
UPU23	1.94	2.51	3.66	0.44	11.49	9.77	−1.72
BUT14DIOL	−0.60	0.71	0.78	0.25	2.14	0.74	−1.40

Table S156: Statistical analysis for the B98 DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−1.47	2.68	4.16	0.01	33.35	4.86	−28.48
G21EA	0.36	1.46	1.96	0.04	7.85	5.77	−2.09
G21IP	0.58	2.97	3.64	0.01	15.01	8.71	−6.30
DIPCS10	−1.89	3.64	4.78	0.01	14.77	4.61	−10.16
PA26	3.57	3.57	4.21	0.02	9.62	9.81	0.19
SIE4x4	16.35	16.35	18.32	0.48	30.94	35.07	4.13
ALKBDE10	−1.29	3.52	4.68	0.03	17.77	8.66	−9.12
YBDE18	−5.26	5.59	6.97	0.11	14.52	1.01	−13.51
AL2X6	−5.73	5.73	6.09	0.16	6.34	−2.24	−8.58
HEAVYSB11	−4.26	4.26	5.03	0.07	8.51	−0.35	−8.86
NBPRC	2.70	3.22	4.32	0.12	11.41	9.69	−1.72
ALK8	−2.47	3.17	4.18	0.05	9.99	2.79	−7.19
RC21	1.55	2.42	2.89	0.07	9.70	5.37	−4.32
G2RC	−0.31	3.43	4.17	0.07	16.31	9.52	−6.79
BH76RC	−0.13	1.67	2.29	0.08	11.62	5.92	−5.70
FH51	1.40	2.63	3.47	0.08	17.81	9.05	−8.75
TAUT15	−0.04	0.97	1.21	0.32	4.03	2.17	−1.86
DC13	1.63	9.57	12.35	0.17	44.71	17.79	−26.92
MB16-43	−38.21	38.21	43.11	0.09	86.72	−1.59	−88.31
DARC	8.63	8.63	9.21	0.27	9.93	11.33	1.40
RSE43	−2.14	2.14	2.34	0.28	3.82	−0.99	−4.81
BSR36	−9.99	9.99	11.43	0.62	22.67	−2.91	−25.57
CDIE20	1.08	1.08	1.23	0.27	2.15	2.08	−0.07
ISO34	−0.33	1.54	2.34	0.11	15.32	7.25	−8.07
ISOL24	−2.93	6.66	10.41	0.30	56.76	21.30	−35.46
C60ISO	−0.43	2.06	2.57	0.02	6.88	1.73	−5.16
PArel	0.24	0.98	1.58	0.21	7.35	5.41	−1.94
BH76	−3.86	4.04	4.50	0.22	11.89	2.57	−9.31
BHPERI	1.07	2.28	2.68	0.11	12.04	5.22	−6.82
BHDIV10	−2.23	3.27	3.53	0.07	9.59	3.92	−5.66
INV24	−1.46	1.82	2.07	0.06	6.61	2.63	−3.98
BHROT27	0.31	0.40	0.55	0.06	1.49	1.20	−0.28
PX13	−3.96	3.96	4.08	0.12	3.90	−2.42	−6.32
WCPT18	−2.09	2.12	2.58	0.06	5.80	0.31	−5.49
RG18	−0.28	0.29	0.44	0.50	1.12	0.06	−1.06
ADIM6	−3.48	3.48	3.86	1.04	4.88	−1.19	−6.07
S22	−2.76	2.76	3.79	0.38	10.44	−0.02	−10.46
S66	−2.25	2.25	2.76	0.41	7.17	0.05	−7.12
HEAVY28	−0.62	0.62	0.69	0.50	1.22	−0.08	−1.31
WATER27	−3.16	3.66	5.97	0.05	19.23	1.60	−17.63
CARBHB12	0.24	0.50	0.69	0.08	2.44	1.71	−0.73
PNICO23	−0.80	0.84	0.95	0.20	2.96	0.45	−2.51
HAL59	−1.05	1.19	1.59	0.26	8.26	2.15	−6.11
AHB21	0.02	0.57	0.70	0.03	2.73	1.64	−1.09
CHB6	0.14	0.88	1.12	0.03	3.23	2.34	−0.89
IL16	2.81	2.81	2.90	0.03	2.93	4.71	1.79
IDISP	3.09	13.03	14.70	0.92	39.23	25.33	−13.90
ICONF	0.07	0.42	0.66	0.13	3.30	1.95	−1.35
ACONF	0.73	0.73	0.82	0.40	1.21	1.47	0.27
AMINO20x4	−0.10	0.54	0.67	0.22	3.32	1.91	−1.41
PCONF21	−0.45	3.13	3.53	1.93	10.29	5.77	−4.52
MCONF	−1.89	1.94	2.20	0.39	3.86	0.42	−3.43
SCONF	−0.42	0.70	0.82	0.15	2.94	1.61	−1.33
UPU23	1.58	2.03	2.90	0.35	8.46	7.27	−1.19
BUT14DIOL	−0.25	0.39	0.43	0.14	1.51	0.70	−0.81

Table S157: Statistical analysis for the HISS DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−7.80	7.96	10.10	0.03	47.20	3.29	−43.91
G21EA	−1.83	3.65	4.22	0.11	12.53	4.41	−8.12
G21IP	1.04	4.19	5.17	0.02	19.89	10.53	−9.36
DIPCS10	0.04	4.42	5.09	0.01	17.40	9.70	−7.70
PA26	3.26	3.26	3.89	0.02	8.39	8.49	0.10
SIE4x4	8.64	8.64	10.22	0.26	19.81	21.96	2.15
ALKBDE10	−5.35	6.12	7.82	0.06	22.57	3.87	−18.70
YBDE18	−2.46	3.07	3.83	0.06	10.01	1.70	−8.32
AL2X6	−1.67	1.89	2.13	0.05	4.04	0.66	−3.38
HEAVYSB11	−4.22	4.22	4.44	0.07	5.14	−1.98	−7.12
NBPRC	0.08	2.80	3.34	0.10	10.63	7.18	−3.45
ALK8	2.75	2.75	4.25	0.04	10.26	10.60	0.33
RC21	3.46	4.16	5.35	0.12	18.89	16.08	−2.82
G2RC	−5.91	7.54	9.59	0.15	32.38	9.66	−22.72
BH76RC	−1.06	2.40	3.10	0.11	10.31	3.75	−6.56
FH51	−2.54	3.53	4.43	0.11	19.13	6.77	−12.35
TAUT15	0.14	1.17	1.56	0.38	5.19	3.17	−2.03
DC13	−2.78	10.22	12.17	0.19	42.57	24.56	−18.01
MB16-43	−4.81	20.40	25.58	0.05	110.93	49.62	−61.31
DARC	−3.90	3.90	4.95	0.12	10.22	−0.92	−11.14
RSE43	−0.66	0.67	0.87	0.09	2.42	0.17	−2.25
BSR36	−7.67	7.67	8.68	0.47	15.85	−2.95	−18.80
CDIE20	1.28	1.34	1.66	0.33	3.83	3.35	−0.48
ISO34	−0.12	1.98	2.58	0.14	10.46	4.24	−6.22
ISOL24	0.33	3.32	4.64	0.15	20.61	10.80	−9.82
C60ISO	5.25	5.25	5.83	0.05	9.26	10.65	1.39
PArel	0.97	1.31	1.98	0.28	7.80	6.21	−1.60
BH76	−0.75	1.55	1.97	0.08	9.86	5.28	−4.58
BHPERI	2.08	2.25	2.84	0.11	10.04	7.81	−2.23
BHDIV10	−0.60	1.75	2.22	0.04	7.62	2.98	−4.64
INV24	−0.50	2.08	3.42	0.07	20.19	12.30	−7.89
BHROT27	0.86	0.89	1.22	0.14	2.60	2.45	−0.15
PX13	−2.87	2.87	3.15	0.09	4.43	−0.32	−4.75
WCPT18	−0.32	2.15	2.34	0.06	7.91	4.44	−3.47
RG18	−0.32	0.32	0.46	0.55	1.16	0.03	−1.13
ADIM6	−3.20	3.20	3.52	0.95	4.30	−1.13	−5.43
S22	−1.86	2.03	2.97	0.28	9.68	1.47	−8.22
S66	−1.63	1.76	2.27	0.32	7.09	1.38	−5.71
HEAVY28	−0.46	0.48	0.57	0.39	1.23	0.11	−1.12
WATER27	1.94	2.39	2.84	0.03	11.92	7.26	−4.66
CARBHB12	0.73	0.78	1.05	0.13	2.72	2.46	−0.26
PNICO23	−0.15	0.49	0.70	0.11	3.91	1.84	−2.07
HAL59	−0.58	0.97	1.30	0.21	7.26	2.31	−4.95
AHB21	−1.32	1.41	1.87	0.06	5.07	0.81	−4.26
CHB6	−1.09	1.36	1.61	0.05	3.83	0.82	−3.01
IL16	1.56	1.56	1.70	0.01	2.77	3.40	0.63
IDISP	0.41	8.70	9.40	0.61	24.05	10.97	−13.08
ICONF	0.27	0.51	0.71	0.16	2.51	1.62	−0.89
ACONF	0.60	0.60	0.67	0.33	0.96	1.17	0.21
AMINO20x4	0.11	0.46	0.61	0.19	3.27	1.93	−1.33
PCONF21	−0.14	2.77	3.16	1.71	8.68	5.10	−3.58
MCONF	−1.30	1.41	1.61	0.28	3.53	0.73	−2.80
SCONF	−0.12	0.35	0.47	0.08	2.01	1.31	−0.70
UPU23	1.58	1.81	2.64	0.32	7.15	6.39	−0.77
BUT14DIOL	−0.08	0.19	0.24	0.07	0.91	0.44	−0.48

Table S158: Statistical analysis for the HSE03 DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−1.81	3.43	5.00	0.01	33.30	6.31	−26.99
G21EA	4.46	4.46	5.31	0.13	9.29	9.79	0.50
G21IP	5.72	6.04	7.21	0.02	18.36	15.03	−3.32
DIPCS10	10.22	10.22	10.80	0.02	10.29	14.56	4.28
PA26	2.88	2.88	3.48	0.02	8.36	8.45	0.09
SIE4x4	14.30	14.30	16.10	0.42	27.80	31.21	3.41
ALKBDE10	−2.39	5.01	5.97	0.05	20.41	8.95	−11.47
YBDE18	−2.76	2.85	3.51	0.06	9.03	0.81	−8.22
AL2X6	−2.84	2.91	3.29	0.08	4.97	0.22	−4.76
HEAVYSB11	−3.17	3.17	3.99	0.05	7.29	−0.21	−7.50
NBPRC	0.73	2.51	3.00	0.09	9.76	5.92	−3.83
ALK8	1.92	2.19	3.27	0.03	8.14	7.34	−0.81
RC21	3.45	3.87	4.72	0.11	12.46	10.48	−1.98
G2RC	−2.85	5.71	7.17	0.11	27.22	9.68	−17.54
BH76RC	−0.16	2.27	3.09	0.11	16.21	9.51	−6.69
FH51	−0.47	2.41	3.26	0.08	16.13	7.95	−8.19
TAUT15	0.34	1.22	1.70	0.40	5.16	3.49	−1.67
DC13	−0.40	8.33	10.97	0.15	44.60	20.71	−23.89
MB16-43	−13.95	18.62	22.84	0.04	82.00	33.96	−48.04
DARC	1.79	3.56	3.92	0.11	11.16	5.04	−6.12
RSE43	−1.58	1.58	1.78	0.21	3.58	−0.57	−4.15
BSR36	−8.09	8.09	9.25	0.50	17.59	−2.74	−20.34
CDIE20	1.41	1.44	1.68	0.35	3.42	3.11	−0.31
ISO34	−0.40	1.54	2.17	0.11	12.17	5.52	−6.65
ISOL24	−1.49	4.44	6.73	0.20	35.46	13.70	−21.76
C60ISO	0.14	2.35	2.73	0.02	7.59	2.53	−5.06
PArel	0.67	1.16	1.79	0.25	7.83	5.90	−1.92
BH76	−4.05	4.25	4.70	0.23	15.71	2.64	−13.08
BHPERI	−0.30	1.18	1.44	0.06	5.48	1.91	−3.58
BHDIV10	−3.32	4.02	4.49	0.09	10.27	3.51	−6.76
INV24	−1.15	1.52	1.97	0.05	9.36	4.11	−5.24
BHROT27	0.58	0.64	0.84	0.10	1.82	1.57	−0.25
PX13	−5.63	5.63	5.77	0.17	5.21	−3.32	−8.53
WCPT18	−3.36	3.36	3.96	0.10	7.31	−0.53	−7.84
RG18	−0.26	0.27	0.43	0.47	1.11	0.08	−1.04
ADIM6	−3.32	3.32	3.67	0.99	4.55	−1.16	−5.71
S22	−2.11	2.22	3.25	0.30	10.07	0.95	−9.12
S66	−1.81	1.90	2.45	0.35	7.26	0.95	−6.32
HEAVY28	−0.46	0.48	0.58	0.39	1.32	0.13	−1.19
WATER27	2.16	2.73	3.36	0.03	16.67	9.47	−7.21
CARBHB12	0.86	0.89	1.21	0.15	2.89	2.72	−0.17
PNICO23	−0.17	0.58	0.84	0.14	4.88	2.67	−2.20
HAL59	−0.52	1.03	1.44	0.22	8.50	3.06	−5.44
AHB21	−1.11	1.22	1.53	0.05	4.22	0.97	−3.24
CHB6	−0.64	1.10	1.30	0.04	3.66	1.37	−2.29
IL16	1.27	1.27	1.45	0.01	2.96	3.03	0.07
IDISP	1.75	9.88	10.88	0.69	28.70	17.12	−11.58
ICONF	0.23	0.41	0.63	0.13	2.72	1.96	−0.76
ACONF	0.61	0.61	0.68	0.33	0.93	1.16	0.22
AMINO20x4	0.05	0.47	0.59	0.19	3.04	1.82	−1.22
PCONF21	−0.45	3.05	3.39	1.88	9.17	5.21	−3.96
MCONF	−1.52	1.60	1.83	0.32	3.83	0.72	−3.11
SCONF	−0.01	0.22	0.29	0.05	1.23	0.76	−0.47
UPU23	1.49	1.86	2.70	0.33	7.84	6.85	−0.99
BUT14DIOL	0.06	0.20	0.26	0.07	1.13	0.76	−0.37

Table S159: Statistical analysis for the HSE06 DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−2.57	3.74	5.40	0.01	32.89	5.82	−27.07
G21EA	−0.60	2.68	2.99	0.08	9.10	4.22	−4.88
G21IP	−0.07	3.70	4.39	0.01	17.28	9.14	−8.14
DIPCS10	−1.63	3.05	3.88	0.00	10.75	3.14	−7.61
PA26	2.36	2.43	3.06	0.01	8.66	7.77	−0.88
SIE4x4	14.30	14.30	16.12	0.42	28.08	31.28	3.19
ALKBDE10	−4.20	5.72	6.56	0.06	18.56	5.62	−12.94
YBDE18	−2.88	2.96	3.60	0.06	8.96	0.76	−8.20
AL2X6	−2.94	2.97	3.36	0.08	4.77	0.08	−4.69
HEAVYSB11	−3.25	3.25	4.07	0.06	7.27	−0.22	−7.50
NBPRC	0.81	2.48	2.97	0.09	9.74	5.94	−3.80
ALK8	1.40	2.05	3.13	0.03	8.34	6.99	−1.35
RC21	3.35	3.79	4.62	0.11	12.11	10.14	−1.97
G2RC	−2.49	5.80	7.15	0.11	27.44	10.41	−17.02
BH76RC	−0.08	2.29	3.09	0.11	16.28	9.78	−6.51
FH51	−0.36	2.35	3.19	0.08	16.02	8.05	−7.97
TAUT15	0.35	1.20	1.70	0.39	5.31	3.53	−1.78
DC13	−0.06	8.04	10.51	0.15	42.26	20.75	−21.51
MB16-43	−14.78	19.02	23.49	0.05	84.57	33.22	−51.35
DARC	1.87	3.55	3.90	0.11	10.91	5.07	−5.83
RSE43	−1.59	1.59	1.79	0.21	3.63	−0.53	−4.16
BSR36	−7.68	7.68	8.77	0.47	16.74	−2.50	−19.24
CDIE20	1.39	1.42	1.65	0.35	3.35	3.06	−0.28
ISO34	−0.42	1.52	2.13	0.10	11.71	5.22	−6.49
ISOL24	−1.50	4.40	6.67	0.20	35.27	13.71	−21.56
C60ISO	−0.28	2.33	2.86	0.02	7.99	2.26	−5.73
PArel	0.68	1.18	1.80	0.25	7.80	5.89	−1.90
BH76	−4.12	4.29	4.77	0.23	15.80	2.35	−13.44
BHPERI	−0.43	1.18	1.48	0.06	5.46	1.70	−3.76
BHDIV10	−3.51	4.18	4.63	0.09	10.14	3.35	−6.79
INV24	−1.19	1.52	1.95	0.05	9.10	3.85	−5.25
BHROT27	0.56	0.62	0.82	0.10	1.77	1.55	−0.22
PX13	−5.80	5.80	5.93	0.17	5.11	−3.62	−8.73
WCPT18	−3.58	3.58	4.12	0.10	7.33	−0.80	−8.12
RG18	−0.29	0.30	0.45	0.52	1.17	0.06	−1.11
ADIM6	−3.38	3.38	3.73	1.01	4.59	−1.19	−5.78
S22	−2.18	2.27	3.27	0.31	9.86	0.73	−9.12
S66	−1.88	1.94	2.49	0.35	7.10	0.74	−6.36
HEAVY28	−0.50	0.51	0.61	0.41	1.29	0.06	−1.22
WATER27	1.38	2.24	2.85	0.03	14.53	7.17	−7.37
CARBHB12	0.76	0.81	1.13	0.13	2.86	2.60	−0.26
PNICO23	−0.20	0.60	0.86	0.14	4.95	2.73	−2.22
HAL59	−0.56	1.04	1.45	0.23	8.47	2.99	−5.48
AHB21	−0.89	1.03	1.30	0.05	3.89	1.07	−2.83
CHB6	−0.59	1.06	1.27	0.04	3.67	1.40	−2.26
IL16	1.50	1.50	1.63	0.01	2.71	3.17	0.46
IDISP	1.70	9.75	10.75	0.69	28.27	17.08	−11.20
ICONF	0.23	0.40	0.61	0.12	2.62	1.92	−0.70
ACONF	0.61	0.61	0.69	0.33	0.94	1.16	0.23
AMINO20x4	0.04	0.47	0.59	0.19	3.00	1.79	−1.21
PCONF21	−0.45	3.03	3.37	1.87	9.13	5.20	−3.93
MCONF	−1.52	1.61	1.83	0.32	3.84	0.73	−3.11
SCONF	0.00	0.22	0.29	0.05	1.27	0.81	−0.46
UPU23	1.48	1.87	2.70	0.33	7.93	6.88	−1.06
BUT14DIOL	0.04	0.20	0.26	0.07	1.15	0.74	−0.40

Table S160: Statistical analysis for the TPSSh DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−1.62	4.41	6.12	0.01	41.69	15.28	−26.42
G21EA	−0.64	2.71	2.96	0.08	10.00	5.43	−4.56
G21IP	−0.88	3.91	4.67	0.02	19.79	11.55	−8.24
DIPCS10	−3.02	3.40	4.72	0.01	11.70	1.38	−10.32
PA26	4.44	4.44	4.96	0.02	9.32	11.09	1.77
SIE4x4	18.07	18.07	20.67	0.54	35.76	40.12	4.36
ALKBDE10	−2.12	4.88	6.18	0.05	22.20	13.82	−8.38
YBDE18	−6.94	6.94	7.50	0.14	9.85	−2.11	−11.96
AL2X6	−3.33	3.46	3.97	0.10	6.24	0.40	−5.84
HEAVYSB11	−4.30	4.37	5.47	0.08	10.66	0.41	−10.25
NBPRC	1.30	2.56	3.38	0.09	10.51	7.07	−3.45
ALK8	−0.37	1.32	1.79	0.02	5.71	1.52	−4.19
RC21	1.59	2.69	3.14	0.08	11.70	6.15	−5.54
G2RC	2.01	5.66	7.16	0.11	26.61	16.07	−10.54
BH76RC	0.01	3.37	4.38	0.16	17.11	8.11	−9.00
FH51	2.60	4.00	5.11	0.13	20.41	12.10	−8.31
TAUT15	0.25	1.33	1.57	0.44	4.67	2.94	−1.73
DC13	1.61	10.43	13.45	0.19	46.56	18.75	−27.81
MB16-43	−45.00	45.00	48.71	0.11	88.44	−0.85	−89.29
DARC	8.55	8.55	9.23	0.26	9.69	11.53	1.84
RSE43	−1.66	1.66	1.89	0.22	4.10	−0.67	−4.77
BSR36	−10.09	10.09	11.32	0.62	23.17	−2.29	−25.46
CDIE20	1.66	1.66	1.83	0.41	3.01	3.18	0.17
ISO34	−1.59	2.30	3.14	0.16	14.95	5.22	−9.73
ISOL24	−4.12	7.19	11.23	0.33	61.65	22.69	−38.96
C60ISO	−4.25	4.40	6.09	0.04	12.64	0.68	−11.96
PArel	0.36	1.32	1.81	0.29	8.96	5.24	−3.72
BH76	−6.65	6.68	7.48	0.36	17.35	1.11	−16.24
BHPERI	−0.74	1.48	1.87	0.07	6.74	2.36	−4.38
BHDIV10	−4.34	4.68	5.06	0.10	8.98	1.66	−7.32
INV24	−1.85	2.00	2.36	0.06	6.39	0.82	−5.56
BHROT27	0.39	0.54	0.70	0.09	2.00	1.41	−0.59
PX13	−6.37	6.37	6.48	0.19	5.18	−3.72	−8.90
WCPT18	−3.69	3.69	3.99	0.11	5.60	−1.22	−6.82
RG18	−0.49	0.49	0.67	0.84	1.49	−0.02	−1.50
ADIM6	−4.59	4.59	5.04	1.37	6.05	−1.73	−7.77
S22	−3.30	3.30	4.41	0.45	11.65	−0.20	−11.85
S66	−2.88	2.88	3.44	0.53	8.37	−0.15	−8.53
HEAVY28	−0.90	0.90	0.99	0.73	1.44	−0.30	−1.74
WATER27	−4.44	5.01	8.16	0.06	26.02	1.76	−24.26
CARBHB12	0.21	0.56	0.82	0.09	2.99	2.08	−0.92
PNICO23	−0.74	0.92	1.11	0.22	4.90	1.90	−3.00
HAL59	−1.06	1.46	1.96	0.32	10.79	3.69	−7.10
AHB21	0.27	0.62	0.81	0.03	3.12	2.24	−0.88
CHB6	0.19	1.05	1.33	0.04	4.07	2.67	−1.41
IL16	2.92	2.92	2.99	0.03	2.68	4.66	1.98
IDISP	3.08	12.21	14.08	0.86	39.57	25.80	−13.77
ICONF	0.09	0.34	0.50	0.10	2.40	1.58	−0.82
ACONF	0.72	0.72	0.81	0.39	1.14	1.39	0.25
AMINO20x4	−0.01	0.52	0.65	0.21	3.03	1.84	−1.20
PCONF21	−0.74	3.78	4.15	2.33	11.15	6.04	−5.12
MCONF	−2.07	2.14	2.41	0.43	4.70	0.76	−3.93
SCONF	0.05	0.27	0.33	0.06	1.21	0.62	−0.59
UPU23	1.77	2.30	3.38	0.40	10.91	9.37	−1.55
BUT14DIOL	−0.21	0.33	0.38	0.12	1.34	0.58	−0.76

Table S161: Statistical analysis for the revTPSSh DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−2.44	5.18	7.09	0.02	48.03	20.00	−28.02
G21EA	−1.44	2.91	3.22	0.09	9.25	3.76	−5.49
G21IP	−1.23	3.94	4.75	0.02	20.01	11.22	−8.78
DIPCS10	−3.65	3.75	5.26	0.01	12.19	0.52	−11.67
PA26	4.27	4.27	4.89	0.02	9.84	11.12	1.28
SIE4x4	17.68	17.68	20.24	0.52	34.96	39.00	4.04
ALKBDE10	−4.07	6.07	6.67	0.06	20.94	10.02	−10.92
YBDE18	−6.02	6.02	6.57	0.12	8.68	−1.16	−9.84
AL2X6	−2.26	2.41	2.72	0.07	4.28	0.46	−3.81
HEAVYSB11	−2.89	3.44	4.33	0.06	10.21	1.68	−8.52
NBPRC	0.53	1.90	2.68	0.07	9.58	6.31	−3.27
ALK8	−0.92	1.42	1.73	0.02	4.43	1.06	−3.37
RC21	2.20	3.40	3.90	0.10	12.93	8.17	−4.76
G2RC	4.07	8.48	10.72	0.17	36.70	22.53	−14.17
BH76RC	0.45	4.49	5.49	0.21	19.97	10.97	−9.00
FH51	2.94	4.63	5.97	0.15	24.88	16.65	−8.23
TAUT15	0.21	1.04	1.32	0.34	4.12	2.62	−1.50
DC13	0.68	9.69	12.90	0.18	52.16	20.76	−31.40
MB16-43	−52.37	52.37	57.00	0.13	94.78	−4.91	−99.69
DARC	5.35	5.42	6.19	0.17	8.71	8.23	−0.47
RSE43	−1.45	1.45	1.68	0.19	3.93	−0.50	−4.43
BSR36	−7.54	7.54	8.37	0.47	16.70	−1.31	−18.02
CDIE20	1.48	1.48	1.59	0.36	2.30	2.78	0.49
ISO34	−2.14	2.85	3.79	0.20	16.52	3.77	−12.74
ISOL24	−3.67	6.23	9.10	0.28	49.44	18.93	−30.51
C60ISO	−5.22	5.29	7.00	0.05	13.98	0.32	−13.66
PArel	0.56	1.33	1.72	0.29	7.89	4.61	−3.28
BH76	−6.45	6.46	7.52	0.35	17.53	0.12	−17.41
BHPERI	−1.62	1.69	2.09	0.08	5.88	0.85	−5.03
BHDIV10	−4.00	4.11	4.52	0.09	7.55	0.58	−6.97
INV24	−1.34	1.74	2.06	0.05	6.88	2.03	−4.85
BHROT27	0.39	0.52	0.67	0.08	1.91	1.43	−0.48
PX13	−3.99	3.99	4.21	0.12	4.59	−1.94	−6.53
WCPT18	−2.99	2.99	3.33	0.09	4.72	−0.83	−5.55
RG18	−0.52	0.52	0.69	0.90	1.62	−0.05	−1.66
ADIM6	−4.13	4.13	4.52	1.23	5.30	−1.58	−6.89
S22	−2.93	2.93	3.83	0.40	9.91	−0.13	−10.04
S66	−2.57	2.57	3.03	0.47	7.21	−0.15	−7.36
HEAVY28	−0.76	0.76	0.84	0.61	1.38	−0.09	−1.47
WATER27	−4.25	4.46	7.40	0.05	22.28	0.81	−21.47
CARBHB12	−0.06	0.47	0.62	0.08	2.29	1.36	−0.92
PNICO23	−0.50	0.74	0.94	0.17	4.63	1.98	−2.65
HAL59	−0.83	1.31	1.76	0.29	10.00	3.71	−6.29
AHB21	0.55	0.60	0.76	0.03	2.21	1.89	−0.32
CHB6	0.12	0.91	1.17	0.03	3.82	2.19	−1.63
IL16	2.76	2.76	2.81	0.03	2.24	3.96	1.72
IDISP	2.81	8.73	10.70	0.61	32.24	20.96	−11.28
ICONF	0.09	0.27	0.38	0.08	1.66	1.20	−0.46
ACONF	0.59	0.59	0.66	0.32	0.91	1.11	0.21
AMINO20x4	0.04	0.43	0.53	0.18	2.40	1.56	−0.84
PCONF21	−0.51	2.94	3.25	1.81	9.04	4.82	−4.22
MCONF	−1.73	1.79	2.02	0.36	4.13	0.79	−3.34
SCONF	0.25	0.36	0.43	0.08	1.36	0.88	−0.47
UPU23	1.36	2.00	2.90	0.35	9.90	8.00	−1.90
BUT14DIOL	−0.32	0.36	0.41	0.13	1.13	0.33	−0.79

Table S162: Statistical analysis for the TPSS0 DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−8.57	10.16	12.64	0.03	53.92	15.68	−38.25
G21EA	−2.11	3.67	4.37	0.11	13.42	4.85	−8.57
G21IP	−0.77	4.06	4.82	0.02	19.75	10.96	−8.79
DIPCS10	−2.19	3.94	5.11	0.01	16.03	4.58	−11.45
PA26	4.58	4.58	5.04	0.02	8.84	10.86	2.02
SIE4x4[a]	13.30	13.30	15.69	0.39	29.02	32.00	2.98
ALKBDE10	−7.20	7.65	8.81	0.08	20.98	2.25	−18.73
YBDE18	−6.47	6.47	6.86	0.13	8.00	−2.81	−10.81
AL2X6	−2.57	2.74	3.12	0.08	5.40	0.50	−4.90
HEAVYSB11	−5.12	5.12	5.60	0.09	7.55	−2.28	−9.83
NBPRC	1.00	2.36	2.92	0.09	8.58	5.37	−3.21
ALK8	0.22	1.18	1.49	0.02	5.28	2.89	−2.39
RC21	1.81	2.56	3.09	0.07	10.35	7.66	−2.69
G2RC	−0.67	4.91	6.02	0.10	23.35	11.03	−12.31
BH76RC	−0.63	3.46	4.39	0.16	18.22	9.27	−8.95
FH51	0.90	2.75	3.54	0.09	14.51	8.11	−6.40
TAUT15	0.31	0.98	1.20	0.32	3.37	2.19	−1.19
DC13	0.09	9.67	11.87	0.18	41.15	20.42	−20.73
MB16-43	−40.77	41.10	44.77	0.10	88.17	7.00	−81.17
DARC	4.23	4.61	5.29	0.14	9.43	7.03	−2.40
RSE43	−1.00	1.00	1.20	0.13	3.05	−0.07	−3.12
BSR36	−9.87	9.87	11.05	0.61	22.07	−2.59	−24.65
CDIE20	1.38	1.39	1.62	0.34	3.25	3.11	−0.13
ISO34	−1.16	2.06	2.64	0.14	11.81	4.29	−7.52
ISOL24	−2.58	5.09	8.08	0.23	43.65	14.43	−29.21
C60ISO	2.23	2.88	3.12	0.03	7.08	5.51	−1.57
PArel	0.64	1.05	1.49	0.23	6.47	4.78	−1.69
BH76	−3.94	4.06	4.89	0.22	14.54	1.73	−12.81
BHPERI	1.13	1.62	1.83	0.08	6.25	3.95	−2.31
BHDIV10	−2.27	2.66	2.81	0.06	6.56	1.95	−4.61
INV24	−0.88	1.94	2.36	0.06	9.98	6.14	−3.83
BHROT27	0.51	0.61	0.79	0.10	1.87	1.50	−0.36
PX13	−3.58	3.58	3.72	0.11	3.85	−1.31	−5.17
WCPT18	−1.23	1.54	1.85	0.04	5.54	2.04	−3.50
RG18	−0.51	0.51	0.66	0.88	1.34	−0.04	−1.37
ADIM6	−4.41	4.41	4.84	1.31	5.80	−1.65	−7.45
S22	−3.06	3.06	4.15	0.42	10.96	−0.17	−11.14
S66	−2.71	2.71	3.26	0.50	7.77	−0.17	−7.95
HEAVY28	−0.94	0.94	1.01	0.76	1.31	−0.38	−1.69
WATER27	−4.78	5.29	8.68	0.07	27.08	1.55	−25.53
CARBHB12	0.09	0.53	0.71	0.09	2.72	1.76	−0.96
PNICO23	−0.83	0.92	1.07	0.22	3.99	1.02	−2.97
HAL59	−1.28	1.46	1.87	0.32	8.72	2.00	−6.72
AHB21	−0.02	0.78	0.94	0.03	3.68	2.06	−1.62
CHB6	−0.28	1.12	1.41	0.04	4.43	2.13	−2.30
IL16	2.85	2.85	2.93	0.03	2.69	4.68	1.99
IDISP	1.88	11.17	12.37	0.79	32.85	20.02	−12.83
ICONF	0.15	0.34	0.50	0.10	2.23	1.42	−0.80
ACONF	0.67	0.67	0.76	0.37	1.09	1.27	0.18
AMINO20x4	0.01	0.50	0.63	0.20	2.97	1.83	−1.14
PCONF21	−0.51	3.45	3.87	2.13	10.64	5.83	−4.80
MCONF	−1.93	2.00	2.26	0.40	4.33	0.68	−3.65
SCONF	−0.09	0.27	0.35	0.06	1.42	0.67	−0.75
UPU23	1.79	2.22	3.26	0.39	9.97	8.80	−1.17
BUT14DIOL	−0.30	0.38	0.43	0.14	1.20	0.42	−0.78

[a] H_2^+ did not converge and was omitted from the statistics

Table S163: Statistical analysis for the revTPSS0 DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−9.09	10.89	13.43	0.04	59.90	20.29	−39.62
G21EA	−2.59	3.75	4.69	0.11	12.71	3.59	−9.13
G21IP	−0.81	4.07	4.90	0.02	19.93	10.84	−9.09
DIPCS10	−2.43	4.24	5.46	0.01	16.87	4.53	−12.34
PA26	4.43	4.43	4.96	0.02	9.23	10.87	1.65
SIE4x4	12.80	12.80	15.09	0.38	28.59	31.22	2.64
ALKBDE10	−8.81	8.81	10.12	0.09	19.74	−1.15	−20.89
YBDE18	−5.77	5.77	6.40	0.12	8.83	−1.28	−10.11
AL2X6	−1.72	1.89	2.12	0.05	3.81	0.51	−3.30
HEAVYSB11	−3.98	3.98	4.52	0.07	7.24	−1.27	−8.51
NBPRC	0.39	1.60	2.16	0.06	7.90	4.81	−3.09
ALK8	−0.30	1.13	1.26	0.02	3.29	1.33	−1.96
RC21	2.28	3.11	3.67	0.09	11.59	8.52	−3.06
G2RC	1.12	6.89	8.02	0.13	27.41	13.48	−13.93
BH76RC	−0.30	4.29	5.31	0.20	21.80	12.18	−9.62
FH51	1.21	3.22	4.22	0.10	20.12	11.70	−8.42
TAUT15	0.28	0.79	0.98	0.26	3.27	1.90	−1.37
DC13	−0.66	10.14	12.18	0.18	47.04	22.82	−24.22
MB16-43	−47.86	47.97	51.70	0.12	85.96	2.32	−83.65
DARC	1.73	2.98	3.30	0.09	7.81	4.50	−3.31
RSE43	−0.86	0.87	1.07	0.11	2.92	0.05	−2.86
BSR36	−7.55	7.55	8.37	0.47	16.34	−1.67	−18.01
CDIE20	1.22	1.22	1.40	0.30	2.55	2.76	0.21
ISO34	−1.64	2.60	3.17	0.18	12.07	4.01	−8.06
ISOL24	−2.24	4.34	6.47	0.20	33.94	11.58	−22.36
C60ISO	1.51	2.59	2.70	0.03	6.62	3.92	−2.70
PArel	0.80	1.13	1.51	0.24	5.72	4.25	−1.47
BH76	−3.84	3.96	5.05	0.21	16.01	0.87	−15.14
BHPERI	0.42	1.01	1.27	0.05	4.63	2.43	−2.20
BHDIV10	−1.94	2.15	2.35	0.05	4.71	1.06	−3.65
INV24	−0.46	1.78	2.40	0.06	10.12	6.90	−3.22
BHROT27	0.51	0.60	0.74	0.10	1.90	1.54	−0.36
PX13	−1.55	1.65	2.00	0.05	3.69	0.37	−3.32
WCPT18	−0.62	1.10	1.39	0.03	5.51	2.77	−2.75
RG18	−0.54	0.54	0.70	0.93	1.59	−0.07	−1.66
ADIM6	−4.02	4.02	4.39	1.20	5.14	−1.54	−6.67
S22	−2.72	2.72	3.63	0.37	9.39	−0.18	−9.57
S66	−2.42	2.42	2.89	0.44	6.83	−0.11	−6.94
HEAVY28	−0.79	0.79	0.86	0.64	1.24	−0.22	−1.45
WATER27	−4.40	4.62	7.78	0.06	23.05	0.67	−22.38
CARBHB12	−0.12	0.45	0.59	0.07	2.15	1.17	−0.98
PNICO23	−0.62	0.73	0.90	0.17	3.71	1.07	−2.64
HAL59	−1.07	1.29	1.66	0.28	8.03	2.03	−5.99
AHB21	0.20	0.60	0.71	0.03	2.80	1.74	−1.06
CHB6	−0.34	1.01	1.32	0.04	4.18	1.71	−2.47
IL16	2.71	2.71	2.76	0.02	2.18	4.07	1.89
IDISP	1.68	8.37	9.42	0.59	26.91	16.07	−10.84
ICONF	0.15	0.26	0.38	0.08	1.60	1.18	−0.43
ACONF	0.61	0.61	0.68	0.33	0.98	1.20	0.21
AMINO20x4	0.05	0.43	0.55	0.18	2.62	1.61	−1.01
PCONF21	−0.31	2.74	3.11	1.69	8.85	4.80	−4.05
MCONF	−1.64	1.69	1.92	0.34	3.83	0.69	−3.15
SCONF	0.08	0.16	0.22	0.03	0.88	0.52	−0.35
UPU23	1.43	1.95	2.83	0.34	9.04	7.58	−1.46
BUT14DIOL	−0.38	0.40	0.45	0.14	1.02	0.19	−0.83

Table S164: Statistical analysis for the TPSS1KCIS DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.10	3.24	4.74	0.01	33.87	12.33	−21.54
G21EA	−1.21	2.33	2.64	0.07	8.54	4.18	−4.36
G21IP	−1.50	3.59	4.49	0.01	17.20	8.56	−8.64
DIPCS10	−5.02	5.02	6.22	0.01	11.26	−0.96	−12.22
PA26	3.83	3.83	4.38	0.02	8.83	10.24	1.41
SIE4x4	17.15	17.15	19.36	0.51	32.39	36.53	4.14
ALKBDE10	−1.62	4.74	5.66	0.05	19.09	12.29	−6.81
YBDE18	−6.21	6.21	7.14	0.13	12.91	−0.73	−13.64
AL2X6	−4.75	4.75	5.31	0.13	7.13	−0.68	−7.81
HEAVYSB11	−5.04	5.04	6.12	0.09	10.24	−0.03	−10.27
NBPRC	2.07	3.00	4.17	0.11	12.04	9.54	−2.50
ALK8	0.02	2.26	3.06	0.04	11.23	5.05	−6.18
RC21	0.93	2.15	2.74	0.06	10.71	4.56	−6.14
G2RC	1.46	4.31	5.69	0.08	23.21	13.94	−9.26
BH76RC	0.38	2.47	3.27	0.12	15.75	9.25	−6.50
FH51	2.50	3.76	4.77	0.12	20.62	10.66	−9.96
TAUT15	0.13	1.23	1.44	0.40	4.25	2.59	−1.66
DC13	1.89	11.35	14.05	0.21	46.30	20.36	−25.95
MB16-43	−41.07	41.07	44.15	0.10	71.71	−8.78	−80.49
DARC	10.10	10.10	10.70	0.31	10.19	13.08	2.89
RSE43	−1.83	1.83	2.07	0.24	4.23	−0.72	−4.94
BSR36	−10.57	10.57	11.94	0.65	23.95	−2.57	−26.52
CDIE20	1.65	1.65	1.85	0.41	3.32	3.37	0.04
ISO34	−1.34	2.13	2.96	0.15	15.19	6.53	−8.66
ISOL24	−4.63	7.83	12.30	0.36	66.44	23.07	−43.37
C60ISO	−3.31	3.61	5.02	0.04	11.11	0.85	−10.26
PArel	0.30	1.12	1.73	0.24	9.10	5.32	−3.78
BH76	−5.32	5.40	6.08	0.29	16.53	2.21	−14.32
BHPERI	0.73	1.92	2.21	0.09	7.61	4.52	−3.09
BHDIV10	−3.53	3.98	4.39	0.09	8.79	2.25	−6.54
INV24	−1.90	1.99	2.33	0.06	6.47	0.63	−5.84
BHROT27	0.37	0.51	0.67	0.08	1.85	1.40	−0.45
PX13	−5.14	5.14	5.24	0.15	4.32	−2.92	−7.24
WCPT18	−2.90	2.90	3.19	0.08	5.11	−0.69	−5.80
RG18	−0.37	0.37	0.55	0.64	1.34	0.04	−1.30
ADIM6	−4.40	4.40	4.85	1.31	5.99	−1.56	−7.55
S22	−3.28	3.28	4.41	0.45	11.87	−0.14	−12.00
S66	−2.79	2.79	3.36	0.51	8.35	−0.11	−8.46
HEAVY28	−0.83	0.83	0.92	0.67	1.44	−0.22	−1.65
WATER27	−4.63	5.06	8.21	0.06	25.86	1.58	−24.28
CARBHB12	0.23	0.55	0.80	0.09	2.87	2.01	−0.86
PNICO23	−0.86	0.98	1.12	0.23	4.33	1.37	−2.96
HAL59	−1.14	1.41	1.89	0.31	10.10	3.08	−7.01
AHB21	0.31	0.60	0.80	0.03	3.02	2.22	−0.80
CHB6	0.23	1.03	1.31	0.04	3.83	2.72	−1.10
IL16	3.14	3.14	3.21	0.03	2.82	4.97	2.15
IDISP	3.45	13.67	15.62	0.96	42.63	27.97	−14.66
ICONF	0.08	0.45	0.68	0.14	3.35	2.06	−1.29
ACONF	0.81	0.81	0.90	0.44	1.29	1.58	0.30
AMINO20x4	−0.05	0.56	0.70	0.23	3.30	2.00	−1.30
PCONF21	−0.64	3.80	4.21	2.35	11.78	6.48	−5.30
MCONF	−2.15	2.21	2.51	0.44	4.65	0.67	−3.98
SCONF	−0.18	0.36	0.48	0.08	1.92	0.91	−1.01
UPU23	1.71	2.27	3.30	0.40	10.52	9.00	−1.51
BUT14DIOL	−0.26	0.40	0.45	0.14	1.51	0.65	−0.85

Table S165: Statistical analysis for the BMK DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.97	3.04	5.00	0.01	43.70	7.77	−35.92
G21EA	−0.71	1.92	2.28	0.06	9.50	5.64	−3.87
G21IP	0.29	3.41	4.53	0.01	23.54	11.96	−11.58
DIPCS10	−4.16	5.20	6.74	0.01	16.85	2.88	−13.97
PA26	1.56	2.01	2.58	0.01	8.36	6.75	−1.62
SIE4x4	10.11	10.11	11.59	0.30	21.58	23.52	1.94
ALKBDE10	−2.69	4.43	5.98	0.04	19.42	3.69	−15.73
YBDE18	−5.02	5.12	5.99	0.10	10.93	0.90	−10.03
AL2X6	−3.20	3.20	3.75	0.09	4.99	−0.65	−5.64
HEAVYSB11	−3.26	3.66	4.22	0.06	7.95	1.78	−6.17
NBPRC	1.26	1.59	2.31	0.06	6.52	5.40	−1.13
ALK8	−1.95	3.13	3.86	0.05	12.15	4.21	−7.95
RC21	1.58	2.21	2.53	0.06	8.61	5.51	−3.10
G2RC	−1.84	3.58	4.81	0.07	20.90	12.94	−7.96
BH76RC	−0.26	1.63	2.04	0.08	9.27	3.85	−5.41
FH51	−0.21	1.65	2.15	0.05	10.35	5.22	−5.12
TAUT15	−0.99	1.09	1.43	0.36	3.42	0.35	−3.07
DC13	−3.31	8.85	12.07	0.16	43.43	13.18	−30.24
MB16-43	−3.20	11.40	14.70	0.03	74.07	22.99	−51.08
DARC	1.36	1.95	2.44	0.06	6.32	4.40	−1.92
RSE43	−1.10	1.13	1.38	0.15	3.64	0.23	−3.41
BSR36	−5.93	5.93	6.70	0.37	14.44	−0.93	−15.37
CDIE20	0.46	0.58	0.67	0.14	1.61	1.19	−0.42
ISO34	−0.66	1.22	1.68	0.08	7.24	2.52	−4.72
ISOL24	−0.65	3.81	5.28	0.17	27.52	14.57	−12.95
C60ISO	4.21	4.21	4.46	0.04	4.29	6.69	2.40
PArel	0.23	0.72	1.21	0.16	6.57	3.91	−2.66
BH76	−0.51	1.22	1.57	0.07	7.60	3.23	−4.37
BHPERI	3.26	3.67	4.00	0.18	10.56	6.02	−4.54
BHDIV10	−0.17	1.19	1.65	0.03	6.51	2.79	−3.72
INV24	−0.34	1.81	2.65	0.06	11.25	7.58	−3.67
BHROT27	0.52	0.58	0.85	0.09	2.35	1.99	−0.36
PX13	0.01	1.00	1.11	0.03	3.32	1.60	−1.72
WCPT18	0.20	0.92	1.23	0.03	5.50	3.61	−1.89
RG18	−2.04	2.04	2.65	3.52	6.40	−0.60	−7.00
ADIM6	−3.86	3.86	4.03	1.15	3.27	−2.15	−5.42
S22	−2.60	2.60	3.05	0.36	5.76	−0.55	−6.31
S66	−2.39	2.39	2.65	0.44	4.65	−0.41	−5.06
HEAVY28	−1.26	1.26	1.29	1.02	1.03	−0.70	−1.73
WATER27	−5.79	5.93	9.63	0.07	26.40	1.80	−24.60
CARBHB12	−0.73	0.79	0.90	0.13	1.95	0.37	−1.58
PNICO23	−1.54	1.54	1.63	0.36	2.29	−0.82	−3.12
HAL59	−1.57	1.58	1.82	0.34	5.76	0.08	−5.68
AHB21	0.59	0.78	0.90	0.03	2.71	1.50	−1.20
CHB6	1.50	1.50	1.76	0.06	2.30	2.77	0.46
IL16	3.53	3.53	3.56	0.03	1.67	4.42	2.75
IDISP	1.24	6.72	7.67	0.47	22.70	13.12	−9.58
ICONF	0.04	0.36	0.45	0.11	1.67	0.99	−0.68
ACONF	0.26	0.26	0.29	0.14	0.47	0.48	0.00
AMINO20x4	0.00	0.32	0.43	0.13	2.49	1.45	−1.03
PCONF21	0.75	1.29	1.80	0.80	5.15	3.69	−1.46
MCONF	−0.77	0.95	1.09	0.19	2.99	1.02	−1.97
SCONF	−0.10	0.19	0.23	0.04	0.73	0.31	−0.42
UPU23	1.43	1.77	2.45	0.31	6.38	5.31	−1.06
BUT14DIOL	−0.11	0.12	0.15	0.04	0.43	0.13	−0.30

Table S166: Statistical analysis for the τHCTHhyb DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	0.12	3.43	4.63	0.01	36.97	13.72	−23.25
G21EA	2.05	2.11	2.81	0.06	8.33	7.65	−0.68
G21IP	2.08	3.45	4.13	0.01	14.93	10.54	−4.39
DIPCS10	1.40	3.74	4.26	0.01	13.30	8.30	−5.01
PA26	3.75	3.75	4.37	0.02	9.33	10.03	0.70
SIE4x4	18.28	18.28	20.22	0.54	32.12	37.35	5.23
ALKBDE10	1.25	4.05	6.00	0.04	20.95	16.19	−4.76
YBDE18	−4.14	5.00	6.39	0.10	16.56	3.57	−12.99
AL2X6	−5.51	5.51	5.87	0.15	6.42	−1.96	−8.38
HEAVYSB11	−2.72	3.05	4.10	0.05	10.06	1.13	−8.93
NBPRC	2.41	2.96	4.05	0.11	10.94	9.39	−1.56
ALK8	−2.48	2.95	3.82	0.05	10.07	1.87	−8.21
RC21	2.36	3.04	3.71	0.09	10.75	7.83	−2.91
G2RC	0.17	3.83	4.72	0.07	19.49	11.00	−8.48
BH76RC	0.22	1.99	3.09	0.09	17.13	11.51	−5.62
FH51	1.48	2.79	3.66	0.09	16.66	9.67	−6.98
TAUT15	0.09	1.30	1.58	0.43	5.01	3.09	−1.92
DC13	2.42	9.33	11.36	0.17	40.42	17.22	−23.20
MB16-43	−32.76	33.45	37.86	0.08	78.03	6.82	−71.21
DARC	7.97	7.97	8.68	0.25	10.59	10.94	0.36
RSE43	−2.60	2.60	2.82	0.34	4.63	−1.36	−5.99
BSR36	−9.39	9.39	10.69	0.58	21.06	−2.75	−23.81
CDIE20	1.28	1.28	1.43	0.32	2.38	2.36	−0.02
ISO34	−0.56	1.52	2.32	0.10	14.83	7.14	−7.69
ISOL24	−3.00	6.43	10.17	0.29	55.63	21.52	−34.11
C60ISO	−3.40	3.62	5.02	0.04	10.86	0.68	−10.17
PArel	0.29	1.20	1.82	0.26	9.02	5.93	−3.09
BH76	−4.91	5.11	5.83	0.27	16.64	3.14	−13.50
BHPERI	−0.56	1.67	2.18	0.08	9.34	2.88	−6.46
BHDIV10	−3.83	4.56	5.09	0.10	11.82	3.69	−8.12
INV24	−1.91	1.97	2.29	0.06	6.11	0.76	−5.36
BHROT27	0.34	0.43	0.59	0.07	1.51	1.23	−0.28
PX13	−6.76	6.76	6.90	0.20	5.90	−3.99	−9.89
WCPT18	−3.85	3.85	4.26	0.11	7.07	−0.95	−8.02
RG18	−0.48	0.48	0.64	0.83	1.46	−0.06	−1.52
ADIM6	−4.10	4.10	4.51	1.22	5.42	−1.51	−6.93
S22	−2.85	2.85	3.88	0.39	10.49	−0.10	−10.59
S66	−2.48	2.48	3.01	0.45	7.47	0.02	−7.44
HEAVY28	−0.71	0.71	0.78	0.57	1.26	−0.19	−1.45
WATER27	−2.54	3.50	5.70	0.04	19.13	2.23	−16.90
CARBHB12	0.36	0.60	0.89	0.10	2.94	2.21	−0.73
PNICO23	−0.63	0.77	0.91	0.18	3.98	1.48	−2.50
HAL59	−0.87	1.23	1.68	0.27	9.60	3.33	−6.27
AHB21	−0.30	0.76	0.91	0.03	3.56	1.71	−1.85
CHB6	0.62	0.75	1.18	0.03	3.00	2.64	−0.36
IL16	2.25	2.25	2.37	0.02	3.17	4.22	1.05
IDISP	3.10	12.13	13.75	0.85	37.26	24.18	−13.09
ICONF	0.12	0.43	0.66	0.13	3.23	1.97	−1.26
ACONF	0.74	0.74	0.82	0.40	1.21	1.47	0.26
AMINO20x4	−0.07	0.52	0.65	0.21	3.19	1.74	−1.45
PCONF21	−0.60	3.41	3.79	2.10	10.52	5.95	−4.57
MCONF	−1.89	1.95	2.20	0.39	4.09	0.59	−3.50
SCONF	−0.15	0.32	0.41	0.07	1.61	0.83	−0.78
UPU23	1.64	2.11	3.05	0.37	9.19	7.82	−1.37
BUT14DIOL	−0.03	0.27	0.34	0.10	1.46	0.85	−0.61

Table S167: Statistical analysis for the M05 DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.78	2.99	4.46	0.01	39.32	20.90	−18.42
G21EA	−2.49	2.93	3.36	0.09	10.60	3.25	−7.35
G21IP	−1.81	3.26	4.17	0.01	18.71	7.14	−11.57
DIPCS10	−5.32	5.55	7.72	0.01	16.48	1.16	−15.32
PA26	2.69	2.79	3.90	0.01	10.39	9.67	−0.71
SIE4x4	14.71	14.71	17.08	0.44	32.64	35.35	2.71
ALKBDE10	−2.57	3.93	4.66	0.04	14.92	4.52	−10.40
YBDE18	−4.80	4.96	6.45	0.10	18.83	1.45	−17.37
AL2X6	−7.79	7.79	7.88	0.22	3.55	−6.54	−10.08
HEAVYSB11	−2.93	3.88	4.84	0.07	11.04	2.21	−8.82
NBPRC	4.04	4.59	6.06	0.17	16.47	15.09	−1.38
ALK8	0.78	2.68	3.36	0.04	10.03	5.54	−4.50
RC21	0.45	2.55	3.26	0.07	11.86	5.99	−5.87
G2RC	−0.32	3.99	5.74	0.08	27.08	15.42	−11.66
BH76RC	−0.45	2.20	3.52	0.10	21.93	13.81	−8.12
FH51	−0.26	3.13	4.23	0.10	24.23	10.11	−14.12
TAUT15	−1.02	1.46	1.65	0.48	4.30	1.30	−2.99
DC13	1.84	10.20	13.29	0.19	52.73	35.84	−16.89
MB16-43	−19.25	20.87	25.58	0.05	68.52	12.18	−56.34
DARC	5.72	5.72	6.18	0.18	7.46	8.75	1.29
RSE43	−1.99	1.99	2.28	0.26	5.54	−0.64	−6.17
BSR36	−9.75	9.75	11.47	0.60	23.65	−2.72	−26.37
CDIE20	1.38	1.49	1.87	0.37	4.64	3.98	−0.66
ISO34	−1.51	2.27	3.35	0.16	12.00	3.13	−8.86
ISOL24	−5.24	7.29	11.06	0.33	53.08	12.95	−40.13
C60ISO	−1.25	2.29	2.90	0.02	8.09	1.91	−6.18
PArel	0.49	1.37	1.91	0.30	7.95	5.21	−2.74
BH76	−1.00	1.89	2.71	0.10	18.78	6.17	−12.61
BHPERI	4.48	4.88	5.32	0.23	12.41	7.69	−4.71
BHDIV10	−1.02	3.15	3.62	0.07	10.01	3.83	−6.19
INV24	−1.67	2.34	3.06	0.07	13.68	6.75	−6.92
BHROT27	0.47	0.52	0.71	0.08	1.72	1.57	−0.15
PX13	0.30	1.53	2.08	0.05	7.31	5.22	−2.10
WCPT18	−1.66	2.26	2.80	0.06	9.28	3.77	−5.51
RG18	−0.01	0.20	0.26	0.34	1.05	0.49	−0.57
ADIM6	−1.87	1.87	2.13	0.56	3.09	−0.47	−3.56
S22	−2.03	2.06	2.81	0.28	8.00	0.32	−7.68
S66	−1.45	1.47	1.83	0.27	5.42	0.44	−4.98
HEAVY28	−0.30	0.42	0.48	0.34	1.47	0.55	−0.92
WATER27	−1.33	1.89	2.99	0.02	12.02	4.07	−7.95
CARBHB12	−0.06	0.49	0.64	0.08	2.38	0.77	−1.61
PNICO23	−0.86	0.86	1.03	0.20	1.99	−0.07	−2.06
HAL59	−0.71	0.80	1.14	0.17	4.77	0.54	−4.24
AHB21	−0.19	0.54	0.75	0.02	2.78	0.91	−1.87
CHB6	−0.71	1.32	1.45	0.05	3.83	1.83	−2.01
IL16	2.78	2.78	2.82	0.03	1.81	3.91	2.10
IDISP	3.30	11.97	13.22	0.84	33.17	19.84	−13.33
ICONF	0.13	0.68	1.07	0.21	5.14	3.31	−1.82
ACONF	0.71	0.71	0.78	0.39	1.15	1.41	0.27
AMINO20x4	−0.19	0.56	0.71	0.23	3.19	1.63	−1.56
PCONF21	0.08	2.23	2.68	1.38	8.75	5.34	−3.42
MCONF	−1.51	1.55	1.78	0.31	3.39	0.40	−2.99
SCONF	−0.77	1.32	1.48	0.29	4.83	2.86	−1.97
UPU23	0.75	1.38	1.82	0.24	5.30	3.96	−1.34
BUT14DIOL	−0.18	0.35	0.40	0.12	1.62	0.89	−0.73

Table S168: Statistical analysis for the M052X DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−2.83	4.05	6.39	0.01	52.75	17.21	−35.54
G21EA	0.30	1.80	2.54	0.05	11.21	8.34	−2.86
G21IP	1.09	3.32	4.50	0.01	19.94	14.04	−5.90
DIPCS10	0.18	4.14	4.76	0.01	14.19	8.51	−5.67
PA26	0.04	1.13	1.50	0.01	6.19	3.63	−2.56
SIE4x4	8.66	8.66	10.10	0.26	19.24	22.33	3.09
ALKBDE10	−2.18	4.51	6.67	0.04	22.88	5.20	−17.68
YBDE18	0.19	0.99	1.12	0.02	3.67	2.12	−1.55
AL2X6	0.31	0.72	1.20	0.02	3.48	2.82	−0.66
HEAVYSB11	−3.48	3.48	4.53	0.06	8.75	−0.15	−8.89
NBPRC	1.04	1.63	2.11	0.06	6.56	5.18	−1.38
ALK8	0.54	2.17	3.00	0.03	9.23	6.50	−2.73
RC21	1.87	2.61	2.87	0.07	7.89	4.76	−3.13
G2RC	−3.27	4.00	4.83	0.08	12.57	3.02	−9.55
BH76RC	−0.73	1.37	1.98	0.06	9.53	2.67	−6.86
FH51	−1.31	1.70	2.11	0.05	8.27	3.26	−5.01
TAUT15	0.65	1.18	1.51	0.39	4.74	3.45	−1.29
DC13	−1.36	8.49	10.94	0.15	37.36	14.05	−23.32
MB16-43	24.42	24.96	31.01	0.06	90.43	78.81	−11.62
DARC	0.46	1.30	1.47	0.04	4.69	1.97	−2.72
RSE43	−0.80	0.83	1.02	0.11	3.33	0.37	−2.95
BSR36	−2.04	2.04	2.36	0.13	4.88	−0.79	−5.68
CDIE20	0.10	0.34	0.55	0.08	1.95	1.47	−0.48
ISO34	0.06	1.06	1.59	0.07	7.88	5.52	−2.36
ISOL24	0.15	2.73	4.27	0.12	22.76	7.13	−15.64
C60ISO	9.71	9.71	10.33	0.10	10.66	14.98	4.32
PArel	0.45	1.02	1.58	0.22	7.27	3.97	−3.30
BH76	−0.47	1.64	2.05	0.09	12.77	8.41	−4.36
BHPERI	−0.66	1.33	1.56	0.06	5.79	3.05	−2.74
BHDIV10	−0.39	1.53	1.82	0.03	5.97	3.32	−2.65
INV24	−0.07	1.60	2.40	0.05	11.55	7.20	−4.36
BHROT27	0.45	0.47	0.64	0.07	1.43	1.31	−0.12
PX13	−7.47	7.47	8.63	0.22	14.14	−0.93	−15.07
WCPT18	−1.34	2.46	3.00	0.07	9.51	4.71	−4.80
RG18	−0.03	0.14	0.19	0.24	0.85	0.36	−0.49
ADIM6	−0.92	0.92	1.06	0.27	1.35	−0.24	−1.59
S22	−0.59	0.79	1.04	0.11	3.34	1.12	−2.23
S66	−0.42	0.57	0.71	0.10	2.51	1.05	−1.46
HEAVY28	−0.26	0.35	0.38	0.28	1.07	0.48	−0.59
WATER27	3.20	3.54	3.92	0.04	11.44	6.83	−4.61
CARBHB12	0.00	0.26	0.33	0.04	1.13	0.73	−0.40
PNICO23	0.14	0.35	0.43	0.08	1.75	0.85	−0.91
HAL59	−0.34	0.62	0.75	0.14	3.66	2.24	−1.42
AHB21	−1.00	1.11	1.69	0.05	5.82	0.73	−5.10
CHB6	−1.96	1.96	2.38	0.07	4.06	−0.60	−4.67
IL16	1.45	1.45	1.52	0.01	1.75	2.28	0.53
IDISP	−0.25	2.01	2.71	0.14	9.04	4.64	−4.39
ICONF	0.12	0.27	0.36	0.08	1.35	0.79	−0.56
ACONF	0.10	0.12	0.15	0.07	0.54	0.37	−0.17
AMINO20x4	0.13	0.29	0.38	0.12	1.77	1.06	−0.70
PCONF21	0.04	0.49	0.57	0.30	1.92	0.97	−0.94
MCONF	0.03	0.17	0.21	0.03	0.92	0.55	−0.38
SCONF	0.14	0.22	0.28	0.05	0.96	0.55	−0.42
UPU23	0.73	0.90	1.19	0.16	3.51	2.96	−0.55
BUT14DIOL	−0.23	0.23	0.27	0.08	0.74	0.05	−0.69

Table S169: Statistical analysis for the M06 DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.16	3.15	5.09		51.53	18.57	−32.96
G21EA	−1.68	2.18	2.42		6.85	2.20	−4.66
G21IP	−1.48	3.09	3.81		15.41	6.58	−8.83
DIPCS10	−6.50	6.50	7.82		11.85	−1.13	−12.98
PA26	2.81	2.85	3.63		9.03	8.69	−0.35
SIE4x4	14.24	14.24	16.48		30.76	33.56	2.80
ALKBDE10	−0.15	3.44	4.40		15.44	5.45	−9.99
YBDE18	−4.81	4.83	5.60		9.98	0.19	−9.79
AL2X6	−3.07	3.07	3.24		3.34	−1.34	−4.68
HEAVYSB11	−0.77	1.83	2.16		5.76	1.86	−3.90
NBPRC	2.14	3.11	3.81		10.58	7.77	−2.81
ALK8	−0.50	3.46	4.25		13.34	5.75	−7.59
RC21	0.57	1.64	2.12		8.15	4.60	−3.55
G2RC	−0.36	3.81	5.34		24.25	14.44	−9.81
BH76RC	−0.09	1.65	2.62		15.50	11.00	−4.50
FH51	−0.20	1.84	2.37		10.40	5.58	−4.82
TAUT15	−0.38	0.80	1.00		3.13	1.07	−2.05
DC13	−0.96	6.65	9.16	0.12	36.91	19.64	−17.27
MB16-43	−34.08	34.42	39.45		95.57	6.08	−89.49
DARC	4.65	4.65	4.93		5.48	6.66	1.17
RSE43	−1.58	1.58	1.90		5.65	−0.36	−6.01
BSR36	−2.52	2.52	3.15		8.38	−0.73	−9.11
CDIE20	1.01	1.04	1.36		3.21	2.84	−0.37
ISO34	−0.70	1.40	1.90		9.35	4.44	−4.92
ISOL24	−2.73	4.01	6.09		27.76	6.90	−20.86
C60ISO	−0.91	2.11	2.67		7.59	1.74	−5.85
PArel	0.65	1.08	1.77		7.46	6.25	−1.22
BH76	−1.00	2.56	4.77		35.31	25.18	−10.13
BHPERI	1.82	2.24	2.59		7.47	4.73	−2.74
BHDIV10	−1.46	1.94	2.50		5.98	1.52	−4.47
INV24	−0.86	1.62	2.28		11.44	6.73	−4.71
BHROT27	0.64	0.69	0.89		2.35	2.09	−0.25
PX13	−0.12	1.47	1.60		4.94	2.73	−2.21
WCPT18	−1.73	1.95	2.48		6.43	1.41	−5.02
RG18	−0.36	0.36	0.48		1.03	0.00	−1.02
ADIM6	0.08	0.23	0.30		0.89	0.57	−0.32
S22	−1.03	1.03	1.25		2.57	−0.04	−2.60
S66	−0.67	0.68	0.83		2.39	0.21	−2.18
HEAVY28	−0.15	0.35	0.41		1.45	0.87	−0.58
WATER27	−1.93	2.59	4.52		20.59	4.88	−15.71
CARBHB12	−0.07	0.31	0.44		1.79	0.65	−1.14
PNICO23	−0.08	0.23	0.27		0.92	0.38	−0.54
HAL59	−0.08	0.57	0.70		3.55	1.57	−1.98
AHB21	0.07	0.32	0.39		1.60	0.86	−0.75
CHB6	1.18	1.26	1.58		2.81	2.56	−0.25
IL16	0.61	0.73	0.82		2.41	1.45	−0.97
IDISP	1.83	3.76	5.62		17.11	12.38	−4.73
ICONF	−0.06	0.35	0.45		1.73	1.10	−0.63
ACONF	−0.35	0.35	0.38		0.48	−0.13	−0.61
AMINO20x4	−0.03	0.36	0.46		2.03	0.85	−1.17
PCONF21	0.31	0.41	0.51		1.33	1.04	−0.30
MCONF	−0.05	0.33	0.40		1.57	0.67	−0.90
SCONF	−0.27	0.31	0.41		1.04	0.22	−0.82
UPU23	0.12	0.53	0.68		2.99	1.67	−1.32
BUT14DIOL	0.14	0.18	0.20		0.69	0.43	−0.26

Table S170: Statistical analysis for the M062X DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−2.32	3.16	5.62	0.01	48.66	17.49	−31.17
G21EA	−0.61	1.76	2.08	0.05	7.49	4.15	−3.35
G21IP	0.12	2.64	3.67	0.01	17.85	11.55	−6.30
DIPCS10	−0.69	3.16	3.58	0.00	11.28	6.58	−4.70
PA26	−0.35	1.24	1.52	0.01	6.68	3.99	−2.69
SIE4x4	8.65	8.65	10.19	0.26	20.91	22.39	1.48
ALKBDE10	−4.04	4.79	7.02	0.05	19.46	1.77	−17.69
YBDE18	−2.48	2.48	2.85	0.05	5.77	−0.18	−5.96
AL2X6	0.55	0.88	1.47	0.02	4.04	3.46	−0.58
HEAVYSB11	−8.21	8.30	9.83	0.14	17.13	0.51	−16.62
NBPRC	−0.03	0.96	1.16	0.03	4.02	2.21	−1.81
ALK8	1.00	2.27	3.13	0.04	9.54	6.02	−3.53
RC21	0.92	1.60	1.92	0.04	7.33	4.90	−2.43
G2RC	−1.23	1.92	2.51	0.04	8.39	2.90	−5.49
BH76RC	−0.48	1.18	1.71	0.06	8.64	2.84	−5.80
FH51	−0.12	1.18	1.53	0.04	6.31	3.26	−3.05
TAUT15	0.36	0.77	0.94	0.25	3.12	1.93	−1.19
DC13	−3.07	7.54	10.34	0.14	38.90	15.24	−23.66
MB16-43	14.97	15.18	18.11	0.04	39.90	37.27	−2.63
DARC	2.25	2.33	2.59	0.07	4.17	3.79	−0.38
RSE43	−0.51	0.63	0.75	0.08	2.47	0.49	−1.98
BSR36	−2.96	2.96	3.77	0.18	9.85	−0.95	−10.80
CDIE20	0.34	0.54	0.83	0.13	2.62	2.09	−0.53
ISO34	−0.62	1.23	1.70	0.08	8.63	4.63	−4.00
ISOL24	−1.22	2.92	4.67	0.13	22.16	4.04	−18.12
C60ISO	6.75	6.75	7.23	0.07	7.88	10.49	2.61
PArel	0.37	0.97	1.49	0.21	6.54	3.90	−2.63
BH76	0.70	2.33	7.29	0.13	47.52	44.30	−3.23
BHPERI	0.75	1.36	1.80	0.07	7.49	4.44	−3.05
BHDIV10	−0.72	1.05	1.32	0.02	4.29	1.29	−3.00
INV24	−0.26	1.29	2.15	0.04	12.73	7.88	−4.85
BHROT27	0.34	0.36	0.52	0.06	1.29	1.18	−0.12
PX13	−5.35	5.35	5.88	0.16	7.82	−1.37	−9.19
WCPT18	−0.97	1.86	2.30	0.05	7.99	3.57	−4.42
RG18	−0.03	0.23	0.31	0.40	1.39	0.80	−0.59
ADIM6	−0.44	0.44	0.47	0.13	0.43	−0.21	−0.64
S22	−0.22	0.39	0.55	0.05	2.18	0.68	−1.50
S66	−0.17	0.26	0.33	0.05	1.48	0.64	−0.84
HEAVY28	−0.17	0.35	0.42	0.28	1.54	0.95	−0.59
WATER27	2.58	2.83	3.21	0.03	9.59	6.26	−3.33
CARBHB12	0.13	0.23	0.33	0.04	1.08	0.87	−0.21
PNICO23	0.12	0.28	0.34	0.07	1.29	0.64	−0.64
HAL59	−0.26	0.40	0.51	0.09	2.83	1.03	−1.80
AHB21	−0.84	0.94	1.32	0.04	4.35	0.72	−3.63
CHB6	−1.42	1.42	1.66	0.05	2.60	−0.49	−3.09
IL16	0.59	0.62	0.69	0.01	1.35	1.12	−0.22
IDISP	1.19	1.92	2.80	0.14	7.34	5.94	−1.41
ICONF	−0.01	0.32	0.43	0.10	1.84	0.79	−1.05
ACONF	−0.25	0.25	0.28	0.14	0.46	−0.05	−0.51
AMINO20x4	−0.03	0.30	0.39	0.12	1.87	1.01	−0.85
PCONF21	0.52	0.88	1.03	0.54	3.20	1.94	−1.27
MCONF	0.32	0.34	0.41	0.07	1.02	0.83	−0.19
SCONF	−0.07	0.25	0.33	0.05	1.35	0.39	−0.96
UPU23	0.37	0.61	0.78	0.11	2.48	1.93	−0.55
BUT14DIOL	−0.06	0.13	0.19	0.05	0.88	0.21	−0.67

Table S171: Statistical analysis for the M08HX DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−2.36	3.12	5.37	0.01	40.43	4.77	−35.66
G21EA	1.62	1.82	2.72	0.05	10.75	9.55	−1.20
G21IP	3.02	3.37	4.69	0.01	18.33	15.51	−2.81
DIPCS10	3.04	3.37	3.97	0.01	9.03	7.37	−1.66
PA26	0.22	0.99	1.26	0.01	5.61	2.66	−2.95
SIE4x4	8.62	8.62	9.94	0.26	19.13	21.78	2.64
ALKBDE10	−3.80	3.86	5.39	0.04	14.17	0.32	−13.85
YBDE18	−2.14	2.18	2.60	0.04	5.32	0.33	−4.99
AL2X6	2.21	2.21	2.30	0.06	1.59	3.13	1.54
HEAVYSB11	−2.28	3.09	4.31	0.05	13.33	1.92	−11.41
NBPRC	0.48	1.96	2.23	0.07	7.20	3.91	−3.29
ALK8	1.71	2.22	3.21	0.04	8.43	7.38	−1.04
RC21	0.59	1.50	1.88	0.04	6.29	4.03	−2.26
G2RC	−2.15	3.29	4.21	0.06	17.29	5.03	−12.26
BH76RC	−0.28	1.19	1.54	0.06	6.46	3.33	−3.12
FH51	−0.35	1.24	1.65	0.04	8.86	5.24	−3.62
TAUT15	0.08	0.65	0.90	0.21	3.18	1.43	−1.75
DC13	−1.30	7.41	9.85	0.13	37.21	15.84	−21.37
MB16-43	−11.22	16.19	20.58	0.04	82.39	24.85	−57.53
DARC	1.01	1.56	1.86	0.05	4.88	3.10	−1.79
RSE43	−0.30	0.56	0.70	0.07	2.28	0.81	−1.47
BSR36	−2.78	2.78	3.27	0.17	7.60	−0.77	−8.37
CDIE20	0.36	0.64	0.93	0.16	3.01	2.35	−0.66
ISO34	−0.15	0.94	1.31	0.06	6.08	3.01	−3.07
ISOL24	−0.17	2.33	3.75	0.11	19.77	5.71	−14.06
C60ISO	7.46	7.46	7.99	0.08	8.48	11.81	3.33
PArel	0.44	0.92	1.35	0.20	5.92	3.39	−2.54
BH76	−0.15	0.99	1.29	0.05	6.83	3.36	−3.47
BHPERI	0.25	1.61	1.96	0.08	7.79	4.95	−2.84
BHDIV10	−0.31	1.04	1.36	0.02	4.79	1.90	−2.89
INV24	0.18	1.92	3.10	0.06	15.11	10.42	−4.69
BHROT27	0.35	0.42	0.57	0.07	1.45	1.15	−0.30
PX13	0.29	2.60	3.00	0.08	9.58	5.14	−4.45
WCPT18	1.01	1.55	1.82	0.04	4.87	3.39	−1.48
RG18	−0.43	0.43	0.67	0.74	1.84	−0.03	−1.87
ADIM6	−0.59	0.59	0.63	0.18	0.65	−0.36	−1.02
S22	−0.22	0.43	0.60	0.06	2.27	0.60	−1.67
S66	−0.11	0.27	0.32	0.05	1.42	0.61	−0.81
HEAVY28	0.15	0.31	0.52	0.25	2.02	1.73	−0.29
WATER27	0.72	1.29	1.63	0.02	6.43	3.69	−2.74
CARBHB12	0.18	0.45	0.51	0.07	1.79	0.87	−0.92
PNICO23	0.44	0.53	0.65	0.12	1.71	1.21	−0.50
HAL59	−0.24	0.52	0.67	0.11	3.80	1.73	−2.07
AHB21	−0.39	0.53	0.73	0.02	2.51	0.53	−1.98
CHB6	−2.51	2.51	2.91	0.09	4.49	−0.91	−5.40
IL16	1.24	1.24	1.32	0.01	1.74	1.81	0.08
IDISP	0.07	2.98	3.42	0.21	8.62	4.56	−4.06
ICONF	−0.08	0.51	0.60	0.16	1.85	0.70	−1.15
ACONF	−0.37	0.37	0.44	0.20	0.63	−0.04	−0.67
AMINO20x4	0.08	0.39	0.53	0.16	2.57	1.52	−1.05
PCONF21	0.57	0.86	1.01	0.53	2.95	1.64	−1.31
MCONF	0.49	0.54	0.66	0.11	1.64	1.37	−0.27
SCONF	0.09	0.32	0.46	0.07	1.95	0.69	−1.26
UPU23	0.46	0.80	1.03	0.14	3.20	2.44	−0.76
BUT14DIOL	−0.19	0.20	0.29	0.07	1.04	0.11	−0.93

Table S172: Statistical analysis for the M11 DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.34	3.44	5.81	0.01	49.18	12.37	−36.81
G21EA	1.44	1.56	2.26	0.05	8.76	8.02	−0.74
G21IP	2.06	3.60	4.83	0.01	19.19	14.32	−4.87
DIPCS10	−2.26	3.27	3.99	0.00	10.68	3.43	−7.26
PA26	0.10	1.22	1.47	0.01	5.46	2.29	−3.17
SIE4x4	9.56	9.56	12.22	0.28	27.78	28.35	0.57
ALKBDE10	0.74	4.32	6.05	0.04	21.52	11.69	−9.83
YBDE18	−0.69	1.76	2.17	0.04	6.85	2.96	−3.89
AL2X6	1.24	1.31	1.71	0.04	3.83	3.62	−0.21
HEAVYSB11	−0.90	1.98	2.67	0.03	9.91	3.11	−6.81
NBPRC	1.28	3.03	3.47	0.11	10.67	6.06	−4.62
ALK8	−1.05	3.41	4.45	0.05	15.18	5.31	−9.87
RC21	−0.04	2.07	2.67	0.06	10.18	5.06	−5.13
G2RC	−2.11	2.89	3.91	0.06	13.38	2.98	−10.40
BH76RC	−0.50	1.44	1.83	0.07	7.61	4.16	−3.45
FH51	−0.54	1.50	1.88	0.05	7.53	3.27	−4.26
TAUT15	−0.27	1.09	1.31	0.36	4.77	2.39	−2.37
DC13	−0.08	9.65	13.79	0.18	57.62	23.78	−33.84
MB16-43	−16.86	21.28	27.28	0.05	93.38	18.94	−74.45
DARC	3.22	3.22	3.64	0.10	5.46	5.74	0.28
RSE43	−1.41	1.42	1.69	0.19	4.06	0.22	−3.83
BSR36	−1.87	1.87	2.09	0.12	4.26	−0.27	−4.53
CDIE20	−0.02	0.78	1.00	0.19	3.61	2.38	−1.23
ISO34	−0.37	1.31	1.95	0.09	8.58	4.25	−4.33
ISOL24	−0.63	3.36	5.82	0.15	31.67	8.54	−23.14
C60ISO	14.60	14.60	15.96	0.15	17.77	22.98	5.21
PArel	0.14	0.78	1.15	0.17	5.51	2.26	−3.26
BH76	−0.67	1.26	1.53	0.07	6.19	2.76	−3.44
BHPERI	1.57	2.16	2.67	0.10	10.14	6.01	−4.13
BHDIV10	−0.18	1.45	1.70	0.03	5.79	1.97	−3.82
INV24	−0.89	2.55	3.34	0.08	14.84	7.53	−7.31
BHROT27	0.54	0.66	0.98	0.11	2.71	2.34	−0.37
PX13	−3.46	3.46	4.34	0.10	7.72	−0.89	−8.60
WCPT18	−0.97	1.69	2.08	0.05	7.93	3.80	−4.13
RG18	−0.41	0.43	0.52	0.74	1.15	0.12	−1.03
ADIM6	−0.32	0.32	0.34	0.10	0.25	−0.19	−0.44
S22	−0.53	0.65	0.83	0.09	2.78	0.70	−2.09
S66	−0.41	0.46	0.54	0.08	1.74	0.63	−1.11
HEAVY28	−0.60	0.61	0.66	0.49	1.09	0.10	−0.99
WATER27	−0.71	1.85	3.01	0.02	10.49	2.51	−7.98
CARBHB12	−0.21	0.36	0.39	0.06	1.17	0.58	−0.59
PNICO23	−0.54	0.58	0.75	0.14	2.27	0.21	−2.05
HAL59	−1.00	1.01	1.14	0.22	3.22	0.25	−2.96
AHB21	−0.19	0.48	0.68	0.02	2.63	0.81	−1.82
CHB6	−2.45	2.45	2.99	0.09	5.13	−0.67	−5.80
IL16	1.93	1.93	1.96	0.02	1.29	2.37	1.08
IDISP	−0.38	3.34	3.69	0.23	10.42	5.44	−4.98
ICONF	0.02	0.49	0.58	0.15	2.00	1.00	−1.00
ACONF	−0.66	0.66	0.74	0.36	1.13	−0.18	−1.31
AMINO20x4	0.11	0.49	0.63	0.20	2.78	1.76	−1.02
PCONF21	0.54	0.98	1.13	0.60	3.75	1.77	−1.98
MCONF	0.83	0.84	0.99	0.17	1.91	1.79	−0.12
SCONF	0.25	0.78	1.04	0.17	4.11	1.30	−2.81
UPU23	0.68	0.84	1.06	0.15	2.91	2.49	−0.42
BUT14DIOL	−0.07	0.25	0.37	0.09	1.70	0.50	−1.19

Table S173: Statistical analysis for the SOGGA11X DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−4.53	4.79	6.86	0.02	37.55	5.56	−31.99
G21EA	0.19	1.92	2.49	0.06	10.00	5.39	−4.61
G21IP	1.95	3.13	4.08	0.01	14.33	9.19	−5.14
DIPCS10	0.72	4.93	5.86	0.01	19.06	7.83	−11.23
PA26	3.45	3.45	4.12	0.02	9.10	9.43	0.33
SIE4x4	10.28	10.28	11.93	0.30	22.91	24.86	1.95
ALKBDE10	−8.20	8.20	9.33	0.08	16.82	−2.03	−18.84
YBDE18	−2.02	3.55	4.18	0.07	12.78	3.51	−9.26
AL2X6	−5.02	5.02	5.39	0.14	5.32	−2.49	−7.82
HEAVYSB11	−3.62	3.62	4.14	0.06	5.59	−0.80	−6.40
NBPRC	1.92	2.57	3.40	0.09	9.36	7.15	−2.21
ALK8	−0.56	1.88	2.44	0.03	8.14	3.89	−4.24
RC21	2.23	2.94	3.56	0.08	12.80	8.49	−4.31
G2RC	−2.57	4.41	5.74	0.09	25.53	11.38	−14.16
BH76RC	0.10	2.14	2.38	0.10	8.97	4.08	−4.89
FH51	−0.45	1.97	2.55	0.06	12.47	7.21	−5.26
TAUT15	0.08	0.46	0.63	0.15	2.77	1.03	−1.75
DC13	−0.45	7.70	9.25	0.14	32.23	20.80	−11.44
MB16-43	−36.82	36.82	40.70	0.09	70.99	−0.54	−71.53
DARC	1.76	2.91	3.22	0.09	8.82	4.05	−4.78
RSE43	−1.46	1.46	1.61	0.19	2.63	−0.56	−3.19
BSR36	−8.88	8.88	10.18	0.55	20.15	−2.83	−22.98
CDIE20	0.97	1.03	1.30	0.25	3.13	2.77	−0.36
ISO34	−0.54	1.45	2.02	0.10	10.94	4.39	−6.55
ISOL24	−1.67	3.53	5.61	0.16	29.49	8.15	−21.34
C60ISO	6.48	6.48	6.93	0.07	7.95	11.57	3.62
PArel	0.69	1.00	1.49	0.22	5.27	4.08	−1.19
BH76	−0.99	1.42	1.83	0.08	7.96	2.61	−5.34
BHPERI	3.60	3.75	4.00	0.18	8.64	6.74	−1.90
BHDIV10	−0.06	1.31	1.60	0.03	5.67	3.15	−2.53
INV24	−0.28	1.45	2.38	0.05	12.91	9.63	−3.27
BHROT27	0.36	0.39	0.52	0.06	1.29	1.12	−0.17
PX13	1.02	1.02	1.23	0.03	2.18	2.27	0.09
WCPT18	1.24	1.34	1.64	0.04	4.44	3.94	−0.49
RG18	−1.32	1.32	1.68	2.28	3.81	−0.25	−4.06
ADIM6	−4.16	4.16	4.41	1.24	4.17	−2.07	−6.24
S22	−2.58	2.58	3.31	0.35	8.10	−0.15	−8.25
S66	−2.34	2.34	2.74	0.43	5.93	−0.12	−6.05
HEAVY28	−1.00	1.00	1.04	0.81	1.07	−0.50	−1.57
WATER27	−4.51	4.64	7.86	0.06	22.47	1.48	−20.99
CARBHB12	−0.27	0.52	0.63	0.09	2.10	1.03	−1.06
PNICO23	−1.16	1.16	1.26	0.27	2.35	−0.57	−2.93
HAL59	−1.46	1.46	1.75	0.32	5.78	−0.07	−5.85
AHB21	0.10	0.70	0.83	0.03	3.54	1.45	−2.09
CHB6	−0.03	1.15	1.39	0.04	4.31	2.37	−1.94
IL16	2.63	2.63	2.69	0.02	1.98	4.02	2.04
IDISP	1.88	9.62	10.70	0.68	29.88	16.92	−12.95
ICONF	0.15	0.41	0.61	0.13	2.82	1.86	−0.96
ACONF	0.45	0.45	0.50	0.25	0.78	0.93	0.15
AMINO20x4	−0.07	0.39	0.50	0.16	2.61	1.55	−1.06
PCONF21	0.25	1.96	2.43	1.21	7.22	4.44	−2.78
MCONF	−1.39	1.47	1.67	0.30	3.31	0.59	−2.73
SCONF	−0.21	0.31	0.37	0.07	1.34	0.72	−0.62
UPU23	1.78	2.07	2.88	0.36	7.34	6.38	−0.96
BUT14DIOL	0.00	0.16	0.21	0.06	0.87	0.54	−0.34

Table S174: Statistical analysis for the N12SX DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−1.30	3.89	5.68	0.01	53.46	20.08	−33.37
G21EA	−2.38	2.87	3.44	0.09	10.75	4.28	−6.47
G21IP	−0.30	3.59	4.65	0.01	22.71	9.94	−12.77
DIPCS10	−4.81	5.77	7.01	0.01	14.88	3.21	−11.67
PA26	3.50	3.58	4.20	0.02	10.60	9.54	−1.07
SIE4x4	14.43	14.43	15.93	0.43	25.23	29.62	4.39
ALKBDE10	0.13	3.68	4.97	0.04	19.22	12.39	−6.83
YBDE18	−1.10	2.39	3.23	0.05	11.91	2.86	−9.05
AL2X6	−2.16	2.46	2.75	0.07	5.26	0.91	−4.35
HEAVYSB11	−0.82	2.96	3.20	0.05	8.54	4.26	−4.28
NBPRC	0.28	2.62	3.09	0.09	9.94	5.77	−4.16
ALK8	3.35	3.85	5.92	0.06	13.91	12.11	−1.80
RC21	4.40	4.90	6.00	0.14	15.24	13.29	−1.95
G2RC	−4.33	6.63	8.67	0.13	28.65	8.78	−19.88
BH76RC	−0.11	2.94	3.71	0.14	17.07	9.99	−7.08
FH51	−1.14	2.89	3.82	0.09	17.61	7.94	−9.67
TAUT15	0.18	1.60	2.20	0.52	7.07	4.47	−2.60
DC13	−2.90	9.84	11.88	0.18	42.71	20.21	−22.50
MB16-43	5.95	17.15	21.73	0.04	89.61	58.08	−31.53
DARC	−0.39	2.92	3.36	0.09	10.76	2.98	−7.79
RSE43	−2.14	2.14	2.40	0.28	4.57	−0.89	−5.46
BSR36	−8.39	8.39	9.53	0.52	18.93	−2.33	−21.25
CDIE20	1.43	1.46	1.68	0.36	3.39	3.09	−0.30
ISO34	−0.32	1.82	2.36	0.12	10.74	3.64	−7.09
ISOL24	−0.73	4.15	5.99	0.19	27.78	10.74	−17.04
C60ISO	0.08	2.38	2.78	0.02	7.76	2.53	−5.23
PArel	0.70	1.34	2.18	0.29	9.50	7.41	−2.09
BH76	−2.89	3.51	4.12	0.19	15.88	5.42	−10.46
BHPERI	−0.10	1.39	1.65	0.07	5.95	2.39	−3.56
BHDIV10	−3.71	4.02	4.57	0.09	8.60	1.54	−7.06
INV24	−2.15	2.59	3.26	0.08	12.37	5.31	−7.06
BHROT27	0.78	0.86	1.19	0.14	2.74	2.47	−0.28
PX13	−5.78	5.78	6.05	0.17	6.73	−3.13	−9.86
WCPT18	−3.18	3.19	3.86	0.09	7.97	0.11	−7.86
RG18	−0.79	0.79	1.05	1.36	2.48	−0.02	−2.49
ADIM6	−3.58	3.58	3.87	1.07	4.27	−1.52	−5.79
S22	−2.18	2.36	3.30	0.32	10.15	1.44	−8.70
S66	−1.91	2.03	2.57	0.37	7.39	1.37	−6.01
HEAVY28	−0.86	0.86	0.95	0.69	1.51	−0.18	−1.69
WATER27	2.69	3.15	3.67	0.04	15.54	9.36	−6.18
CARBHB12	0.64	0.78	1.03	0.13	2.83	2.36	−0.48
PNICO23	−0.58	0.87	1.16	0.20	6.09	3.27	−2.81
HAL59	−0.91	1.17	1.57	0.25	7.94	2.37	−5.57
AHB21	−1.20	1.33	1.74	0.06	4.47	1.04	−3.43
CHB6	−0.93	1.36	1.51	0.05	3.46	1.31	−2.15
IL16	1.74	1.74	1.88	0.02	3.07	3.47	0.40
IDISP	1.87	9.90	10.82	0.70	28.68	16.29	−12.40
ICONF	0.24	0.54	0.77	0.17	3.13	2.01	−1.12
ACONF	0.54	0.54	0.60	0.30	0.87	1.06	0.19
AMINO20x4	0.12	0.49	0.65	0.20	3.46	2.19	−1.26
PCONF21	0.01	2.86	3.25	1.77	8.65	5.29	−3.37
MCONF	−1.46	1.58	1.81	0.32	4.09	0.92	−3.17
SCONF	−0.15	0.28	0.35	0.06	1.30	0.72	−0.57
UPU23	1.56	1.88	2.72	0.33	7.24	6.21	−1.02
BUT14DIOL	0.16	0.19	0.25	0.07	0.88	0.70	−0.17

Table S175: Statistical analysis for the MN12SX DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−3.43	4.56	6.47	0.01	39.46	9.33	−30.13
G21EA	−0.81	2.39	3.06	0.07	10.51	3.71	−6.80
G21IP	−0.75	3.66	4.71	0.01	20.08	9.16	−10.91
DIPCS10	−8.15	8.15	10.38	0.01	18.14	−1.19	−19.33
PA26	0.86	1.61	1.99	0.01	5.94	4.16	−1.77
SIE4x4	8.85	8.96	10.67	0.27	20.46	19.56	−0.90
ALKBDE10	−0.60	3.86	5.37	0.04	18.91	5.57	−13.34
YBDE18	−3.31	3.90	4.64	0.08	10.94	1.53	−9.41
AL2X6	−3.15	3.15	3.31	0.09	2.84	−0.93	−3.78
HEAVYSB11	−0.34	1.92	2.53	0.03	9.64	4.97	−4.67
NBPRC	1.04	2.74	3.13	0.10	9.32	5.72	−3.60
ALK8	−5.12	7.10	9.78	0.11	27.19	5.85	−21.34
RC21	0.27	1.44	1.89	0.04	8.17	4.50	−3.67
G2RC	0.15	2.72	3.40	0.05	14.26	9.10	−5.16
BH76RC	−0.08	1.55	2.35	0.07	12.41	4.25	−8.16
FH51	1.47	2.07	3.12	0.07	16.21	11.28	−4.93
TAUT15	0.79	1.58	1.91	0.52	5.72	3.47	−2.26
DC13	−1.00	8.77	10.83	0.16	39.80	19.98	−19.82
MB16-43	−6.21	12.89	16.15	0.03	71.69	31.95	−39.74
DARC	4.81	4.81	5.32	0.15	6.53	7.18	0.64
RSE43	−1.62	1.62	1.85	0.21	4.95	−0.17	−5.12
BSR36	−4.25	4.25	4.81	0.26	9.43	−1.22	−10.65
CDIE20	1.30	1.33	1.58	0.33	3.30	3.07	−0.23
ISO34	−0.32	1.19	1.55	0.08	7.46	4.15	−3.31
ISOL24	−1.69	4.11	5.53	0.19	27.32	14.80	−12.52
C60ISO	−0.23	2.26	2.83	0.02	8.25	2.56	−5.69
PArel	1.21	1.51	2.39	0.33	7.97	6.96	−1.00
BH76	−0.15	1.14	1.59	0.06	8.66	4.26	−4.40
BHPERI	2.50	2.80	3.19	0.13	9.01	5.54	−3.47
BHDIV10	0.20	1.69	1.84	0.04	5.08	2.37	−2.71
INV24	−0.08	1.44	2.24	0.05	12.08	7.28	−4.80
BHROT27	0.58	0.59	0.86	0.09	2.47	2.39	−0.09
PX13	2.34	2.43	2.82	0.07	4.95	4.32	−0.63
WCPT18	0.73	1.17	1.33	0.03	3.89	2.30	−1.59
RG18	−0.81	0.81	1.09	1.40	2.56	−0.16	−2.72
ADIM6	−1.22	1.22	1.26	0.36	0.89	−0.71	−1.60
S22	−1.16	1.16	1.43	0.16	2.93	−0.25	−3.18
S66	−0.96	0.96	1.04	0.18	1.72	−0.10	−1.81
HEAVY28	−0.48	0.49	0.55	0.40	1.17	0.10	−1.07
WATER27	−7.02	7.24	11.05	0.09	31.35	2.97	−28.38
CARBHB12	−0.99	0.99	1.12	0.16	1.77	−0.42	−2.19
PNICO23	−0.61	0.61	0.75	0.14	1.57	0.05	−1.52
HAL59	−1.09	1.09	1.24	0.24	3.54	−0.22	−3.76
AHB21	0.94	0.97	1.11	0.04	2.41	2.14	−0.28
CHB6	−0.10	0.54	0.66	0.02	2.06	0.94	−1.12
IL16	2.02	2.02	2.04	0.02	1.27	2.52	1.25
IDISP	2.83	3.49	6.77	0.25	17.63	16.41	−1.21
ICONF	−0.01	0.24	0.34	0.07	1.49	0.57	−0.92
ACONF	−0.04	0.06	0.09	0.03	0.34	0.08	−0.26
AMINO20x4	−0.02	0.50	0.65	0.20	3.10	1.46	−1.64
PCONF21	0.81	0.85	1.09	0.52	2.99	2.59	−0.41
MCONF	−0.13	0.38	0.46	0.08	1.80	0.71	−1.09
SCONF	−0.37	0.56	0.66	0.12	2.26	1.31	−0.96
UPU23	0.01	0.76	0.98	0.13	3.75	2.32	−1.43
BUT14DIOL	−0.61	0.61	0.62	0.22	0.72	−0.10	−0.81

Table S176: Statistical analysis for the MN15 DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.03	2.72	4.23	0.01	40.01	12.03	−27.98
G21EA	0.82	1.37	1.76	0.04	7.19	4.53	−2.66
G21IP	0.30	2.75	3.70	0.01	17.36	8.97	−8.40
DIPCS10	−3.62	4.35	5.71	0.01	15.10	2.60	−12.50
PA26	0.84	1.64	1.94	0.01	6.61	4.58	−2.03
SIE4x4	10.97	11.30	13.47	0.34	32.21	29.56	−2.65
ALKBDE10	−1.13	2.88	4.31	0.03	14.66	4.01	−10.65
YBDE18	−1.63	3.38	3.92	0.07	11.45	3.62	−7.83
AL2X6	1.45	1.45	1.70	0.04	2.78	3.06	0.29
HEAVYSB11	−4.97	5.09	5.79	0.09	8.93	0.66	−8.28
NBPRC	−1.18	1.78	2.08	0.06	5.95	2.66	−3.29
ALK8	−0.80	3.72	4.82	0.06	16.10	9.67	−6.43
RC21	0.64	1.74	2.14	0.05	8.56	4.74	−3.82
G2RC	−1.02	2.63	3.13	0.05	11.63	6.98	−4.65
BH76RC	0.12	1.57	2.28	0.07	11.59	4.84	−6.75
FH51	0.27	1.61	2.17	0.05	10.79	5.52	−5.27
TAUT15	0.68	1.19	1.60	0.39	5.26	3.70	−1.56
DC13	−1.61	5.10	7.19	0.09	28.84	16.50	−12.34
MB16-43	16.67	20.19	23.68	0.05	89.95	57.21	−32.75
DARC	1.67	1.71	2.06	0.05	3.66	3.44	−0.22
RSE43	−1.35	1.35	1.54	0.18	3.35	−0.40	−3.75
BSR36	0.22	0.57	0.76	0.04	3.09	2.03	−1.06
CDIE20	0.55	0.64	0.89	0.16	2.61	2.20	−0.42
ISO34	−0.94	1.50	1.86	0.10	5.64	1.91	−3.73
ISOL24	−1.24	2.64	3.62	0.12	16.96	5.02	−11.94
C60ISO	1.95	1.95	2.24	0.02	3.41	3.45	0.04
PArel	0.80	1.34	2.03	0.29	8.36	6.39	−1.97
BH76	−1.07	1.50	2.00	0.08	9.20	2.56	−6.63
BHPERI	0.78	1.26	1.76	0.06	7.97	4.84	−3.13
BHDIV10	−1.70	1.70	2.01	0.04	3.41	−0.01	−3.43
INV24	−1.33	2.68	3.55	0.08	15.19	8.14	−7.04
BHROT27	0.46	0.48	0.67	0.08	1.48	1.37	−0.10
PX13	−1.91	2.03	2.17	0.06	4.28	0.73	−3.55
WCPT18	−1.28	1.50	1.72	0.04	5.89	1.98	−3.91
RG18	0.02	0.10	0.12	0.17	0.45	0.26	−0.19
ADIM6	1.27	1.27	1.41	0.38	1.69	2.14	0.45
S22	−0.16	0.56	0.82	0.08	2.91	0.65	−2.27
S66	0.14	0.43	0.55	0.08	2.92	1.59	−1.34
HEAVY28	0.21	0.33	0.41	0.27	1.31	0.85	−0.47
WATER27	1.07	1.22	1.46	0.02	4.36	3.45	−0.91
CARBHB12	−0.03	0.24	0.34	0.04	1.48	0.61	−0.88
PNICO23	0.28	0.30	0.35	0.07	0.84	0.68	−0.16
HAL59	0.17	0.54	0.69	0.12	3.32	1.97	−1.34
AHB21	−0.25	0.33	0.43	0.01	1.26	0.24	−1.01
CHB6	−0.18	0.32	0.41	0.01	1.20	0.40	−0.80
IL16	0.95	1.03	1.12	0.01	2.63	1.96	−0.68
IDISP	0.74	3.58	4.32	0.25	11.80	6.23	−5.56
ICONF	0.13	0.51	0.61	0.16	2.00	1.15	−0.85
ACONF	−0.50	0.50	0.57	0.27	0.87	−0.14	−1.01
AMINO20x4	0.08	0.52	0.68	0.21	3.39	1.99	−1.40
PCONF21	0.52	1.09	1.28	0.67	4.10	1.98	−2.12
MCONF	0.51	0.57	0.69	0.11	1.84	1.48	−0.36
SCONF	0.11	0.50	0.68	0.11	2.96	1.23	−1.73
UPU23	0.15	0.54	0.69	0.09	3.16	1.48	−1.68
BUT14DIOL	−0.36	0.36	0.45	0.13	1.26	0.11	−1.14

Table S177: Statistical analysis for the LC-ωhPBE DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−3.09	4.43	7.42	0.01	47.72	6.55	−41.17
G21EA	0.08	2.84	3.22	0.08	10.90	5.08	−5.82
G21IP	2.78	4.59	5.64	0.02	18.54	11.73	−6.81
DIPCS10	3.01	3.15	4.11	0.00	7.27	6.91	−0.37
PA26	2.51	2.61	3.01	0.01	6.46	5.13	−1.33
SIE4x4	9.35	9.35	12.27	0.28	26.11	28.50	2.39
ALKBDE10	−1.18	5.50	7.15	0.05	24.27	11.81	−12.46
YBDE18	−2.61	2.87	3.57	0.06	8.72	1.12	−7.60
AL2X6	−2.29	2.29	2.55	0.06	3.72	−0.30	−4.01
HEAVYSB11	−6.64	6.64	6.96	0.11	6.73	−3.32	−10.05
NBPRC	0.25	2.31	2.90	0.08	9.65	6.04	−3.61
ALK8	0.52	0.67	0.83	0.01	2.00	1.38	−0.62
RC21	2.71	3.46	4.71	0.10	15.62	11.32	−4.29
G2RC	−3.65	5.45	6.93	0.11	25.39	11.51	−13.88
BH76RC	−0.65	2.29	2.81	0.11	10.61	5.14	−5.46
FH51	−1.80	2.98	3.95	0.10	19.91	6.02	−13.88
TAUT15	−0.25	0.90	1.06	0.30	3.44	1.69	−1.75
DC13	−3.42	10.47	14.14	0.19	55.44	26.97	−28.47
MB16-43	−25.48	29.26	35.22	0.07	111.44	38.31	−73.12
DARC	−5.98	5.98	6.35	0.18	7.13	−3.34	−10.46
RSE43	−0.58	0.66	0.85	0.09	2.71	0.46	−2.25
BSR36	−5.84	5.84	6.45	0.36	12.93	−1.25	−14.18
CDIE20	0.14	0.95	1.31	0.23	4.69	2.90	−1.79
ISO34	−0.74	2.03	2.94	0.14	12.08	5.17	−6.90
ISOL24	0.54	4.71	6.28	0.21	28.01	12.19	−15.82
C60ISO	17.27	17.27	19.02	0.18	22.29	28.03	5.74
PArel	0.40	1.00	1.26	0.22	5.19	1.85	−3.34
BH76	0.35	1.61	2.22	0.09	10.72	6.00	−4.72
BHPERI	4.60	4.75	5.54	0.23	17.33	15.40	−1.94
BHDIV10	0.02	1.46	1.89	0.03	7.17	4.13	−3.04
INV24	−0.20	2.33	3.89	0.07	21.72	12.71	−9.01
BHROT27	0.40	0.60	0.86	0.10	2.88	2.04	−0.84
PX13	−4.51	4.51	4.87	0.14	5.93	−0.95	−6.89
WCPT18	−0.54	1.89	2.57	0.05	11.48	8.08	−3.40
RG18	−0.63	0.63	0.79	1.09	1.67	−0.12	−1.79
ADIM6	−3.87	3.87	4.22	1.15	4.87	−1.50	−6.37
S22	−2.79	2.79	3.59	0.38	8.81	−0.39	−9.20
S66	−2.44	2.44	2.82	0.45	6.43	−0.28	−6.71
HEAVY28	−0.97	0.97	1.02	0.78	1.24	−0.29	−1.53
WATER27	−5.75	6.14	10.03	0.08	29.17	1.58	−27.59
CARBHB12	−0.25	0.45	0.56	0.07	1.95	0.80	−1.15
PNICO23	−1.15	1.15	1.22	0.27	2.25	−0.45	−2.70
HAL59	−1.63	1.63	1.88	0.36	5.49	0.06	−5.43
AHB21	0.16	0.79	0.92	0.04	3.34	1.85	−1.50
CHB6	−0.72	1.30	1.67	0.05	4.93	1.44	−3.49
IL16	3.04	3.04	3.12	0.03	2.65	4.77	2.12
IDISP	−2.18	6.97	7.76	0.49	20.27	9.47	−10.80
ICONF	0.26	0.46	0.59	0.14	1.76	1.24	−0.52
ACONF	0.57	0.57	0.63	0.31	0.93	1.13	0.20
AMINO20x4	−0.01	0.47	0.60	0.19	2.98	1.53	−1.44
PCONF21	−0.17	2.72	3.11	1.68	8.86	5.16	−3.70
MCONF	−1.37	1.46	1.68	0.29	3.55	0.69	−2.86
SCONF	−0.13	0.40	0.51	0.09	1.94	1.13	−0.81
UPU23	2.01	2.14	3.07	0.37	8.07	7.51	−0.56
BUT14DIOL	−0.39	0.40	0.45	0.14	0.94	0.14	−0.79

SI.7.8 Results for dispersion-uncorrected double-hybrid functionals

Table S178: Statistical analysis for the B2PLYP DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−1.21	2.31	3.10	0.01	20.45	8.33	−12.11
G21EA	−0.53	1.30	1.66	0.04	7.06	4.21	−2.85
G21IP	−0.91	2.28	2.78	0.01	13.01	5.78	−7.23
DIPCS10	−3.12	3.97	4.56	0.01	13.41	4.23	−9.18
PA26	0.92	1.14	1.86	0.01	6.85	5.96	−0.89
SIE4x4	9.89	9.89	11.26	0.29	19.53	21.39	1.86
ALKBDE10	−0.11	3.19	3.88	0.03	12.68	5.92	−6.76
YBDE18	−3.28	3.71	4.39	0.08	11.67	2.94	−8.73
AL2X6	−5.57	5.57	5.82	0.16	5.04	−3.30	−8.34
HEAVYSB11	−3.94	3.94	4.16	0.07	4.65	−2.10	−6.75
NBPRC	2.45	2.96	4.14	0.11	11.61	10.33	−1.28
ALK8	−3.28	3.28	4.35	0.05	7.04	−0.15	−7.19
RC21	−1.39	1.75	2.20	0.05	7.51	1.78	−5.73
G2RC	0.68	1.45	2.00	0.03	9.82	6.02	−3.80
BH76RC	−0.22	1.18	1.58	0.06	8.14	4.67	−3.47
FH51	1.32	2.17	2.88	0.07	17.56	8.83	−8.72
TAUT15	0.03	0.71	0.87	0.23	2.81	1.55	−1.26
DC13	3.88	9.14	10.94	0.17	37.61	20.58	−17.02
MB16-43	−34.39	34.39	37.64	0.08	88.90	−3.10	−92.00
DARC	8.69	8.69	8.89	0.27	5.85	10.64	4.79
RSE43	−0.61	0.67	0.82	0.09	3.35	1.12	−2.23
BSR36	−6.11	6.11	6.88	0.38	12.91	−2.05	−14.96
CDIE20	0.86	0.86	0.94	0.21	1.51	1.64	0.13
ISO34	−0.03	1.38	2.04	0.09	12.45	7.79	−4.66
ISOL24	−2.49	5.63	8.59	0.26	47.09	19.52	−27.57
C60ISO	−7.02	7.02	9.30	0.07	17.56	−0.38	−17.94
PArel	0.07	0.75	1.18	0.16	6.15	3.16	−2.99
BH76	−2.17	2.28	2.65	0.12	6.75	1.12	−5.63
BHPERI	0.52	1.61	1.93	0.08	8.51	3.53	−4.98
BHDIV10	−0.56	1.97	2.43	0.04	8.29	4.12	−4.17
INV24	−0.82	0.96	1.17	0.03	3.77	1.20	−2.57
BHROT27	0.22	0.25	0.37	0.04	1.22	1.04	−0.17
PX13	−2.42	2.42	2.52	0.07	2.55	−1.03	−3.58
WCPT18	−1.18	1.18	1.43	0.03	2.79	−0.07	−2.86
RG18	−0.44	0.45	0.55	0.78	1.13	0.03	−1.10
ADIM6	−2.87	2.87	3.15	0.85	3.75	−1.10	−4.85
S22	−1.94	1.94	2.50	0.27	6.38	−0.06	−6.44
S66	−1.71	1.71	2.04	0.31	4.71	0.04	−4.67
HEAVY28	−0.75	0.75	0.79	0.60	0.98	−0.32	−1.30
WATER27	−2.56	2.76	4.42	0.03	13.83	0.96	−12.87
CARBHB12	−0.10	0.37	0.46	0.06	1.65	0.85	−0.79
PNICO23	−0.98	0.98	1.04	0.23	1.63	−0.42	−2.04
HAL59	−0.82	0.89	1.14	0.19	5.28	1.42	−3.86
AHB21	0.30	0.39	0.49	0.02	1.70	1.31	−0.39
CHB6	−0.35	0.85	0.98	0.03	2.84	1.50	−1.33
IL16	2.22	2.22	2.26	0.02	1.54	3.20	1.66
IDISP	2.42	7.84	9.36	0.55	25.67	18.01	−7.65
ICONF	0.05	0.35	0.46	0.11	2.04	0.94	−1.11
ACONF	0.35	0.37	0.44	0.20	0.85	0.79	−0.06
AMINO20x4	−0.07	0.35	0.45	0.14	2.25	1.27	−0.97
PCONF21	−0.17	1.94	2.19	1.20	6.50	3.73	−2.78
MCONF	−1.10	1.12	1.27	0.23	2.25	0.28	−1.97
SCONF	−0.14	0.32	0.40	0.07	1.64	1.04	−0.59
UPU23	1.18	1.44	2.02	0.25	5.54	4.89	−0.65
BUT14DIOL	−0.10	0.21	0.23	0.07	0.85	0.49	−0.36

Table S179: Statistical analysis for the B2GPPLYP DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−3.13	3.30	4.36	0.01	18.75	2.15	−16.60
G21EA	−1.13	1.72	1.93	0.05	6.70	3.34	−3.36
G21IP	−0.81	2.01	2.51	0.01	12.84	5.08	−7.76
DIPCS10	−2.95	3.40	4.21	0.01	11.47	2.27	−9.19
PA26	0.80	1.03	1.68	0.01	6.92	5.33	−1.59
SIE4x4	6.56	6.56	7.50	0.19	13.14	14.51	1.37
ALKBDE10	−1.33	3.13	3.59	0.03	11.28	4.04	−7.24
YBDE18	−1.80	2.18	2.43	0.04	7.33	2.03	−5.30
AL2X6	−4.22	4.22	4.42	0.12	3.79	−2.64	−6.42
HEAVYSB11	−3.11	3.11	3.22	0.05	3.20	−1.74	−4.94
NBPRC	1.71	2.09	2.87	0.08	8.24	7.06	−1.19
ALK8	−2.18	2.24	3.06	0.04	6.25	0.23	−6.03
RC21	−1.43	1.70	2.11	0.05	5.56	1.38	−4.18
G2RC	−0.51	1.16	1.58	0.02	7.31	3.78	−3.53
BH76RC	−0.39	1.00	1.37	0.05	6.83	3.08	−3.75
FH51	0.32	1.41	1.96	0.05	11.08	5.10	−5.98
TAUT15	0.14	0.55	0.70	0.18	2.46	1.27	−1.18
DC13	2.80	5.95	7.50	0.11	26.95	16.75	−10.20
MB16-43	−25.81	26.08	30.73	0.06	102.84	5.62	−97.22
DARC	5.23	5.23	5.45	0.16	4.77	7.02	2.25
RSE43	0.05	0.42	0.75	0.06	4.47	3.22	−1.26
BSR36	−4.86	4.86	5.43	0.30	9.60	−1.90	−11.50
CDIE20	0.71	0.71	0.79	0.17	1.37	1.40	0.04
ISO34	0.17	0.92	1.54	0.06	9.89	6.58	−3.30
ISOL24	−1.36	3.90	5.89	0.18	32.30	13.96	−18.35
C60ISO	−6.05	6.14	8.39	0.06	17.06	0.39	−16.68
PArel	0.20	0.56	0.92	0.12	4.06	2.44	−1.62
BH76	−0.62	1.23	1.71	0.07	11.41	6.97	−4.43
BHPERI	0.11	0.87	1.19	0.04	5.89	2.43	−3.47
BHDIV10	0.12	1.40	1.81	0.03	6.50	3.88	−2.61
INV24	−0.25	0.76	1.02	0.02	4.41	2.84	−1.57
BHROT27	0.30	0.31	0.48	0.05	1.77	1.66	−0.11
PX13	−1.48	1.48	1.63	0.04	2.16	−0.18	−2.34
WCPT18	−0.48	0.80	0.98	0.02	3.37	1.53	−1.84
RG18	−0.32	0.33	0.41	0.57	0.92	0.06	−0.86
ADIM6	−2.20	2.20	2.42	0.65	2.91	−0.82	−3.73
S22	−1.31	1.31	1.74	0.18	4.53	0.04	−4.49
S66	−1.19	1.20	1.48	0.22	3.50	0.18	−3.32
HEAVY28	−0.57	0.57	0.60	0.46	0.71	−0.27	−0.98
WATER27	−1.12	1.54	2.47	0.02	8.80	1.16	−7.64
CARBHB12	0.05	0.32	0.41	0.05	1.54	0.98	−0.56
PNICO23	−0.70	0.70	0.76	0.16	1.31	−0.25	−1.56
HAL59	−0.57	0.64	0.81	0.14	3.63	1.00	−2.64
AHB21	−0.06	0.39	0.47	0.02	1.76	0.88	−0.88
CHB6	−0.74	0.99	1.05	0.04	2.20	0.76	−1.45
IL16	1.65	1.65	1.69	0.02	1.34	2.47	1.13
IDISP	1.54	5.25	6.23	0.37	16.90	11.70	−5.20
ICONF	0.07	0.30	0.37	0.09	1.45	0.57	−0.88
ACONF	0.19	0.24	0.28	0.13	0.70	0.53	−0.17
AMINO20x4	−0.04	0.26	0.34	0.11	1.79	0.99	−0.80
PCONF21	−0.04	1.36	1.56	0.84	4.66	2.78	−1.88
MCONF	−0.69	0.71	0.81	0.14	1.56	0.23	−1.33
SCONF	−0.09	0.25	0.32	0.05	1.28	0.89	−0.39
UPU23	0.95	1.14	1.56	0.20	3.96	3.45	−0.51
BUT14DIOL	−0.07	0.15	0.17	0.05	0.68	0.39	−0.30

Table S180: Statistical analysis for the MPW2PLYP DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−2.47	2.95	4.01	0.01	21.54	4.42	−17.13
G21EA	−0.71	1.48	1.81	0.04	7.46	4.56	−2.90
G21IP	−0.66	2.33	2.82	0.01	12.84	6.10	−6.73
DIPCS10	−2.38	3.49	4.51	0.01	15.15	5.57	−9.58
PA26	0.81	1.12	1.82	0.01	7.09	5.86	−1.23
SIE4x4	9.09	9.09	10.38	0.27	18.46	20.06	1.61
ALKBDE10	−1.35	3.27	3.70	0.03	11.45	3.85	−7.60
YBDE18	−2.80	3.06	3.63	0.06	9.27	1.72	−7.55
AL2X6	−4.54	4.54	4.83	0.13	4.53	−2.63	−7.16
HEAVYSB11	−3.81	3.81	3.96	0.07	3.87	−2.31	−6.17
NBPRC	1.89	2.56	3.43	0.09	10.18	8.16	−2.01
ALK8	−2.32	2.50	3.61	0.04	7.45	0.73	−6.73
RC21	−0.62	1.25	1.60	0.04	6.10	1.92	−4.18
G2RC	−0.40	1.43	1.74	0.03	7.50	4.32	−3.18
BH76RC	−0.40	1.28	1.59	0.06	6.93	2.86	−4.07
FH51	0.62	1.56	2.17	0.05	12.81	5.20	−7.62
TAUT15	0.06	0.66	0.86	0.22	2.96	1.59	−1.37
DC13	2.78	7.81	9.87	0.14	35.73	18.88	−16.85
MB16-43	−30.89	31.02	35.32	0.07	81.05	2.76	−78.29
DARC	6.95	6.95	7.19	0.21	5.89	8.80	2.92
RSE43	−0.50	0.56	0.70	0.07	2.98	1.00	−1.97
BSR36	−6.19	6.19	7.11	0.38	13.09	−2.54	−15.63
CDIE20	0.77	0.77	0.85	0.19	1.48	1.58	0.10
ISO34	0.07	1.22	1.89	0.08	12.05	7.81	−4.24
ISOL24	−2.05	5.00	7.58	0.23	41.43	17.39	−24.04
C60ISO	−4.34	4.66	6.50	0.05	14.13	0.85	−13.28
PArel	0.16	0.69	1.08	0.15	5.09	3.30	−1.79
BH76	−1.97	2.12	2.47	0.11	7.12	1.58	−5.54
BHPERI	0.73	1.35	1.66	0.06	6.94	3.42	−3.52
BHDIV10	−0.09	1.62	2.12	0.04	7.52	4.38	−3.14
INV24	−0.38	0.78	0.98	0.02	4.04	2.14	−1.90
BHROT27	0.29	0.31	0.45	0.05	1.29	1.12	−0.17
PX13	−1.96	1.96	2.09	0.06	2.42	−0.61	−3.03
WCPT18	−0.77	1.12	1.37	0.03	3.88	1.32	−2.56
RG18	0.01	0.24	0.31	0.41	1.26	0.72	−0.55
ADIM6	−1.99	1.99	2.24	0.59	2.99	−0.59	−3.58
S22	−1.27	1.34	1.91	0.18	5.58	0.38	−5.20
S66	−1.05	1.15	1.46	0.21	4.08	0.50	−3.58
HEAVY28	−0.43	0.43	0.49	0.35	0.85	−0.06	−0.91
WATER27	1.66	1.90	2.47	0.02	11.25	8.02	−3.23
CARBHB12	0.31	0.40	0.53	0.07	1.59	1.28	−0.31
PNICO23	−0.51	0.52	0.62	0.12	1.65	0.08	−1.57
HAL59	−0.39	0.57	0.82	0.12	4.64	1.66	−2.99
AHB21	−0.33	0.44	0.56	0.02	1.63	0.62	−1.01
CHB6	−1.14	1.39	1.49	0.05	2.87	0.76	−2.11
IL16	1.55	1.55	1.61	0.01	1.47	2.40	0.92
IDISP	2.13	7.08	8.46	0.50	23.89	16.09	−7.80
ICONF	0.07	0.34	0.44	0.10	1.95	0.92	−1.03
ACONF	0.27	0.30	0.36	0.16	0.75	0.65	−0.10
AMINO20x4	−0.03	0.31	0.40	0.13	2.05	1.25	−0.80
PCONF21	−0.11	1.60	1.82	0.99	5.39	3.12	−2.27
MCONF	−0.88	0.91	1.04	0.18	1.86	0.21	−1.65
SCONF	−0.14	0.29	0.36	0.06	1.45	0.96	−0.49
UPU23	1.04	1.24	1.71	0.22	4.41	3.87	−0.55
BUT14DIOL	0.00	0.14	0.17	0.05	0.70	0.48	−0.22

Table S181: Statistical analysis for the PWPB95 DFA for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−0.54	1.83	2.86	0.01	24.79	11.14	−13.66
G21EA	−1.64	1.71	1.84	0.05	3.39	0.65	−2.73
G21IP	−1.29	1.94	2.37	0.01	10.15	3.61	−6.54
DIPCS10	−4.04	4.09	4.62	0.01	8.90	0.21	−8.68
PA26	1.77	1.79	2.21	0.01	6.20	5.93	−0.27
SIE4x4	9.93	9.93	11.37	0.29	20.89	22.64	1.75
ALKBDE10	−2.52	3.26	3.70	0.03	8.63	3.10	−5.52
YBDE18	−1.66	2.53	3.10	0.05	7.90	2.22	−5.68
AL2X6	−1.85	1.85	2.00	0.05	2.27	−0.39	−2.66
HEAVYSB11	−1.75	1.78	2.34	0.03	5.22	0.16	−5.06
NBPRC	0.89	1.45	2.02	0.05	5.58	4.32	−1.26
ALK8	0.71	1.75	2.44	0.03	7.67	5.76	−1.91
RC21	0.15	1.06	1.34	0.03	5.86	2.62	−3.23
G2RC	0.31	2.02	2.58	0.04	9.86	5.91	−3.96
BH76RC	0.14	1.14	1.61	0.05	9.18	5.06	−4.12
FH51	0.78	1.47	1.82	0.05	8.56	4.15	−4.40
TAUT15	−0.05	0.63	0.74	0.21	2.30	1.24	−1.06
DC13	0.54	4.81	6.06	0.09	22.28	10.74	−11.54
MB16-43	−13.09	13.09	16.05	0.03	55.08	−2.31	−57.39
DARC	3.59	3.59	3.92	0.11	4.39	5.38	0.99
RSE43	−1.01	1.01	1.18	0.13	2.58	−0.33	−2.91
BSR36	−4.63	4.63	5.05	0.29	9.51	−1.03	−10.53
CDIE20	0.72	0.76	0.90	0.19	1.89	1.73	−0.16
ISO34	−0.59	0.90	1.11	0.06	4.31	1.46	−2.84
ISOL24	−1.70	3.19	4.50	0.15	22.95	8.64	−14.31
C60ISO	−3.21	3.50	4.88	0.04	10.76	0.75	−10.01
PArel	0.36	0.69	1.09	0.15	5.15	3.70	−1.45
BH76	−1.52	1.62	1.94	0.09	5.68	1.02	−4.66
BHPERI	1.14	1.40	1.54	0.07	4.43	2.58	−1.86
BHDIV10	−1.31	1.33	1.58	0.03	2.92	0.06	−2.87
INV24	−0.63	0.99	1.21	0.03	4.78	2.24	−2.54
BHROT27	0.27	0.32	0.42	0.05	1.08	0.81	−0.27
PX13	−1.13	1.19	1.31	0.04	2.58	0.43	−2.14
WCPT18	−0.87	0.93	1.14	0.03	2.56	0.30	−2.26
RG18	−0.16	0.29	0.40	0.50	1.52	0.68	−0.84
ADIM6	−1.69	1.69	1.81	0.50	1.85	−0.73	−2.58
S22	−1.65	1.65	2.02	0.23	4.14	−0.05	−4.18
S66	−1.36	1.36	1.51	0.25	3.43	−0.18	−3.61
HEAVY28	−0.61	0.61	0.64	0.49	0.73	−0.19	−0.92
WATER27	−5.77	5.79	9.24	0.07	24.65	0.28	−24.38
CARBHB12	−0.34	0.40	0.52	0.07	1.62	0.35	−1.27
PNICO23	−0.71	0.71	0.78	0.17	1.64	−0.22	−1.86
HAL59	−0.81	0.85	1.00	0.19	3.56	0.75	−2.81
AHB21	0.51	0.51	0.61	0.02	1.24	1.29	0.05
CHB6	−0.83	1.07	1.31	0.04	3.07	0.62	−2.45
IL16	2.17	2.17	2.19	0.02	1.12	2.75	1.63
IDISP	1.34	3.84	5.15	0.27	15.38	11.01	−4.38
ICONF	0.00	0.14	0.20	0.04	0.73	0.47	−0.26
ACONF	0.00	0.06	0.07	0.03	0.26	0.12	−0.13
AMINO20x4	−0.03	0.27	0.33	0.11	1.43	0.68	−0.75
PCONF21	0.16	0.90	1.10	0.56	3.17	2.10	−1.07
MCONF	−0.56	0.63	0.75	0.13	1.94	0.50	−1.43
SCONF	−0.09	0.19	0.22	0.04	0.67	0.30	−0.37
UPU23	1.03	1.21	1.65	0.21	4.19	3.70	−0.49
BUT14DIOL	−0.47	0.47	0.48	0.17	0.57	−0.07	−0.64

Table S182: Statistical analysis for the DSD-BLYP DFA (no dispersion correction) for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−2.72	3.06	4.00	0.01	21.40	3.91	−17.49
G21EA	−1.26	1.76	2.00	0.05	7.37	3.85	−3.52
G21IP	−1.12	2.02	2.51	0.01	12.60	4.75	−7.85
DIPCS10	−3.82	4.00	4.62	0.01	10.04	0.91	−9.13
PA26	0.70	0.95	1.55	0.01	6.52	4.81	−1.71
SIE4x4	5.75	5.75	6.57	0.17	11.26	12.47	1.21
ALKBDE10	−0.72	2.92	3.47	0.03	11.62	4.92	−6.70
YBDE18	−1.30	1.94	2.18	0.04	7.71	3.27	−4.44
AL2X6	−4.23	4.23	4.39	0.12	3.42	−2.79	−6.21
HEAVYSB11	−2.64	2.64	2.77	0.05	3.12	−1.18	−4.30
NBPRC	1.76	2.07	2.86	0.07	7.95	7.12	−0.83
ALK8	−2.19	2.20	3.04	0.04	5.74	0.03	−5.72
RC21	−2.29	2.50	2.93	0.07	6.05	1.26	−4.79
G2RC	0.02	1.04	1.48	0.02	6.94	4.08	−2.86
BH76RC	−0.23	0.87	1.26	0.04	7.30	3.90	−3.39
FH51	0.52	1.51	2.04	0.05	11.50	5.83	−5.67
TAUT15	0.05	0.46	0.54	0.15	1.89	0.85	−1.03
DC13	3.04	5.70	6.93	0.10	23.22	14.87	−8.35
MB16-43	−25.73	25.94	30.88	0.06	117.69	4.52	−113.17
DARC	5.19	5.19	5.35	0.16	3.83	6.82	2.99
RSE43	0.42	0.58	1.19	0.08	5.75	4.93	−0.82
BSR36	−4.33	4.33	4.80	0.27	8.36	−1.65	−10.01
CDIE20	0.64	0.64	0.70	0.16	1.20	1.22	0.02
ISO34	0.13	0.89	1.39	0.06	8.60	5.76	−2.84
ISOL24	−1.35	3.63	5.53	0.17	30.35	13.02	−17.33
C60ISO	−7.93	7.93	10.34	0.08	19.39	−0.45	−19.84
PArel	0.10	0.52	0.86	0.11	4.30	2.06	−2.24
BH76	−0.11	1.14	1.90	0.06	13.40	9.05	−4.35
BHPERI	−0.22	0.73	1.16	0.03	5.96	1.98	−3.98
BHDIV10	0.11	1.35	1.69	0.03	6.01	3.36	−2.65
INV24	−0.27	0.72	1.04	0.02	5.39	2.58	−2.81
BHROT27	0.20	0.22	0.31	0.04	0.93	0.85	−0.07
PX13	−1.34	1.34	1.47	0.04	1.90	−0.17	−2.07
WCPT18	−0.51	0.65	0.82	0.02	2.57	0.92	−1.64
RG18	−0.32	0.32	0.41	0.55	0.87	0.05	−0.82
ADIM6	−2.08	2.08	2.28	0.62	2.74	−0.78	−3.52
S22	−1.26	1.26	1.59	0.17	3.93	−0.06	−3.99
S66	−1.16	1.16	1.38	0.21	3.14	0.07	−3.07
HEAVY28	−0.54	0.54	0.56	0.44	0.65	−0.23	−0.88
WATER27	−2.24	2.38	3.82	0.03	11.84	0.68	−11.16
CARBHB12	−0.04	0.29	0.37	0.05	1.38	0.78	−0.61
PNICO23	−0.74	0.74	0.78	0.17	1.12	−0.30	−1.42
HAL59	−0.57	0.62	0.75	0.14	3.06	0.80	−2.26
AHB21	0.15	0.32	0.39	0.01	1.54	0.96	−0.58
CHB6	−0.59	0.82	0.87	0.03	1.85	0.69	−1.15
IL16	1.71	1.71	1.74	0.02	1.24	2.51	1.26
IDISP	1.44	4.42	5.33	0.31	14.92	10.21	−4.72
ICONF	0.04	0.27	0.33	0.08	1.21	0.38	−0.84
ACONF	0.14	0.21	0.24	0.11	0.67	0.46	−0.20
AMINO20x4	−0.07	0.25	0.32	0.10	1.66	0.85	−0.81
PCONF21	−0.03	1.19	1.36	0.73	4.14	2.50	−1.63
MCONF	−0.59	0.61	0.69	0.12	1.33	0.20	−1.14
SCONF	−0.11	0.27	0.33	0.06	1.28	0.87	−0.42
UPU23	0.87	1.06	1.42	0.19	3.57	3.13	−0.44
BUT14DIOL	−0.12	0.18	0.20	0.06	0.71	0.36	−0.35

Table S183: Statistical analysis for the DSD-PBEP86 DFA (no dispersion correction) for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−3.22	3.30	4.27	0.01	21.60	2.01	−19.59
G21EA	−1.01	1.51	1.80	0.04	7.70	4.72	−2.98
G21IP	−1.06	2.10	2.62	0.01	13.63	6.58	−7.05
DIPCS10	−3.91	3.91	4.36	0.01	6.75	−0.96	−7.71
PA26	0.85	0.98	1.40	0.01	5.38	4.25	−1.13
SIE4x4	4.92	4.92	5.71	0.15	10.40	11.44	1.05
ALKBDE10	−2.43	3.19	3.79	0.03	9.10	2.05	−7.05
YBDE18	−0.22	1.23	1.54	0.02	6.77	4.15	−2.62
AL2X6	−2.52	2.52	2.60	0.07	2.01	−1.43	−3.44
HEAVYSB11	−2.09	2.09	2.17	0.04	2.34	−0.91	−3.25
NBPRC	0.79	1.08	1.35	0.04	3.82	2.90	−0.92
ALK8	−0.60	1.57	2.04	0.03	7.32	3.88	−3.44
RC21	−1.44	1.86	2.32	0.05	5.65	1.49	−4.16
G2RC	−0.51	1.51	1.98	0.03	8.95	4.98	−3.98
BH76RC	−0.23	0.84	1.38	0.04	8.53	4.90	−3.63
FH51	−0.15	0.85	1.15	0.03	5.95	2.66	−3.29
TAUT15	0.02	0.45	0.50	0.15	1.44	0.76	−0.68
DC13	1.50	2.94	3.74	0.05	14.44	7.15	−7.29
MB16-43	−17.19	17.40	23.17	0.04	112.42	4.55	−107.86
DARC	1.04	1.25	1.55	0.04	3.30	2.55	−0.75
RSE43	0.84	0.86	1.68	0.11	7.14	7.04	−0.10
BSR36	−3.55	3.55	3.95	0.22	6.57	−1.52	−8.09
CDIE20	0.55	0.56	0.64	0.14	1.26	1.20	−0.06
ISO34	−0.03	0.53	0.78	0.04	4.44	2.54	−1.90
ISOL24	−0.53	1.88	2.87	0.09	15.53	6.68	−8.85
C60ISO	−7.86	7.86	10.06	0.08	18.49	−0.66	−19.14
PArel	0.21	0.50	0.77	0.11	3.60	1.81	−1.79
BH76	0.00	1.20	2.04	0.06	13.94	9.89	−4.05
BHPERI	−1.03	1.08	1.17	0.05	2.71	0.67	−2.03
BHDIV10	−0.73	1.30	1.49	0.03	4.12	1.92	−2.21
INV24	−0.13	0.64	1.00	0.02	5.73	3.47	−2.26
BHROT27	0.18	0.19	0.25	0.03	0.69	0.64	−0.05
PX13	−2.27	2.27	2.35	0.07	2.45	−1.00	−3.44
WCPT18	−1.40	1.41	1.62	0.04	3.21	0.11	−3.10
RG18	−0.20	0.23	0.30	0.40	0.80	0.16	−0.64
ADIM6	−1.40	1.40	1.55	0.42	1.98	−0.47	−2.45
S22	−0.79	0.80	1.06	0.11	2.81	0.06	−2.75
S66	−0.73	0.74	0.91	0.14	2.35	0.17	−2.19
HEAVY28	−0.25	0.25	0.28	0.20	0.40	−0.04	−0.44
WATER27	−0.57	1.04	1.67	0.01	6.17	0.98	−5.19
CARBHB12	0.24	0.30	0.44	0.05	1.41	1.14	−0.26
PNICO23	−0.26	0.28	0.33	0.07	1.11	0.21	−0.90
HAL59	−0.23	0.38	0.49	0.08	2.55	1.04	−1.52
AHB21	−0.13	0.28	0.38	0.01	1.67	0.54	−1.13
CHB6	−0.52	0.59	0.66	0.02	1.27	0.22	−1.06
IL16	1.05	1.05	1.10	0.01	1.33	1.67	0.34
IDISP	0.66	2.21	2.59	0.16	7.15	4.41	−2.74
ICONF	0.05	0.18	0.22	0.06	0.76	0.33	−0.43
ACONF	0.01	0.12	0.14	0.07	0.49	0.23	−0.26
AMINO20x4	−0.06	0.18	0.22	0.07	1.10	0.53	−0.57
PCONF21	−0.05	0.85	0.95	0.52	2.74	1.76	−0.97
MCONF	−0.30	0.32	0.37	0.06	0.89	0.26	−0.64
SCONF	−0.06	0.14	0.18	0.03	0.76	0.52	−0.24
UPU23	0.68	0.85	1.11	0.15	2.80	2.40	−0.40
BUT14DIOL	−0.10	0.14	0.15	0.05	0.48	0.22	−0.26

Table S184: Statistical analysis for the DSD-PBEB95 DFA (no dispersion correction) for all 55 test sets of the GMTKN55 database. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), normalised MAD (NMAD), deviation span (Δ_{err}), maximum (max) and minimum deviation (min). The NMAD is defined as the ratio between the MAD for a set and its average absolute reaction energy. For all test sets, the def2-QZVP atomic-orbital basis set was used, with additional diffuse functions for the G21EA, WATER27, AHB21, and IL16 sets. All values are in kcal/mol, except for the dimensionless NMAD.

Set	MD	MAD	RMSD	NMAD	Δ_{err}	max	min
W4-11	−2.17	2.68	3.66	0.01	25.39	7.91	−17.48
G21EA	−2.76	2.89	2.97	0.09	5.92	1.59	−4.34
G21IP	−2.18	2.58	2.89	0.01	10.89	3.22	−7.68
DIPCS10	−6.03	6.03	6.33	0.01	7.80	−2.50	−10.30
PA26	1.34	1.35	1.72	0.01	4.91	4.72	−0.19
SIE4x4	5.84	5.84	6.74	0.17	12.51	13.61	1.11
ALKBDE10	−3.21	3.26	3.92	0.03	6.64	0.25	−6.38
YBDE18	−0.18	1.11	1.31	0.02	4.56	1.74	−2.82
AL2X6	−1.78	1.78	1.85	0.05	1.52	−0.84	−2.36
HEAVYSB11	−1.22	1.22	1.45	0.02	2.89	−0.19	−3.08
NBPRC	0.72	1.04	1.44	0.04	3.64	2.84	−0.80
ALK8	0.87	1.68	2.89	0.03	8.80	7.66	−1.15
RC21	−0.90	1.20	1.58	0.03	5.96	1.60	−4.36
G2RC	−0.14	1.49	2.00	0.03	8.63	4.43	−4.20
BH76RC	0.13	1.09	1.51	0.05	8.56	4.66	−3.89
FH51	0.14	0.98	1.22	0.03	5.41	2.77	−2.64
TAUT15	−0.14	0.41	0.48	0.13	1.51	0.54	−0.97
DC13	0.50	3.86	4.54	0.07	15.26	9.05	−6.21
MB16-43	−12.45	12.48	17.51	0.03	87.62	0.61	−87.01
DARC	1.46	1.46	1.83	0.04	2.97	2.98	0.01
RSE43	−0.02	0.47	0.73	0.06	3.85	2.46	−1.39
BSR36	−3.70	3.70	4.02	0.23	7.01	−1.02	−8.04
CDIE20	0.56	0.61	0.73	0.15	1.65	1.45	−0.20
ISO34	−0.39	0.69	0.89	0.05	3.50	1.47	−2.02
ISOL24	−1.01	2.05	2.92	0.09	14.26	4.90	−9.36
C60ISO	−4.75	4.87	6.57	0.05	13.51	0.44	−13.07
PArel	0.31	0.55	0.80	0.12	3.61	2.41	−1.20
BH76	0.35	1.04	1.65	0.06	10.85	7.63	−3.22
BHPERI	0.97	1.13	1.26	0.05	3.75	2.17	−1.58
BHDIV10	−0.33	0.56	0.72	0.01	2.20	0.78	−1.42
INV24	−0.10	0.74	1.15	0.02	5.95	4.34	−1.61
BHROT27	0.22	0.24	0.33	0.04	0.78	0.66	−0.11
PX13	0.05	0.56	0.65	0.02	2.24	1.41	−0.83
WCPT18	−0.11	0.55	0.61	0.02	1.93	0.85	−1.07
RG18	−0.12	0.22	0.29	0.38	0.97	0.34	−0.63
ADIM6	−1.21	1.21	1.30	0.36	1.39	−0.47	−1.86
S22	−1.14	1.15	1.41	0.16	2.78	0.08	−2.70
S66	−0.95	0.95	1.05	0.17	2.43	−0.07	−2.50
HEAVY28	−0.45	0.45	0.47	0.36	0.52	−0.13	−0.65
WATER27	−4.64	4.64	7.34	0.06	19.37	0.02	−19.35
CARBHB12	−0.25	0.31	0.44	0.05	1.44	0.34	−1.10
PNICO23	−0.59	0.59	0.64	0.14	1.09	−0.26	−1.35
HAL59	−0.61	0.63	0.72	0.14	1.93	0.22	−1.71
AHB21	0.39	0.42	0.49	0.02	1.17	1.01	−0.16
CHB6	−0.91	0.97	1.23	0.04	2.26	0.18	−2.08
IL16	1.81	1.81	1.83	0.02	0.85	2.29	1.44
IDISP	0.75	2.17	2.78	0.15	8.16	5.70	−2.46
ICONF	0.01	0.14	0.19	0.04	0.75	0.42	−0.33
ACONF	−0.07	0.09	0.11	0.05	0.31	0.07	−0.24
AMINO20x4	−0.05	0.23	0.28	0.09	1.26	0.61	−0.65
PCONF21	0.21	0.58	0.72	0.36	2.10	1.42	−0.68
MCONF	−0.28	0.34	0.41	0.07	1.15	0.37	−0.78
SCONF	−0.15	0.25	0.30	0.05	1.05	0.59	−0.45
UPU23	0.75	0.91	1.19	0.16	3.04	2.66	−0.38
BUT14DIOL	−0.43	0.43	0.44	0.15	0.56	−0.01	−0.57

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