ELECTRONIC SUPPLEMENTARY INFORMATION

PpF: A Density Functional Fine-Tuned for Noncovalent Interactions of Protein and Peptide Residues

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Supplementary Table S1. The optimized parameters of PpF. The parameters shown in the table correspond to X in equation (1), a_{ijk} in equation (2), b_i and c_i in equation (3), and $s_{r,6}$ in equation (5).

Nonseparable terms				Correlation terms	
a_{000}	0.299938742	a_{102}	-0.478206219	b_0	0.847844158
a_{001}	-0.172177576	a_{103}	0.175131824	b_1	-0.446743709
a_{002}	-0.230713056	a_{104}	-0.78214315	b_2	2.651157441
a_{003}	0.02832559	a_{110}	-2.594696308	b_3	-0.40206795
a_{004}	0.772464711	a_{111}	2.485383353	b_4	-4.375100339
a_{005}	0.597848025	a_{112}	2.155460062	b_5	-0.870229495
a_{010}	1.721784595	a_{113}	2.453851081	b_6	-1.100915595
a_{011}	-1.982181999	a_{120}	2.335456849	b_7	-3.309440201
a_{012}	-4.989794582	a_{121}	-1.078985645	b_8	5.210543232
a_{013}	0.370783141	a_{122}	1.584827496		
a_{014}	0.551650128	a_{200}	-0.814084182	c_0	0.710701177
a_{020}	-1.059864769	a_{201}	-0.055000108	c_1	-1.941499329
a_{021}	-3.279728742	a_{202}	0.837087648	c_2	-0.820386618
a_{022}	-4.357572238	a_{203}	-1.165170805	c_3	-2.160021538
a_{023}	-0.400672749	a_{210}	1.169855634	c_4	1.184473418
a_{030}	-0.284525701	a_{211}	-3.048643977	c_5	0.561395141
a_{031}	-2.539921881	a_{212}	6.018704766	c_6	-1.200071513
a_{032}	-1.81154969	a_{300}	0.08433292	c_7	2.41042793
a_{100}	0.920088229	a_{301}	-1.155597218	c_8	-3.397253208
a_{101}	0.72264503	a_{302}	0.341332712		
HF exchange				Damped dispersion	
X	41.7050			$s_{r,6}$	1.53

Supplementary Table S2. Training sets and the final inverse weights.

Index	Database	Description	Source	Number of data	Inverse weight
1	BHPERI26[1, 2]	Barrier heights of pericyclic reactions	MGCDB84	26	0.1343
2	CR20[3]	Cycloreversion reaction energies	MGCDB84	20	0.3165
3	CRBH20[4]	Barrier heights for cycloreversion of heterocyclic rings	MGCDB84	20	0.5913
4	PX13[5, 6]	Barrier heights for proton exchange in water, ammonia, and hydrogen fluoride clusters	MGCDB84	13	1.7577
5	WCPT27[7]	Barrier heights of water-catalyzed proton-transfer reactions	MGCDB84	27	0.2839
6	HTBH38/18[8]	Hydrogen transfer barrier heights	MDB2019	38	0.2085
7	NHTBH38/18[9]	Non-hydrogen transfer barrier heights	MDB2019	38	0.1557
8	NCCE30/18[10-14]	Noncovalent complexation energies	MDB2019	30	0.0694
9	NGD21/18[10, 15]	Noble gas dimer weak interactions	MDB2019	21	0.2699
10	A21x12[16]	PECs for the 21 equilibrium complexes from A24	MGCDB84	252	0.0571
11	A24[17]	Binding energies of small noncovalent complexes	MGCDB84	24	0.0633
12	Bauza30[18, 19]	Binding energies of halogen-, chalcogen-, and pnicogen-bonded dimers	MGCDB84	30	0.0845
13	BzDC215[20]	PECs for benzene interacting with two rare-gas atoms and eight first- and second-row hydrides	MGCDB84	215	0.2209
14	CT20[21]	Binding energies of charge-transfer complexes	MGCDB84	20	0.1062
15	DS14[22]	Binding energies of complexes containing divalent sulfur	MGCDB84	14	0.1020
16	FmH2O10[23, 24]	Binding energies of isomers of $F^-(H_2O)_{10}$	MGCDB84	10	0.5567
17	WATER27[1, 25]	Binding energies of neutral and charged water clusters	MGCDB84	23	0.6808
18	H2O6Bind8[23, 24]	Binding energies of isomers of $(H_2O)_6$	MGCDB84	8	0.1140
19	HB15[26]	Binding energies of hydrogen-bonded dimers featuring ionic groups common in biomolecules	MGCDB84	15	0.1698
20	HW30[27]	Binding energies of hydrocarbon-water dimers	MGCDB84	30	0.2215
21	HW6Cl[23, 24]	Binding energies of $Cl^-(H_2O)_n$(n=1-6)	MGCDB84	6	1.1148
22	HW6F[23, 24]	Binding energies of $F^-(H_2O)_n$(n=1-6)	MGCDB84	6	0.0989
23	Shields38[28]	Binding energies of $(H_2O)_n$(n=2-10)	MGCDB84	38	0.3371
24	SW49Bind345[29]	Binding energies of $SO_4^{2-}(H_2O)_n$(n=3-5)	MGCDB84	31	0.1327
25	SW49Bind6[29]	Binding energies of $SO_4^{2-}(H_2O)_6$	MGCDB84	18	0.1513
26	TA13[30]	Binding energies of dimers involving radicals	MGCDB84	13	0.2056
27	AlkBind12[31]	Binding energies of saturated and	MGCDB84	12	0.1888

Index	Database	Description	Source	Number of data	Inverse weight
		unsaturated hydrocarbon dimers			
28	HB49[32-34]	Binding energies of small- and medium-sized hydrogen-bonded systems	MGCDB84	49	0.1607
29	Ionic43[35]	Binding energies of anion-neutral, cation-neutral, and anion-cation dimers	MGCDB84	43	0.4545
30	H2O20Bind4[1, 25, 36, 37]	Binding energies of isomers of $(H_2O)_{20}$(dod, fc, fs, and es)	MGCDB84	4	0.4451
31	H2O20Bind10[23]	Binding energies of isomers of $(H_2O)_{20}$(low-energy structures)	MGCDB84	10	0.3135
32	CE20[5, 6]	Binding energies of water, ammonia, and hydrogen fluoride clusters	MGCDB84	20	0.1550
33	NC15[38]	Binding energies of very small noncovalent complexes	MGCDB84	15	0.0674
34	IsoL6/11[10]	Isomerization energies of large molecules	MDB2019	6	1.1202
35	2pIsoE4[39]	2p isomerization energies	MDB2019	4	1.3452
36	4pIsoE4[39]	4p isomerization energies	MDB2019	4	1.2523
37	AlkIsomer11[40]	Isomerization energies of $n = 4 - 8$ alkanes	MGCDB84	11	0.0622
38	Butanediol65[41]	Isomerization energies of butane-1,4-diol	MGCDB84	65	0.0073
39	DIE60[42]	Isomerization energies of reactions involving double-bond migration in conjugated dienes	MGCDB84	60	0.3867
40	EIE22[43]	Isomerization energies of enecarbonyls	MGCDB84	22	0.4046
41	ACONF[1, 44]	Isomerization energies of alkane conformers	MGCDB84	15	0.0471
42	CYCONF[1, 45]	Isomerization energies of cysteine conformers	MGCDB84	11	0.1077
43	Pentane14[46]	Isomerization energies of stationary points on the n-pentane torsional surface	MGCDB84	14	0.0252
44	SW49Rel345[29]	Isomerization energies of $SO_4^{2-}(H_2O)_n$(n=3-5)	MGCDB84	31	0.0867
45	SW49Rel6[29]	Isomerization energies of $SO_4^{2-}(H_2O)_6$	MGCDB84	18	0.0615
46	H2O20Rel4[1, 25, 36, 37]	Isomerization energies of isomers of $(H_2O)_{20}$(dod, fc, fs, and es)	MGCDB84	4	0.1484
47	H2O20Rel10[23]	Isomerization energies of isomers of $(H_2O)_{20}$(low-energy structures)	MGCDB84	10	0.1456
48	H2O16Rel5[47]	Isomerization energies of $(H_2O)_{16}$(boat and fused cube structures)	MGCDB84	5	0.0362
49	AlkAtom19[40]	$n = 1-8$ alkane atomization energies	MGCDB84	19	0.1080
50	AlkIsod14[40]	$n = 3-8$ alkane isodesmic reaction energies	MGCDB84	14	0.0994
51	G21EA[1, 48]	Adiabatic electron affinities of atoms and small molecules	MGCDB84	25	1.9061
52	G21IP[1, 48]	Adiabatic ionization potentials of atoms and small molecules	MGCDB84	36	2.8200
53	NBPRC[1, 49, 50]	Reactions involving NH_3/BH_3 and	MGCDB84	12	1.2623

Index	Database	Description	Source	Number of data	Inverse weight
		PH_3/BH_3			
54	BSR36[50, 51]	Hydrocarbon bond separation reaction energies	MGCDB84	36	0.3311
55	HNBrBDE18[52]	Homolytic N–Br bond dissociation energies	MGCDB84	18	1.1192
56	PlatonicTAE6[53]	Total atomization energies of platonic hydrocarbon cages, C_nH_n (n =4,6,8,10,12,20)	MGCDB84	6	0.5139
57	PlatonicIG6[53]	Isogyric reactions of platonic hydrocarbon cages, C_nH_n (n =4,6,8,10,12,20)	MGCDB84	6	4.0677
58	PlatonicID6[53]	Isodesmic reactions of platonic hydrocarbon cages, C_nH_n (n =4,6,8,10,12,20)	MGCDB84	6	0.3028
59	PlatonicHD6[53]	Homodesmotic reactions of platonic hydrocarbon cages, C_nH_n (n =4,6,8,10,12,20)	MGCDB84	6	4.6747
60	WCPT6[7]	Tautomerization energies for water-catalyzed proton-transfer reactions	MGCDB84	6	0.1488
61	SR-MGM-BE8[10, 54, 55]	Single-reference main-group metal bond energies	MDB2019	8	0.8401
62	SR-MGN-BE107[10]	Single-reference main-group non-metal bond energies	MDB2019	107	0.9376
63	MR-MGM-BE4[10]	Multi-reference main-group metal bond energies	MDB2019	4	0.7942
64	MR-MGN-BE17[10]	Multi-reference main-group non-metal bond energies	MDB2019	17	3.3421
65	SR-TML-BE11[10, 55-57]	Single-reference TM^g bond energies	MDB2019	11	3.2198
66	SR-TMD-BE4[10]	multi-reference TM bond energies	MDB2019	4	3.2198
67	MR-TML-BE12[10, 55, 57]	single-reference TM dimer bond energies (Cu_2, CuAg, Zr_2, Ag_2)	MDB2019	12	3.4096
68	MR-TMD-BE3[10, 58]	multi-reference TM dimer bond energies (V_2, Cr_2, Fe_2)	MDB2019	3	1.0968
69	πTC13[10]	Thermochemistry of π systems	MDB2019	13	4.0142
70	HC7/11[10]	Hydrocarbon chemistry	MDB2019	7	1.9148
71	IP23[10, 59]	Ionization potentials	MDB2019	23	1.7727
72	EA13/03[10]	Electron affinities	MDB2019	13	1.1354
73	PA8[10]	Proton affinities	MDB2019	8	0.9259
74	AE17[10]	Atomic energies	MDB2019	17	4.6426
75	DC9/19[10]	Difficult cases	MDB2019	9	4.8733
76	SMAE3/19[60-62]	Sulfur molecules atomization energies	MDB2019	3	0.9361
77	3dEE8[10, 58, 59]	3d TM atomic excitation energies and first excitation energy of Fe_2	MDB2019	8	1.7215
78	4dAEE5[63]	4d TM atomic excitation energies	MDB2019	5	0.8205
79	pAEE5[64]	p-block atomic excitation energies	MDB2019	5	3.1988
80	DBH24[65, 66]	Diverse barrier heights	MGCDB84	24	0.0550

Index	Database	Description	Source	Number of data	Inverse weight
81	BH76RC[1, 8, 9]	Reaction energies from HTBH38 and NHTBH38	MGCDB84	30	0.0813
82	ISOMERIZATION20[60]	Isomerization energies	MGCDB84	20	0.2786
83	BDE99MR[60]	Bond dissociation energies (MR)	MGCDB84	16	0.2346
84	BDE99nonMR[60]	Bond dissociation energies (SR)	MGCDB84	83	0.2933
85	HAT707MR[60]	Heavy-atom transfer energies (MR)	MGCDB84	202	0.1092
86	HAT707nonMR[60]	Heavy-atom transfer energies (SR)	MGCDB84	505	0.1366
87	SN13[60]	Nucleophilic substitution energies	MGCDB84	13	0.1067
88	TAE140MR[60]	Total atomization energies (MR)	MGCDB84	16	0.4876
89	TAE140nonMR[60]	Total atomization energies (SR)	MGCDB84	124	0.1625
90	AAIE12	Amino-acid interaction energies	Present	12	0.0006

Supplementary Table S3. Functionals compared in this work.

Functionals	Ref(s)	Type	Damped dispersion
Local functionals			
PBE	[67]	GGA[a]	none
PBE-D3(BJ)	[67]	GGA	D3(BJ)[b,68]
TPSS	[69]	meta-GGA	none
TPSS-D3(BJ)	[69]	meta-GGA	D3(BJ)[68]
M06-L	[70]	meta-GGA	none
M06-L-D3(0)	[70]	meta-GGA	D3(0)[c,71]
MN15-L	[72]	meta-NGA	none
revM06-L	[73]	meta-GGA	none
SCAN-D3(0)	[74]	meta-GGA	D3(0)[75]
r2SCAN	[76]	meta-GGA	none
r2SCAN-3c	[77]	meta-GGA	D4[d,78]
Range-separated hybrid functionals			
ωB97X-D	[79]	range-separated hybrid	D2[e,80]
M11	[81]	range-separated hybrid	none
M11-D3(BJ)	[81]	range-separated hybrid	D3(BJ)[82]
revM11	[83]	range-separated hybrid	none
M11plus	[84]	range-separated hybrid	none
ωB97X-V	[85]	range-separated hybrid	VV10[f,85]
ωB97M-V	[86]	range-separated hybrid	VV10[86]
M06-SX	[87]	range-separated hybrid	none
DM21	[88]	range-separated hybrid	D3(BJ)[68]
Global hybrid functionals			
B3LYP	[89, 90]	global hybrid GGA	none
B3LYP-D3(BJ)	[89, 90]	global hybrid GGA	D3(BJ)[68]
PBE0	[91, 92]	global hybrid GGA	none
PBE0-D3(BJ)	[91, 92]	global hybrid GGA	D3(BJ)[68]
M05-2X	[93]	global hybrid meta-GGA	none

M05-2X-D3(0)	[93]	global hybrid meta-GGA	D3(0)[71]
PW6B95-D3(BJ)	[94]	global hybrid meta-GGA	D3(BJ)[68]
M06-2X	[95]	global hybrid meta-GGA	none
M06-2X-D3(0)	[95]	global hybrid meta-GGA	D3(0)[71]
M06	[95]	global hybrid meta-GGA	none
M06-D3(0)	[95]	global hybrid meta-GGA	D3(0)[71]
M08-HX	[96]	global hybrid meta-GGA	none
MN15	[97]	global hybrid meta-NGA	none
MN15-D3(BJ)	[97]	global hybrid meta-NGA	D3(BJ)[68]
revM06	[98]	global hybrid meta-GGA	none
CF22D	[99]	global hybrid meta-NGA	D3(0)[100]
PpF	present	global hybrid meta-NGA	D3(0)[100]
Doubly hybrid functionals			
DSD-BLYP-D3(BJ)	[71, 101]	doubly hybrid functional	D3(BJ)[71]
B2GPPLYP-D3(BJ)	[66, 71]	doubly hybrid functional	D3(BJ)[71]
B2PLYP-D3(BJ)	[71, 102]	doubly hybrid functional	D3(BJ)[71]
MPW2PLYP-D3(BJ)	[103, 104]	doubly hybrid functional	D3(BJ)[103]
PWPB95-D3(BJ)	[50, 71]	doubly hybrid functional	D3(BJ)[71]

[a]GGA denotes generalized gradient approximations; NGA denotes nonseparable gradient approximation.

[b]D3(BJ) refers to D3 molecular mechanics dispersion term with empirical Becke-Johnson damping.

[c]D3(0) refers to the original D3 molecular mechanics dispersion term that is empirically damped to zero.

[d]D4 refers to an atomic-charge-dependent London dispersion correction with empirical damping.

[e]D2 refers to a pairwise-additive molecular mechanics dispersion correction with empirical damping.

[f]VV10 is a density-based nonlocal correlation term.

Supplementary Table S4. Interaction energies (kcal/mol) of the amino-acid pair training and test sets for 28 functionals and the reference method.

Dataset	System	DLPNO-CCSD(T)	PpF	ω B97X-V	PBE0-D3(BJ)	ω B97X-D	ω B97M-V	B3LYP-D3(BJ)
Training set	1	-21.78	-21.81	-22.03	-21.88	-21.91	-22.14	-22.06
	2	-9.75	-9.89	-9.84	-9.84	-9.83	-9.86	-9.82
	3	-9.75	-9.64	-9.73	-9.69	-9.64	-9.77	-9.65
	4	-11.79	-11.95	-11.87	-11.77	-12.27	-12.01	-11.87
	5	-15.93	-15.98	-16.04	-15.93	-16.01	-16.28	-16.08
	6	-71.71	-71.94	-71.81	-72.43	-71.89	-71.99	-72.49
	7	-105.93	-105.90	-105.68	-105.87	-105.62	-105.81	-105.86
	8	-9.35	-9.52	-9.31	-9.25	-9.32	-9.49	-9.21
	9	-14.39	-14.23	-14.11	-14.29	-14.28	-14.62	-14.49
	10	-0.61	-0.58	-0.47	-0.86	-0.77	-0.51	-0.76
	11	-26.21	-26.04	-26.03	-26.42	-26.40	-26.47	-26.87
	12	-14.51	-14.47	-14.43	-14.55	-15.04	-14.87	-14.77
Test set	1	-9.19	-9.29	-9.16	-9.31	-9.37	-9.28	-9.29
	2	-21.16	-21.21	-21.36	-21.04	-21.09	-21.59	-21.54
	3	-14.43	-14.43	-14.25	-14.52	-14.84	-14.63	-14.70
	4	-15.59	-15.58	-15.74	-15.75	-15.73	-15.83	-15.83
	5	-10.02	-10.00	-9.85	-10.16	-10.17	-10.10	-10.29

6	-10.86	-10.69	-10.42	-11.16	-11.27	-11.15	-11.16
7	-1.14	-1.16	-1.06	-1.22	-1.33	-0.98	-1.20
8	-7.04	-7.13	-7.08	-7.38	-7.27	-7.19	-7.37
9	-14.70	-14.59	-14.65	-14.96	-14.48	-14.86	-15.00
10	-15.15	-15.07	-15.07	-15.16	-15.10	-15.33	-15.34
11	-8.75	-8.70	-8.81	-9.30	-8.70	-8.82	-9.24
12	-6.24	-5.89	-5.93	-6.78	-6.21	-6.03	-6.61
13	-7.04	-7.00	-6.91	-7.20	-7.23	-7.03	-7.22
14	-10.11	-9.87	-9.84	-10.14	-9.96	-10.06	-10.17
15	-7.40	-7.45	-7.49	-7.17	-6.96	-7.52	-7.21
16	-12.95	-13.13	-13.02	-13.02	-13.12	-13.23	-13.00
17	-10.17	-10.08	-10.00	-10.21	-10.15	-10.15	-10.28
18	-8.80	-8.66	-8.59	-8.73	-8.53	-8.79	-8.74
19	-6.71	-6.61	-6.66	-7.37	-6.92	-6.79	-7.18
20	-20.32	-20.09	-20.21	-20.47	-20.19	-20.40	-20.74
21	-6.69	-6.72	-6.03	-6.56	-6.56	-6.65	-6.71
22	-11.82	-11.57	-11.60	-11.52	-12.12	-12.12	-11.92
23	-16.02	-16.02	-15.84	-16.36	-16.70	-16.27	-16.48
24	-9.71	-9.73	-9.64	-10.10	-9.63	-9.70	-10.04

Dataset	System	M06-2X-D3(0)	CF22D	PBE-D3(BJ)	M06-L-D3(0)	revM11	PW6B95-D3(BJ)	revM06
Training set	1	-21.92	-21.19	-21.05	-21.80	-21.18	-20.85	-20.90
	2	-9.84	-9.56	-9.44	-10.01	-9.12	-9.23	-9.04
	3	-9.60	-9.36	-9.48	-10.45	-8.50	-9.08	-8.49
	4	-11.98	-11.47	-11.40	-12.84	-11.11	-11.24	-10.91
	5	-16.34	-15.27	-15.21	-16.52	-15.75	-14.85	-15.31
	6	-72.09	-71.80	-73.15	-72.33	-71.22	-71.64	-71.19
	7	-106.08	-105.37	-105.17	-106.17	-104.92	-105.02	-105.06
	8	-9.66	-9.08	-9.02	-10.42	-8.74	-8.65	-8.58
	9	-14.75	-13.26	-13.42	-14.79	-13.26	-12.84	-12.81
	10	-0.36	-0.53	-1.15	-0.71	0.44	-0.56	0.37
	11	-26.64	-24.87	-26.00	-27.24	-25.75	-24.78	-25.31
	12	-15.11	-13.60	-13.80	-15.86	-14.05	-13.16	-13.48
Test set	1	-9.37	-8.87	-8.84	-9.58	-8.47	-8.54	-8.33
	2	-22.06	-20.60	-20.45	-21.69	-21.64	-20.38	-21.17
	3	-14.90	-13.52	-13.77	-15.46	-14.03	-13.33	-13.64
	4	-15.83	-15.04	-15.06	-15.89	-15.56	-14.79	-15.21
	5	-10.34	-9.47	-9.98	-10.68	-9.32	-9.21	-9.16
	6	-11.71	-9.41	-10.53	-12.55	-9.95	-9.10	-9.38
	7	-0.95	-1.15	-1.36	-1.17	-0.79	-1.20	-0.76
	8	-7.25	-6.84	-7.33	-7.76	-6.61	-6.54	-6.61

9	-14.85	-14.02	-14.52	-15.01	-13.66	-13.61	-13.74
10	-15.27	-14.32	-14.45	-15.51	-14.36	-13.93	-14.13
11	-8.68	-8.48	-9.09	-8.68	-8.16	-8.30	-7.92
12	-5.79	-5.66	-6.89	-6.35	-5.12	-5.58	-5.04
13	-7.11	-6.58	-7.05	-7.58	-6.37	-6.46	-6.32
14	-10.04	-9.35	-9.76	-10.40	-9.32	-9.14	-8.98
15	-7.58	-7.17	-7.03	-7.77	-7.48	-7.10	-7.23
16	-13.36	-12.55	-12.32	-13.97	-12.29	-12.07	-12.15
17	-10.23	-9.64	-9.99	-10.63	-9.23	-9.45	-9.16
18	-8.80	-8.20	-8.42	-8.94	-8.29	-8.03	-8.00
19	-7.02	-6.27	-7.08	-7.09	-6.38	-6.15	-6.10
20	-20.38	-19.41	-20.07	-20.25	-19.68	-19.38	-19.49
21	-7.49	-5.94	-6.21	-7.38	-6.26	-5.69	-5.90
22	-12.49	-10.75	-10.76	-13.17	-11.20	-10.63	-10.75
23	-16.40	-15.07	-15.63	-16.78	-15.16	-15.00	-14.94
24	-9.74	-9.35	-9.89	-9.65	-9.31	-9.22	-9.18

Dataset	System	TPSS-D3(BJ)	M11	M06-L	MN15-L	MN15	M06-2X	M06
Training set	1	-20.48	-20.87	-19.96	-20.79	-20.42	-20.22	-20.04
	2	-9.14	-8.70	-8.67	-9.14	-8.78	-8.60	-8.49
	3	-9.19	-7.78	-8.60	-9.52	-8.44	-7.90	-8.28
	4	-11.07	-9.87	-10.90	-12.46	-11.10	-10.20	-10.74
	5	-14.46	-15.41	-14.81	-15.31	-14.88	-14.78	-14.77
	6	-72.50	-71.19	-70.68	-69.86	-70.84	-71.27	-70.51
	7	-104.82	-104.96	-104.99	-104.12	-104.55	-104.99	-104.22
	8	-8.53	-8.22	-8.73	-9.83	-8.58	-8.11	-8.54
	9	-12.84	-13.52	-12.87	-11.75	-12.24	-13.00	-12.69
	10	-1.02	0.97	0.25	0.17	0.24	0.54	0.40
	11	-25.17	-26.14	-25.51	-24.13	-24.51	-25.08	-24.80
	12	-13.10	-13.91	-13.91	-13.63	-13.31	-13.34	-13.97
Test set	1	-8.57	-8.24	-8.23	-7.99	-8.06	-8.13	-8.03
	2	-19.67	-21.54	-20.18	-21.37	-20.67	-20.70	-19.72
	3	-13.21	-14.19	-13.93	-13.43	-13.40	-13.52	-13.69
	4	-14.50	-15.37	-14.52	-15.38	-15.00	-14.58	-14.43
	5	-9.59	-9.23	-9.39	-8.86	-8.91	-9.17	-9.01
	6	-9.69	-10.14	-10.78	-7.88	-8.95	-10.12	-9.85
	7	-1.24	-0.18	-0.52	-1.44	-0.98	-0.34	-0.26
	8	-6.81	-5.80	-6.59	-7.09	-6.38	-6.20	-6.18

9	-13.83	-13.17	-13.42	-13.13	-12.86	-13.41	-12.97
10	-13.88	-14.18	-13.89	-13.54	-13.57	-13.79	-13.72
11	-8.76	-7.88	-7.64	-6.50	-7.61	-7.71	-7.23
12	-6.42	-4.50	-5.33	-4.16	-4.92	-4.84	-2.78
13	-6.72	-6.14	-6.52	-6.44	-6.14	-6.13	-6.18
14	-9.28	-9.18	-9.02	-8.80	-8.86	-8.77	-8.97
15	-6.55	-6.78	-6.56	-8.34	-7.14	-6.48	-6.35
16	-11.95	-12.11	-12.37	-12.45	-11.96	-11.89	-12.10
17	-9.69	-9.07	-9.26	-9.11	-8.90	-8.99	-8.83
18	-7.92	-8.00	-7.69	-7.98	-7.87	-7.66	-7.58
19	-6.65	-6.11	-6.07	-5.01	-6.02	-6.08	-5.72
20	-19.48	-19.85	-18.91	-18.37	-18.76	-19.15	-18.46
21	-5.74	-6.42	-5.95	-6.38	-6.27	-6.21	-5.30
22	-10.42	-11.33	-11.29	-11.67	-10.80	-10.81	-10.92
23	-15.17	-15.33	-15.17	-14.46	-14.60	-14.94	-14.62
24	-9.55	-9.25	-8.94	-7.88	-8.73	-9.08	-8.64

Dataset	System	revM06-L	M06-SX	M08-HX	M05-2X	PBE0	PBE	B3LYP	TPSS
Training set	1	-20.45	-20.44	-20.40	-20.26	-17.13	-16.28	-15.49	-14.56
	2	-8.95	-8.75	-8.28	-8.62	-6.59	-6.19	-5.39	-5.12
	3	-8.48	-8.12	-6.95	-7.80	-5.21	-5.04	-3.64	-3.68
	4	-10.86	-10.50	-9.87	-9.82	-6.49	-6.11	-4.57	-4.48
	5	-14.79	-14.80	-14.92	-14.39	-10.83	-10.05	-8.83	-8.01
	6	-70.80	-70.98	-71.19	-71.37	-70.38	-71.09	-69.67	-69.96
	7	-104.87	-104.75	-104.91	-104.85	-102.44	-101.65	-100.87	-100.44
	8	-8.44	-8.20	-7.66	-7.71	-4.77	-4.52	-3.01	-2.93
	9	-11.85	-12.22	-12.97	-12.14	-8.60	-7.64	-6.36	-5.63
	10	0.24	0.39	0.83	0.63	1.03	0.73	1.69	1.26
	11	-24.39	-24.61	-25.34	-24.52	-20.49	-19.93	-18.20	-17.55
	12	-12.63	-12.85	-13.21	-12.35	-8.18	-7.33	-5.61	-4.98
Test set	1	-8.04	-8.00	-7.78	-7.93	-5.81	-5.32	-4.43	-4.20
	2	-20.60	-20.54	-20.78	-20.30	-15.86	-15.15	-13.97	-13.01
	3	-13.00	-13.08	-13.46	-12.70	-8.98	-8.12	-6.62	-6.10
	4	-14.83	-14.75	-14.67	-14.42	-11.29	-10.54	-9.46	-8.83
	5	-8.62	-8.74	-8.87	-8.76	-6.11	-5.86	-4.45	-4.43
	6	-8.12	-8.66	-9.56	-8.60	-4.40	-3.54	-1.05	-0.91
	7	-1.04	-0.72	-0.05	-0.37	0.47	0.34	1.13	0.86
	8	-6.85	-6.36	-5.49	-5.98	-3.76	-3.66	-2.23	-2.22

9	-13.53	-13.31	-12.70	-13.28	-10.46	-9.99	-8.68	-8.17
10	-13.71	-13.68	-13.72	-13.44	-10.40	-9.63	-8.58	-7.86
11	-7.64	-7.69	-7.27	-7.91	-6.80	-6.58	-5.79	-5.66
12	-5.11	-4.91	-4.41	-4.80	-4.07	-4.13	-2.78	-3.00
13	-6.35	-6.07	-5.84	-5.84	-3.88	-3.68	-2.47	-2.50
14	-8.58	-8.61	-8.79	-8.42	-6.09	-5.67	-4.42	-4.17
15	-7.42	-6.97	-6.47	-6.32	-3.95	-3.80	-2.73	-2.53
16	-11.86	-11.67	-11.33	-11.49	-8.26	-7.50	-6.23	-5.92
17	-8.84	-8.78	-8.50	-8.75	-6.44	-6.19	-5.00	-4.96
18	-7.62	-7.66	-7.82	-7.40	-5.11	-4.76	-3.61	-3.35
19	-5.64	-5.77	-5.57	-5.91	-4.08	-3.71	-2.32	-2.43
20	-18.91	-18.99	-19.42	-19.16	-16.44	-15.99	-14.99	-14.37
21	-4.81	-5.34	-6.14	-5.19	-0.37	0.26	2.77	2.39
22	-10.16	-10.04	-10.16	-9.44	-4.42	-3.55	-1.58	-1.29
23	-14.28	-14.41	-14.98	-14.21	-10.69	-9.84	-8.18	-7.88
24	-8.88	-8.99	-8.97	-9.16	-8.08	-7.83	-7.14	-6.99

Supplementary Table S5. MUEs (kcal/mol) of 28 functionals for the amino-acid pair training and test sets.

Dataset	System	PpF	ω B97X-V	PBE0-D3(BJ)	ω B97X-D	ω B97M-V	B3LYP-D3(BJ)	M06-2X-D3(0)
Training set	1	0.03	0.25	0.10	0.13	0.36	0.28	0.14
	2	0.14	0.09	0.09	0.08	0.11	0.07	0.09
	3	0.11	0.02	0.06	0.11	0.02	0.10	0.15
	4	0.16	0.08	0.02	0.48	0.22	0.08	0.19
	5	0.05	0.11	0.00	0.08	0.35	0.15	0.41
	6	0.23	0.10	0.72	0.18	0.28	0.78	0.38
	7	0.03	0.25	0.06	0.31	0.12	0.07	0.15
	8	0.17	0.04	0.10	0.03	0.14	0.14	0.31
	9	0.16	0.27	0.10	0.11	0.23	0.10	0.36
	10	0.03	0.14	0.25	0.16	0.10	0.15	0.25
	11	0.17	0.18	0.21	0.19	0.26	0.66	0.43
	12	0.04	0.08	0.04	0.53	0.35	0.26	0.60
	Mean	0.11	0.14	0.15	0.20	0.21	0.24	0.29
Test set	1	0.10	0.03	0.12	0.18	0.09	0.10	0.18
	2	0.05	0.20	0.12	0.07	0.43	0.38	0.90
	3	0.00	0.17	0.09	0.41	0.20	0.27	0.47
	4	0.01	0.15	0.16	0.14	0.25	0.24	0.24
	5	0.02	0.17	0.14	0.15	0.08	0.27	0.32

6	0.17	0.44	0.30	0.41	0.29	0.30	0.85
7	0.02	0.08	0.08	0.19	0.16	0.06	0.19
8	0.09	0.05	0.34	0.23	0.16	0.33	0.21
9	0.11	0.04	0.26	0.22	0.17	0.30	0.15
10	0.08	0.08	0.01	0.05	0.19	0.19	0.12
11	0.05	0.06	0.55	0.05	0.07	0.49	0.07
12	0.35	0.31	0.54	0.03	0.21	0.37	0.45
13	0.04	0.14	0.16	0.19	0.02	0.18	0.07
14	0.24	0.27	0.03	0.15	0.05	0.06	0.07
15	0.05	0.09	0.23	0.44	0.13	0.19	0.18
16	0.18	0.07	0.07	0.17	0.28	0.05	0.41
17	0.09	0.17	0.04	0.02	0.02	0.11	0.06
18	0.14	0.21	0.07	0.27	0.00	0.06	0.00
19	0.10	0.05	0.66	0.21	0.09	0.47	0.31
20	0.23	0.10	0.15	0.13	0.09	0.42	0.06
21	0.03	0.65	0.13	0.13	0.03	0.02	0.80
22	0.25	0.22	0.30	0.30	0.30	0.10	0.67
23	0.00	0.19	0.34	0.68	0.25	0.46	0.38
24	0.02	0.07	0.39	0.08	0.01	0.33	0.03
Mean	0.10	0.17	0.22	0.20	0.15	0.24	0.30

Dataset	System	CF22D	PBE-D3(BJ)	M06-L-D3(0)	revM11	PW6B95-D3(BJ)	revM06	TPSS-D3(BJ)
Training set	1	0.59	0.73	0.02	0.61	0.93	0.89	1.30
	2	0.19	0.31	0.26	0.63	0.52	0.72	0.61
	3	0.39	0.27	0.70	1.25	0.67	1.26	0.56
	4	0.32	0.39	1.05	0.68	0.55	0.88	0.72
	5	0.66	0.72	0.59	0.18	1.08	0.62	1.47
	6	0.09	1.44	0.62	0.49	0.07	0.52	0.79
	7	0.56	0.76	0.24	1.01	0.91	0.87	1.11
	8	0.27	0.33	1.07	0.61	0.70	0.78	0.82
	9	1.13	0.97	0.40	1.12	1.55	1.58	1.55
	10	0.08	0.54	0.10	1.05	0.05	0.98	0.41
	11	1.34	0.21	1.03	0.46	1.43	0.90	1.04
	12	0.91	0.71	1.35	0.46	1.35	1.03	1.41
	Mean	0.55	0.62	0.62	0.71	0.82	0.92	0.98
Test set	1	0.32	0.35	0.39	0.73	0.65	0.86	0.62
	2	0.56	0.71	0.53	0.48	0.78	0.01	1.49
	3	0.91	0.66	1.03	0.40	1.10	0.78	1.22
	4	0.55	0.53	0.30	0.03	0.80	0.38	1.09
	5	0.55	0.04	0.66	0.70	0.81	0.86	0.43
	6	1.45	0.33	1.69	0.92	1.76	1.48	1.17
	7	0.01	0.22	0.03	0.35	0.06	0.37	0.10

8	0.20	0.29	0.72	0.43	0.50	0.42	0.23
9	0.68	0.18	0.31	1.04	1.09	0.96	0.87
10	0.83	0.70	0.36	0.78	1.22	1.02	1.27
11	0.27	0.34	0.07	0.59	0.45	0.83	0.01
12	0.58	0.65	0.11	1.13	0.66	1.20	0.18
13	0.46	0.01	0.54	0.67	0.58	0.72	0.32
14	0.76	0.35	0.29	0.79	0.97	1.13	0.83
15	0.23	0.37	0.37	0.08	0.30	0.17	0.85
16	0.40	0.63	1.02	0.66	0.88	0.81	1.00
17	0.53	0.18	0.46	0.94	0.72	1.02	0.48
18	0.60	0.38	0.14	0.50	0.77	0.79	0.88
19	0.44	0.37	0.38	0.33	0.56	0.61	0.06
20	0.91	0.25	0.07	0.64	0.94	0.83	0.84
21	0.75	0.48	0.69	0.43	1.00	0.78	0.95
22	1.07	1.06	1.35	0.62	1.19	1.07	1.40
23	0.95	0.39	0.76	0.86	1.02	1.09	0.85
24	0.36	0.18	0.06	0.41	0.49	0.53	0.16
Mean	0.60	0.40	0.51	0.60	0.80	0.78	0.72

Dataset	System	M11	M06-L	MN15-L	MN15	M06-2X	M06	revM06-L
Training set	1	0.91	1.82	0.99	1.36	1.56	1.74	1.34
	2	1.05	1.08	0.61	0.97	1.15	1.26	0.81
	3	1.97	1.15	0.23	1.31	1.85	1.47	1.27
	4	1.92	0.89	0.67	0.69	1.59	1.05	0.93
	5	0.52	1.12	0.62	1.05	1.15	1.16	1.14
	6	0.52	1.03	1.85	0.87	0.44	1.20	0.91
	7	0.97	0.94	1.81	1.38	0.94	1.71	1.07
	8	1.13	0.62	0.48	0.77	1.24	0.81	0.91
	9	0.87	1.52	2.64	2.15	1.39	1.70	2.54
	10	1.58	0.86	0.78	0.85	1.15	1.01	0.85
	11	0.07	0.70	2.08	1.70	1.13	1.41	1.82
	12	0.60	0.60	0.88	1.20	1.17	0.54	1.89
	Mean	1.01	1.03	1.14	1.19	1.23	1.26	1.29
Test set	1	0.95	0.96	1.20	1.13	1.06	1.16	1.15
	2	0.38	0.98	0.21	0.49	0.46	1.44	0.56
	3	0.24	0.50	1.00	1.03	0.91	0.74	1.42
	4	0.22	1.07	0.21	0.59	1.01	1.16	0.76
	5	0.79	0.63	1.16	1.11	0.85	1.01	1.40
	6	0.72	0.08	2.98	1.91	0.74	1.01	2.74
	7	0.96	0.62	0.30	0.16	0.80	0.88	0.10

8	1.24	0.45	0.05	0.66	0.84	0.86	0.19
9	1.53	1.28	1.57	1.84	1.29	1.73	1.16
10	0.97	1.26	1.61	1.58	1.36	1.43	1.44
11	0.87	1.11	2.25	1.14	1.04	1.52	1.12
12	1.74	0.91	2.08	1.32	1.40	3.46	1.13
13	0.90	0.52	0.60	0.90	0.91	0.86	0.69
14	0.93	1.09	1.31	1.25	1.34	1.14	1.53
15	0.62	0.84	0.94	0.26	0.92	1.05	0.02
16	0.84	0.58	0.50	0.99	1.06	0.85	1.09
17	1.10	0.91	1.06	1.27	1.18	1.34	1.34
18	0.80	1.11	0.82	0.93	1.14	1.22	1.17
19	0.60	0.64	1.70	0.69	0.63	0.99	1.06
20	0.47	1.41	1.95	1.56	1.17	1.86	1.40
21	0.27	0.74	0.31	0.42	0.48	1.39	1.87
22	0.49	0.53	0.15	1.02	1.01	0.90	1.66
23	0.69	0.85	1.56	1.42	1.08	1.40	1.75
24	0.46	0.77	1.83	0.98	0.63	1.07	0.83
Mean	0.78	0.83	1.14	1.03	0.97	1.27	1.15

Dataset	System	M06-SX	M08-HX	M05-2X	PBE0	PBE	B3LYP	TPSS
Training set	1	1.34	1.38	1.52	4.65	5.50	6.29	7.22
	2	1.01	1.47	1.13	3.16	3.56	4.36	4.63
	3	1.63	2.80	1.95	4.54	4.71	6.11	6.07
	4	1.29	1.92	1.97	5.30	5.68	7.22	7.31
	5	1.12	1.01	1.54	5.10	5.88	7.10	7.92
	6	0.73	0.52	0.34	1.33	0.62	2.04	1.75
	7	1.19	1.02	1.08	3.49	4.28	5.06	5.49
	8	1.16	1.69	1.64	4.58	4.83	6.34	6.42
	9	2.17	1.42	2.25	5.79	6.75	8.03	8.76
	10	1.00	1.44	1.24	1.64	1.34	2.30	1.87
	11	1.60	0.87	1.69	5.72	6.28	8.01	8.66
	12	1.66	1.30	2.16	6.33	7.18	8.90	9.53
	Mean	1.32	1.40	1.54	4.30	4.72	5.98	6.30
Test set	1	1.20	1.41	1.26	3.38	3.87	4.76	4.99
	2	0.62	0.38	0.86	5.30	6.01	7.19	8.15
	3	1.35	0.97	1.73	5.45	6.31	7.81	8.33
	4	0.84	0.92	1.17	4.30	5.05	6.13	6.76
	5	1.28	1.15	1.26	3.91	4.16	5.57	5.59
	6	2.20	1.30	2.26	6.46	7.32	9.81	9.95
	7	0.42	1.09	0.77	1.61	1.48	2.27	2.00

	8	0.68	1.55	1.06	3.28	3.38	4.81	4.82
	9	1.39	2.00	1.42	4.24	4.71	6.02	6.53
	10	1.47	1.43	1.71	4.75	5.52	6.57	7.29
	11	1.06	1.48	0.84	1.95	2.17	2.96	3.09
	12	1.34	1.83	1.44	2.17	2.11	3.46	3.24
	13	0.97	1.20	1.20	3.16	3.36	4.57	4.54
	14	1.50	1.32	1.69	4.02	4.44	5.69	5.94
	15	0.43	0.93	1.08	3.45	3.60	4.67	4.87
	16	1.28	1.62	1.46	4.69	5.45	6.72	7.03
	17	1.39	1.67	1.42	3.73	3.98	5.17	5.21
	18	1.13	0.98	1.40	3.69	4.04	5.19	5.45
	19	0.94	1.14	0.80	2.63	3.00	4.39	4.28
	20	1.33	0.90	1.16	3.88	4.33	5.33	5.95
	21	1.34	0.55	1.50	6.32	6.95	9.46	9.08
	22	1.78	1.66	2.38	7.40	8.27	10.24	10.53
	23	1.62	1.04	1.81	5.33	6.18	7.84	8.14
	24	0.72	0.74	0.55	1.63	1.88	2.57	2.72
	Mean	1.18	1.22	1.34	4.03	4.48	5.80	6.02

Supplementary Table S6. Mean MUEs (kcal/mol) of 28 functionals for the amino-acid pair training and test sets.

Functionals	PpF	ωB97X-V	PBE0-D3(BJ)	ω B97X-D	ωB97M-V	B3LYP-D3(BJ)	M06-2X-D3(0)
Training set	0.11	0.14	0.15	0.20	0.21	0.24	0.29
Test set	0.10	0.17	0.22	0.20	0.15	0.24	0.30

Functionals	CF22D	PBE-D3(BJ)	M06-L-D3(0)	revM11	PW6B95-D3(BJ)	revM06	TPSS-D3(BJ)
Training set	0.55	0.62	0.62	0.71	0.82	0.92	0.98
Test set	0.60	0.40	0.51	0.60	0.80	0.78	0.72

Functionals	M11	M06-L	MN15-L	MN15	M06-2X	M06	revM06-L
Training set	1.01	1.03	1.14	1.19	1.23	1.26	1.29
Test set	0.78	0.83	1.14	1.03	0.97	1.27	1.15

Functionals	M06-SX	M08-HX	M05-2X	PBE0	PBE	B3LYP	TPSS	Mean MUE
Training set	1.32	1.40	1.54	4.30	4.72	5.98	6.30	1.44
Test set	1.18	1.22	1.34	4.03	4.48	5.80	6.02	1.32

Supplementary Table S7. Computational time (single-core CPU) for 22 functionals on the ALA-VAL residue pair system.

Rank	Functionals	Time [h]	Rank	Functionals	Time [h]
1	**PBE-D3(BJ)**	5.196	**12**	**M06-2X**	6.224
2	**PBE**	5.228	**13**	**PW6B95-D3(BJ)**	6.274
3	**TPSS**	5.337	**14**	**CF22D**	6.311
4	**TPSS-D3(BJ)**	5.347	**15**	**M05-2X**	6.321
5	**MN15-L**	5.574	**16**	**M08-HX**	6.364
6	**B3LYP**	5.702	**17**	**M06-2X-D3(0)**	6.390
7	**PBE0-D3(BJ)**	5.799	**18**	**MN15**	6.856
8	**PBE0**	5.838	**19**	**PpF**	6.939
9	**M06-L**	5.854	**20**	**M06**	7.088
10	**M06-L-D3(0)**	5.867	**21**	**ωB97X-D**	8.381
11	**B3LYP-D3(BJ)**	5.879	**22**	**M11**	10.128

Supplementary Table S8. Interaction energies (kcal/mol) of 260 amino-acid pair systems calculated with the PpF functional.

System name	Energy	System name	Energy	System name	Energy	System name	Energy
1_ARG_GLU	-64.09	66_LYS_ASP	-220.25	131_VAL_VAL	-13.87	196_ARG_ASP	-95.59
2_GLN_ARG	-21.39	67_TRP_LEU	-4.60	132_PHE_LYS	-116.07	197_ARG_GLN	-20.14
3_VAL_ASP	32.85	68_TRP_ASP	-83.56	133_VAL_ALA	-15.22	198_GLU_LYS	-129.05
4_THR_LEU	-18.12	69_TRP_VAL	-0.13	134_PHE_SER	-6.02	199_GLU_ARG	-61.57
5_ASN_ASN	-16.10	70_ALA_ILE	-39.75	135_THR_ASN	-21.64	200_ASP_ARG	-164.97
6_ASP_ARG	-57.51	71_TRP_MET	-20.26	136_PHE_ASN	-24.31	201_ILE_GLU	-35.68
7_ASP_LYS	-86.35	72_ALA_TYR	-8.49	137_THR_SER	-11.06	202_LEU_GLU	-31.43
8_ASP_GLY	-28.14	73_LEU_ARG	-26.53	138_THR_SER	-33.77	203_ARG_ASP	-118.88
9_VAL_LEU	-41.40	74_THR_LYS	-25.59	139_LYS_ASN	-21.01	204_PHE_ILE	-16.73
10_ASN_SER	-23.92	75_ARG_ARG	29.70	140_LYS_TYR	-13.54	205_ARG_GLU	-117.84
11_TYR_SER	1.36	76_ILE_LEU	-5.67	141_LYS_ARG	-55.17	206_SER_VAL	-16.42
12_TYR_SER	-6.58	77_ILE_GLU	-101.64	142_LYS_GLY	-5.75	207_THR_ALA	-10.05
13_ARG_TYR	-14.42	78_ILE_TYR	6.15	143_PHE_MET	-21.35	208_ARG_TRP	-7.25
14_PRO_TYR	-11.16	79_ALA_TYR	-7.40	144_PHE_GLN	-12.65	209_GLN_THR	-14.23

15_TYR_ARG	-16.87	80_GLY_GLY	-8.86	145_ASP_LEU	6.50	210_GLN_HIE	-8.22
16_ASP_SER	-38.07	81_ALA_THR	-6.03	146_ASP_HID	-22.12	211_THR_GLY	-7.05
17_LEU_LEU	-42.72	82_SER_HID	-16.44	147_ASP_ARG	-105.82	212_THR_ARG	-6.66
18_LEU_ILE	-12.05	83_LYS_VAL	-16.24	148_ASP_HIE	-21.97	213_TYR_ILE	-16.72
19_LEU_ILE	-12.96	84_THR_GLY	-11.18	149_LEU_ASN	-16.61	214_SER_VAL	-1.97
20_ILE_LEU	-44.24	85_THR_SER	-15.38	150_GLY_TRP	-16.39	215_TRP_GLY	-12.41
21_TYR_LEU	-8.63	86_ASP_ILE	-26.75	151_ASP_LYS	-122.40	216_PHE_TRP	-10.33
22_ARG_TYR	-26.88	87_GLN_SER	-22.29	152_ALA_SER	-6.56	217_GLU_ARG	-83.19
23_ILE_GLY	-37.45	88_ILE_TYR	-9.36	153_ALA_ASN	-6.98	218_PRO_TYR	-25.70
24_ILE_PHE	-17.17	89_GLN_THR	-9.46	154_ILE_ASP	-28.43	219_PRO_ALA	-17.10
25_GLU_SER	-24.92	90_ILE_LYS	-17.04	155_ASP_LYS	-76.70	220_ILE_ALA	-14.64
26_GLU_LYS	-75.12	91_LEU_GLU	-19.71	156_PRO_ARG	-27.03	221_GLY_PHE	-15.67
27_TYR_TYR	-6.83	92_LEU_VAL	-10.84	157_GLU_ASN	-27.64	222_GLN_ARG	-5.84
28_ASN_LYS	51.07	93_LEU_TYR	-8.85	158_VAL_THR	-9.74	223_GLN_HID	3.94
29_TYR_ALA	-31.59	94_LEU_THR	-11.36	159_VAL_VAL	-10.22	224_GLN_SER	-9.89
30_GLU_TYR	-27.65	95_LEU_MET	-13.87	160_VAL_VAL	-15.40	225_GLN_HIE	-17.94

31_SER_VAL	-14.55	96_ARG_MET	-23.99	161_ALA_VAL	-9.92	226_GLN_SER	-32.83
32_ILE_SER	-16.08	97_ALA_LEU	-9.51	162_THR_ALA	-9.11	227_ALA_SER	-20.32
33_GLN_ARG	-19.67	98_VAL_TRP	-15.04	163_GLN_THR	-1.05	228_TRP_MET	-12.30
34_PRO_PHE	-26.13	99_ALA_GLU	23.36	164_LYS_CYS	-21.51	229_SER_THR	-27.00
35_GLN_ASP	-27.60	100_ALA_TRP	-6.81	165_LYS_GLN	-27.01	230_GLY_ARG	-119.64
36_TYR_GLY	-9.88	101_ARG_GLN	1.00	166_LYS_ASP	-108.90	231_GLY_ASN	-31.29
37_VAL_GLY	-14.44	102_ARG_PHE	-8.43	167_LYS_GLN	-31.83	232_ASN_VAL	5.16
38_PRO_ARG	-27.34	103_LEU_ASN	-4.30	168_ARG_GLY	-13.73	233_ASN_ILE	-8.14
39_ILE_VAL	-9.71	104_LEU_PHE	-1.00	169_GLN_HID	-6.60	234_ASN_GLY	-8.19
40_ASN_THR	-10.02	105_LEU_ASN	-4.04	170_GLY_ARG	19.22	235_ASN_PRO	-17.44
41_ASN_GLY	-15.31	106_ILE_ASN	-10.69	171_GLN_MET	-6.82	236_VAL_TYR	-5.27
42_ARG_VAL	-12.00	107_ILE_PHE	-1.77	172_ASN_TRP	-13.48	237_VAL_TYR	-12.48
43_LYS_TYR	-18.27	108_ILE_GLN	-3.54	173_ASN_HIE	-7.44	238_VAL_SER	-34.70
44_ASP_ASN	-27.54	109_PHE_TYR	-2.07	174_ILE_MET	-15.49	239_VAL_GLY	-30.25
45_LYS_ASN	-14.39	110_PHE_ASN	-1.19	175_ILE_ARG	-16.07	240_VAL_ILE	-11.17
46_LEU_LYS	-31.80	111_PHE_GLU	-9.88	176_LYS_GLY	-5.57	241_VAL_VAL	-4.27

47_LEU_GLY	-33.06	112_PHE_TYR	-1.62	177_VAL_ALA	-12.78	242_ASN_GLN	-6.80
48_LEU_PHE	-14.28	113_ARG_GLN	-6.26	178_LYS_ASP	-125.30	243_ASN_ASP	-30.84
49_VAL_PHE	-10.70	114_ILE_PRO	-4.88	179_LEU_MET	-17.05	244_ARG_LEU	-5.16
50_GLU_ARG	-122.46	115_SER_TYR	-13.28	180_LEU_ILE	-14.94	245_SER_HID	8.48
51_GLU_TRP	-13.09	116_VAL_GLN	-14.91	181_ALA_ILE	-41.62	246_SER_ARG	-8.31
52_LEU_SER	-10.07	117_GLU_TRP	-4.94	182_ALA_GLY	-36.82	247_CYS_LEU	-37.66
53_LEU_SER	-22.79	118_PRO_THR	-1.84	183_ALA_ALA	-17.93	248_CYS_GLY	-35.87
54_LEU_LYS	-133.74	119_PRO_THR	-2.07	184_ALA_GLN	-6.84	249_CYS_ILE	-19.14
55_LEU_ASN	-28.34	120_PRO_PRO	-0.66	185_ILE_ILE	-18.45	250_VAL_VAL	1.01
56_LEU_TYR	-31.58	121_PRO_PHE	-5.12	186_PHE_ALA	-13.87	251_VAL_LEU	-3.02
57_LYS_TYR	-18.32	122_PRO_THR	-8.08	187_ARG_THR	-15.28	252_GLU_GLN	-15.20
58_TRP_LEU	0.20	123_TYR_HIE	-8.48	188_VAL_VAL	-11.92	253_GLY_ILE	-12.53
59_ALA_GLU	-92.70	124_TYR_LYS	-12.49	189_VAL_GLY	7.45	254_LEU_GLY	-17.79
60_SER_LEU	-9.10	125_TYR_THR	-6.45	190_LEU_HIE	-11.96	255_PRO_ASN	-10.29
61_ASN_TYR	-3.87	126_SER_ASN	-15.48	191_ALA_GLN	-32.00	256_VAL_TYR	-12.03
62_PRO_ASP	-97.99	127_ALA_SER	-7.96	192_GLN_ARG	-11.84	257_ARG_GLN	-16.18

63_SER_VAL	-25.41	128_VAL_ARG	-88.12	193_ASN_ASP	-83.86	258_ALA_TRP	-9.27
64_ALA_HID	-153.84	129_VAL_PHE	-9.36	194_LEU_VAL	-13.83	259_LEU_GLU	-43.67
65_ALA_GLU	-82.80	130_VAL_ILE	-9.11	195_VAL_VAL	-16.22	260_ARG_GLU	-164.61

Supplementary Table S9. MUEs (kcal/mol) of 23 functionals for the SCAI dataset.

Functionals	PpF	CF22D	PW6B95-D3(BJ)	MN15	M06-L-D3(0)	M06-SX
MUE	1.28	1.29	1.38	1.39	1.46	1.47

Functionals	revM06	M06	M06-2X-D3(0)	PBE0-D3(BJ)	revM11	B3LYP-D3(BJ)
MUE	1.48	1.49	1.50	1.52	1.61	1.63

Functionals	ωB97M-V	ω B97X-D	MN15-L	M06-2X	TPSS-D3(BJ)	M08-HX
MUE	1.65	1.77	1.84	1.84	1.90	1.97

Functionals	M05-2X	ωB97X-V	M06-L	M11	revM06-L	Mean MUE
MUE	1.99	2.45	2.52	2.70	3.49	1.81

Supplementary Table S10. MUEs (kcal/mol) of 24 functionals for the 4 datasets of JSCH database.

Dataset	CF22D	PpF	M06-2X	ω B97X-V	M06-L-D3(0)	M08-HX	M06
Hydrogen-bonded DNA	0.39	0.45	0.63	0.48	0.65	0.46	0.72
Interstrand	0.60	0.58	0.84	0.67	0.63	1.04	1.05
Stacked	0.47	0.53	0.67	0.98	0.54	0.80	0.86
Amino	2.03	2.56	1.73	1.70	2.88	2.48	1.76
JSCH	0.69	0.79	0.84	0.88	0.90	0.99	0.99

Dataset	M06-SX	revM06	M06-2X-D3(0)	ω B97M-V	revM11	MN15	ω B97X-D
Hydrogen-bonded DNA	1.40	1.22	0.41	0.58	0.46	0.81	1.04
Interstrand	0.88	0.85	0.63	0.68	0.77	0.72	0.70
Stacked	0.49	0.47	1.26	1.35	1.07	1.32	1.09
Amino	1.86	2.33	2.12	1.85	2.81	2.19	2.54
JSCH	1.00	1.00	1.01	1.06	1.08	1.17	1.18

Dataset	M11	PBE0-D3(BJ)	M06-L	revM06-L	M05-2X	B3LYP-D3(BJ)
Hydrogen-bonded DNA	0.56	1.76	1.14	2.31	0.85	1.69
Interstrand	1.11	0.73	1.00	0.83	0.94	0.68
Stacked	0.83	0.47	0.86	0.52	1.27	0.91
Amino	3.59	3.12	2.81	2.14	3.01	3.67
JSCH	1.19	1.22	1.22	1.27	1.32	1.43

Dataset	TPSS-D3(BJ)	MN15-L	PW6B95-D3(BJ)	B3LYP	Number	Mean MUE
Hydrogen-bonded DNA	1.24	3.97	0.43	2.84	38	1.10
Interstrand	0.78	0.92	0.62	2.31	32	0.86
Stacked	0.49	3.50	0.84	8.43	54	1.25
Amino	14.41	4.06	20.07	7.18	19	3.95
JSCH	2.61	3.12	3.26	5.43	143	1.49

Supplementary Table S11. MUEs (kcal/mol) of 28 functionals for the 35 datasets of MGCDB84_NC database.

Database	Dataset	ωB97M-V	ωB97X-V	PpF	CF22D	ω B97X-D	M06-L-D3(0)	M11-D3(BJ)
NCED	A24	0.07	0.05	0.13	0.13	0.13	0.26	0.24
	DS14	0.13	0.09	0.17	0.18	0.21	0.27	0.29
	HB15	0.17	0.22	0.33	0.38	0.35	0.39	0.36
	HSG	0.09	0.12	0.15	0.15	0.27	0.25	0.32
	NBC10	0.10	0.18	0.36	0.37	0.17	0.21	0.19
	S22	0.21	0.20	0.38	0.54	0.19	0.39	0.40
	X40	0.18	0.19	0.24	0.27	0.47	0.40	0.37
	A21x12	0.03	0.02	0.07	0.05	0.05	0.11	0.09
	BzDC215	0.14	0.15	0.19	0.16	0.22	0.19	0.33
	HW30	0.13	0.11	0.16	0.20	0.27	0.38	0.29
	NC15	0.04	0.04	0.08	0.06	0.13	0.20	0.16
	S66	0.12	0.09	0.19	0.29	0.30	0.34	0.33
	S66x8	0.07	0.12	0.15	0.20	0.21	0.29	0.27
	3B-69-DIM	0.12	0.14	0.33	0.31	0.26	0.35	0.36
	AlkBind12	0.12	0.10	0.16	0.17	0.86	0.54	0.53
	CO2Nitrogen1	0.07	0.09	0.46	0.49	0.80	0.84	0.29
	HB49	0.18	0.20	0.29	0.30	0.30	0.48	0.42
	Ionic43	0.51	0.61	0.63	0.50	0.79	0.78	1.09

	Mean	0.10	0.13	0.21	0.22	0.23	0.28	0.29
NCEC	H2O6Bind8	0.29	0.43	0.32	0.19	0.83	0.91	0.55
	HW6Cl	0.18	0.32	0.81	0.71	0.36	0.96	0.98
	HW6F	0.12	0.11	1.84	1.12	0.45	1.25	1.80
	FmH2O10	0.42	0.13	4.96	2.13	2.85	4.85	2.99
	Shields38	0.40	0.59	0.82	0.59	0.59	0.76	0.53
	SW49Bind345	0.22	0.25	0.16	0.22	0.61	0.39	0.50
	SW49Bind6	0.59	0.61	0.08	0.63	0.49	0.41	1.16
	WATER27	0.43	0.80	0.85	0.84	0.54	0.88	0.86
	3B-69-TRIM	0.27	0.31	0.67	0.88	0.65	0.79	0.76
	CE20	0.42	0.38	0.57	0.47	0.32	0.81	1.05
	H2O20Bind10	0.96	1.17	1.23	3.78	1.92	1.64	6.03
	H2O20Bind4	1.05	1.85	2.32	1.41	0.96	3.21	5.76
	Mean	0.38	0.47	0.84	0.85	0.73	0.98	1.17
NCD	TA13	1.67	1.75	2.02	1.63	2.03	2.73	1.14
	XB18	0.40	0.49	0.31	0.29	0.97	0.36	0.97
	Bauza30	0.45	0.66	0.69	0.44	1.14	1.39	0.72
	CT20	0.07	0.08	0.11	0.11	0.43	0.31	0.41
	XB51	0.46	0.53	0.42	0.34	0.84	0.63	1.00
	Mean	0.54	0.64	0.66	0.50	1.03	1.09	0.80
Overall mean		0.16	0.19	0.31	0.31	0.32	0.40	0.41

Database	Dataset（3	MN15-D3(BJ)	MN15	B3LYP-D3(BJ)	M06-2X-D3(0)	PW6B95-D3(BJ)	TPSS-D3(BJ)	M06-D3(0)
NCED	A24	0.20	0.19	0.12	0.16	0.09	0.11	0.16
	DS14	0.20	0.20	0.19	0.15	0.15	0.17	0.17
	HB15	0.49	0.50	0.60	0.28	0.27	0.57	0.32
	HSG	0.22	0.22	0.14	0.17	0.24	0.18	0.33
	NBC10	0.27	0.28	0.19	0.19	0.22	0.25	0.37
	S22	0.57	0.57	0.30	0.33	0.36	0.30	0.30
	X40	0.27	0.27	0.22	0.19	0.24	0.32	0.38
	A21x12	0.09	0.09	0.05	0.08	0.07	0.08	0.11
	BzDC215	0.42	0.42	0.14	0.27	0.27	0.22	0.23
	HW30	0.32	0.31	0.18	0.28	0.10	0.19	0.28
	NC15	0.09	0.09	0.07	0.11	0.10	0.13	0.19
	S66	0.53	0.52	0.25	0.25	0.27	0.27	0.49
	S66x8	0.35	0.35	0.18	0.20	0.22	0.24	0.37
	3B-69-DIM	0.31	0.33	0.22	0.22	0.23	0.29	0.29
	AlkBind12	1.07	1.03	0.14	0.36	0.26	0.30	1.38
	CO2Nitrog	0.30	0.32	0.06	0.12	0.36	0.54	0.62
	HB49	0.42	0.42	0.42	0.30	0.42	0.60	0.34
	Ionic43	0.56	0.56	0.64	0.79	0.81	0.63	0.48
	Mean	0.32	0.32	0.19	0.21	0.23	0.25	0.31
NCEC	H2O6Bind8	0.38	0.40	2.35	1.91	1.07	1.25	0.80

	HW6Cl	1.86	1.85	0.89	2.70	0.56	0.62	1.57
	HW6F	2.15	2.13	0.32	4.03	0.97	1.34	1.61
	FmH2O10	3.49	3.40	2.60	9.86	4.36	1.09	7.34
	Shields38	0.53	0.49	2.85	2.13	1.77	2.45	0.85
	SW49Bind	0.16	0.16	0.68	0.59	1.05	0.67	0.85
	SW49Bind	0.40	0.44	1.40	1.31	2.71	0.73	1.59
	WATER27	0.91	0.89	2.35	2.70	1.33	2.66	1.20
	3B-69-	0.88	0.80	0.59	0.49	0.60	0.70	0.70
	CE20	0.77	0.78	1.62	1.13	1.00	1.81	0.56
	H2O20Bind	6.41	6.71	8.84	7.51	11.61	0.87	3.42
	H2O20Bind	1.67	1.97	11.90	6.77	10.31	9.85	3.97
	Mean	1.08	1.07	1.93	2.05	1.89	1.45	1.33
NCD	TA13	1.57	1.57	2.73	1.07	1.99	3.84	1.80
	XB18	0.25	0.25	0.28	0.51	0.28	0.79	0.30
	Bauza30	0.63	0.62	1.30	0.94	1.55	2.65	1.59
	CT20	0.15	0.15	0.22	0.15	0.08	0.25	0.47
	XB51	0.42	0.43	0.70	0.50	0.41	1.40	0.44
	Mean	0.58	0.58	1.05	0.65	0.93	1.85	1.01
Overall mean		0.42	0.42	0.43	0.45	0.45	0.46	0.46

Database	Dataset	M06-2X	M08-HX	M05-2X-D3(0)	M06-L	M05-2X	PBE0-D3(BJ)	M11	M06
NCED	A24	0.20	0.16	0.20	0.33	0.21	0.20	0.33	0.34
	DS14	0.20	0.15	0.16	0.40	0.27	0.28	0.51	0.49
	HB15	0.28	0.39	0.43	0.47	0.35	0.89	0.46	0.54
	HSG	0.48	0.59	0.25	0.59	0.56	0.14	0.85	0.68
	NBC10	0.44	0.55	0.22	0.51	0.89	0.15	0.73	0.74
	S22	0.38	0.46	0.34	0.73	0.79	0.45	0.70	1.02
	X40	0.27	0.40	0.27	0.53	0.41	0.30	0.62	0.69
	A21x12	0.06	0.09	0.09	0.15	0.08	0.10	0.11	0.12
	BzDC215	0.22	0.35	0.34	0.27	0.25	0.28	0.21	0.36
	HW30	0.29	0.25	0.33	0.46	0.25	0.25	0.32	0.42
	NC15	0.11	0.12	0.08	0.21	0.09	0.12	0.18	0.22
	S66	0.26	0.31	0.24	0.55	0.57	0.29	0.54	0.69
	S66x8	0.30	0.43	0.25	0.44	0.45	0.27	0.47	0.59
	3B-69-DIM	0.43	0.61	0.21	0.61	0.48	0.29	0.74	0.81
	AlkBind12	0.25	0.22	0.24	0.31	0.93	0.10	0.41	0.39
	CO2Nitrogen1	0.29	0.50	0.16	1.13	0.58	0.28	0.84	1.39
	HB49	0.35	0.38	0.36	0.60	0.41	0.61	0.54	0.63
	Ionic43	0.83	1.01	1.18	0.73	1.31	0.94	1.21	0.58
	Mean	0.30	0.40	0.26	0.43	0.44	0.27	0.47	0.54
NCEC	H2O6Bind8	1.47	0.56	2.93	1.19	1.87	3.92	0.87	1.46

	HW6Cl	2.56	2.09	2.72	0.81	2.27	2.45	0.73	0.78
	HW6F	3.88	1.82	4.39	1.08	3.92	2.21	1.55	0.88
	FmH2O10	8.51	2.95	10.45	3.28	7.28	7.28	1.56	2.57
	Shields38	1.62	0.42	3.10	1.21	1.84	3.86	0.96	1.58
	SW49Bind345	0.47	0.52	0.42	0.35	0.05	0.77	0.76	0.32
	SW49Bind6	0.88	1.12	1.00	0.28	0.14	1.61	1.87	0.36
	WATER27	2.38	0.89	3.42	1.09	2.62	3.65	0.98	1.37
	3B-69-TRIM	1.12	1.68	0.56	1.47	1.31	0.71	1.94	2.13
	CE20	1.16	0.34	1.56	1.10	1.51	2.30	1.31	1.32
	H2O20Bind10	3.35	3.86	11.47	6.24	3.05	13.61	9.83	8.31
	H2O20Bind4	2.71	4.67	12.08	7.52	3.97	14.75	9.36	10.69
	Mean	1.76	1.28	2.60	1.47	1.75	2.90	1.84	1.87
NCD	TA13	1.06	1.04	1.64	2.72	1.60	2.45	1.13	1.77
	XB18	0.55	0.74	0.45	0.36	0.52	0.29	1.17	0.32
	Bauza30	0.93	0.89	1.51	1.38	1.49	2.43	0.88	1.52
	CT20	0.20	0.31	0.10	0.35	0.12	0.18	0.49	0.64
	XB51	0.56	0.66	0.43	0.65	0.53	0.71	1.28	0.51
	Mean	0.67	0.72	0.89	1.09	0.91	1.37	0.94	1.03
Overall mean		0.48	0.52	0.56	0.58	0.62	0.62	0.66	0.72

Database	Dataset	PBE-D3(BJ)	PBE0	PBE	MN15-L	TPSS	B3LYP	Number	Mean MUE
NCED	A24	0.31	0.46	0.39	0.42	0.82	0.97	24	0.26
	DS14	0.40	0.86	0.79	0.60	1.43	1.67	14	0.39
	HB15	0.80	0.48	0.67	2.15	1.10	1.15	15	0.55
	HSG	0.21	1.67	1.64	0.66	2.40	2.58	21	0.58
	NBC10	0.15	2.37	2.35	0.94	2.97	3.50	184	0.71
	S22	0.43	2.40	2.61	1.95	3.51	3.78	22	0.88
	X40	0.35	1.25	1.22	0.91	1.77	1.93	31	0.53
	A21x12	0.13	0.14	0.13	0.17	0.25	0.34	252	0.11
	BzDC215	0.22	0.81	0.89	0.61	1.25	1.61	215	0.39
	HW30	0.29	0.42	0.44	0.45	0.92	1.02	30	0.33
	NC15	0.21	0.11	0.14	0.06	0.18	0.27	15	0.13
	S66	0.30	2.07	2.17	1.85	3.08	3.26	66	0.73
	S66x8	0.28	1.50	1.56	1.14	2.17	2.39	528	0.55
	3B-69-DIM	0.30	1.32	1.38	0.89	1.93	2.01	207	0.56
	AlkBind12	0.11	3.37	3.36	3.18	4.67	4.96	12	1.05
	CO2Nitrogen16	0.39	2.42	2.57	0.64	3.40	3.36	16	0.83
	HB49	0.88	0.72	0.83	1.71	1.13	1.15	49	0.55
	Ionic43	0.95	1.24	1.08	2.11	1.60	1.96	43	0.93
	Mean	0.28	1.25	1.29	0.93	1.79	2.02	1744	0.50
NCEC	H2O6Bind8	4.14	0.89	0.76	9.90	3.70	3.75	8	1.75

	HW6Cl	2.99	0.83	0.78	4.52	3.85	4.81	6	1.66
	HW6F	0.77	1.04	2.04	5.45	4.80	4.24	6	2.05
	FmH2O10	6.20	3.62	6.20	17.56	16.30	16.10	10	5.73
	Shields38	5.86	0.67	1.30	9.45	3.21	4.09	38	1.95
	SW49Bind345	1.39	1.23	1.02	1.71	2.35	2.58	31	0.73
	SW49Bind6	2.79	3.12	2.45	5.01	6.09	6.53	18	1.64
	WATER27	5.15	1.58	2.16	7.79	2.87	3.22	23	2.01
	3B-69-TRIM	0.71	3.94	4.17	2.24	5.84	5.95	69	1.53
	CE20	3.86	1.06	1.45	5.38	2.17	2.64	20	1.39
	H2O20Bind10	14.32	9.60	11.56	46.41	31.28	29.51	10	9.45
	H2O20Bind4	24.57	6.18	3.21	39.83	18.57	22.30	4	8.69
	Mean	3.79	2.57	2.90	7.74	5.96	6.25	243	2.18
NCD	TA13	4.66	2.01	4.14	1.44	3.21	2.05	13	2.09
	XB18	1.06	0.61	0.66	0.58	0.71	1.25	8	0.56
	Bauza30	3.21	1.77	2.62	1.73	2.02	1.32	30	1.37
	CT20	0.31	0.37	0.36	0.31	0.58	0.65	20	0.28
	XB51	1.64	0.80	1.25	0.68	1.21	1.18	20	0.74
	Mean	2.25	1.18	1.87	1.04	1.58	1.24	91	1.02
Overall mean		0.78	1.40	1.51	1.73	2.27	2.48	2078	0.72

Supplementary Table S12. MUEs (kcal/mol) of 38 functionals for the 55 datasets of the GMTKN55 database.

Database	Dataset	DSD-BLYP-D3(BJ)	PWPB95-D3(BJ)	DM21	B2GPPLYP-D3(BJ)	B2PLYP-D3(BJ)
Small	W4-11	2.51	1.86	3.04	2.77	1.98
	G21EA	1.76	1.71	1.34	1.71	1.29
	G21IP	2.02	1.94	1.81	2.01	2.28
	DIPCS10	3.99	4.09	2.07	3.40	3.96
	PA26	1.02	1.90	1.74	1.13	1.30
	SIE4x4	5.88	10.02	4.92	6.69	10.08
	ALKBDE10	2.78	3.13	4.22	2.91	3.17
	YBDE18	0.95	1.91	2.84	0.93	2.12
	AL2X6	0.54	0.91	0.82	0.63	2.21
	HEAVYSB1	2.10	0.73	3.42	1.91	1.70
	NBPRC	0.88	0.85	1.64	0.93	1.36
	ALK8	2.71	4.23	3.42	2.60	1.07
	RC21	1.84	1.32	1.02	1.39	1.16
	G2RC	1.03	2.17	1.38	1.36	1.44

	BH76RC	0.81	1.14	1.22	0.96	1.13
	FH51	1.11	1.16	1.04	1.05	1.50
	TAUT15	0.46	0.62	0.45	0.54	0.72
	DC13	3.94	3.71	4.23	4.13	6.77
	Mean	1.98	2.07	2.24	2.08	2.16
Large	MB16-43	7.92	6.71	6.65	9.44	16.62
	DARC	2.38	1.72	1.04	2.58	5.03
	RSE43	0.59	0.97	1.45	0.41	0.57
	BSR36	1.49	2.42	0.51	2.08	2.42
	CDIE20	0.56	0.70	0.35	0.64	0.75
	ISO34	0.69	0.79	0.58	0.74	1.13
	ISOL24	2.38	2.09	1.56	2.66	3.83
	C60ISO	7.63	3.48	11.35	6.04	6.76
	PArel	0.53	0.68	0.84	0.55	0.74
	Mean	2.57	2.38	2.32	2.89	4.60
BH	BH76	1.22	1.76	2.08	1.38	2.59

	BHPERI	1.88	0.80	0.77	1.47	1.67
	BHDIV10	1.35	1.59	1.34	1.45	2.13
	INV24	0.80	0.78	0.90	0.79	0.69
	BHROT27	0.23	0.32	0.19	0.33	0.26
	PX13	1.58	1.25	0.90	1.68	2.74
	WCPT18	1.04	1.10	1.57	1.15	1.71
	Mean	1.13	1.21	1.33	1.18	1.81
Inter-NC	RG18	0.16	0.19	0.57	0.16	0.15
	ADIM6	0.37	0.18	0.11	0.44	0.25
	S22	0.17	0.41	0.20	0.14	0.15
	S66	0.17	0.26	0.18	0.23	0.18
	HEAVY28	0.19	0.17	0.17	0.20	0.17
	WATER27	0.94	3.59	1.96	1.87	2.03
	CARBHB12	0.42	0.22	0.51	0.51	0.56
	PNICO23	0.21	0.14	0.17	0.23	0.19
	HAL59	0.43	0.30	0.58	0.44	0.41

	AHB21	0.26	0.31	0.24	0.42	0.25
	CHB6	1.70	1.53	1.06	1.81	1.18
	IL16	0.56	1.25	0.49	0.53	0.61
	Mean	0.36	0.63	0.49	0.48	0.45
Intra-NC	IDISP	1.02	1.38	1.37	1.16	1.96
	ICONF	0.18	0.18	0.18	0.20	0.20
	ACONF	0.19	0.25	0.13	0.14	0.13
	AMINO20x4	0.13	0.23	0.19	0.13	0.15
	PCONF21	0.23	0.45	0.27	0.28	0.34
	MCONF	0.30	0.34	0.22	0.21	0.23
	SCONF	0.06	0.18	0.36	0.07	0.12
	UPU23	0.43	0.53	0.50	0.47	0.48
	BUT14DIOL	0.06	0.36	0.17	0.09	0.13
	Mean	0.19	0.33	0.25	0.19	0.23
Overall mean		1.29	1.38	1.40	1.41	1.79

Database	Dataset	MPW2PLYP-D3(BJ)	CF22D	PpF	ωB97M-V	M08-HX	PW6B95-D3(BJ)
Small	W4-11	2.66	1.85	2.36	3.73	3.12	2.50
	G21EA	1.48	1.24	3.44	2.91	1.82	1.27
	G21IP	2.34	2.77	3.40	3.41	3.37	2.77
	DIPCS10	3.49	5.73	7.62	5.25	3.37	2.74
	PA26	1.19	1.27	1.24	1.37	0.99	2.52
	SIE4x4	9.22	10.95	11.34	10.88	8.62	15.36
	ALKBDE10	3.23	3.30	4.07	5.43	3.86	3.96
	YBDE18	2.10	2.55	3.40	3.19	2.18	3.26
	AL2X6	2.66	1.23	0.87	1.30	2.21	0.61
	HEAVYSB1	2.44	2.34	1.17	1.73	3.09	1.38
	NBPRC	1.71	1.27	1.13	0.90	1.96	1.46
	ALK8	1.40	3.61	4.48	2.53	2.22	4.48
	RC21	1.05	1.56	1.94	2.14	1.50	2.83
	G2RC	1.59	2.08	2.71	1.94	3.29	3.08
	BH76RC	1.26	1.25	1.28	1.29	1.19	1.48

	FH51	1.18	1.11	1.53	1.04	1.24	1.67
	TAUT15	0.65	0.81	0.70	0.34	0.65	0.88
	DC13	6.42	4.21	5.15	5.40	7.41	6.90
	Mean	2.34	2.23	2.75	2.98	2.72	2.87
Large	MB16-43	22.08	10.99	9.16	14.82	16.19	8.97
	DARC	4.64	1.42	1.46	0.64	1.56	3.66
	RSE43	0.49	0.76	0.93	1.26	0.56	2.16
	BSR36	3.76	0.18	0.77	0.81	2.78	3.20
	CDIE20	0.70	0.55	0.68	0.60	0.64	1.14
	ISO34	1.08	0.61	0.88	0.62	0.94	1.28
	ISOL24	3.78	1.86	2.08	1.59	2.33	3.67
	C60ISO	4.65	3.95	5.90	11.47	7.46	1.65
	PArel	0.68	0.99	1.00	0.59	0.92	0.95
	Mean	5.63	2.73	2.67	3.77	4.23	3.43
BH	BH76	2.32	1.70	2.00	1.60	0.99	4.02
	BHPERI	0.85	1.12	1.00	1.13	1.61	1.06

	BHDIV10	1.73	1.15	1.07	1.28	1.04	2.62
	INV24	0.71	1.69	1.39	1.30	1.92	1.15
	BHROT27	0.32	0.24	0.48	0.22	0.42	0.56
	PX13	2.15	0.83	1.34	1.89	2.60	1.45
	WCPT18	1.45	1.16	0.97	1.38	1.55	1.39
	Mean	1.52	1.28	1.39	1.29	1.27	2.30
Inter-NC	RG18	0.27	0.14	0.19	0.08	0.43	0.22
	ADIM6	0.10	0.04	0.10	0.11	0.59	0.32
	S22	0.31	0.51	0.54	0.24	0.43	0.32
	S66	0.29	0.23	0.18	0.12	0.27	0.19
	HEAVY28	0.12	0.23	0.35	0.20	0.31	0.17
	WATER27	4.99	1.70	3.42	0.76	1.29	2.19
	CARBHB12	0.75	0.32	0.25	0.18	0.45	0.38
	PNICO23	0.22	0.37	0.41	0.26	0.53	0.25
	HAL59	0.34	0.37	0.43	0.28	0.52	0.34
	AHB21	0.63	0.24	0.69	0.22	0.53	0.37

	CHB6	1.55	0.57	0.49	0.93	2.51	1.51
	IL16	0.50	0.87	0.65	0.89	1.24	1.28
	Mean	0.77	0.45	0.64	0.30	0.58	0.52
Intra-NC	IDISP	2.78	1.70	2.69	1.71	2.98	2.90
	ICONF	0.25	0.28	0.26	0.17	0.51	0.23
	ACONF	0.08	0.04	0.21	0.13	0.37	0.13
	AMINO20x4	0.14	0.28	0.28	0.19	0.39	0.32
	PCONF21	0.39	0.28	0.57	0.60	0.86	0.51
	MCONF	0.10	0.19	0.43	0.38	0.54	0.37
	SCONF	0.12	0.16	0.62	0.15	0.32	0.19
	UPU23	0.50	0.44	0.42	0.50	0.80	0.58
	BUT14DIOL	0.15	0.21	0.15	0.05	0.20	0.34
	Mean	0.24	0.27	0.37	0.27	0.49	0.40
Overall mean		2.04	1.45	1.68	1.82	1.91	1.93

Database	Dataset	M06-2X	M06-2X-D3(0)	MN15	MN15-D3(BJ)	M11-D3(BJ)	M11	M05-2X
Small	W4-11	3.16	3.16	2.72	2.72	3.42	3.44	4.05
	G21EA	1.76	1.76	1.37	1.37	1.56	1.56	1.80
	G21IP	2.64	2.64	2.75	2.75	3.61	3.60	3.32
	DIPCS10	3.16	3.16	4.35	4.35	3.26	3.27	4.14
	PA26	1.24	1.23	1.64	1.64	1.23	1.22	1.13
	SIE4x4	8.65	8.67	11.30	11.30	9.59	9.56	8.66
	ALKBDE10	4.79	4.79	2.88	2.88	4.30	4.32	4.51
	YBDE18	2.48	2.40	3.38	3.37	1.56	1.76	0.99
	AL2X6	0.88	0.90	1.45	1.47	2.39	1.31	0.72
	HEAVYSB11	8.30	8.16	5.09	5.07	1.96	1.98	3.48
	NBPRC	0.96	0.95	1.78	1.78	2.76	3.03	1.63
	ALK8	2.27	2.31	3.72	3.72	3.74	3.41	2.17
	RC21	1.60	1.63	1.74	1.74	2.06	2.07	2.61
	G2RC	1.92	1.92	2.63	2.63	2.81	2.89	4.00
	BH76RC	1.18	1.18	1.57	1.57	1.44	1.44	1.37

	FH51	1.18	1.20	1.61	1.61	1.47	1.50	1.70
	TAUT15	0.77	0.78	1.19	1.19	1.09	1.09	1.18
	DC13	7.54	7.51	5.10	5.09	9.11	9.65	8.49
	Mean	2.73	2.72	2.75	2.75	2.96	2.99	3.16
Large	MB16-43	15.18	15.68	20.19	20.23	18.01	21.28	24.96
	DARC	2.33	2.16	1.71	1.70	2.60	3.22	1.30
	RSE43	0.63	0.63	1.35	1.35	1.41	1.42	0.83
	BSR36	2.96	2.48	0.57	0.57	1.05	1.87	2.04
	CDIE20	0.54	0.54	0.64	0.64	0.78	0.78	0.34
	ISO34	1.23	1.23	1.50	1.50	1.32	1.31	1.06
	ISOL24	2.92	2.74	2.64	2.63	3.40	3.36	2.73
	C60ISO	6.75	6.88	1.95	1.96	14.75	14.60	9.71
	PArel	0.97	0.97	1.34	1.34	0.77	0.78	1.02
	Mean	4.21	4.20	4.70	4.71	4.94	5.66	5.83
BH	BH76	2.33	2.34	1.50	1.50	1.28	1.26	1.64
	BHPERI	1.36	1.35	1.26	1.26	1.89	2.16	1.33

	BHDIV10	1.05	1.05	1.70	1.70	1.42	1.45	1.53
	INV24	1.29	1.28	2.68	2.68	2.49	2.55	1.60
	BHROT27	0.36	0.36	0.48	0.48	0.66	0.66	0.47
	PX13	5.35	5.32	2.03	2.03	3.47	3.46	7.47
	WCPT18	1.86	1.88	1.50	1.50	1.76	1.69	2.46
	Mean	1.89	1.89	1.52	1.52	1.62	1.65	1.89
Inter-NC	RG18	0.23	0.32	0.10	0.10	0.31	0.43	0.14
	ADIM6	0.44	0.27	1.27	1.32	0.58	0.32	0.92
	S22	0.39	0.34	0.56	0.56	0.41	0.65	0.79
	S66	0.26	0.22	0.43	0.44	0.28	0.46	0.57
	HEAVY28	0.35	0.33	0.33	0.34	0.27	0.61	0.35
	WATER27	2.83	3.70	1.22	1.23	1.34	1.85	3.54
	CARBHB12	0.23	0.25	0.24	0.24	0.22	0.36	0.26
	PNICO23	0.28	0.29	0.30	0.30	0.32	0.58	0.35
	HAL59	0.40	0.35	0.54	0.54	0.65	1.01	0.62
	AHB21	0.94	0.95	0.33	0.33	0.46	0.48	1.11

	CHB6	1.42	1.42	0.32	0.32	2.75	2.45	1.96
	IL16	0.62	0.47	1.03	1.02	1.53	1.93	1.45
	Mean	0.62	0.67	0.52	0.53	0.59	0.84	0.90
Intra-NC	IDISP	1.92	2.07	3.58	3.60	3.65	3.34	2.01
	ICONF	0.32	0.32	0.51	0.51	0.53	0.49	0.27
	ACONF	0.25	0.27	0.50	0.50	0.72	0.66	0.12
	AMINO20x4	0.30	0.30	0.52	0.52	0.51	0.49	0.29
	PCONF21	0.88	1.09	1.09	1.10	1.34	0.98	0.49
	MCONF	0.34	0.55	0.57	0.57	1.24	0.84	0.17
	SCONF	0.25	0.26	0.50	0.50	0.80	0.78	0.22
	UPU23	0.61	0.50	0.54	0.53	0.69	0.84	0.90
	BUT14DIOL	0.13	0.13	0.36	0.36	0.26	0.25	0.23
	Mean	0.36	0.40	0.59	0.59	0.74	0.64	0.34
Overall mean		1.97	1.99	2.04	2.04	2.20	2.36	2.43

Database	Dataset	M05-2X-D3(0)	ωB97X-D	ωB97X-V	M11plus	M06-D3(0)	PBE0-D3(BJ)	M06
Small	W4-11	4.04	2.35	2.78	3.51	3.15	3.70	3.15
	G21EA	1.80	1.57	1.84	1.98	2.18	2.62	2.18
	G21IP	3.32	2.95	2.96	3.62	3.09	3.68	3.09
	DIPCS10	4.14	5.42	4.10	4.21	6.51	2.99	6.50
	PA26	1.13	4.20	2.65	2.12	2.90	2.88	2.85
	SIE4x4	8.71	13.37	11.49	7.20	14.32	14.39	14.24
	ALKBDE10	4.51	3.86	4.07	2.93	3.44	5.66	3.44
	YBDE18	0.93	2.81	2.03	1.96	4.54	0.98	4.83
	AL2X6	0.77	3.08	1.21	0.52	2.46	1.48	3.07
	HEAVYSB11	3.20	2.17	1.39	0.78	1.78	1.37	1.83
	NBPRC	1.53	1.76	1.43	1.66	2.82	3.18	3.11
	ALK8	2.18	3.12	0.95	3.65	3.37	4.61	3.46
	RC21	2.71	2.95	3.53	2.00	1.69	5.50	1.64
	G2RC	4.02	3.71	3.92	4.50	3.79	6.75	3.81
	BH76RC	1.37	1.98	1.81	1.68	1.65	2.46	1.65

	FH51	1.76	1.85	2.30	2.35	1.85	2.77	1.84
	TAUT15	1.17	0.79	0.72	2.14	0.78	1.13	0.80
	DC13	8.40	5.48	6.52	6.36	6.51	8.01	6.65
	Mean	3.16	3.00	2.96	3.06	3.29	3.90	3.32
Large	MB16-43	26.32	31.11	32.51	32.60	32.43	15.86	34.42
	DARC	0.96	1.61	4.31	1.42	3.83	3.76	4.65
	RSE43	0.81	1.40	0.98	0.34	1.54	1.45	1.58
	BSR36	1.04	3.79	2.11	0.49	1.29	3.25	2.52
	CDIE20	0.34	0.57	0.63	0.78	1.03	1.24	1.04
	ISO34	1.05	0.90	1.17	1.27	1.43	1.42	1.40
	ISOL24	2.54	1.97	2.98	2.47	3.52	2.11	4.01
	C60ISO	9.78	8.50	13.74	13.12	2.10	2.35	2.11
	PArel	1.02	0.66	0.63	0.76	1.08	1.21	1.08
	Mean	5.88	7.14	7.56	7.02	7.22	4.46	7.86
BH	BH76	1.66	1.56	1.83	1.31	2.61	5.00	2.56
	BHPERI	1.47	2.16	2.07	2.50	1.90	3.27	2.24

	BHDIV10	1.51	1.22	0.85	1.84	1.94	4.81	1.94
	INV24	1.60	1.79	1.22	2.41	1.54	1.17	1.62
	BHROT27	0.46	0.39	0.31	0.29	0.67	0.58	0.69
	PX13	7.43	1.51	2.56	4.98	1.45	6.55	1.47
	WCPT18	2.52	1.23	1.71	2.45	2.01	4.33	1.95
	Mean	1.92	1.45	1.56	1.84	1.94	3.71	1.98
Inter-NC	RG18	0.16	0.29	0.10	0.14	0.32	0.11	0.36
	ADIM6	0.36	1.03	0.16	0.38	1.82	0.06	0.23
	S22	0.35	0.21	0.22	0.54	0.27	0.48	1.03
	S66	0.31	0.34	0.12	0.31	0.44	0.36	0.68
	HEAVY28	0.30	0.25	0.18	0.28	0.31	0.31	0.35
	WATER27	5.42	1.31	1.30	5.67	1.52	5.92	2.59
	CARBHB12	0.24	0.52	0.33	0.62	0.31	1.44	0.31
	PNICO23	0.40	0.28	0.19	0.45	0.25	0.94	0.23
	HAL59	0.46	0.56	0.30	0.41	0.47	0.61	0.57
	AHB21	1.14	0.30	0.34	1.04	0.31	1.24	0.32

	CHB6	1.95	0.50	0.87	1.69	1.28	1.37	1.26
	IL16	1.04	1.53	1.02	1.02	0.41	0.34	0.73
	Mean	0.92	0.53	0.36	0.95	0.52	1.05	0.74
Intra-NC	IDISP	1.37	2.63	2.59	1.83	4.08	1.54	3.76
	ICONF	0.27	0.46	0.26	0.44	0.36	0.28	0.35
	ACONF	0.07	0.23	0.03	0.22	0.52	0.06	0.35
	AMINO20x4	0.28	0.32	0.19	0.38	0.41	0.28	0.36
	PCONF21	0.36	0.50	0.30	0.82	1.19	0.90	0.41
	MCONF	0.51	0.31	0.24	0.16	0.71	0.27	0.33
	SCONF	0.27	0.31	0.15	0.33	0.32	0.27	0.31
	UPU23	0.48	0.72	0.59	0.78	0.83	0.54	0.53
	BUT14DIOL	0.19	0.17	0.04	0.12	0.25	0.22	0.18
	Mean	0.33	0.38	0.25	0.37	0.58	0.34	0.40
Overall mean		2.44	2.46	2.47	2.60	2.67	2.70	2.79

Database	Dataset	r2SCAN-3c	B3LYP-D3(BJ)	PBE0	MN15-L	r2SCAN	SCAN-	TPSS-D3(BJ)
Small	W4-11	3.79	3.40	3.62	3.41	3.85	4.02	5.91
	G21EA	4.83	1.91	2.62	2.40	5.12	3.64	2.20
	G21IP	4.65	3.55	3.68	3.46	4.66	4.69	3.95
	DIPCS10	5.08	4.73	2.99	10.46	5.09	4.93	3.69
	PA26	1.96	2.87	2.56	2.25	2.54	3.14	4.87
	SIE4x4	17.80	18.06	14.15	10.99	18.07	17.99	21.91
	ALKBDE10	5.13	4.39	5.83	4.48	5.12	19.21	4.16
	YBDE18	3.65	4.72	2.55	4.20	3.84	3.36	4.67
	AL2X6	1.58	2.71	2.76	1.35	0.96	1.95	2.24
	HEAVYSB11	3.47	3.30	3.58	6.47	3.93	6.79	2.57
	NBPRC	2.05	2.00	2.55	1.93	1.60	2.28	1.46
	ALK8	3.22	2.48	1.87	3.23	2.70	3.12	3.73
	RC21	5.36	2.44	4.22	2.00	4.64	6.53	4.44
	G2RC	5.70	2.73	6.21	6.73	5.50	6.29	7.11
	BH76RC	3.18	2.25	2.37	2.43	3.14	3.38	3.57

	FH51	2.74	2.61	2.47	2.55	2.49	2.69	4.30
	TAUT15	1.28	1.16	1.15	0.70	1.57	1.72	1.63
	DC13	9.32	10.57	8.87	7.83	8.60	7.30	8.91
	Mean	4.34	3.73	3.82	3.75	4.32	4.83	5.27
Large	MB16-43	14.75	24.84	17.55	20.42	13.25	16.56	25.88
	DARC	2.52	8.03	3.10	2.78	3.68	2.13	5.42
	RSE43	1.40	1.72	1.59	1.23	1.54	1.29	1.97
	BSR36	0.79	3.35	7.59	3.55	2.23	1.48	4.32
	CDIE20	1.35	1.00	1.38	1.78	1.64	1.48	1.67
	ISO34	1.50	1.78	1.64	1.88	1.37	1.30	2.31
	ISOL24	3.40	5.80	3.96	3.54	4.88	3.34	5.84
	C60ISO	4.85	2.22	2.16	5.94	5.39	6.05	8.40
	PArel	1.59	1.18	1.22	2.19	1.55	1.48	1.54
	Mean	4.09	6.74	5.60	5.68	4.30	4.48	7.36
BH	BH76	6.06	5.70	4.62	1.81	7.16	7.71	9.22
	BHPERI	4.18	1.18	1.30	1.78	3.87	5.17	5.51

	BHDIV10	5.38	3.22	4.27	2.08	5.98	6.51	6.90
	INV24	1.21	1.05	1.54	2.02	1.21	1.16	1.79
	BHROT27	0.85	0.41	0.59	0.87	0.76	0.82	0.53
	PX13	5.29	4.33	6.18	6.38	8.86	8.23	8.92
	WCPT18	3.94	2.27	3.72	1.81	5.94	6.12	6.34
	Mean	4.20	3.24	3.24	2.02	5.03	5.43	6.19
Inter-NC	RG18	0.19	0.13	0.34	0.17	0.23	0.24	0.13
	ADIM6	0.50	0.11	3.44	3.88	1.97	0.05	0.16
	S22	0.40	0.31	2.37	1.82	1.16	0.44	0.32
	S66	0.29	0.26	2.03	1.66	1.01	0.45	0.29
	HEAVY28	0.28	0.34	0.58	0.58	0.49	0.32	0.35
	WATER27	2.77	4.07	2.21	12.01	7.72	10.65	4.43
	CARBHB12	1.04	0.88	0.72	1.20	0.92	1.35	1.42
	PNICO23	0.71	0.48	0.65	0.40	0.66	0.98	1.11
	HAL59	0.73	0.57	1.09	0.59	0.99	0.99	0.99
	AHB21	1.11	0.33	0.94	2.29	2.48	1.61	0.67

	CHB6	0.42	1.41	1.08	0.64	0.42	0.44	0.94
	IL16	0.56	0.76	1.73	2.40	1.04	0.91	0.34
	Mean	0.74	0.75	1.42	2.19	1.60	1.61	0.94
Intra-NC	IDISP	3.27	3.57	9.51	7.55	6.03	2.45	3.22
	ICONF	1.39	0.29	0.40	0.53	0.33	0.31	0.19
	ACONF	0.33	0.05	0.63	0.69	0.41	0.15	0.09
	AMINO20x4	0.26	0.21	0.48	0.92	0.26	0.22	0.34
	PCONF21	0.66	0.53	3.06	4.10	1.02	0.49	1.08
	MCONF	0.39	0.22	1.65	1.61	0.63	0.47	0.42
	SCONF	0.42	0.30	0.28	0.92	0.39	0.60	1.05
	UPU23	0.46	0.61	1.90	1.68	0.97	0.44	0.49
	BUT14DIOL	0.39	0.31	0.23	1.10	0.16	0.41	0.28
	Mean	0.49	0.36	1.08	1.44	0.54	0.41	0.48
Overall mean		2.81	2.90	3.02	3.08	3.13	3.35	3.92

Database	Dataset	M06-L-D3(0)	M06-L	PBE-D3(BJ)	B3LYP	TPSS	PBE	Number	Mean
Small	W4-11	4.46	4.46	15.68	4.22	5.11	14.96	140	3.97
	G21EA	3.80	3.80	3.43	1.91	2.21	3.43	25	2.13
	G21IP	4.46	4.46	3.85	3.55	3.95	3.85	36	3.21
	DIPCS10	8.42	8.42	4.50	4.75	3.69	4.51	10	4.62
	PA26	5.11	5.09	2.19	2.28	4.38	1.97	26	2.23
	SIE4x4	17.96	17.94	23.72	17.63	21.56	23.44	16	12.80
	ALKBDE10	5.59	5.59	6.30	4.57	4.26	6.21	10	4.64
	YBDE18	4.82	4.90	4.93	8.47	7.29	5.91	18	3.20
	AL2X6	0.62	0.80	1.63	9.05	3.96	4.26	6	1.86
	HEAVYSB11	2.56	2.71	3.55	7.91	4.44	4.58	11	3.25
	NBPRC	3.97	4.04	2.41	5.19	2.78	2.82	12	2.05
	ALK8	3.70	3.76	4.14	6.07	1.61	2.78	8	3.11
	RC21	3.11	3.04	6.85	2.30	3.14	5.48	21	2.63
	G2RC	5.90	5.89	6.92	2.56	6.57	6.29	25	3.74
	BH76RC	2.92	2.92	4.18	2.38	3.63	4.09	30	1.93

	FH51	2.64	2.67	3.17	3.97	5.09	3.40	51	2.06
	TAUT15	1.44	1.45	1.84	1.13	1.61	1.81	15	1.04
	DC13	10.41	10.47	8.63	15.14	12.56	10.14	13	7.49
	Mean	4.71	4.72	8.26	4.66	5.26	8.07	473	3.51
Large	MB16-43	63.27	63.92	24.26	57.89	47.14	22.78	43	23.75
	DARC	8.07	8.30	3.31	15.75	11.39	6.94	14	3.80
	RSE43	2.67	2.68	2.94	1.96	2.17	3.10	43	1.37
	BSR36	5.09	5.64	3.17	10.70	10.21	7.67	36	3.03
	CDIE20	2.22	2.22	1.65	1.26	1.86	1.81	20	0.99
	ISO34	2.32	2.31	1.49	2.31	2.64	1.80	34	1.36
	ISOL24	6.52	6.71	4.39	9.53	8.87	6.83	24	3.70
	C60ISO	7.07	7.20	10.72	2.01	8.80	11.06	9	6.95
	PArel	1.62	1.63	1.81	1.17	1.54	1.81	20	1.09
	Mean	14.43	14.67	6.80	14.62	12.75	7.75	243	6.10
BH	BH76	3.93	3.92	9.62	4.94	8.63	9.15	76	3.31
	BHPERI	1.86	1.91	6.69	4.42	2.26	3.95	26	2.10

	BHDIV10	3.08	3.09	8.87	2.76	6.09	8.23	10	2.66
	INV24	1.46	1.47	2.07	1.87	2.72	2.67	24	1.61
	BHROT27	0.98	0.98	0.47	0.40	0.54	0.47	27	0.49
	PX13	0.94	0.92	12.02	3.54	8.35	11.54	13	4.02
	WCPT18	2.10	2.09	9.34	1.11	5.45	8.61	18	2.56
	Mean	2.52	2.52	7.12	3.30	5.47	6.51	194	2.49
Inter-NC	RG18	0.32	0.32	0.26	0.80	0.48	0.28	18	0.25
	ADIM6	0.94	0.17	0.21	5.06	4.70	3.38	6	0.94
	S22	0.44	0.81	0.48	3.78	3.44	2.55	22	0.75
	S66	0.35	0.59	0.40	3.24	2.99	2.11	66	0.61
	HEAVY28	0.53	0.56	0.42	1.30	0.86	0.47	28	0.37
	WATER27	1.11	1.95	8.92	5.79	4.65	2.83	27	3.41
	CARBHB12	0.44	0.46	1.91	0.62	0.63	1.09	12	0.58
	PNICO23	0.33	0.40	1.32	1.78	0.94	0.82	23	0.48
	HAL59	0.49	0.56	1.18	1.78	1.55	1.30	59	0.64
	AHB21	0.49	0.49	1.15	0.86	0.71	0.83	21	0.66

	CHB6	1.90	1.90	0.93	1.21	1.02	0.79	6	1.30
	IL16	0.75	0.62	0.59	4.02	2.92	1.49	16	1.10
	Mean	0.54	0.69	1.51	2.56	2.13	1.53	304	0.87
Intra-NC	IDISP	6.33	6.37	2.76	16.42	12.85	10.78	6	3.93
	ICONF	0.30	0.30	0.32	0.58	0.37	0.43	17	0.33
	ACONF	0.50	0.46	0.07	0.96	0.75	0.61	15	0.31
	AMINO20x4	0.35	0.35	0.34	0.66	0.53	0.51	80	0.35
	PCONF21	1.28	1.02	1.25	3.81	3.99	3.48	18	1.12
	MCONF	0.90	0.81	0.49	2.49	2.23	1.80	51	0.64
	SCONF	0.42	0.41	0.80	0.73	0.42	0.35	17	0.39
	UPU23	0.73	0.50	0.53	2.49	2.36	1.99	23	0.79
	BUT14DIOL	0.22	0.21	0.46	0.38	0.30	0.26	64	0.25
	Mean	0.64	0.58	0.53	1.60	1.39	1.18	291	0.53
Overall mean		4.37	4.43	5.02	5.08	5.11	5.16	1505	2.69

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