Supporting Information

Small basis set density-functional theory methods corrected with atom-centered potentials

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Section S1. Sample input file demonstrating the use of atom-centered potentials in Gaussian16 software

The 6-31G* basis set file (in .gbs extension) and the corresponding ACP files (in .acp extension) are provided separately in the supporting information ZIP file accompanying this document. An externally specified basis set file named **"631gs.gbs"** and the additional ACP file **"631gs.acp"** is defined and invoked by adding the keyword **"genECP"** to the route section of the Gaussian input file. Note that the ACP are not transferable and are proposed to be used with their underlying methods only.

```
%mem=4GB
%nprocs=8
# BLYP empiricaldispersion=gd3bj genECP

Title: Sample water dimer input using BLYP-D3/6-31G*-ACP method

0 1
O   -0.702196054   -0.056060256    0.009942262
H   -1.022193224    0.846775782   -0.011488714
H    0.257521062    0.042121496    0.005218999
O    2.220871067    0.026716792    0.000620476
H    2.597492682   -0.411663274    0.766744858
H    2.593135384   -0.449496183   -0.744782026

@631gs.gbs/N

@631gs.acp/N
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Section S2. Formulas for all the statistical error measures

a) Mean absolute error (MAE)

$$MAE = \frac{1}{n}\sum_{i=1}^{n} x_i$$

where, $x_i = \left|x_{calc,i} - x_{ref,i}\right|$

b) Mean signed error (MSE)

$$MSE = \frac{1}{n}\sum_{i=1}^{n} x_i$$

where, $x_i = x_{calc,i} - x_{ref,i}$

c) Maximum absolute error (MAXE)

$$MAXE = \max_i \left| x_{calc,i} - x_{ref,i} \right|$$

d) Root-mean-square error (RMSE)

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n} x_i^2}$$

where, $x_i = x_{calc,i} - x_{ref,i}$

e) Standard deviation (SD)

$$SD = \sigma = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n} (x_i - \overline{x})^2}$$

where, $x_i = x_{calc,i} - x_{ref,i}$

$$\overline{x} = \frac{1}{n}(x_{calc,i} - x_{ref,i})$$

Table S1. Detailed list of data sets in the ACP training set.

Data set(s)	Data points	Data set description	Reference energy level	Reference # in article
Non-covalent interaction energies:				
HBC6	118	Interaction energies of doubly hydrogen-bonded dimer complexes at various intermolecular distances	CCSD(T)/CBS	77, 78
MiriyalaHB104	104	Interaction energies of hydrogen-bonded dimer complexes	CCSD(T)/CBS	79, 80
IonicHB	96	Interaction energies of charged (both positive and negative) hydrogen-bonded dimer complexes at various intermolecular distances	CCSD(T)/CBS	81
HB375x10	3749	Interaction energies of neutral hydrogen-bonded dimer complexes at various intermolecular distances	CCSD(T)/CBS	82
IHB100x10	350	Interaction energies of charged (both positive and negative) hydrogen-bonded dimer complexes at various intermolecular distances	CCSD(T)/CBS	82
HB300SPXx10	1980	Interaction energies of neutral hydrogen-bonded dimer complexes in an extended	CCSD(T)/CBS	83

		chemical space (excluding iodine and bromine containing systems) at various intermolecular distances.		
CARBHB12	12	Interaction energies of dimer complexes between singlet carbene analogues and H_2O, NH_3, HCl	W2-F12	14
S22x5	110	Interaction energies of small non-covalently bound dimer complexes at various intermolecular distances	CCSD(T)/CBS	78,84,85
S66x8	528	Interaction energies of small non-covalently bound dimer complexes at various intermolecular distances	CCSD(T)/CBS	86–88
S66a8	528	Interaction energies of small non-covalently bound dimer complexes at various intermolecular angular displacements	CCSD(T)/CBS	87
A21x12	228	Interaction energies of small non-covalently bound dimer complexes (excluding argon containing systems) at various intermolecular distances	CCSD(T)/CBS	89–91
NBC10ext	195	Interaction energies of non-covalently interacting dimer complexes at various intermolecular distances	CCSD(T)/CBS	78,92–95
3B-69-DIM	207	Interaction energies of all relevant pairs of monomers from 3B-69-TRIM	CCSD(T)/CBS	96
3B-69-TRIM	69	Interaction energies of trimer complexes of small organic molecules	CCSD(T)/CBS	96
HW30	30	Interaction energies of dimer complexes of hydrocarbons and water	CCSD(T)/CBS	97
B-set	160	Interaction energies of dimer complexes containing boron at various intermolecular distances	DLPNO-CCSD(T)/CBS	58, 64
F-set	160	Interaction energies of dimer complexes containing fluorine at various intermolecular distances	DLPNO-CCSD(T)/CBS	58, 64
Si-set	152	Interaction energies of dimer complexes containing silicon at various intermolecular distances	DLPNO-CCSD(T)/CBS	58, 64
P-set	120	Interaction energies of dimer complexes containing phosphorus at various intermolecular distances	DLPNO-CCSD(T)/CBS	58, 64
S-set	144	Interaction energies of dimer complexes containing sulfur at various intermolecular distances	DLPNO-CCSD(T)/CBS	58, 64
Cl-set	160	Interaction energies of dimer complexes containing chlorine at various intermolecular distances	DLPNO-CCSD(T)/CBS	58, 64
Sulfurx8	104	Interaction energies of dimer complexes containing divalent sulfur at various intermolecular distances	CCSD(T)/CBS	98
Pisub	105	Interaction energies of non-covalently bound substituted aromatic dimer complexes	DLPNO-CCSD(T)/CBS	58, 99, 100
Pi29n	29	Interaction energies of neutral π-conjugated dimer complexes	CCSD(T)/CBS	101

		representing organic electronic precursors		
BzDC215	170	Interaction energies of dimer complexes (excluding neon and argon containing systems) of benzene with small molecules	CCSD(T)/CBS	102
C2H4NT	75	Interaction energies of dimer complexes of ethene and coronene	CCSD(T)/CBS	95
Hill18	18	Interaction energies of hydrogen-bonded and halogen-bonded dimer complexes	CCSD(T)/CBS	103
X40x10	220	Interaction energies of dimer complexes (excluding iodine and bromine containing systems) representing halogen-bonding at various intermolecular distances	CCSD(T)/CBS	104
PNICO23	23	Interaction energies of dimer complexes representing pnictogen-bonding	W1-F12, W2-F12	14, 105
ADIM6	6	Interaction energies of six alkane dimer complexes ranging from ethane to n-heptane	W1-F12	14, 25, 106
HC12	12	Interaction energies of saturated and unsaturated hydrocarbon dimer complexes	CCSD(T)/CBS	107
BBI	100	Interaction energies of peptide backbone-backbone dimer complexes	DW-CCSD(T)-F12/aug-cc-pV(D+d)z	108
SSI	2805	Interaction energies of peptide sidechain-sidechain dimer complexes	DW-CCSD(T)-F12/aug-cc-pV(D+d)z	108
NucTAA	454	Interaction energies of dimer complexes of amino acid and nucleotide	DLPNO-CCSD(T)/CBS	58, 109–112
CarbhydBz	34	Interaction energies of carbohydrate-benzene dimer complexes	CCSD(T)/CBS	113
CarbhydNaph	46	Interaction energies of carbohydrate-naphthalene dimer complexes	CCSD(T)/CBS	114
CarbhydAroAA	48	Interaction energies of dimer complexes representing carbohydrate and aromatic amino acids	DLPNO-CCSD(T)/CBS	58, 115
CarbhydAro	161	Interaction energies of dimer complexes representing carbohydrate and substituted aromatic molecule	DLPNO-CCSD(T)/CBS	58, 116
WatAA	259	Interaction energies of dimer complexes representing interactions between water and amino acids	DLPNO-CCSD(T)/CBS	58, 117
HSG	17	Interaction energies of dimer complexes representing protein-ligand interactions	CCSD(T)/CBS	78, 118
PLF547	392	Interaction energies of dimer complexes representing protein-ligand interactions	DLPNO-CCSD(T)/CBS	119
JSCH	124	Interaction energies of dimer complexes of nucleotide base pairs	CCSD(T)/CBS	84
DNAstack	40	Interaction energies of stacked DNA base-pair steps	CBS(T)-F12-CP	120
DNA2body	10	Interaction energies of nucleobase pairs	CBS(T)-F12-CP	120
ACHC	54	Interaction energies of nucleobase stacking configurations	DW-CCSD(T**)-F12/aug-cc-pVDZ	121
BDNA	71	Interaction energies of nucleobase stacking configurations	CCSD(T)/CBS	122

NucBTrimer	141	Interaction energies of complexes of nucleobase trimers	DLPNO-CCSD(T)/CBS	58, 123
Water38	38	Interaction energies of water clusters $(H_2O)_n$ (where n = 2-10)	CCSD(T)/CBS	124
Water1888	1888	Interaction energies of various water dimer configurations with reference data lying between -5 to +5 kcal/mol	CCSD(T)/CBS	95,125–127
Water-2body	410	Interaction energies of various water dimer configurations	CCSD(T)/CBS	54, 58
CH4PAH	382	Interaction energies of dimer complexes of methane and polycyclic aromatic hydrocarbons	CCSD(T)/CBS	128, 129
CO2MOF	20	Interaction energies of dimer complexes of carbon dioxide and organic building units of metal-organic frameworks	inc-CCSD(T)|MP2+F12+INT/cc-pVDZ-F12	130
CO2PAH	249	Interaction energies of dimer complexes of carbon dioxide and polycyclic aromatic hydrocarbons	CCSD(T**)-F12avg/CBS	131
CO2NPHAC	96	Interaction energies of dimer complexes of carbon dioxide and nitrogen-doped poly-heterocyclic aromatic compounds	CCSD(T)/CBS	132
BzGas	129	Interaction energies of nine benzene-gas dimer complexes at various intermolecular distances (where gas = CO_2, CH_4, N_2)	CCSD(T)/CBS	133
SSI-anionic, WatAA-anionic, HSG-anionic, PLF547-anionic, IonicHB-anionic, IHB100x10-anionic	575, 64, 4, 155, 24, 650	Interaction energies of only anion-neutral and anion-cation dimer complexes from earlier described datasets	Various	58, 78, 81, 82, 108, 117–119
Ionic43-anionic	37	Interaction energies of anion-neutral and anion-cation dimer complexes (excluding sodium, potassium, and lithium containing complexes)	CCSD(T)/CBS	134
Molecular conformational energies:				
37Conf8	258	Relative energies of conformers of organic molecule isomers	DLPNO-CCSD(T)/cc-pVTZ	135
DCONF	2142	Relative energies of conformers of 62 model systems representing drug-like molecules at various intramolecular torsion angles	CCSD(T)/CBS	136
ICONF	17	Relative energies of conformers of 10 molecules containing H, N, O, Si, P, and S	W1-F12	14
MCONF	51	Relative energies of conformers of melatonin	CCSD(T)/CBS	137
Torsion21	189	Relative energies of conformers of Glyoxal, Oxalyl halides, and their thiocarbonyl derivatives (excluding bromine containing systems) at various intramolecular torsion angles	CCSD(T)/CBS	138
MolCONF	5623	Relative energies of conformers of molecules taken from crystal structure database and protein-ligand database (only containing our 10 target elements)	DLPNO-CCSD(T)/cc-pVTZ	139

PEPCONF-Dipeptide	875	Relative energies of conformers of various model dipeptide systems	DLPNO-CCSD(T)/CBS	58, 140
TPCONF	8	Relative energies of conformers of two model tetrapeptides	CCSD(T)/CBS	141
P76	71	Relative energies of conformers of five isolated small peptides containing aromatic side chains	CCSD(T)/CBS	142
YMPJ	495	Relative energies of conformers of proteinogenic amino acid monomers	MP2-F12/cc-pVTZ-F12+[CCSD(Ts)-F12b – MP2-F12]/cc-pVDZ-F12	143
SPS	17	Relative energies of conformers of DNA sugar-phosphate-sugar backbone	CCSD(T)/CBS	144
rSPS	45	Relative energies of conformers of RNA sugar-phosphate-sugar backbone	CCSD(T)/CBS	145
UpU46	45	Relative energies of conformers of model RNA backbone	DLPNO-CCSD(T)/CBS*	146
SCONF	17	Relative energies of conformers of two model carbohydrates	CCSD(T)/CBS	14, 147
DSCONF	27	Relative energies of conformers of three disaccharides	CCSD(T)/CBS	148
SacchCONF	56	Relative energies of conformers of monosaccharides	CCSD(T)/CBS	149
CCONF	426	Relative energies of conformers of glucose and α-maltose isomers	DLPNO-CCSD(T)/CBS	150
ACONF	15	Relative energies of conformers of n-alkane chains	W1h-val	151
BCONF	64	Relative energies of conformers of butane-1,4-diol	CCSD(T)-F12b/cc-pVTZ-F12	152
PentCONF	342	Relative energies of conformers of n-pentane	CCSD(T)-F12/CBS	153
Undecamer125	124	Relative energies of conformers of $(H_2O)_{11}$	CCSD(T)/CBS	154
PEPCONF-Dipeptide-anionic, MolCONF-anionic	175, 79	Relative energies of conformers of systems containing only negative charge from earlier described datasets	Various	58, 139, 140
Reaction energies:				
MN-RE	7555	Automatically generated reactions using molecules from Minnesota Database2015B[156]	Various	155
BH9-RE	449	From BH9 set comprising chemical reactions belonging to nine types common in organic chemistry and biochemistry	DLPNO-CCSD(T)/CBS	74
DIE60	60	Double-bond migration reactions in conjugated dienes	W*n*-F12	157
FH51	51	Reactions involving various organic and inorganic molecules	CCSD(T)-F12/CBS	158, 159
BSR36	36	Hydrocarbon bond separation reactions	CCSD(T)/CBS	160, 161
BH76RC	30	Hydrogen and non-hydrogen atom transfer reactions of small molecules	W*n*	162–164
G2RC	23	Reactions whose reactants and products had been taken from the G2/97 set	W2-F12	141, 164, 165
RC21	21	Organic radical fragmentation and rearrangement reactions	W1-F12	14

CR20	20	Cyclo-reversion reactions	W1-F12	166
PlatonicHD6	6	Homodesmotic reactions involving platonic hydrocarbon cages, C_nH_n (where n = 4,6,8,10,12,20)	W*n*-F12	167
PlatonicID6	6	Isodesmic reactions involving platonic hydrocarbon cages, C_nH_n (where n = 4,6,8,10,12,20)	W*n*-F12	167
PlatonicIG6	6	Isogyric reactions involving platonic hydrocarbon cages, C_nH_n (where n = 4,6,8,10,12,20)	W*n*-F12	167
AlkIsod14	14	Isodesmic reactions involving C_nH_{2n+2} alkanes (where n=3-8)	W*n*	168
DARC	14	Diels-Alder reactions	W1-F12	14, 164, 169
DC13	12	Reactions that were known to be difficult for DFT methods	Various	14,63,178,179,170–177
WCPT6	6	Tautomeric water-catalyzed proton transfer reactions	W*n*	180
NBPRC	6	Reactions involving NH_3/BH_3 and PH_3/BH_3	CCSD(T)/CBS	161, 164, 181
Barrier height energies:				
Grambow2020-B97D3	32722	Reactions involving H, C, N, and O generated using automated potential energy surface exploration	DLPNO-CCSD(T)/CBS	182, This work
Grambow2020-ωB97XD3	23922	Reactions involving H, C, N, and O generated using automated potential energy surface exploration	DLPNO-CCSD(T)/CBS	182, This work
BH9	898	Chemical reactions belonging to nine types common in organic chemistry and biochemistry	DLPNO-CCSD(T)/CBS	74
E2SN2	418	Competing E2 and S_N2 reactions	DLPNO-CCSD(T)/CBS	183, This work
HTBH38	38	Hydrogen atom transfer reactions of small molecules	W1 and theoretical estimate	163
NHTBH38	38	Non-hydrogen atom transfer reactions of small molecules	W1 and theoretical estimate	162
WCPT27	27	Water-catalyzed proton-transfer reactions	W*n*	180
BHROT27	27	Rotation around single bonds	W*n*-F12	14
BHPERI26	26	Pericyclic reactions	W*n*-F12	164, 184
DBH24	24	Diverse reactions involving small molecules	W1 and theoretical estimate	185, 186
INV24	24	Inversion and racemization reactions	W*n*-F12 and DLPNO-CCSD(T)/CBS	187
CRBH20	20	Cyclo-reversion reactions of heterocyclic rings	W*n*	188
PX13	13	Proton exchange reactions in small clusters of H_2O, NH_3, and HF	W1-F12	189, 190
Bond separation energies:				
BSE49	4502	Breaking of 49 unique X-Y type single bonds (except H-H, H-F, and H-Cl) into corresponding radical fragments, where X and Y are H, B, C, N, O, F, Si, P, S, Cl	(RO)CBS-QB3	76
Molecular deformation energies:				

MOLdef	9298	Molecular deformation energies relative to the equilibrium geometry of systems containing our 10 target elements	DLPNO-CCSD(T)/CBS	43, 58
MOLdef-H2O	990	Molecular deformation energies relative to the equilibrium geometry of water containing systems	CCSD(T)/CBS	58, 191, 192
MOLdef-TS	6294	Molecular deformation energies relative to the transition structure of BH9 data set. Molecules were deformed along the imaginary normal mode only.	DLPNO-CCSD(T)/CBS	74, This work
Isomerization energies:				
ISO34	34	Relative energies of isomers of small and medium-sized organic molecules	W1-F12	14, 193
ISOL24	24	Relative energies of isomers of large organic molecules	DLPNO-CCSD(T)/CBS	14, 194
IDISP	6	Relative energies of isomers of hydrocarbon molecules	DLPNO-CCSD(T)/CBS	14, 161, 164, 193, 195, 196
EIE22	22	Relative energies of isomers of enecarbonyls	W1-F12	197
PArel	20	Relative energies of protonated isomers	CCSD(T)/CBS	14
AlkIsomer11	11	Relative energies of isomers of C_nH_{2n+2} where n=4–8	W*n*	168
PAH6	6	Relative energies of polycyclic aromatic hydrocarbon isomers	CCSD(T)/CBS	198
Styrene45	44	Relative energies of isomers of C_8H_8	W1-F12	170
TAUT15	15	Relative energies in tautomeric molecules	W1-F12	14
H2O16Rel15	4	Relative energies of isomers of $(H_2O)_{16}$ (boat and fused cube structures)	CCSD(T)/aug-cc-pVTZ	199
H2O20Rel10	9	Relative energies of isomers of $(H_2O)_{20}$ (lowest-energy structures)	CCSD(T)/CBS	200
SW49Rel6	17	Relative energies of isomers of $SO_4^{2-}(H_2O)_6$	CCSD(T)/CBS	201
SW49Rel345	28	Relative energies of isomers of $SO_4^{2-}(H_2O)_n$ where n=3–5	CCSD(T)/CBS	201
Total atomization energies:				
W4-17	194	First- and second-row molecules and radicals with up to eight non-hydrogen atoms	W4	202
PlatonicTAE6	6	Platonic hydrocarbon cages, C_nH_n (where n = 4,6,8,10,12,20)	W*n*-F12	167
AlkAtom19	19	C_nH_{2n+2} where n=1–8	W*n*	168

Table S2. Detailed list of data sets in the ACP validation set.

Data set(s)	Data points	Data set description	Reference energy level	Reference # in article
Non-covalent interaction energies:				
BlindNCI	80	Interaction energies of 10 dimer complexes at various intermolecular distances used previously for blind test	CCSD(T)/CBS	203
DES15K	11474	Interaction energies of various non-covalently bound dimer complexes	CCSD(T)/CBS	204

NENCI-2021	5859	Interaction energies of non-equilibrium dimer complexes	CCSD(T)/CBS	205
CE20	20	Interaction energies of water, ammonia, and hydrogen fluoride clusters	W1-F12	189, 190
WaterOrg	2,376	Interaction energies of hydrogen-bonding interactions between water clusters and organic molecule complexes	DLPNO-CCSD(T)/CBS	206
R160x6	960	Interaction energies of small dimer complexes at short intermolecular distances	CCSD(T)/CBS	207
R739x5	4330	Interaction energies of small dimer complexes at short intermolecular distances	CCSD(T)/CBS	208
CHAL336	48	Interaction energies of chalcogen-bonded dimer complexes	W1-F12 or DLPNO-CCSD(T)/CBS	209
XB45	33	Interaction energies of halogen-bonded dimer complexes	CCSD(T)/aug-cc-pVTZ	210
L7	7	Interaction energies of seven relatively large non-covalently bound complexes	DLPNO-CCSD(T)/CBS	211, 212
S12L	10	Interaction energies of supramolecular host-guest complexes	DLPNO-CCSD(T)/CBS	9, 11, 212
S30L	26	Interaction energies of supramolecular host-guest complexes	Experimental back-corrected	213
Ni2021	11	Interaction energies of large non-covalently bound complexes ranging in size between 126-1027 atoms	CIM-DLPNO-CCSD(T)||RI-MP2	214
C60dimer	14	Interaction energies of the C_{60} dimer complex at various intermolecular distances	DLPNO-CCSD(T)/CBS	215
H2O20Bind10	10	Interaction energies of clusters of $(H_2O)_{20}$	CCSD(T)/CBS	200
HW6Cl-anionic	6	Interaction energies of clusters of $Cl^-(H_2O)_n$ (where n = 1-6)	CCSD(T)/CBS	200, 216
HW6F-anionic	6	Interaction energies of clusters of $F^-(H_2O)_n$ (where n = 1-6)	CCSD(T)/CBS	200, 216
FmH2O10-anionic	10	Interaction energies of clusters of $F^-(H_2O)_{10}$	CCSD(T)/CBS	200, 216
SW49Bind345-anionic	30	Interaction energies of clusters of $SO_4^{2-}(H_2O)_n$ (where n = 3-5)	CCSD(T)/CBS	201
SW49Bind6-anionic	18	Interaction energies of clusters of $SO_4^{2-}(H_2O)_6$	CCSD(T)/CBS	201
Anionpi-anionic	16	Interaction energies of anion-π type non-covalently interacting dimer complexes	DLPNO-CCSD(T)/CBS	217
IL236-anionic	236	Interaction energies of ion pair dimer complexes representing model ionic liquids	CCSD(T)/CBS	218
DES15K-anionic, NENCI-2021-anionic, CHAL336-anionic, XB45-anionic, S30L-anionic	1281, 889, 19, 12, 2	Interaction energies of only anion-neutral and anion-cation dimer complexes from earlier described datasets	Various	204, 205, 209, 210, 213
Molecular conformational energies:				
SafroleCONF	5	Relative energies of safrole conformers	CCSD(T)/CBS	219
AlcoholCONF	31	Relative energies of small alcohol conformers	CCSD(T)/aug-cc-pVTZ	220
BeranCONF	50	Relative energies of flexible organic molecule conformers relevant in crystal structure prediction	CCSD(T)/CBS or MP2D/CBS	221
Torsion30	2107	Relative energies of conformers of model systems representing biaryl drug-like molecules at various intramolecular torsion angles	CCSD(T)*/CBS	222

		(excluding many datapoints for which geometries were missing).		
ANI1ccxCONF	5254	Relative energies with respect to the energy minimum of organic molecules generated using normal mode sampling, dimer sampling, and torsion sampling	CCSD(T)*/CBS	223
MPCONF196	112	Relative energies of medium-sized macrocyclic peptide conformers	DLPNO-CCSD(T)/CBS	224
PEPCONF-Tripeptide	647	Relative energies of conformers of various model tripeptide systems	DLPNO-CCSD(T)/CBS	58, 140
PEPCONF-Disulfide	620	Relative energies of conformers of various model peptide systems containing disulfide linkages	LC-ωPBE-XDM/aug-cc-pVTZ	140
PEPCONF-Cyclic	320	Relative energies of conformers of various macrocyclic peptides	LC-ωPBE-XDM/aug-cc-pVTZ	140
PEPCONF-Bioactive	175	Relative energies of conformers of various polypeptides that show bioactive function	LC-ωPBE-XDM/aug-cc-pVTZ	140
PEPCONF-Disulfide-anionic, PEPCONF-Bioactive-anionic	150, 20	Relative energies of conformers of systems containing only negative charge from earlier described datasets	LC-ωPBE-XDM/aug-cc-pVTZ	140
Reaction energies:				
W4-17-RE	5205	Automatically generated reactions using molecules from the W4-17[202]	W4	155
Barrier height energies:				
WaterOrgBH	88	Pericyclic reactions in absence and presence of water clusters	DLPNO-CCSD(T)/CBS	unpublished data

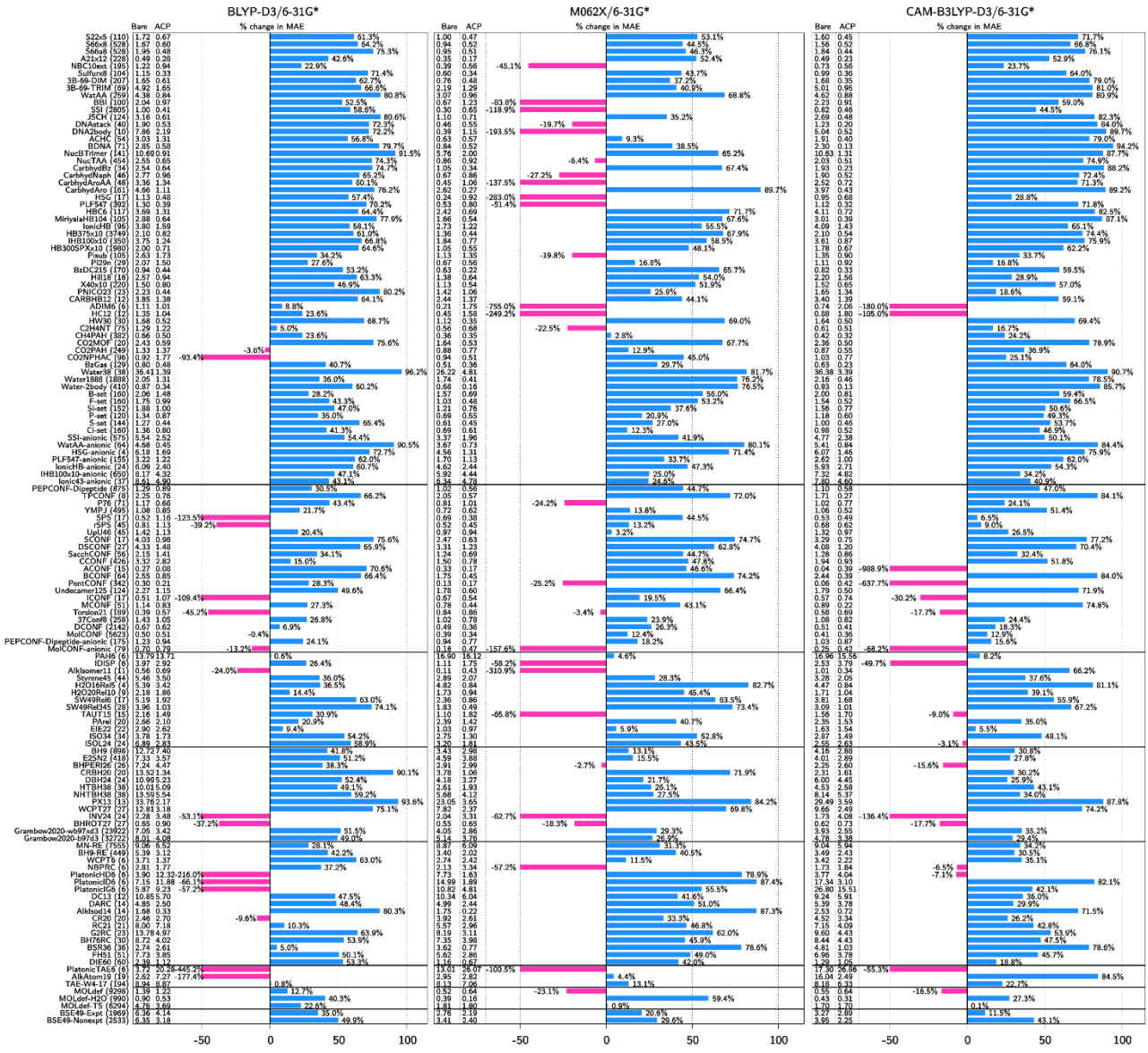

Figure S1. Mean absolute errors (MAEs, in kcal/mol) of uncorrected methods ("Bare") and ACP-corrected methods ("ACP") along with percentage change in MAEs on application of ACPs to the training set. The various shorthand notations are as follows: NCI = non-covalent interaction energies, CONF = molecular conformational energies, ISOM = isomerization energies, BH = barrier heights, RE = reaction energies, TAE = total atomization energies, DEF = molecular deformation energies, and BSE = bond separation energies. The % change in MAE is calculated as [MAE of ACP-corrected method] – [MAE of uncorrected method] / [MAE of uncorrected method] x 100%.

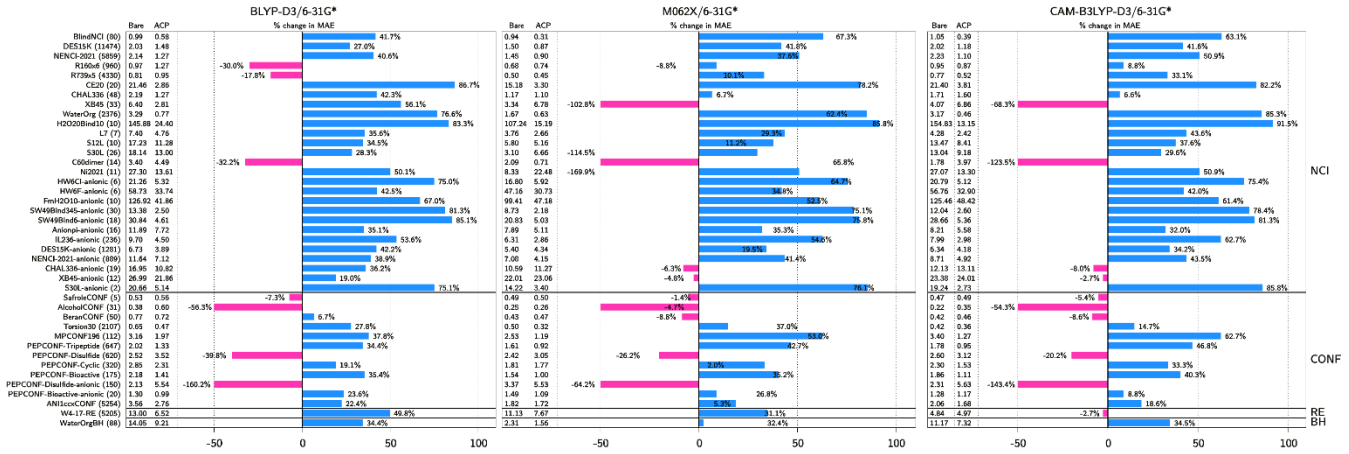

Figure S2. Mean absolute errors (MAEs) of uncorrected methods ("bare") and ACP-corrected methods ("ACP") along with percentage change in MAEs on application of ACPs to the validation set. The various shorthand notations are as follows: NCI = non-covalent interaction energies, CONF = molecular conformational energies, RE = reaction energies, and BH = barrier heights. The % change in MAE is calculated as [MAE of ACP-corrected method] – [MAE of uncorrected method] / [MAE of uncorrected method] x 100%.

Table S3. Detailed error analysis with respect to reference data in the training set. The numbers in bracket in the first column indicates the number of data points. The various shorthand notations are as follows: MAE = mean absolute error in kcal/mol, MSE = mean signed error in kcal/mol, MAXE = maximum absolute error in kcal/mol, RMSE = root-mean-square error in kcal/mol, and SD = standard deviation in kcal/mol.

Data set (# of data points)		BLYP-D3/6-31G*	BLYP-D3/6-31G*-ACP	M062X/6-31G*	M062X/6-31G*-ACP	CAMB3LYP-D3/6-31G*	CAMB3LYP-D3/6-31G*-ACP
S22x5 (110)	MAE	1.72	0.67	1.00	0.47	1.60	0.45
	MSE	-1.72	-0.38	-0.75	0.12	-1.59	-0.20
	MAXE	5.73	5.08	4.05	2.49	6.87	2.30
	RMSE	2.46	1.09	1.45	0.66	2.48	0.68
	SD	1.77	1.03	1.25	0.65	1.91	0.65
S66x8 (528)	MAE	1.67	0.60	0.94	0.52	1.56	0.52
	MSE	-1.67	-0.12	-0.79	0.22	-1.56	0.03
	MAXE	5.57	5.33	3.48	2.82	6.47	4.25
	RMSE	2.08	0.90	1.25	0.77	2.08	0.77
	SD	1.23	0.89	0.98	0.74	1.38	0.77
S66a8 (528)	MAE	1.95	0.48	0.95	0.51	1.84	0.44
	MSE	-1.95	-0.10	-0.81	0.32	-1.84	-0.04
	MAXE	5.62	2.35	3.83	2.10	6.43	1.77
	RMSE	2.18	0.61	1.28	0.67	2.18	0.55
	SD	0.96	0.60	0.99	0.59	1.16	0.55
A21x12 (228)	MAE	0.49	0.28	0.35	0.17	0.49	0.23
	MSE	-0.47	-0.07	-0.32	-0.04	-0.48	-0.11
	MAXE	4.72	3.09	3.62	1.71	5.54	2.24
	RMSE	0.96	0.61	0.72	0.29	1.01	0.43
	SD	0.84	0.61	0.65	0.29	0.88	0.42
NBC10ext (195)	MAE	1.22	0.94	0.39	0.56	0.73	0.56
	MSE	-1.22	-0.89	-0.11	-0.26	-0.73	-0.45

	MAXE	3.25	3.74	1.44	2.26	1.40	1.37
	RMSE	1.56	1.31	0.52	0.80	0.88	0.70
	SD	0.97	0.97	0.51	0.76	0.49	0.54
Sulfurx8 (104)	MAE	1.15	0.33	0.60	0.34	0.99	0.36
	MSE	-1.15	-0.08	-0.54	0.10	-0.99	-0.07
	MAXE	3.07	1.53	2.15	1.20	3.00	1.42
	RMSE	1.43	0.44	0.82	0.44	1.28	0.49
	SD	0.86	0.44	0.61	0.43	0.80	0.48
3B-69-DIM (207)	MAE	1.65	0.61	0.76	0.48	1.68	0.35
	MSE	-1.64	0.31	-0.69	0.38	-1.67	0.09
	MAXE	6.34	4.16	3.30	2.05	6.44	1.62
	RMSE	2.09	0.99	1.11	0.62	2.18	0.49
	SD	1.29	0.94	0.87	0.48	1.40	0.49
3B-69-TRIM (69)	MAE	4.92	1.65	2.19	1.29	5.01	0.95
	MSE	-4.92	0.92	-2.14	1.08	-5.01	0.27
	MAXE	12.00	6.14	10.01	4.13	12.69	3.59
	RMSE	5.41	2.20	2.76	1.60	5.58	1.21
	SD	2.26	2.01	1.76	1.20	2.47	1.19
WatAA (259)	MAE	4.38	0.84	3.07	0.96	4.62	0.88
	MSE	-4.38	0.08	-3.07	-0.35	-4.62	-0.40
	MAXE	8.70	2.37	7.00	2.51	9.14	2.49
	RMSE	4.57	1.07	3.32	1.13	4.80	1.11
	SD	1.28	1.06	1.26	1.07	1.28	1.04
BBI (100)	MAE	2.04	0.97	0.67	1.23	2.23	0.91
	MSE	-2.04	0.93	-0.64	1.23	-2.23	0.91
	MAXE	2.79	2.89	1.57	2.04	3.19	2.03
	RMSE	2.06	1.13	0.77	1.29	2.31	1.03
	SD	0.30	0.64	0.42	0.38	0.59	0.49
SSI (2805)	MAE	1.00	0.41	0.30	0.65	0.82	0.46
	MSE	-1.00	0.18	-0.12	0.63	-0.82	0.35
	MAXE	5.06	8.23	3.96	3.63	5.29	4.31
	RMSE	1.22	0.59	0.53	0.73	1.08	0.58
	SD	0.71	0.57	0.52	0.36	0.70	0.46
JSCH (124)	MAE	3.16	0.61	1.10	0.71	2.69	0.48
	MSE	-3.16	-0.05	-0.84	0.51	-2.69	0.34
	MAXE	7.75	1.87	4.88	2.41	9.29	1.94
	RMSE	3.68	0.79	1.57	0.90	3.52	0.66
	SD	1.90	0.79	1.33	0.74	2.27	0.56
DNAstack (40)	MAE	1.90	0.53	0.46	0.55	1.23	0.20
	MSE	-1.90	-0.41	0.05	0.35	-1.22	0.13
	MAXE	3.88	1.41	1.14	1.40	2.60	1.12
	RMSE	2.27	0.71	0.52	0.63	1.46	0.33
	SD	1.26	0.59	0.52	0.53	0.82	0.30
DNA2body (10)	MAE	7.86	2.19	0.39	1.15	5.04	0.52
	MSE	-7.86	-2.19	-0.14	1.05	-5.04	0.23
	MAXE	8.80	3.21	0.91	1.90	5.68	1.24
	RMSE	7.87	2.29	0.48	1.28	5.05	0.63
	SD	0.42	0.70	0.48	0.77	0.30	0.61
ACHC (54)	MAE	3.03	1.31	0.63	0.57	1.91	0.40
	MSE	-3.03	-1.31	-0.31	-0.38	-1.91	-0.40
	MAXE	4.55	1.76	3.66	1.86	2.26	0.64
	RMSE	3.10	1.34	0.86	0.70	1.94	0.43
	SD	0.62	0.27	0.80	0.59	0.37	0.16
BDNA (71)	MAE	2.85	0.58	0.84	0.52	2.30	0.13
	MSE	-2.85	-0.51	-0.57	0.36	-2.30	0.00

	MAXE	6.06	1.31	2.68	1.05	6.21	0.49
	RMSE	3.45	0.73	1.29	0.55	3.07	0.19
	SD	1.95	0.53	1.16	0.42	2.04	0.19
NucBTrimer (141)	MAE	10.69	0.91	5.76	2.00	10.63	1.31
	MSE	-10.69	0.01	-5.76	1.53	-10.63	1.17
	MAXE	14.95	4.14	9.79	4.58	16.76	4.01
	RMSE	10.84	1.17	6.01	2.30	10.86	1.58
	SD	1.82	1.18	1.72	1.72	2.23	1.07
NucTAA (454)	MAE	2.55	0.65	0.86	0.92	2.03	0.51
	MSE	-2.53	-0.07	-0.45	0.79	-2.02	0.03
	MAXE	13.86	7.50	7.56	3.60	10.01	4.66
	RMSE	3.19	1.00	1.33	1.07	2.61	0.73
	SD	1.94	1.00	1.25	0.73	1.66	0.73
CarbhydBz (34)	MAE	2.54	0.64	1.05	0.34	1.93	0.23
	MSE	-2.54	-0.62	-1.03	0.34	-1.93	0.23
	MAXE	4.30	1.14	2.47	1.32	3.37	1.02
	RMSE	2.62	0.67	1.15	0.44	2.01	0.30
	SD	0.65	0.26	0.53	0.29	0.56	0.21
CarbhydNaph (46)	MAE	2.77	0.96	0.67	0.86	1.90	0.52
	MSE	-2.77	-0.96	-0.62	0.86	-1.90	0.52
	MAXE	3.88	1.53	2.00	1.44	2.72	0.88
	RMSE	2.81	1.00	0.81	0.93	1.95	0.56
	SD	0.51	0.28	0.52	0.37	0.44	0.20
CarbhydAroAA (48)	MAE	3.36	1.34	0.45	1.06	2.52	0.72
	MSE	-3.36	-1.34	0.15	1.06	-2.52	-0.72
	MAXE	6.45	3.27	1.24	1.76	4.88	1.65
	RMSE	3.60	1.49	0.52	1.12	2.70	0.81
	SD	1.30	0.67	0.50	0.36	0.98	0.37
CarbhydAro (161)	MAE	4.66	1.11	2.62	0.27	3.97	0.43
	MSE	-4.66	-1.01	-2.62	0.03	-3.97	-0.36
	MAXE	8.89	2.73	6.32	1.18	7.80	1.43
	RMSE	4.93	1.23	2.93	0.37	4.26	0.51
	SD	1.61	0.70	1.31	0.37	1.56	0.36
HSG (17)	MAE	1.13	0.48	0.24	0.92	0.95	0.68
	MSE	-1.13	0.30	-0.08	0.90	-0.95	0.63
	MAXE	2.65	1.40	1.40	1.90	2.84	2.02
	RMSE	1.27	0.64	0.40	1.02	1.13	0.88
	SD	0.59	0.58	0.40	0.48	0.62	0.64
PLF547 (392)	MAE	1.30	0.39	0.53	0.80	1.12	0.32
	MSE	-1.28	0.14	0.03	0.79	-1.10	0.17
	MAXE	6.45	4.63	3.14	3.41	5.84	1.96
	RMSE	1.83	0.66	0.75	1.01	1.64	0.48
	SD	1.31	0.64	0.75	0.63	1.22	0.45
HBC6 (117)	MAE	3.69	1.31	2.42	0.69	4.11	0.72
	MSE	-3.66	-0.13	-2.39	-0.36	-4.10	-0.59
	MAXE	6.92	6.84	5.20	3.61	7.64	2.39
	RMSE	4.37	1.87	2.92	0.95	4.92	0.93
	SD	2.39	1.88	1.69	0.88	2.73	0.72
MiriyalaHB 104(105)	MAE	2.88	0.64	1.66	0.54	3.01	0.39
	MSE	-2.88	0.45	-1.65	0.30	-3.01	0.03
	MAXE	5.53	3.03	3.60	1.74	6.86	1.64
	RMSE	3.01	0.85	1.88	0.66	3.17	0.50
	SD	0.88	0.73	0.91	0.58	1.02	0.50
IonicHB (96)	MAE	3.80	1.59	2.73	1.22	4.09	1.43
	MSE	-3.76	-1.35	-2.72	-1.02	-4.08	-1.36

	MAXE	7.14	4.10	6.44	3.32	7.81	3.23
	RMSE	4.27	1.90	3.14	1.49	4.51	1.68
	SD	2.03	1.34	1.59	1.09	1.93	0.98
HB375x10 (3749)	MAE	2.10	0.82	1.36	0.44	2.10	0.54
	MSE	-2.10	0.35	-1.33	0.16	-2.10	0.06
	MAXE	6.46	9.37	5.64	3.46	7.59	5.08
	RMSE	2.44	1.26	1.68	0.62	2.49	0.73
	SD	1.25	1.21	1.04	0.60	1.35	0.73
IHB100x10 (350)	MAE	3.75	1.24	1.84	0.77	3.61	0.87
	MSE	-3.74	-0.62	-1.81	-0.20	-3.60	-0.65
	MAXE	7.74	6.05	6.52	4.16	7.67	4.32
	RMSE	4.14	1.58	2.24	1.08	3.93	1.14
	SD	1.79	1.45	1.32	1.07	1.56	0.94
HB300SPXx10 (1980)	MAE	2.00	0.71	1.05	0.55	1.78	0.67
	MSE	-1.99	-0.21	-0.98	0.20	-1.77	-0.01
	MAXE	8.54	6.18	6.77	4.33	9.39	4.28
	RMSE	2.48	1.05	1.56	0.80	2.36	0.98
	SD	1.48	1.03	1.22	0.77	1.56	0.98
Pisub (105)	MAE	2.63	1.73	1.13	1.35	1.35	0.90
	MSE	-2.63	-1.72	-0.97	-1.27	-1.35	-0.84
	MAXE	5.49	3.87	2.98	3.14	3.07	2.10
	RMSE	2.83	1.96	1.33	1.63	1.43	1.02
	SD	1.07	0.93	0.92	1.02	0.48	0.58
Pi29n (29)	MAE	2.07	1.50	0.67	0.56	1.11	0.92
	MSE	-2.07	-1.48	0.57	0.02	-1.11	-0.91
	MAXE	7.57	6.55	1.97	3.82	2.07	3.89
	RMSE	2.46	1.96	0.83	0.89	1.19	1.18
	SD	1.34	1.32	0.61	0.90	0.42	0.76
BzDC215 (170)	MAE	0.94	0.44	0.63	0.22	0.82	0.33
	MSE	-0.94	-0.42	-0.59	-0.14	-0.82	-0.27
	MAXE	2.99	1.88	3.17	0.77	3.03	1.33
	RMSE	1.19	0.61	0.93	0.29	1.05	0.43
	SD	0.73	0.44	0.72	0.26	0.65	0.34
Hill18 (18)	MAE	2.57	0.94	1.38	0.64	2.20	1.56
	MSE	-2.57	-0.31	-0.82	-0.54	-1.76	-1.56
	MAXE	3.91	1.85	5.01	1.67	3.95	3.83
	RMSE	2.68	1.07	1.69	0.83	2.34	1.84
	SD	0.78	1.06	1.52	0.65	1.58	1.00
X40x10 (220)	MAE	1.50	0.80	1.13	0.54	1.52	0.65
	MSE	-1.49	0.12	-1.06	-0.12	-1.51	-0.21
	MAXE	6.89	3.87	6.03	3.90	7.38	4.08
	RMSE	2.21	1.13	1.74	0.90	2.31	0.99
	SD	1.64	1.13	1.38	0.90	1.75	0.97
PNICO23 (23)	MAE	2.23	0.44	1.42	1.06	1.65	1.34
	MSE	2.23	0.38	1.25	1.05	1.54	1.34
	MAXE	4.95	1.26	4.49	3.92	4.61	4.25
	RMSE	2.50	0.57	2.00	1.49	2.12	1.81
	SD	1.16	0.43	1.60	1.08	1.49	1.25
CARBHB12 (12)	MAE	3.85	1.38	2.44	1.37	3.40	1.39
	MSE	3.85	0.14	2.44	1.07	3.40	1.08
	MAXE	7.41	2.78	4.86	3.51	6.48	3.42
	RMSE	4.58	1.59	2.98	1.79	3.96	1.85
	SD	2.58	1.66	1.79	1.50	2.11	1.56
ADIM6 (6)	MAE	1.11	1.01	0.21	1.75	0.74	2.06
	MSE	-1.11	1.01	-0.21	1.75	-0.74	2.06

	MAXE	1.65	1.67	0.32	2.87	1.02	3.48
	RMSE	1.20	1.11	0.21	1.93	0.78	2.27
	SD	0.52	0.51	0.07	0.88	0.29	1.05
HC12 (12)	MAE	1.35	1.04	0.45	1.58	0.88	1.80
	MSE	-1.35	0.33	-0.40	0.96	-0.88	1.23
	MAXE	2.37	1.70	1.21	2.78	1.96	3.69
	RMSE	1.44	1.13	0.54	1.70	0.96	2.01
	SD	0.50	1.13	0.37	1.47	0.41	1.67
HW30 (30)	MAE	1.68	0.52	1.12	0.35	1.64	0.50
	MSE	-1.68	-0.44	-1.12	-0.11	-1.64	-0.33
	MAXE	3.66	1.70	2.95	0.97	3.16	1.11
	RMSE	1.81	0.64	1.28	0.46	1.74	0.58
	SD	0.70	0.47	0.62	0.46	0.60	0.49
C2H4NT (75)	MAE	1.29	1.22	0.56	0.68	0.61	0.51
	MSE	-1.29	-1.22	0.45	0.23	-0.56	-0.43
	MAXE	2.92	4.23	1.83	1.62	1.22	1.79
	RMSE	1.51	1.56	0.65	0.78	0.71	0.67
	SD	0.79	0.98	0.47	0.75	0.44	0.52
CH4PAH (382)	MAE	0.66	0.50	0.36	0.35	0.42	0.32
	MSE	-0.65	-0.48	0.02	0.20	-0.33	0.27
	MAXE	2.15	4.48	2.62	1.36	1.34	2.72
	RMSE	0.79	0.88	0.46	0.42	0.50	0.61
	SD	0.46	0.74	0.46	0.37	0.37	0.54
CO2MOF (20)	MAE	2.43	0.59	1.64	0.53	2.36	0.50
	MSE	-2.43	-0.23	-1.64	-0.30	-2.36	-0.34
	MAXE	4.12	2.01	3.39	1.39	3.84	1.89
	RMSE	2.55	0.74	1.90	0.70	2.51	0.67
	SD	0.77	0.72	0.98	0.65	0.87	0.60
CO2PAH (249)	MAE	1.33	1.37	0.88	0.77	0.87	0.55
	MSE	-1.33	0.86	-0.33	0.73	-0.87	0.26
	MAXE	4.29	9.84	4.93	3.55	2.71	3.27
	RMSE	1.71	2.50	1.23	0.99	1.10	0.89
	SD	1.09	2.35	1.18	0.67	0.68	0.85
CO2NPHAC (96)	MAE	0.92	1.77	0.94	0.51	1.03	0.77
	MSE	-0.92	1.52	-0.67	0.50	-1.03	0.64
	MAXE	2.19	9.96	2.80	3.07	2.81	5.24
	RMSE	1.11	2.97	1.21	0.78	1.33	1.33
	SD	0.63	2.57	1.01	0.61	0.85	1.17
BzGas (129)	MAE	0.80	0.48	0.51	0.36	0.63	0.23
	MSE	-0.80	0.31	-0.41	-0.06	-0.62	0.04
	MAXE	2.40	3.66	2.43	1.31	1.50	1.07
	RMSE	0.95	0.88	0.77	0.48	0.73	0.29
	SD	0.51	0.83	0.65	0.48	0.37	0.29
Water38 (38)	MAE	36.41	1.39	26.22	4.81	36.38	3.39
	MSE	-36.41	0.77	-26.22	-4.81	-36.38	-3.39
	MAXE	71.87	2.88	50.33	8.44	71.53	6.24
	RMSE	39.56	1.60	28.29	5.13	39.46	3.71
	SD	15.67	1.42	10.77	1.82	15.47	1.53
Water1888 (1888)	MAE	2.05	1.31	1.74	0.41	2.16	0.46
	MSE	-2.05	0.63	-1.71	-0.14	-2.14	0.00
	MAXE	6.72	7.76	5.88	2.10	6.51	2.15
	RMSE	2.41	1.83	2.10	0.52	2.55	0.61
	SD	1.28	1.72	1.21	0.50	1.39	0.61
Water-2body (410)	MAE	0.87	0.34	0.68	0.16	0.93	0.13
	MSE	-0.85	0.10	-0.63	-0.09	-0.90	-0.06

	MAXE	4.92	2.28	3.69	1.30	4.61	1.46
	RMSE	1.59	0.59	1.25	0.24	1.75	0.21
	SD	1.34	0.59	1.08	0.23	1.51	0.21
B-set (160)	MAE	2.06	1.48	1.57	0.69	2.00	0.81
	MSE	-1.94	-0.84	-1.31	-0.06	-1.90	-0.49
	MAXE	7.48	12.19	7.49	3.84	7.71	3.32
	RMSE	2.80	2.30	2.26	0.94	2.83	1.17
	SD	2.02	2.15	1.85	0.94	2.10	1.06
F-set (160)	MAE	1.75	0.99	1.03	0.48	1.54	0.52
	MSE	-1.74	0.11	-0.85	0.30	-1.52	0.13
	MAXE	6.86	13.42	4.01	3.93	7.17	2.85
	RMSE	2.38	1.69	1.49	0.75	2.30	0.72
	SD	1.63	1.70	1.23	0.69	1.73	0.71
Si-set (152)	MAE	1.88	1.00	1.21	0.76	1.56	0.77
	MSE	-1.20	-0.65	-1.10	-0.36	-1.52	-0.53
	MAXE	6.46	6.80	5.41	6.38	5.21	5.02
	RMSE	2.54	1.61	1.83	1.38	2.13	1.30
	SD	2.25	1.47	1.46	1.34	1.50	1.19
P-set (120)	MAE	1.34	0.87	0.69	0.55	1.18	0.60
	MSE	-1.29	0.02	-0.56	0.31	-1.15	0.14
	MAXE	5.89	11.29	3.88	3.90	7.02	2.68
	RMSE	1.86	1.59	1.10	0.87	1.85	0.89
	SD	1.35	1.59	0.95	0.81	1.46	0.88
S-set (144)	MAE	1.27	0.44	0.61	0.45	1.00	0.46
	MSE	-1.27	-0.18	-0.48	0.08	-0.99	-0.13
	MAXE	4.03	2.98	2.41	2.07	3.26	3.10
	RMSE	1.61	0.64	0.84	0.60	1.29	0.66
	SD	0.99	0.62	0.69	0.60	0.82	0.65
Cl-set (160)	MAE	1.36	0.80	0.69	0.61	0.98	0.52
	MSE	-1.34	-0.02	-0.20	0.38	-0.93	-0.07
	MAXE	6.14	14.09	4.12	5.22	6.40	2.71
	RMSE	1.97	1.88	1.13	1.00	1.63	0.80
	SD	1.45	1.89	1.11	0.93	1.35	0.80
SSI-anionic (575)	MAE	5.54	2.52	3.37	1.96	4.77	2.38
	MSE	-5.53	-1.91	-3.23	-1.52	-4.74	-2.03
	MAXE	13.92	8.07	9.76	6.28	13.06	7.42
	RMSE	6.70	3.35	4.31	2.55	5.95	3.10
	SD	3.79	2.75	2.85	2.05	3.60	2.35
WatAA-anionic (64)	MAE	4.68	0.45	3.67	0.73	5.41	0.84
	MSE	-4.68	0.29	-3.67	-0.60	-5.41	-0.75
	MAXE	8.18	1.58	6.86	2.25	8.53	2.29
	RMSE	4.77	0.54	3.77	0.82	5.49	0.95
	SD	0.92	0.46	0.87	0.57	0.92	0.59
HSG-anionic (4)	MAE	6.18	1.69	4.56	1.31	6.07	1.46
	MSE	-6.18	-0.82	-4.56	-1.31	-6.07	-1.46
	MAXE	8.53	2.47	7.84	2.23	8.91	2.41
	RMSE	6.56	1.76	5.17	1.52	6.63	1.64
	SD	2.53	1.80	2.79	0.90	3.07	0.86
PLF547-anionic (155)	MAE	3.22	1.22	1.70	1.13	2.62	1.00
	MSE	-3.17	-0.88	-1.21	-0.04	-2.57	-0.62
	MAXE	19.38	16.95	12.06	6.08	15.83	6.69
	RMSE	5.18	2.60	3.14	1.69	4.47	1.87
	SD	4.11	2.45	2.90	1.70	3.66	1.77
IonicHB-anionic (24)	MAE	6.09	2.40	4.62	2.44	5.93	2.71
	MSE	-6.09	-2.39	-4.62	-2.43	-5.93	-2.71

	MAXE	8.49	5.32	7.95	3.58	9.58	4.07
	RMSE	6.59	2.76	5.16	2.63	6.52	2.90
	SD	2.57	1.41	2.34	1.03	2.77	1.05
IHB100x10-anionic (650)	MAE	8.17	4.32	5.92	4.44	7.32	4.82
	MSE	-8.16	-4.08	-5.91	-4.42	-7.31	-4.81
	MAXE	25.34	18.53	22.15	20.19	23.33	20.49
	RMSE	9.43	5.63	7.08	5.76	8.48	6.08
	SD	4.73	3.88	3.91	3.68	4.30	3.73
Ionic43-anionic (37)	MAE	8.61	4.90	6.34	4.78	7.80	4.60
	MSE	-8.61	-4.82	-6.34	-4.78	-7.80	-4.53
	MAXE	23.57	19.69	20.99	18.99	23.04	19.85
	RMSE	10.28	6.75	8.16	6.73	9.63	6.79
	SD	5.69	4.80	5.21	4.80	5.73	5.13
PEPCONF-Dipeptide (875)	MAE	1.29	0.89	1.02	0.56	1.10	0.58
	MSE	0.63	0.05	0.55	0.08	0.61	0.11
	MAXE	7.05	3.94	4.78	2.53	6.47	2.77
	RMSE	1.63	1.19	1.30	0.72	1.40	0.74
	SD	1.51	1.19	1.18	0.72	1.26	0.73
TPCONF (8)	MAE	2.25	0.76	2.05	0.57	1.71	0.27
	MSE	-2.00	0.18	-1.27	0.03	-0.98	0.08
	MAXE	4.53	1.53	4.34	1.11	3.05	0.74
	RMSE	2.92	0.83	2.48	0.72	1.99	0.34
	SD	2.28	0.86	2.27	0.77	1.85	0.35
P76 (71)	MAE	1.17	0.66	0.81	1.01	1.02	0.77
	MSE	1.01	-0.12	0.41	-0.19	0.98	-0.34
	MAXE	3.41	2.59	3.09	2.82	2.64	2.25
	RMSE	1.48	0.84	1.16	1.25	1.25	0.97
	SD	1.10	0.83	1.09	1.25	0.77	0.91
YMPJ (495)	MAE	1.08	0.85	0.72	0.62	1.06	0.52
	MSE	0.56	0.03	0.21	-0.44	0.92	-0.25
	MAXE	4.92	3.29	2.86	3.05	3.97	2.64
	RMSE	1.43	1.06	0.92	0.80	1.42	0.71
	SD	1.31	1.06	0.89	0.66	1.08	0.67
SPS (17)	MAE	0.52	1.16	0.69	0.38	0.53	0.49
	MSE	0.31	-0.86	0.57	0.30	0.33	-0.18
	MAXE	1.47	2.78	1.32	1.30	1.21	1.24
	RMSE	0.63	1.42	0.76	0.52	0.63	0.62
	SD	0.57	1.16	0.53	0.44	0.56	0.61
rSPS (45)	MAE	0.81	1.13	0.52	0.45	0.68	0.62
	MSE	0.69	0.70	0.27	-0.23	0.57	0.18
	MAXE	1.89	3.70	1.85	1.37	2.17	2.65
	RMSE	0.97	1.48	0.61	0.57	0.86	0.79
	SD	0.69	1.32	0.56	0.53	0.65	0.78
UpU46 (45)	MAE	1.42	1.13	0.97	0.94	1.32	0.97
	MSE	-1.03	-0.41	-0.34	0.29	-0.42	-0.02
	MAXE	6.42	2.97	3.24	3.87	5.45	3.61
	RMSE	1.87	1.38	1.25	1.17	1.63	1.23
	SD	1.58	1.34	1.22	1.14	1.59	1.24
SCONF (17)	MAE	4.03	0.98	2.47	0.63	3.29	0.75
	MSE	1.60	-0.65	0.94	-0.27	1.38	-0.36
	MAXE	10.39	2.25	6.25	3.21	7.94	2.51
	RMSE	4.67	1.22	2.86	1.05	3.75	1.03
	SD	4.52	1.07	2.78	1.04	3.60	0.99
DSCONF (27)	MAE	4.33	1.48	3.31	1.23	4.08	1.20
	MSE	3.26	1.00	2.88	0.44	3.46	0.42

	MAXE	11.13	3.53	8.84	3.57	10.31	3.80
	RMSE	5.65	1.78	4.17	1.52	5.13	1.55
	SD	4.71	1.51	3.07	1.48	3.87	1.52
SacchCONF (56)	MAE	2.15	1.41	1.24	0.69	1.28	0.86
	MSE	0.03	0.89	0.88	0.14	0.79	0.58
	MAXE	7.64	5.38	4.11	1.92	3.46	2.35
	RMSE	2.81	1.93	1.50	0.82	1.57	1.04
	SD	2.84	1.73	1.22	0.81	1.37	0.87
CCONF (426)	MAE	3.32	2.82	1.50	0.78	1.94	0.93
	MSE	-1.61	2.70	0.09	-0.23	-0.42	0.28
	MAXE	16.20	8.83	6.27	3.08	8.64	3.88
	RMSE	4.40	3.44	1.90	1.00	2.50	1.17
	SD	4.10	2.14	1.90	0.98	2.47	1.13
ACONF (15)	MAE	0.27	0.08	0.33	0.17	0.04	0.39
	MSE	-0.27	-0.02	-0.33	-0.17	-0.02	0.39
	MAXE	0.63	0.18	0.66	0.32	0.07	0.89
	RMSE	0.31	0.09	0.36	0.19	0.04	0.45
	SD	0.16	0.10	0.17	0.08	0.04	0.23
BCONF (64)	MAE	2.55	0.85	1.75	0.45	2.44	0.39
	MSE	2.51	-0.74	1.66	0.34	2.42	0.02
	MAXE	4.30	2.03	2.80	1.29	3.61	1.01
	RMSE	2.70	0.97	1.83	0.56	2.56	0.47
	SD	1.01	0.64	0.79	0.44	0.84	0.48
PentCONF (342)	MAE	0.30	0.21	0.13	0.17	0.06	0.42
	MSE	-0.30	0.16	-0.05	-0.16	0.00	0.42
	MAXE	1.06	1.09	0.50	0.51	0.27	0.81
	RMSE	0.39	0.31	0.17	0.20	0.08	0.46
	SD	0.25	0.27	0.16	0.12	0.08	0.18
Undecamer125 (124)	MAE	2.27	1.15	1.78	0.60	1.79	0.50
	MSE	1.38	0.83	0.85	-0.58	1.19	-0.44
	MAXE	4.89	2.49	4.76	2.21	3.64	1.73
	RMSE	2.59	1.37	2.04	0.75	2.06	0.65
	SD	2.20	1.09	1.86	0.48	1.69	0.48
ICONF (17)	MAE	0.51	1.07	0.67	0.54	0.57	0.74
	MSE	0.17	-0.04	0.16	0.08	0.34	0.53
	MAXE	2.66	3.45	1.63	2.31	1.67	1.71
	RMSE	0.81	1.42	0.85	0.81	0.73	0.94
	SD	0.82	1.47	0.86	0.83	0.66	0.81
MCONF (51)	MAE	1.14	0.83	0.78	0.44	0.89	0.22
	MSE	0.99	-0.65	0.75	0.21	0.83	-0.01
	MAXE	2.31	2.15	1.43	1.20	1.41	0.55
	RMSE	1.31	0.96	0.85	0.55	0.95	0.27
	SD	0.87	0.72	0.40	0.51	0.47	0.27
Torsion21 (189)	MAE	0.39	0.57	0.84	0.86	0.58	0.69
	MSE	0.12	0.47	0.65	0.54	0.46	0.49
	MAXE	1.87	1.85	2.93	2.34	2.15	2.39
	RMSE	0.56	0.73	1.07	1.07	0.74	0.88
	SD	0.54	0.56	0.84	0.92	0.58	0.73
37Conf8 (258)	MAE	1.43	1.05	1.02	0.78	1.08	0.82
	MSE	0.19	-0.51	0.19	-0.40	0.51	-0.20
	MAXE	10.35	5.93	7.43	4.31	9.13	3.50
	RMSE	2.01	1.36	1.49	1.03	1.63	1.04
	SD	2.00	1.27	1.48	0.95	1.55	1.02
DCONF (2142)	MAE	0.67	0.62	0.49	0.36	0.51	0.41
	MSE	0.50	0.46	0.41	0.16	0.44	0.26

	MAXE	3.30	3.77	2.35	1.67	2.21	2.11
	RMSE	0.93	0.90	0.70	0.51	0.70	0.59
	SD	0.79	0.78	0.56	0.48	0.55	0.53
MolCONF (5623)	MAE	0.50	0.51	0.39	0.34	0.41	0.36
	MSE	0.07	0.04	-0.04	-0.10	0.01	-0.07
	MAXE	10.64	6.66	4.63	6.26	6.37	6.41
	RMSE	0.91	0.87	0.63	0.55	0.73	0.60
	SD	0.91	0.86	0.63	0.54	0.73	0.60
PEPCONF-Dipeptide-anionic (175)	MAE	1.23	0.94	0.94	0.77	1.03	0.87
	MSE	-0.07	-0.19	0.05	-0.17	0.07	-0.03
	MAXE	4.53	4.19	3.03	2.66	3.80	2.59
	RMSE	1.59	1.21	1.21	0.97	1.33	1.07
	SD	1.60	1.20	1.21	0.96	1.33	1.07
MolCONF-anionic (79)	MAE	0.70	0.79	0.18	0.47	0.25	0.42
	MSE	0.41	0.53	0.05	0.05	0.08	0.01
	MAXE	4.50	4.12	0.75	2.94	1.06	2.25
	RMSE	1.48	1.41	0.27	0.84	0.40	0.70
	SD	1.43	1.31	0.26	0.84	0.39	0.71
PAH6 (6)	MAE	13.79	13.71	16.90	16.12	16.96	15.56
	MSE	-13.79	-13.71	-16.90	-16.12	-16.96	-15.56
	MAXE	34.80	34.60	41.28	40.20	41.27	39.46
	RMSE	17.95	17.86	21.55	20.80	21.59	20.29
	SD	12.58	12.54	14.65	14.40	14.62	14.26
IDISP (6)	MAE	3.97	2.92	1.11	1.75	2.53	3.79
	MSE	3.97	1.99	0.18	-0.88	0.14	-1.84
	MAXE	10.34	9.33	3.41	3.46	4.16	8.00
	RMSE	5.28	4.21	1.53	2.06	2.91	4.82
	SD	3.81	4.07	1.66	2.04	3.18	4.88
AlkIsomer11 (11)	MAE	0.56	0.69	0.11	0.43	1.01	0.34
	MSE	0.56	0.69	0.09	-0.43	1.01	0.33
	MAXE	1.35	2.09	0.25	1.05	2.74	1.21
	RMSE	0.67	0.88	0.12	0.52	1.22	0.47
	SD	0.39	0.58	0.09	0.29	0.72	0.34
Styrene45 (44)	MAE	5.46	3.50	2.89	2.07	3.28	2.05
	MSE	3.63	1.01	-0.15	-0.80	2.69	0.59
	MAXE	16.29	10.56	13.84	6.76	10.41	5.58
	RMSE	7.01	4.25	3.91	2.54	3.92	2.45
	SD	6.07	4.18	3.96	2.44	2.88	2.41
H2O16Rel5 (4)	MAE	5.39	3.42	4.82	0.84	4.47	0.84
	MSE	5.11	3.42	4.51	0.84	4.15	0.84
	MAXE	7.71	4.47	6.96	1.50	6.37	1.38
	RMSE	6.08	3.73	5.41	0.97	5.00	0.93
	SD	3.81	1.72	3.46	0.58	3.22	0.45
H2O20Rel10 (9)	MAE	2.18	1.86	1.73	0.94	1.71	1.04
	MSE	-1.82	-1.74	-1.71	-0.41	-1.20	-0.43
	MAXE	10.05	6.60	8.45	2.50	7.91	2.82
	RMSE	3.70	2.60	3.07	1.19	2.87	1.30
	SD	3.42	2.05	2.71	1.18	2.77	1.30
SW49Rel6 (17)	MAE	5.19	1.92	2.36	0.86	3.81	1.68
	MSE	5.16	1.92	2.34	0.85	3.76	1.67
	MAXE	19.60	3.34	9.73	3.34	15.78	5.54
	RMSE	6.85	2.31	3.22	1.12	5.34	2.04
	SD	4.64	1.33	2.27	0.75	3.91	1.21
SW49Rel345 (28)	MAE	3.96	1.03	1.83	0.49	3.09	1.01
	MSE	-0.28	0.10	-0.14	0.01	-0.17	0.02

	MAXE	9.37	1.84	4.67	1.60	7.55	2.74
	RMSE	4.61	1.19	2.14	0.62	3.63	1.27
	SD	4.69	1.21	2.18	0.63	3.70	1.30
TAUT15 (15)	MAE	2.16	1.49	1.10	1.82	1.56	1.70
	MSE	-0.90	-0.62	-0.41	0.94	-0.56	0.71
	MAXE	5.92	4.56	3.37	4.38	5.28	4.42
	RMSE	2.61	1.83	1.45	2.20	1.93	1.96
	SD	2.53	1.79	1.44	2.06	1.91	1.90
PArel (20)	MAE	2.66	2.10	2.39	1.42	2.35	1.53
	MSE	-0.45	0.94	0.17	0.53	-0.02	0.71
	MAXE	11.15	8.83	9.61	3.92	9.06	4.86
	RMSE	3.87	2.99	3.53	1.84	3.37	2.02
	SD	3.94	2.92	3.62	1.81	3.46	1.94
EIE22 (22)	MAE	2.90	2.62	1.03	0.97	1.63	1.54
	MSE	2.85	2.62	0.96	0.88	1.58	1.54
	MAXE	5.91	5.10	2.30	1.85	3.53	2.91
	RMSE	3.20	2.88	1.24	1.09	1.89	1.71
	SD	1.48	1.21	0.80	0.65	1.07	0.75
ISO34 (34)	MAE	3.78	1.73	2.75	1.30	2.87	1.49
	MSE	-1.67	-0.68	-1.58	-0.93	-1.33	-0.72
	MAXE	20.99	5.85	9.98	5.62	13.46	6.94
	RMSE	5.48	2.17	3.54	1.82	3.90	2.10
	SD	5.30	2.10	3.22	1.59	3.72	2.00
ISOL24 (24)	MAE	6.89	2.83	3.20	1.81	2.55	2.63
	MSE	-3.33	0.17	-0.49	-0.53	-0.42	0.20
	MAXE	22.58	8.60	11.87	5.31	6.80	10.74
	RMSE	8.86	3.82	4.14	2.32	3.33	3.70
	SD	8.38	3.89	4.20	2.31	3.38	3.77
BH9 (898)	MAE	12.72	7.40	3.43	2.98	4.16	2.88
	MSE	-12.27	-6.64	-1.71	-1.56	-2.39	-1.56
	MAXE	96.05	78.89	89.84	91.90	87.14	92.36
	RMSE	15.25	10.09	6.98	6.57	7.57	6.55
	SD	9.06	7.61	6.77	6.38	7.19	6.37
E2SN2 (418)	MAE	7.33	3.57	4.59	3.88	4.01	2.89
	MSE	-7.17	-0.84	-2.10	-2.25	-1.98	-1.46
	MAXE	18.98	14.11	19.45	18.74	17.28	14.77
	RMSE	8.32	4.55	5.71	5.11	4.97	3.93
	SD	4.23	4.47	5.32	4.59	4.56	3.65
BHPERI26 (26)	MAE	7.24	4.47	2.91	2.99	2.25	2.60
	MSE	-7.24	-4.21	-1.97	-2.67	-1.17	-2.14
	MAXE	12.15	9.67	6.44	5.48	5.90	4.70
	RMSE	7.66	5.17	3.30	3.50	2.82	3.00
	SD	2.57	3.05	2.70	2.30	2.61	2.14
CRBH20 (20)	MAE	13.52	1.34	3.78	1.06	2.31	1.61
	MSE	-13.52	-0.08	3.78	0.04	2.03	-1.26
	MAXE	16.42	3.47	6.75	4.29	4.29	4.05
	RMSE	13.59	1.73	4.47	1.53	2.66	2.01
	SD	1.33	1.77	2.44	1.57	1.76	1.60
DBH24 (24)	MAE	10.99	5.23	4.18	3.27	6.00	4.45
	MSE	-10.36	-3.90	-1.21	-1.14	-3.97	-3.00
	MAXE	33.88	20.20	18.30	15.53	22.72	16.60
	RMSE	13.84	7.16	6.54	5.01	8.23	6.01
	SD	9.37	6.13	6.57	4.98	7.37	5.32
HTBH38 (38)	MAE	10.01	5.09	2.61	1.93	4.53	2.58
	MSE	-10.01	-4.93	-1.41	-0.47	-4.31	-2.13

	MAXE	21.52	15.16	9.21	5.08	15.97	7.46
	RMSE	11.14	6.10	3.42	2.40	5.67	3.10
	SD	4.96	3.63	3.16	2.39	3.74	2.28
NHTBH38 (38)	MAE	13.59	5.54	5.68	4.12	8.14	5.37
	MSE	-12.91	-3.40	-2.43	-1.65	-5.55	-3.04
	MAXE	41.16	21.28	25.28	15.54	30.16	19.01
	RMSE	17.22	7.52	8.37	5.86	10.85	7.10
	SD	11.55	6.80	8.12	5.70	9.44	6.50
PX13 (13)	MAE	33.76	2.17	23.05	3.65	29.49	3.59
	MSE	-33.76	-0.25	-23.05	-3.56	-29.49	-3.35
	MAXE	60.70	5.12	43.79	5.97	58.58	5.41
	RMSE	36.57	2.73	25.74	3.96	33.23	3.76
	SD	14.63	2.83	11.94	1.80	15.94	1.79
WCPT27 (27)	MAE	12.81	3.18	7.82	2.37	9.66	2.49
	MSE	-12.81	1.11	-5.54	0.81	-7.31	1.36
	MAXE	28.78	7.17	15.89	9.91	19.22	9.52
	RMSE	15.19	3.77	9.10	3.20	11.36	3.36
	SD	8.31	3.67	7.36	3.15	8.86	3.13
INV24 (24)	MAE	2.28	3.48	2.04	3.31	1.73	4.08
	MSE	-1.26	-2.17	0.80	-1.93	0.25	-1.33
	MAXE	8.17	10.82	11.57	16.90	8.48	11.56
	RMSE	3.08	4.70	3.21	5.10	2.42	5.33
	SD	2.87	4.26	3.17	4.82	2.46	5.27
BHROT27 (27)	MAE	0.65	0.90	0.55	0.65	0.62	0.73
	MSE	0.44	0.86	0.53	0.34	0.59	0.62
	MAXE	1.80	2.98	1.81	2.08	1.81	2.81
	RMSE	0.84	1.25	0.74	0.91	0.84	1.07
	SD	0.73	0.92	0.53	0.86	0.62	0.88
Grambow2020-ωB97xD3 (23922)	MAE	7.05	3.42	4.05	2.86	3.93	2.55
	MSE	-6.61	-1.74	3.26	0.72	3.10	0.75
	MAXE	38.51	33.49	40.04	32.16	39.24	30.32
	RMSE	8.67	4.48	5.39	4.03	4.99	3.60
	SD	5.61	4.13	4.30	3.97	3.90	3.52
Grambow2020-B97D3(32722)	MAE	8.01	4.08	5.14	3.76	4.78	3.38
	MSE	-7.46	-2.31	4.32	1.43	3.88	1.32
	MAXE	193.94	190.51	212.07	212.66	210.23	210.74
	RMSE	9.86	5.67	7.59	6.22	6.96	5.75
	SD	6.44	5.17	6.24	6.06	5.78	5.60
MN-RE (7555)	MAE	9.06	6.52	8.87	6.09	9.04	5.94
	MSE	2.29	1.04	1.30	1.11	1.95	1.36
	MAXE	61.18	53.95	80.84	53.88	82.57	52.34
	RMSE	12.03	8.81	13.02	8.74	13.50	8.33
	SD	11.81	8.75	12.96	8.67	13.36	8.22
BH9-RE (449)	MAE	5.39	3.12	3.40	2.02	3.49	2.43
	MSE	1.79	-1.02	-1.41	-0.64	-1.56	-1.21
	MAXE	42.25	38.22	38.24	39.52	37.53	38.04
	RMSE	7.31	4.84	5.00	3.82	5.23	4.08
	SD	7.10	4.74	4.81	3.77	5.00	3.90
WCPT6 (6)	MAE	3.71	1.37	2.74	2.42	3.42	2.22
	MSE	3.04	0.84	2.74	1.66	3.12	1.77
	MAXE	6.24	2.08	4.37	4.50	6.01	4.47
	RMSE	3.95	1.51	3.06	2.74	3.75	2.64
	SD	2.77	1.38	1.49	2.39	2.28	2.15
NBPRC (6)	MAE	2.81	1.77	2.13	3.34	1.73	1.84
	MSE	2.67	0.53	1.98	2.95	0.83	1.73

	MAXE	7.56	2.67	3.66	7.99	3.09	5.34
	RMSE	3.64	1.93	2.44	4.08	2.00	2.51
	SD	2.71	2.03	1.56	3.09	1.99	2.00
PlatonicHD6 (6)	MAE	3.90	12.32	7.73	1.63	3.77	4.04
	MSE	-3.65	-12.32	5.93	0.21	3.44	-1.19
	MAXE	8.19	17.60	17.41	3.28	6.02	7.85
	RMSE	4.78	13.45	9.11	1.91	4.17	4.52
	SD	3.38	5.90	7.58	2.07	2.57	4.77
PlatonicID6 (6)	MAE	7.15	11.88	14.99	1.89	17.34	3.10
	MSE	7.15	-11.88	14.30	-1.46	17.34	2.33
	MAXE	13.71	17.16	34.15	2.76	26.81	5.77
	RMSE	8.49	12.98	18.11	2.04	18.23	3.91
	SD	5.00	5.73	12.17	1.56	6.15	3.43
PlatonicIG6 (6)	MAE	5.87	9.23	10.82	4.81	26.80	15.51
	MSE	-5.87	-9.23	9.49	4.75	26.80	15.51
	MAXE	12.63	14.51	24.52	11.19	45.72	25.55
	RMSE	7.03	10.23	12.86	6.16	28.75	16.58
	SD	4.23	4.83	9.51	4.29	11.39	6.42
DC13 (12)	MAE	10.85	5.70	10.34	6.04	9.24	5.91
	MSE	5.66	1.00	-2.52	-3.19	-0.98	-2.40
	MAXE	27.88	11.09	24.49	20.09	30.50	17.53
	RMSE	13.33	6.84	13.20	8.21	12.43	7.93
	SD	12.60	7.06	13.53	7.90	12.94	7.89
DARC (14)	MAE	4.85	2.50	4.99	2.44	5.39	3.78
	MSE	4.58	-2.03	-4.99	-2.44	-5.39	-3.78
	MAXE	7.53	4.96	8.43	4.14	11.51	5.85
	RMSE	5.46	3.08	5.38	2.81	5.94	4.11
	SD	3.09	2.41	2.09	1.46	2.58	1.68
AlkIsod14 (14)	MAE	1.68	0.33	1.75	0.22	2.53	0.72
	MSE	-1.68	-0.02	-1.75	-0.09	-2.53	-0.72
	MAXE	2.92	0.81	3.01	0.62	4.89	1.48
	RMSE	1.81	0.40	1.90	0.28	2.77	0.79
	SD	0.72	0.42	0.76	0.28	1.17	0.34
CR20 (20)	MAE	2.46	2.70	3.92	2.61	4.52	3.34
	MSE	-1.93	2.70	3.92	2.28	4.52	3.27
	MAXE	3.84	7.10	9.42	4.04	9.99	5.05
	RMSE	2.70	3.18	4.64	2.77	5.15	3.55
	SD	1.93	1.72	2.56	1.62	2.53	1.39
RC21 (21)	MAE	8.00	7.18	5.57	2.96	7.15	4.09
	MSE	6.98	5.96	5.24	1.91	7.00	3.85
	MAXE	18.89	15.25	12.76	5.99	17.31	8.03
	RMSE	9.46	8.52	6.30	3.37	8.27	4.70
	SD	6.53	6.23	3.59	2.85	4.51	2.77
G2RC (23)	MAE	13.78	4.97	8.19	3.11	9.60	4.43
	MSE	6.08	0.20	-0.54	-0.11	-0.76	-0.66
	MAXE	42.11	16.73	21.83	7.17	29.37	10.95
	RMSE	17.21	6.50	10.41	3.66	13.09	5.68
	SD	16.47	6.64	10.63	3.74	13.37	5.77
BH76RC (30)	MAE	8.72	4.02	7.35	3.98	8.44	4.43
	MSE	0.21	-0.94	-1.06	-1.85	-1.33	-2.21
	MAXE	46.48	20.72	42.05	21.73	45.54	23.84
	RMSE	13.07	6.12	11.07	5.74	12.12	6.43
	SD	13.29	6.16	11.20	5.52	12.25	6.14
BSR36 (36)	MAE	2.74	2.61	3.62	0.77	4.81	1.03
	MSE	-2.74	2.55	-3.62	0.77	-4.81	0.17

	MAXE	7.01	12.32	12.62	3.15	13.06	5.07
	RMSE	3.15	3.70	4.53	0.99	5.58	1.45
	SD	1.58	2.72	2.76	0.62	2.86	1.46
FH51 (51)	MAE	7.73	3.85	5.62	2.86	6.96	3.78
	MSE	4.12	1.00	0.24	1.22	0.21	0.85
	MAXE	29.45	19.12	20.83	19.86	23.35	20.72
	RMSE	10.86	5.50	8.01	4.82	9.50	5.52
	SD	10.15	5.46	8.09	4.71	9.59	5.51
DIE60 (60)	MAE	2.39	1.12	1.16	0.67	1.29	1.05
	MSE	2.39	1.05	1.11	0.46	1.24	0.85
	MAXE	4.76	2.52	3.07	1.92	3.14	3.05
	RMSE	2.55	1.35	1.44	0.89	1.56	1.43
	SD	0.90	0.85	0.92	0.76	0.95	1.16
PlatonicTAE6 (6)	MAE	3.72	20.28	13.01	26.07	17.30	26.86
	MSE	-3.72	20.28	13.01	-26.07	17.30	-26.86
	MAXE	9.77	32.99	20.16	54.13	42.17	48.56
	RMSE	5.04	22.04	13.52	30.05	21.29	29.25
	SD	3.73	9.46	4.05	16.37	13.59	12.68
AlkAtom19 (19)	MAE	2.62	7.27	2.95	2.82	16.04	2.49
	MSE	2.62	-7.27	-2.74	2.46	-16.04	-2.49
	MAXE	4.62	11.08	5.09	5.60	23.95	4.07
	RMSE	2.78	7.65	3.25	3.19	16.90	2.62
	SD	0.96	2.47	1.80	2.08	5.46	0.86
TAE-W4-17 (194)	MAE	8.94	8.87	8.13	7.06	8.18	6.33
	MSE	3.67	8.02	-6.54	-3.75	-4.46	-1.19
	MAXE	58.07	45.96	76.36	35.76	73.67	45.05
	RMSE	12.85	11.33	13.11	9.19	13.41	8.84
	SD	12.35	8.03	11.39	8.41	12.68	8.79
MOLdef (9298)	MAE	1.39	1.22	0.52	0.64	0.55	0.64
	MSE	-0.53	0.28	0.33	0.22	0.34	0.29
	MAXE	31.78	24.92	15.02	19.46	15.37	15.86
	RMSE	2.47	1.98	0.95	1.31	0.98	1.27
	SD	2.41	1.96	0.90	1.29	0.92	1.24
MOLdef-H2O (990)	MAE	0.90	0.53	0.39	0.16	0.43	0.31
	MSE	-0.30	-0.24	-0.03	0.09	-0.05	0.15
	MAXE	5.52	3.97	3.11	2.03	3.56	2.53
	RMSE	1.40	0.79	0.62	0.27	0.68	0.47
	SD	1.37	0.76	0.61	0.25	0.68	0.45
MOLdef-TS (6294)	MAE	4.76	3.69	1.81	1.80	1.70	1.70
	MSE	4.37	2.44	0.69	0.68	0.71	0.62
	MAXE	101.46	100.80	97.83	98.84	97.79	98.60
	RMSE	7.04	5.71	3.87	3.81	3.77	3.74
	SD	5.52	5.16	3.81	3.74	3.71	3.69
BSE49-expt (1969)	MAE	6.36	4.14	2.76	2.19	3.27	2.89
	MSE	5.96	3.23	-0.16	-0.37	2.84	1.79
	MAXE	26.03	41.84	22.06	18.52	26.34	91.18
	RMSE	7.40	5.30	3.61	3.02	4.36	4.84
	SD	4.37	4.20	3.60	3.00	3.31	4.50
BSE49-non-expt (2533)	MAE	6.35	3.18	3.41	2.40	3.95	2.25
	MSE	5.37	1.08	1.78	0.29	3.43	0.84
	MAXE	26.23	17.78	58.40	59.36	36.18	49.03
	RMSE	7.46	3.98	5.64	4.54	4.99	3.50
	SD	5.18	3.84	5.35	4.53	3.63	3.40

Table S4. Detailed error analysis with respect to reference data in the validation set. The numbers in bracket in the first column indicates the number of data points. The various shorthand notations are as follows: MAE = mean absolute error in kcal/mol, MSE = mean signed error in kcal/mol, MAXE = maximum absolute error in kcal/mol, RMSE = root-mean-square error in kcal/mol, and SD = standard deviation in kcal/mol.

Data set (# of data points)		BLYP-D3/6-31G*	BLYP-D3/6-31G*-ACP	M062X/6-31G*	M062X/6-31G*-ACP	CAMB3LYP-D3/6-31G*	CAMB3LYP-D3/6-31G*-ACP
BlindNCI (80)	MAE	0.99	0.58	0.94	0.31	1.05	0.39
	MSE	-0.96	0.27	-0.80	0.11	-1.04	0.18
	MAXE	5.40	6.72	7.42	2.10	5.92	4.57
	RMSE	1.73	1.30	1.78	0.52	1.82	0.84
	SD	1.45	1.28	1.61	0.51	1.51	0.82
DES15K (11474)	MAE	2.03	1.48	1.50	0.87	2.02	1.18
	MSE	-1.98	0.72	-1.33	0.58	-1.90	0.77
	MAXE	10.74	14.53	10.96	10.07	12.64	14.29
	RMSE	2.44	2.46	1.98	1.25	2.60	1.82
	SD	1.43	2.36	1.47	1.11	1.78	1.64
NENCI-2021 (5859)	MAE	2.14	1.27	1.45	0.90	2.23	1.10
	MSE	-2.02	0.61	-1.16	0.54	-1.97	0.55
	MAXE	8.38	14.77	6.92	12.02	8.59	19.88
	RMSE	2.50	2.07	1.92	1.56	2.77	2.12
	SD	1.48	1.98	1.53	1.46	1.94	2.05
R160x6 (960)	MAE	0.97	1.27	0.68	0.74	0.95	0.87
	MSE	-0.80	1.03	-0.22	0.45	-0.66	0.50
	MAXE	4.73	8.04	6.01	6.68	6.51	7.12
	RMSE	1.27	1.85	1.03	1.06	1.28	1.24
	SD	0.99	1.54	1.00	0.96	1.09	1.13
R739x5 (4330)	MAE	0.81	0.95	0.50	0.45	0.77	0.52
	MSE	-0.77	0.75	-0.29	0.28	-0.72	0.26
	MAXE	5.56	8.51	4.35	4.11	6.40	3.47
	RMSE	1.05	1.39	0.76	0.62	1.08	0.74
	SD	0.72	1.17	0.70	0.56	0.80	0.69
CE20 (20)	MAE	21.46	2.86	15.18	3.30	21.40	3.81
	MSE	21.46	0.88	15.18	3.30	21.40	3.81
	MAXE	45.15	9.01	29.85	5.98	45.16	8.49
	RMSE	24.74	4.08	17.37	3.70	24.69	4.56
	SD	12.62	4.09	8.67	1.72	12.63	2.57
CHAL336 (48)	MAE	2.19	1.27	1.17	1.10	1.71	1.60
	MSE	-1.96	-1.05	-0.97	-1.09	-1.52	-1.60
	MAXE	3.68	9.71	4.88	9.28	3.58	10.91
	RMSE	2.37	2.73	1.36	1.70	1.85	2.22
	SD	1.34	2.55	0.97	1.32	1.07	1.56
XB45 (33)	MAE	6.40	2.81	3.34	6.78	4.07	6.86
	MSE	6.40	2.31	3.21	6.71	4.01	6.76
	MAXE	14.58	11.27	8.47	22.70	8.97	23.53
	RMSE	7.47	4.46	3.96	9.72	4.71	9.94
	SD	3.92	3.87	2.36	7.14	2.50	7.39
WaterOrg (2376)	MAE	3.29	0.77	1.67	0.63	3.17	0.46
	MSE	-3.29	0.50	-1.67	0.61	-3.17	0.34
	MAXE	8.56	2.47	5.02	1.77	7.63	1.83
	RMSE	3.53	0.99	1.87	0.72	3.41	0.56
	SD	1.29	0.86	0.86	0.37	1.26	0.44

H2O20Bind10 (10)	MAE	145.88	24.40	107.24	15.19	154.83	13.15
	MSE	-145.88	24.40	-107.24	-15.19	-154.83	-13.15
	MAXE	154.29	26.52	114.15	17.32	161.66	15.59
	RMSE	145.91	24.47	107.27	15.22	154.85	13.20
	SD	3.27	2.01	2.61	1.12	2.64	1.23
L7 (7)	MAE	7.40	4.76	3.76	2.66	4.28	2.42
	MSE	-7.40	-3.45	1.24	1.98	-4.28	-0.50
	MAXE	10.95	8.46	6.17	10.86	11.51	6.71
	RMSE	7.91	5.36	4.17	4.32	5.54	3.05
	SD	3.03	4.43	4.30	4.16	3.79	3.25
S12L (10)	MAE	17.23	11.28	5.80	5.16	13.47	8.41
	MSE	-17.23	-10.87	-5.80	-4.39	-13.47	-8.25
	MAXE	25.94	33.28	9.61	16.89	20.28	26.51
	RMSE	18.08	16.26	6.13	7.88	14.19	12.62
	SD	5.76	12.74	2.07	6.90	4.71	10.07
S30L (26)	MAE	18.14	13.00	3.10	6.66	13.04	9.18
	MSE	-18.14	-11.38	-2.78	-1.89	-13.04	-7.06
	MAXE	34.15	41.65	12.18	16.21	34.84	30.15
	RMSE	19.56	18.21	4.24	8.08	14.33	12.98
	SD	7.48	14.50	3.27	8.02	6.05	11.11
C60dimer (14)	MAE	3.40	4.49	2.09	0.71	1.78	3.97
	MSE	-3.40	-4.49	2.08	0.05	-1.78	-3.97
	MAXE	7.17	9.74	4.61	1.62	3.12	9.29
	RMSE	3.78	5.10	2.36	0.88	1.99	4.57
	SD	1.73	2.51	1.16	0.91	0.92	2.35
Ni2021 (11)	MAE	27.30	13.61	8.33	22.48	27.07	13.30
	MSE	-26.04	12.91	-2.11	22.48	-25.44	13.16
	MAXE	81.62	57.74	13.91	80.46	78.22	53.41
	RMSE	33.99	19.75	9.62	30.79	33.23	18.87
	SD	22.91	15.67	9.85	22.06	22.42	14.17
HW6Cl-anionic (6)	MAE	21.26	5.32	16.80	5.92	20.79	5.12
	MSE	-21.26	-5.32	-16.80	-5.92	-20.79	-5.12
	MAXE	39.46	8.37	29.18	9.04	38.89	8.15
	RMSE	24.77	5.93	19.26	6.56	24.25	5.77
	SD	13.92	2.86	10.31	3.08	13.66	2.93
HW6F-anionic (6)	MAE	58.73	33.74	47.16	30.73	56.76	32.90
	MSE	-58.73	-33.74	-47.16	-30.73	-56.76	-32.90
	MAXE	87.17	41.57	68.21	39.25	84.79	42.02
	RMSE	62.62	35.13	50.01	31.76	60.53	34.06
	SD	23.80	10.70	18.22	8.80	23.04	9.64
FmH2O10-anionic (10)	MAE	126.92	41.86	99.41	47.18	125.46	48.42
	MSE	-126.92	-41.86	-99.41	-47.18	-125.46	-48.42
	MAXE	128.35	45.12	100.71	47.86	127.16	49.41
	RMSE	126.93	41.90	99.42	47.18	125.47	48.43
	SD	1.68	1.94	1.47	0.53	1.53	0.67
SW49Bind345-anionic (30)	MAE	13.38	2.50	8.73	2.18	12.04	2.60
	MSE	-13.38	-2.50	-8.71	-2.17	-12.03	-2.60
	MAXE	24.84	5.33	16.15	4.05	22.72	4.91
	RMSE	15.90	2.88	10.44	2.57	14.40	3.02
	SD	8.74	1.46	5.84	1.40	8.06	1.55
SW49Bind6-anionic (18)	MAE	30.84	4.61	20.83	5.03	28.66	5.36
	MSE	-30.84	-4.61	-20.83	-5.03	-28.66	-5.36
	MAXE	35.90	6.43	23.16	5.95	32.41	7.05
	RMSE	31.17	4.79	20.95	5.08	28.91	5.49
	SD	4.66	1.36	2.28	0.75	3.89	1.23

Anionpi-anionic (16)	MAE	11.89	7.72	7.89	5.11	8.21	5.58
	MSE	-11.28	-7.09	-7.63	-4.12	-7.78	-3.83
	MAXE	29.83	20.84	23.82	15.59	24.00	16.16
	RMSE	16.08	10.74	10.71	7.12	11.37	7.56
	SD	11.84	8.33	7.76	6.00	8.56	6.73
IL236-anionic (236)	MAE	9.70	4.50	6.31	2.86	7.99	2.98
	MSE	-9.70	-4.47	-6.31	-2.80	-7.99	-2.93
	MAXE	16.78	10.38	12.07	6.74	14.85	7.24
	RMSE	10.09	5.02	6.71	3.31	8.52	3.45
	SD	2.79	2.29	2.27	1.76	2.96	1.81
DES15K-anionic (1281)	MAE	6.73	3.89	5.40	4.34	6.34	4.18
	MSE	-6.63	-2.70	-5.38	-4.27	-6.29	-4.07
	MAXE	46.04	39.88	38.09	35.37	43.60	36.56
	RMSE	10.19	6.73	8.22	6.75	9.52	6.88
	SD	7.73	6.16	6.22	5.23	7.14	5.54
NENCI-2021-anionic (889)	MAE	11.64	7.12	7.08	4.15	8.71	4.92
	MSE	-10.83	-5.99	-5.93	-3.28	-7.25	-3.41
	MAXE	41.36	24.91	37.45	19.90	40.92	20.60
	RMSE	16.31	10.01	9.90	5.93	11.96	6.73
	SD	12.20	8.03	7.94	4.94	9.52	5.80
CHAL336-anionic (19)	MAE	16.95	10.82	10.59	11.27	12.13	13.11
	MSE	-16.95	-10.82	-10.58	-11.27	-12.00	-13.11
	MAXE	40.20	23.96	32.20	30.32	36.18	34.04
	RMSE	22.94	14.09	14.97	14.55	17.56	17.17
	SD	15.88	9.28	10.89	9.46	13.16	11.39
XB45-anionic (12)	MAE	26.99	21.86	22.01	23.06	23.38	24.01
	MSE	26.99	21.86	22.01	23.06	23.38	24.01
	MAXE	73.46	56.63	52.90	47.01	62.09	52.22
	RMSE	35.00	28.57	28.91	28.25	31.40	29.93
	SD	23.28	19.21	19.57	17.04	21.90	18.67
S30L-anionic (2)	MAE	20.66	5.14	14.22	3.40	19.24	2.73
	MSE	-20.66	-5.14	-14.22	-3.40	-19.24	-2.73
	MAXE	21.66	5.54	16.83	5.07	20.30	3.15
	RMSE	20.69	5.15	14.46	3.79	19.27	2.76
	SD	1.41	0.56	3.69	2.36	1.50	0.59
SafroleCONF (5)	MAE	0.53	0.56	0.49	0.50	0.47	0.49
	MSE	-0.53	-0.56	-0.49	-0.50	-0.47	-0.49
	MAXE	1.13	1.26	1.07	1.10	1.08	1.08
	RMSE	0.71	0.78	0.68	0.69	0.68	0.68
	SD	0.53	0.60	0.53	0.54	0.55	0.53
AlcoholCONF (31)	MAE	0.38	0.60	0.25	0.26	0.22	0.35
	MSE	-0.23	-0.48	0.09	-0.03	0.00	0.01
	MAXE	1.23	1.32	0.65	0.74	0.69	0.81
	RMSE	0.48	0.70	0.29	0.30	0.28	0.41
	SD	0.42	0.51	0.28	0.30	0.28	0.42
BeranCONF (50)	MAE	0.77	0.72	0.43	0.47	0.42	0.46
	MSE	-0.04	0.45	-0.02	-0.02	0.12	0.19
	MAXE	2.62	1.70	1.61	1.79	2.68	1.98
	RMSE	0.98	0.81	0.63	0.66	0.62	0.65
	SD	0.99	0.68	0.63	0.66	0.61	0.62
Torsion30 (2107)	MAE	0.65	0.47	0.50	0.32	0.42	0.36
	MSE	0.34	0.32	0.32	0.11	0.26	0.15
	MAXE	9.50	11.50	10.46	11.08	10.81	12.05
	RMSE	1.00	0.90	0.90	0.72	0.84	0.79
	SD	0.95	0.84	0.84	0.72	0.80	0.78

MPCONF196 (112)	MAE	3.16	1.97	2.53	1.19	3.40	1.27
	MSE	1.80	-0.64	1.64	0.50	2.60	0.90
	MAXE	14.12	7.59	12.37	4.12	15.05	4.08
	RMSE	4.44	2.47	3.61	1.53	4.75	1.59
	SD	4.07	2.40	3.23	1.45	4.00	1.32
PEPCONF-Tripeptide (647)	MAE	2.02	1.33	1.61	0.92	1.78	0.95
	MSE	1.35	-0.31	0.97	0.01	1.29	-0.14
	MAXE	9.56	5.05	7.75	3.64	8.32	4.38
	RMSE	2.61	1.67	2.09	1.17	2.30	1.19
	SD	2.23	1.64	1.85	1.17	1.91	1.19
PEPCONF-Disulfide (620)	MAE	2.52	3.52	2.42	3.05	2.60	3.12
	MSE	0.95	-2.46	0.26	-1.98	1.10	-2.11
	MAXE	10.30	20.04	13.57	20.63	9.90	20.97
	RMSE	3.18	4.69	3.16	4.28	3.29	4.34
	SD	3.04	3.99	3.15	3.80	3.10	3.79
PEPCONF-Cyclic (320)	MAE	2.85	2.31	1.81	1.77	2.30	1.53
	MSE	-0.80	-0.06	-0.09	-1.21	1.48	0.64
	MAXE	14.00	12.41	8.78	11.54	14.85	6.55
	RMSE	3.69	2.94	2.31	2.30	3.14	1.92
	SD	3.60	2.94	2.31	1.96	2.77	1.82
PEPCONF-Bioactive (175)	MAE	2.18	1.41	1.54	1.00	1.86	1.11
	MSE	1.39	-0.12	0.66	-0.32	1.30	-0.38
	MAXE	8.14	7.48	6.06	3.61	7.19	4.02
	RMSE	2.78	1.91	1.99	1.28	2.40	1.41
	SD	2.41	1.91	1.89	1.24	2.02	1.36
PEPCONF-Disulfide-anionic (150)	MAE	2.13	5.54	3.37	5.53	2.31	5.63
	MSE	-1.15	-4.84	-2.38	-4.65	-1.30	-4.70
	MAXE	8.44	22.17	13.67	22.47	8.38	22.48
	RMSE	2.73	7.06	4.50	7.36	2.91	7.38
	SD	2.48	5.15	3.83	5.72	2.61	5.70
PEPCONF-Bioactive-anionic (20)	MAE	1.30	0.99	1.49	1.09	1.28	1.17
	MSE	0.76	-0.01	0.77	-0.24	0.84	-0.25
	MAXE	3.94	2.40	3.36	3.75	2.67	3.37
	RMSE	1.58	1.25	1.72	1.51	1.47	1.50
	SD	1.42	1.28	1.58	1.53	1.24	1.52
ANI1ccxCONF (5254)	MAE	3.56	2.76	1.82	1.72	2.06	1.68
	MSE	-0.57	-0.29	0.76	0.61	1.09	0.90
	MAXE	29.37	20.68	17.24	12.10	22.80	11.12
	RMSE	5.04	3.71	2.97	2.28	3.64	2.25
	SD	5.01	3.70	2.87	2.20	3.47	2.06
W4-17-RE (5205)	MAE	13.00	6.52	11.13	7.67	11.17	7.32
	MSE	-0.52	-0.28	0.38	0.39	0.04	0.35
	MAXE	91.81	32.79	76.44	54.11	78.35	54.91
	RMSE	18.27	8.14	16.59	10.64	16.77	10.40
	SD	18.27	8.14	16.58	10.64	16.77	10.40
WaterOrgBH (88)	MAE	14.05	9.21	2.31	1.56	1.70	1.66
	MSE	-14.05	-9.21	0.80	-1.52	0.87	-1.36
	MAXE	18.89	12.70	5.12	4.51	5.02	4.40
	RMSE	14.46	9.34	2.63	1.82	2.12	1.90
	SD	3.46	1.56	2.52	1.00	1.95	1.33