The Transferability Limits of Static Benchmarks

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Supplementary Information

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Table 1: Overview of the individual subsets present in the data set compiled by Mardirossian and Head-Gordon.[1] "Uncertainty Labels" (UL, see main text for their definition) are given for selected generalized gradient approximation (GGA) and meta-GGA density functionals. The descriptions of the subsets have been adapted from Ref. 1.

Subset	Description	#	UL (PBE)	UL (B97-D3(0))	UL (TPSS)	UL (B97M-rV)
3B-69-DIM	Binding energies of all relevant pairs of monomers from 3B-69-TRIM	207	0.0, 2.0	0.0, 2.1	0.0, 1.6	0.0, 2.1
3B-69-TRIM	Binding energies of trimers (three different orientations of 23 distinct molecular crystals)	69	0.0, 0.4	0.0, 0.7	−0.1, −0.5	0.0, 0.7
A21x12	Potential energy curves (PECS) for the 21 equilibrium complexes from A24	252	0.0, 2.6	0.0, 2.6	0.0, 2.6	0.0, 2.6
A24	Binding energies of small non-covalent complexes	24	0.0, 0.2	0.0, 0.2	0.0, 0.2	0.0, 0.2
ACONF	Isomerisation energies of alkane conformers	15	0.0, 0.1	0.0, 0.2	0.0, 0.1	0.0, 0.2
AE18	Absolute atomic energies of hydrogen through argon	18	−3.0, −15.2	−0.7, −1.6	−0.3, −2.7	−6.6, −23.0
AlkAtom19	n = 1 − 8 alkane atomisation energies	19	−0.1, −0.6	−0.1, −0.8	0.0, 0.1	0.0, 0.2

AlkBind12	Binding energies of saturated and unsaturated hydrocarbon dimers	12	0.0, 0.1	0.0, 0.1	0.0, 0.0	0.0, 0.1
AlkIsod14	n = 3−8 alkane isodesmic reaction energies	14	0.0, 0.1	0.0, 0.1	−0.1, −0.1	0.0, 0.1
AlkIsomer11	Isomerisation energies of n = 4−8 alkanes	11	0.0, 0.1	0.0, 0.1	0.0, 0.1	0.0, 0.1
Bauza30	Binding energies of halogen-, chalcogen-, and pnicogen-bonded dimers	30	0.0, 0.2	0.0, 0.2	0.0, 0.2	0.0, 0.2
BDE99MR	Bond dissociation energies (multi-reference cases)	16	−0.1, −0.4	0.0, −0.2	0.0, −0.1	0.0, 0.0
BDE99nonMR	Bond dissociation energies (single-reference cases)	83	−0.1, −0.5	−0.1, 0.1	0.0, 0.0	−0.2, −0.2
BH76RC	Reaction energies from HTBH38 and NHTBH38	30	−0.1, 0.1	−0.1, 0.1	0.0, 0.0	−0.1, 0.1
BHPERI26	Barrier heights of pericyclic reactions	26	0.0, 0.2	0.0, 0.1	0.0, 0.2	0.0, 0.2
BSR36	Hydrocarbon bond separation reaction energies	36	−0.1, −0.3	−0.2, −0.7	−0.3, −1.8	0.0, 0.4
Butanediol65	Isomerisation energies of butane-1,4-diol	65	0.0, 0.7	0.0, 0.7	0.0, 0.7	0.0, 0.7
BzDC215	PECs for benzene interacting with two rare-gas atoms and eight first- and second-row hydrides	215	0.0, 2.2	0.0, 2.2	0.0, 2.0	0.0, 2.2
C20C24	Isomerisation energies of the ground state structures of C_{20} and C_{24}	8	−0.6, −0.9	−4.1, −9.1	−2.3, −3.7	−3.3, −5.2

CE20	Binding energies of water, ammonia, and hydrogen fluoride clusters	20	0.0, 0.2	0.0, 0.2	0.0, 0.1	0.0, 0.2
CO2Nitrogen16	Binding energies of CO_2 to molecular models of pyridinic N-doped graphene	16	0.0, 0.1	0.0, 0.2	0.0, 0.1	0.0, 0.2
CR20	Cycloreversion reaction energies	20	0.0, 0.2	−0.1, −1.3	0.0, −0.1	0.0, 0.1
CRBH20	Barrier heights for cycloreversion of heterocyclic rings	20	0.0, −0.1	−0.2, −2.4	−0.1, −0.6	−0.1, −1.0
CT20	Binding energies of charge-transfer complexes	20	0.0, 0.2	0.0, 0.2	0.0, 0.2	0.0, 0.2
CYCONF	Isomerisation energies of cysteine conformers	11	0.0, 0.1	0.0, 0.1	0.0, 0.1	0.0, 0.1
DBH24	Diverse barrier heights	24	−0.2, −0.2	−0.2, −0.4	−0.2, −0.6	−0.1, −0.4
DIE60	Isomerisation energies of reactions involving double-bond migration in conjugated dienes	60	0.0, 0.6	0.0, 0.5	0.0, 0.5	0.0, 0.4
DS14	Binding energies of complexes containing divalent sulfur	14	0.0, 0.1	0.0, 0.1	0.0, 0.1	0.0, 0.1
EA13	Adiabatic electron affinities	13	0.0, 0.1	0.0, 0.0	0.0, 0.1	0.0, 0.1
EIE22	Isomerisation energies of enecarbonyls	22	0.0, 0.2	0.0, 0.2	0.0, 0.2	0.0, 0.1
FmH2O10	Binding energies of isomers of $F^-(H_2O)_{10}$	10	0.0, 0.0	0.0, −0.2	−0.1, −1.0	0.0, 0.1
G21EA	Adiabatic electron affinities of atoms and small molecules	25	0.0, 0.2	0.0, 0.1	0.0, 0.1	0.0, 0.1

G21IP	Adiabatic ionisation potentials of atoms and small molecules	36	0.0, 0.2	0.0, 0.0	0.0, 0.0	−0.1, −0.1
H2O16Rel5	Isomerisation energies of $(H_2O)_{16}$ (boat and fused cube structures)	5	0.0, 0.0	0.0, 0.0	0.0, 0.0	0.0, 0.0
H2O20Bind10	Binding energies of isomers of $(H_2O)_{20}$ (low-energy structures)	10	0.0, −0.2	−0.1, −1.3	−0.5, −3.9	0.0, 0.1
H2O20Bind4	Binding energies of isomers of $(H_2O)_{20}$ (dod, fc, fs, and es)	4	0.0, 0.0	0.0, −0.1	−0.2, −0.6	0.0, 0.0
H2O20Rel10	Isomerisation energies of $(H_2O)_{20}$ (low-energy structures)	10	0.0, 0.1	0.0, 0.1	0.0, 0.1	0.0, 0.1
H2O20Rel4	Isomerisation energies of $(H_2O)_{20}$ (dod, fc, fs, and es)	4	0.0, 0.0	0.0, 0.0	0.0, 0.0	0.0, 0.0
H2O6Bind8	Binding energies of isomers of $(H_2O)_6$	8	0.0, 0.1	0.0, 0.0	0.0, 0.0	0.0, 0.1
HAT707MR	Heavy-atom transfer energies (multi-reference cases)	202	−0.1, −1.4	−0.2, −3.8	−0.1, −3.1	−0.1, −0.3
HAT707nonMR	Heavy-atom transfer energies (single-reference cases)	505	−0.1, −0.8	−0.1, −2.1	−0.1, −2.6	−0.1, −3.0
HB15	Binding energies of hydrogen-bonded dimers featuring ionic groups common in biomolecules	15	0.0, 0.1	0.0, 0.1	0.0, 0.1	0.0, 0.1
HB49	Binding energies of small- and medium-sized hydrogen-bonded systems	49	0.0, 0.5	0.0, 0.5	0.0, 0.5	0.0, 0.5
HNBrBDE18	Homolytic N–Br bond dissociation energies	18	0.0, 0.2	0.0, −0.2	0.0, 0.1	0.0, −0.1

HSG	Binding energies of small ligands interacting with protein receptors	21	0.0, 0.2	0.0, 0.2	0.0, 0.2	0.0, 0.2
HTBH38	Hydrogen transfer barrier heights	38	−0.1, −0.4	−0.1, −0.9	−0.1, −0.7	−0.1, −0.4
HW30	Binding energies of hydrocarbon-water dimers	30	0.0, 0.3	0.0, 0.3	0.0, 0.3	0.0, 0.3
HW6Cl	Binding energies of Cl–$(H_2O)_n$ (n = 1 – 6	6	0.0, 0.1	0.0, 0.1	0.0, 0.0	0.0, 0.1
HW6F	Binding energies of F–$(H_2O)_n$ (n = 1 – 6)	6	0.0, 0.1	0.0, 0.0	0.0, 0.0	0.0, 0.1
Ionic43	Binding energies of anion-neutral, cation-neutral, and anion-cation dimers	43	0.0, 0.4	0.0, 0.4	0.0, 0.4	0.0, 0.4
IP13	Adiabatic ionisation potentials	13	0.0, 0.1	0.0, 0.0	0.0, 0.0	0.0, −0.1
ISOMERIZATION20	Isomerisation energies	20	0.0, 0.1	0.0, 0.1	0.0, 0.1	0.0, 0.0
Melatonin52	Isomerisation energies of melatonin	52	0.0, 0.5	0.0, 0.5	0.0, 0.4	0.0, 0.5
NBC10	PECs for methane dimer and dimers of small aromatic systems	184	0.0, 1.6	0.0, 1.9	0.0, 0.9	0.0, 1.9
NBPRC	Reactions involving NH3/BH3 and PH3/BH3	12	0.0, 0.1	−0.1, 0.0	0.0, 0.1	0.0, 0.1
NC15	Binding energies of very small non-covalent complexes	15	0.0, 0.2	0.0, 0.2	0.0, 0.2	0.0, 0.2
NHTBH38	Non-hydrogen transfer barrier heights	38	−0.2, −0.4	−0.2, −0.7	−0.2, −1.2	−0.2, −0.7
Pentane14	Isomerisation energies of stationary points on the n-pentane torsional surface	14	0.0, 0.1	0.0, 0.1	0.0, 0.1	0.0, 0.1

PlatonicHD6	Homodesmotic reactions involving platonic hydrocarbon cages, C_nH_n (n = 4, 6, 8, 10, 12, 20)	6	−0.1, −0.5	−0.2, −0.3	−0.7, −3.2	−0.1, −0.1
PlatonicID6	Isodesmic reactions involving platonic hydrocarbon cages, C_nH_n (n = 4, 6, 8, 10, 12, 20)	6	−0.1, −0.1	−0.5, −0.7	−0.2, −0.4	−0.1, −0.1
PlatonicIG6	Isogyric reactions involving platonic hydrocarbon cages, C_nH_n (n = 4, 6, 8, 10, 12, 20)	6	−0.3, −0.3	−0.2, −0.4	−0.4, −0.5	−1.7, −2.6
PlatonicTAE6	Total atomisation energies of platonic hydrocarbon cages, C_nH_n (n = 4, 6, 8, 10, 12, 20)	6	−2.0, −4.9	−3.9, −6.1	−0.8, −0.9	0.0, −0.1
PX13	Barrier heights for proton exchange in water, ammonia, and hydrogen fluoride clusters	13	−0.1, −0.3	0.0, −0.1	−0.1, −0.2	0.0, 0.1
RG10	PECs for the 10 rare-gas dimers involving helium through krypton	569	0.0, 6.2	0.0, 6.2	0.0, 6.2	0.0, 6.2
S22	Binding energies of hydrogen-bonded and dispersion-bound non-covalent complexes	22	0.0, 0.2	0.0, 0.2	−0.1, 0.0	0.0, 0.2
S66	Binding energies of non-covalent interactions found in organic molecules and biomolecules	66	0.0, 0.6	0.0, 0.7	0.0, 0.3	0.0, 0.7
S66x8	PECs for the 66 complexes from S66	528	0.0, 5.2	0.0, 5.7	0.0, 3.8	0.0, 5.7
Shields38	Binding energies of $(H_2O)_n$ (n = 2−10)	38	0.0, 0.4	0.0, 0.3	0.0, 0.2	0.0, 0.4

SN13	Nucleophilic substitution energies	13	0.0, 0.0	0.0, 0.0	0.0, 0.0	0.0, 0.1
Styrene45	Isomerisation energies of C_8H_8	45	0.0, 0.3	−0.1, −0.7	−0.1, 0.1	−0.1, −0.4
SW49Bind345	Binding energies of isomers of $SO_4^{2-}(H_2O)_n$ (n = 3 − 5)	31	0.0, 0.3	0.0, 0.3	0.0, 0.2	0.0, 0.3
SW49Bind6	Binding energies of isomers of $SO_4^{2-}(H_2O)_6$	18	0.0, 0.2	0.0, 0.2	0.0, −0.1	0.0, 0.2
SW49Rel345	Isomerisation energies of $SO_4^{2-}(H_2O)_n$ (n = 3 − 5)	31	0.0, 0.3	0.0, 0.3	0.0, 0.3	0.0, 0.3
SW49Rel6	Isomerisation energies of $SO_4^{2-}(H_2O)_6$	18	0.0, 0.2	0.0, 0.2	0.0, 0.2	0.0, 0.2
TA13	Binding energies of dimers involving radicals	13	0.0, 0.0	−0.1, −0.1	−0.1, 0.0	−0.1, −0.1
TAE140MR	Total atomisation energies (multi-reference cases)	16	−0.6, −2.7	−0.3, −1.0	−0.2, −0.7	−0.1, −0.4
TAE140nonMR	Total atomisation energies (single-reference cases)	124	−0.3, −5.9	−0.2, −0.1	−0.1, −0.3	−0.7, −0.7
WATER27	Binding energies of neutral and charged water clusters	23	0.0, 0.2	0.0, 0.2	0.0, 0.1	0.0, 0.2
WCPT27	Barrier heights of water-catalysed proton-transfer reactions	27	−0.1, −0.3	−0.1, −0.2	0.0, −0.1	0.0, 0.1
WCPT6	Tautomerisation energies for water-catalysed proton-transfer reactions	6	0.0, 0.1	0.0, 0.1	0.0, 0.1	0.0, 0.1
X40	Binding energies of non-covalent interactions involving halogenated molecules	31	0.0, 0.3	0.0, 0.3	0.0, 0.2	0.0, 0.3

XB18	Binding energies of small halogen-bonded dimers	8	0.0, 0.1	0.0, 0.1	0.0, 0.1	0.0, 0.1
XB51	Binding energies of large halogen-bonded dimers	20	0.0, 0.2	0.0, 0.2	0.0, 0.2	0.0, 0.2
YMPJ519	Isomerisation energies of the proteinogenic amino acids	519	0.0, 5.6	0.0, 5.5	0.0, 5.4	0.0, 5.6

Table 2: Overview of the individual subsets present in the data set compiled by Mardirossian and Head-Gordon.[1] "Uncertainty Labels" (UL, see main text for their definition) are given for selected generalized gradient approximation (GGA) and meta-GGA density functionals. The descriptions of the subsets have been adapted from Ref. 1.

Subset	Description	#	UL (PBE0)	UL (ωB97M-V)
3B-69-DIM	Binding energies of all relevant pairs of monomers from 3B-69-TRIM	207	0.0, 1.8	0.0, 2.1
3B-69-TRIM	Binding energies of trimers (three different orientations of 23 distinct molecular crystals)	69	0.0, 0.0	0.0, 0.7
A21x12	Potential energy curves (PECS) for the 21 equilibrium complexes from A24	252	0.0, 2.6	0.0, 2.6
A24	Binding energies of small non-covalent complexes	24	0.0, 0.2	0.0, 0.2
ACONF	Isomerisation energies of alkane conformers	15	0.0, 0.1	0.0, 0.2
AE18	Absolute atomic energies of hydrogen through argon	18	−4.7, −25.9	−0.4, −2.3
AlkAtom19	n = 1−8 alkane atomisation energies	19	0.0, 0.2	0.0, 0.1

AlkBind12	Binding energies of saturated and unsaturated hydrocarbon dimers	12	0.0, 0.0	0.0, 0.1
AlkIsod14	n = 3 – 8 alkane isodesmic reaction energies	14	0.0, 0.0	0.0, 0.1
AlkIsomer11	Isomerisation energies of n = 4 – 8 alkanes	11	0.0, 0.1	0.0, 0.1
Bauza30	Binding energies of halogen-, chalcogen-, and pnicogen-bonded dimers	30	0.0, 0.2	0.0, 0.3
BDE99MR	Bond dissociation energies (multi-reference cases)	16	0.0, 0.0	−0.3, −1.0
BDE99nonMR	Bond dissociation energies (single-reference cases)	83	−0.1, 0.1	−0.5, −1.2
BH76RC	Reaction energies from HTBH38 and NHTBH38	30	0.0, 0.2	0.0, 0.1
BHPERI26	Barrier heights of pericyclic reactions	26	0.0, 0.2	−0.1, 0.0
BSR36	Hydrocarbon bond separation reaction energies	36	−0.2, −1.2	0.0, 0.2
Butanediol65	Isomerisation energies of butane-1,4-diol	65	0.0, 0.7	0.0, 0.7
BzDC215	PECs for benzene interacting with two rare-gas atoms and eight first- and second-row hydrides	215	0.0, 2.1	0.0, 2.2
C20C24	Isomerisation energies of the ground state structures of C_{20} and C_{24}	8	−0.5, −0.8	−0.7, −1.5

CE20	Binding energies of water, ammonia, and hydrogen fluoride clusters	20	0.0, 0.2	0.0, 0.2
CO2Nitrogen16	Binding energies of CO_2 to molecular models of pyridinic N-doped graphene	16	0.0, 0.1	0.0, 0.2
CR20	Cycloreversion reaction energies	20	0.0, 0.2	0.0, 0.2
CRBH20	Barrier heights for cycloreversion of heterocyclic rings	20	0.0, 0.2	0.0, 0.1
CT20	Binding energies of charge-transfer complexes	20	0.0, 0.2	0.0, 0.2
CYCONF	Isomerisation energies of cysteine conformers	11	0.0, 0.1	0.0, 0.1
DBH24	Diverse barrier heights	24	−0.1, 0.0	0.0, 0.0
DIE60	Isomerisation energies of reactions involving double-bond migration in conjugated dienes	60	0.0, 0.5	0.0, 0.5
DS14	Binding energies of complexes containing divalent sulfur	14	0.0, 0.1	0.0, 0.1
EA13	Adiabatic electron affinities	13	0.0, 0.1	−0.1, −0.1
EIE22	Isomerisation energies of enecarbonyls	22	0.0, 0.2	0.0, 0.2
FmH2O10	Binding energies of isomers of $F^-(H_2O)_{10}$	10	0.0, 0.0	0.0, 0.1
G21EA	Adiabatic electron affinities of atoms and small molecules	25	0.0, 0.1	−0.2, −0.5

G21IP	Adiabatic ionisation potentials of atoms and small molecules	36	0.0, 0.0	−0.3, −1.6
H2O16Rel5	Isomerisation energies of $(H_2O)_{16}$ (boat and fused cube structures)	5	0.0, 0.0	0.0, 0.1
H2O20Bind10	Binding energies of isomers of $(H_2O)_{20}$ (low-energy structures)	10	−0.1, −0.4	0.0, 0.1
H2O20Bind4	Binding energies of isomers of $(H_2O)_{20}$ (dod, fc, fs, and es)	4	0.0, −0.1	0.0, 0.0
H2O20Rel10	Isomerisation energies of $(H_2O)_{20}$ (low-energy structures)	10	0.0, 0.1	0.0, 0.1
H2O20Rel4	Isomerisation energies of $(H_2O)_{20}$ (dod, fc, fs, and es)	4	0.0, 0.0	0.0, 0.0
H2O6Bind8	Binding energies of isomers of $(H_2O)_6$	8	0.0, 0.1	0.0, 0.1
HAT707MR	Heavy-atom transfer energies (multi-reference cases)	202	−0.1, 0.2	−0.4, −13.2
HAT707nonMR	Heavy-atom transfer energies (single-reference cases)	505	−0.1, −1.4	−0.4, −10.3
HB15	Binding energies of hydrogen-bonded dimers featuring ionic groups common in biomolecules	15	0.0, 0.1	0.0, 0.1
HB49	Binding energies of small- and medium-sized hydrogen-bonded systems	49	0.0, 0.5	0.0, 0.5
HNBrBDE18	Homolytic N–Br bond dissociation energies	18	0.0, 0.1	−0.1, −0.3

HSG	Binding energies of small ligands interacting with protein receptors	21	0.0, 0.2	0.0, 0.2
HTBH38	Hydrogen transfer barrier heights	38	0.0, 0.0	−0.1, −0.1
HW30	Binding energies of hydrocarbon-water dimers	30	0.0, 0.3	0.0, 0.3
HW6Cl	Binding energies of Cl–$(H_2O)_n$ (n = 1–6	6	0.0, 0.1	0.0, 0.1
HW6F	Binding energies of F–$(H_2O)_n$ (n = 1–6)	6	0.0, 0.1	0.0, 0.1
Ionic43	Binding energies of anion-neutral, cation-neutral, and anion-cation dimers	43	0.0, 0.4	0.0, 0.4
IP13	Adiabatic ionisation potentials	13	0.0, 0.0	−0.1, −0.4
ISOMERIZATION20	Isomerisation energies	20	0.0, 0.1	−0.1, −0.1
Melatonin52	Isomerisation energies of melatonin	52	0.0, 0.4	0.0, 0.5
NBC10	PECs for methane dimer and dimers of small aromatic systems	184	0.0, 1.1	0.0, 1.9
NBPRC	Reactions involving NH3/BH3 and PH3/BH3	12	0.0, 0.1	0.0, 0.1
NC15	Binding energies of very small non-covalent complexes	15	0.0, 0.2	0.0, 0.2
NHTBH38	Non-hydrogen transfer barrier heights	38	−0.1, 0.0	−0.1, −0.2
Pentane14	Isomerisation energies of stationary points on the n-pentane torsional surface	14	0.0, 0.1	0.0, 0.1

PlatonicHD6	Homodesmotic reactions involving platonic hydrocarbon cages, C_nH_n (n = 4, 6, 8, 10, 12, 20)	6	−0.1, −0.6	−0.1, −0.4
PlatonicID6	Isodesmic reactions involving platonic hydrocarbon cages, C_nH_n (n = 4, 6, 8, 10, 12, 20)	6	−0.4, −0.4	0.0, 0.0
PlatonicIG6	Isogyric reactions involving platonic hydrocarbon cages, C_nH_n (n = 4, 6, 8, 10, 12, 20)	6	−1.3, −1.9	−0.7, −1.0
PlatonicTAE6	Total atomisation energies of platonic hydrocarbon cages, C_nH_n (n = 4, 6, 8, 10, 12, 20)	6	−1.1, −2.8	−0.1, −0.3
PX13	Barrier heights for proton exchange in water, ammonia, and hydrogen fluoride clusters	13	0.0, −0.2	−0.1, −0.2
RG10	PECs for the 10 rare-gas dimers involving helium through krypton	569	0.0, 6.2	0.0, 6.2
S22	Binding energies of hydrogen-bonded and dispersion-bound non-covalent complexes	22	0.0, 0.1	0.0, 0.2
S66	Binding energies of non-covalent interactions found in organic molecules and biomolecules	66	0.0, 0.5	0.0, 0.7
S66x8	PECs for the 66 complexes from S66	528	0.0, 4.4	0.0, 5.7
Shields38	Binding energies of $(H_2O)_n$ (n = 2 – 10)b	38	0.0, 0.4	0.0, 0.3

SN13	Nucleophilic substitution energies	13	0.0, 0.1	0.0, 0.1
Styrene45	Isomerisation energies of C_8H_8	45	0.0, 0.2	−0.1, −0.2
SW49Bind345	Binding energies of isomers of $SO_4{}^{2-}(H_2O)_n$ (n = 3−5)	31	0.0, 0.3	0.0, 0.3
SW49Bind6	Binding energies of isomers of $SO_4{}^{2-}(H_2O)_6$	18	0.0, 0.1	0.0, 0.2
SW49Rel345	Isomerisation energies of $SO_4{}^{2-}(H_2O)_n$ (n = 3−5)	31	0.0, 0.3	0.0, 0.3
SW49Rel6	Isomerisation energies of $SO_4{}^{2-}(H_2O)_6$	18	0.0, 0.2	0.0, 0.2
TA13	Binding energies of dimers involving radicals	13	0.0, 0.1	−0.2, −0.3
TAE140MR	Total atomisation energies (multi-reference cases)	16	0.0, 0.1	−1.1, −1.6
TAE140nonMR	Total atomisation energies (single-reference cases)	124	−0.2, 0.0	−0.3, −1.2
WATER27	Binding energies of neutral and charged water clusters	23	0.0, 0.2	0.0, 0.2
WCPT27	Barrier heights of water-catalysed proton-transfer reactions	27	0.0, −0.1	−0.1, −0.1
WCPT6	Tautomerisation energies for water-catalysed proton-transfer reactions	6	0.0, 0.1	0.0, 0.1
X40	Binding energies of non-covalent interactions involving halogenated molecules	31	0.0, 0.3	0.0, 0.3

XB18	Binding energies of small halogen-bonded dimers	8	0.0, 0.1	0.0, 0.1
XB51	Binding energies of large halogen-bonded dimers	20	0.0, 0.2	0.0, 0.2
YMPJ519	Isomerisation energies of the proteinogenic amino acids	519	0.0, 5.4	0.0, 5.4

References

[1] Mardirossian, N.; Head-Gordon, M. Thirty years of density functional theory in computational chemistry: an overview and extensive assessment of 200 density functionals. *Mol. Phys.* **2017**, *115*, 2315–2372.