

Supporting Information for: “Simplified tuning of long-range corrected density functionals for use in symmetry-adapted perturbation theory”

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Table S1: Range-separation parameters (in units of bohr<sup>-1</sup>) for monomers *A* and *B* of the S66 data set.

Dimer	$\omega_{\text{GDD}A}$	$\omega_{\text{IE}A}$	$\omega_{\text{GDD}B}$	$\omega_{\text{IE}B}$
Water–Water	0.505	0.513	0.503	0.513
Water–MeOH	0.505	0.513	0.430	0.445
Water–MeNH <sub>2</sub>	0.504	0.512	0.412	0.403
Water–Peptide	0.505	0.512	0.351	0.357
MeOH–MeOH	0.429	0.446	0.430	0.445
MeOH–MeNH <sub>2</sub>	0.428	0.445	0.412	0.403
MeOH–Peptide	0.429	0.446	0.352	0.345
MeOH–Water	0.429	0.446	0.503	0.513
MeNH <sub>2</sub> –MeOH	0.411	0.403	0.427	0.446
MeNH <sub>2</sub> –MeNH <sub>2</sub>	0.413	0.403	0.411	0.403
MeNH <sub>2</sub> –Peptide	0.413	0.403	0.352	0.345
MeNH <sub>2</sub> –Water	0.412	0.403	0.505	0.512
Peptide–MeOH	0.352	0.363	0.429	0.445
Peptide–MeNH <sub>2</sub>	0.351	0.366	0.410	0.403
Peptide–Peptide	0.350	0.358	0.350	0.358
Peptide–Water	0.351	0.356	0.507	0.513
Uracil–Uracil	0.341	0.305	0.342	0.307
Water–Pyridine	0.502	0.512	0.354	0.336
MeOH–Pyridine	0.428	0.446	0.355	0.337
AcOH–AcOH	0.391	0.383	0.391	0.383
AcNH <sub>2</sub> –AcNH <sub>2</sub>	0.377	0.477	0.377	0.477
AcOH–Uracil	0.392	0.383	0.342	0.307
AcNH <sub>2</sub> –Uracil	0.378	0.477	0.342	0.307
Benzene–Benzene	0.344	0.288	0.344	0.288
Pyridine–Pyridine	0.352	0.329	0.351	0.329
Uracil–Uracil	0.343	0.306	0.343	0.306
Benzene–Pyridine	0.339	0.287	0.353	0.329
Benzene–Uracil	0.345	0.287	0.343	0.306
Pyridine–Uracil	0.354	0.330	0.343	0.306
Benzene–Ethene	0.341	0.287	0.425	0.364
Uracil–Ethene	0.342	0.306	0.423	0.364
Uracil–Ethyne	0.342	0.306	0.438	0.403
Pyridine–Ethene	0.348	0.329	0.418	0.364
Pentane–Pentane	0.323	0.375	0.323	0.375
Neopentane–Pentane	0.323	0.375	0.328	0.296
Neopentane–Neopentane	0.329	0.297	0.329	0.297
Cyclopentane–Neopentane	0.338	0.346	0.327	0.281
Cyclopentane–Cyclopentane	0.337	0.346	0.338	0.346
Benzene–Cyclopentane	0.341	0.287	0.336	0.346
Benzene–Neopentane	0.342	0.287	0.328	0.281
Uracil–Pentane	0.341	0.306	0.322	0.375

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**Table S1 – continued from previous page**

Dimer	$\omega_{\text{GDD}A}$	$\omega_{\text{IE}A}$	$\omega_{\text{GDD}B}$	$\omega_{\text{IE}B}$
Uracil–Cyclopentane	0.343	0.306	0.338	0.346
Uracil–Neopentane	0.343	0.306	0.327	0.281
Ethene–Pentane	0.424	0.364	0.324	0.379
Ethyne–Pentane	0.435	0.403	0.324	0.386
Peptide–Pentane	0.351	0.353	0.323	0.383
Benzene–Benzene	0.338	0.288	0.340	0.288
Pyridine–Pyridine	0.350	0.331	0.353	0.329
Benzene–Pyridine	0.338	0.288	0.349	0.329
Benzene–Ethyne	0.342	0.287	0.437	0.403
Ethyne–Ethyne	0.435	0.100	0.437	0.403
Benzene–AcOH	0.337	0.288	0.391	0.386
Benzene–AcNH <sub>2</sub>	0.339	0.287	0.379	0.470
Benzene–Water	0.341	0.287	0.502	0.513
Benzene–MeOH	0.343	0.287	0.429	0.446
Benzene–MeNH <sub>2</sub>	0.343	0.288	0.411	0.403
Benzene–Peptide	0.344	0.288	0.351	0.348
Pyridine–Pyridine	0.355	0.332	0.355	0.332
Ethyne–Water	0.436	0.403	0.504	0.513
Ethyne–AcOH	0.437	0.403	0.391	0.386
Pentane–AcOH	0.322	0.375	0.394	0.387
Pentane–AcNH <sub>2</sub>	0.323	0.382	0.377	0.472
Benzene–AcOH	0.340	0.288	0.391	0.388
Peptide–Ethene	0.350	0.347	0.424	0.364
Pyridine–Ethyne	0.353	0.333	0.437	0.402
MeNH <sub>2</sub> –Pyridine	0.412	0.403	0.349	0.331

Table S2: Range-separation parameters (in units of bohr<sup>-1</sup>) for monomers *A* and *B* of the L7 data set.

Dimer	$\omega_{\text{GDD}A}$	$\omega_{\text{IE}A}$	$\omega_{\text{GDD}B}$	$\omega_{\text{IE}B}$
Coronene–Coronene (C2C2PD)	0.273	0.211	0.273	0.211
GC Base Pair–GC Base Pair (GCGC)	0.296	0.254	0.296	0.254
Guanine Trimer (GGG)	0.321	0.271	0.297	0.248
Octadecane–Octadecane (CBH)	0.260	0.254	0.260	0.254
Phenylalanine Trimer (PHE)	0.295	0.245	0.272	0.241
Circumcoronene–Adenine (C3A)	0.321	0.280	0.248	0.171
Circumcoronene–GC Base Pair (C3GC)	0.295	0.248	0.248	0.171

Table S3: Range-separation parameters (in units of bohr<sup>-1</sup>) for monomers *A* and *B* of the DNA–ellipticine complex.

Dimer	$\omega_{\text{GDD}A}$	$\omega_{\text{IE}A}$
DNA Double Strand	0.242	0.308
Ellipticine	0.282	0.205

Table S4: Error statistics (in kcal/mol) for SAPT0(KS) methods applied to the S66 database and three subsets thereof, using the aug-cc-pVTZ basis set.

Method	H-Bonded		Disp.-Bound		Mixed		All S66	
	MAE <sup>a</sup>	Max <sup>b</sup>	MAE <sup>a</sup>	Max <sup>b</sup>	MAE <sup>a</sup>	Max <sup>b</sup>	MAE <sup>a</sup>	Max <sup>b</sup>
SAPT0(HF)	1.00	3.26	0.72	2.02	0.34	0.87	0.70	3.26
SAPT0(HF) + $\delta$ HF	1.03	3.27	1.09	2.70	0.84	1.34	0.99	3.27
SAPT(B3LYP)	0.64	2.66	3.89	8.32	1.82	3.34	2.13	8.32
SAPT0(B3LYP) + $\delta$ HF	1.91	4.77	4.27	8.91	2.32	3.98	2.86	8.91
SAPT0(LRC- $\omega$ PBE)	2.22	7.15	1.39	3.45	0.59	1.14	1.43	7.15
SAPT0(LRC- $\omega$ PBE) + $\delta$ HF	0.28	0.63	1.77	4.03	0.85	1.77	0.97	4.03

<sup>a</sup>Mean absolute error, with respect to complete-basis CCSD(T) benchmarks.

<sup>b</sup>Maximum deviation with respect to the benchmarks.

Table S5: Error statistics for SAPT0(KS) methods applied to the S66 database and three subsets thereof. (These are complementary to the statistics presented in Table 1, encompassing the same set of methods.)

Method <sup>a</sup>	H-Bonded		Disp.-Bound		Mixed		All S66	
	MAPE <sup>b</sup> (%)	Std. Dev. <sup>c</sup> (kcal/mol)	MAPE <sup>b</sup> (%)	Std. Dev. <sup>c</sup> (kcal/mol)	MAPE <sup>b</sup> (%)	Std. Dev. <sup>c</sup> (kcal/mol)	MAPE <sup>b</sup> (%)	Std. Dev. <sup>c</sup> (kcal/mol)
SAPT0(HF)	24	1.47	31	0.81	22	0.44	26	1.14
SAPT0(HF) + $\delta$ HF	5	0.24	22	0.41	12	0.36	13	0.38
SAPT0(B3LYP)	17	1.02	40	1.43	19	0.43	26	1.12
SAPT0(B3LYP) + $\delta$ HF	7	0.64	48	1.58	22	0.59	26	1.19
SAPT0(LRC- $\omega$ PBE) <sup>d</sup>	31	2.01	29	1.26	19	0.81	27	1.64
SAPT0(LRC- $\omega$ PBE) <sup>d</sup> + $\delta$ HF	12	0.55	30	0.61	14	0.60	19	0.62
XSAPT <sup>d</sup> + <i>ai</i> D3	21	1.49	6	0.87	7	0.16	11	1.24
XSAPT <sup>d</sup> + <i>ai</i> D3 + $\delta$ HF	2	0.12	12	0.19	15	0.27	10	0.24
XSAPT <sup>d</sup> + MBD	10	1.12	7	0.22	9	0.18	9	0.80
XSAPT <sup>d</sup> + MBD + $\delta$ HF	10	0.66	13	0.27	21	0.29	14	0.49

<sup>a</sup>Basis set is jun-cc-pVDZ for SAPT0(KS) and def2-TZVPPD for XSAPT.

<sup>b</sup>Mean absolute percentage error, with respect to complete-basis CCSD(T) benchmarks.

<sup>c</sup>Standard deviation in kcal/mol.

<sup>d</sup>Uses LRC- $\omega$ PBE with  $\omega_{\text{GDD}}$  tuning.

Table S6: Error statistics for SAPT0(KS) methods applied to the S66 database and three subsets thereof, using the aug-cc-pVTZ basis set. (These are complementary to the statistics presented in Table S4, encompassing the same set of methods.)

Method	H-Bonded		Disp.-Bound		Mixed		All S66	
	MAPE <sup>a</sup> (%)	Std. Dev. <sup>b</sup> (kcal/mol)	MAPE <sup>a</sup> (%)	Std. Dev. <sup>b</sup> (kcal/mol)	MAPE <sup>a</sup> (%)	Std. Dev. <sup>b</sup> (kcal/mol)	MAPE <sup>a</sup> (%)	Std. Dev. <sup>b</sup> (kcal/mol)
SAPT0(HF)	10	0.86	19	0.67	10	0.28	13	0.71
SAPT0(HF) + $\delta$ HF	10	0.97	30	0.81	24	0.31	21	0.76
SAPT0(B3LYP)	8	0.59	114	1.88	52	0.95	58	1.88
SAPT0(B3LYP) + $\delta$ HF	21	1.31	126	2.04	65	0.94	71	1.82
SAPT0(LRC- $\omega$ PBE) <sup>c</sup>	22	1.85	39	1.00	17	0.35	26	1.42
SAPT0(LRC- $\omega$ PBE) <sup>c</sup> + $\delta$ HF	4	0.20	51	1.14	24	0.52	26	0.96

<sup>a</sup>Mean absolute percentage error, with respect to complete-basis CCSD(T) benchmarks.

<sup>b</sup>Standard deviation.

<sup>c</sup>Uses LRC- $\omega$ PBE with  $\omega_{\text{GDD}}$  tuning.

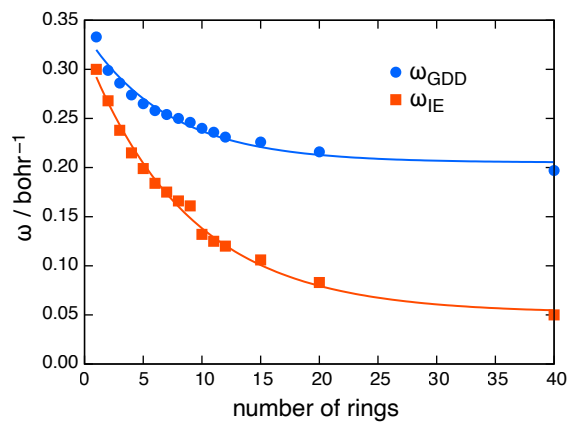


Fig. S1: Tuned values of  $\omega$  for the linear acene sequence of benzene, naphthalene, anthracene, ..., computed at the LRC- $\mu$ BOP/def2-TZVP level of theory. As with the analogous results using LRC- $\omega$ PBE (Fig. 1), the IE-tuning procedure tends toward a very small value of  $\omega_{\text{IE}}$  in the large-system limit, such that the functional in question is essentially a GGA on the length scale of dynamical correlation in chemical bonds.