Supporting Information for:

Quick-and-Easy Construction and Validation of Protein–Ligand Binding Models Using Fragment-Based Semi-Empirical Quantum Chemistry

Paige E. Bowling,[1,2] Dustin R. Broderick,[2] and John M. Herbert[1,2*]
[1] *Biophysics Graduate Program, The Ohio State University, Columbus, Ohio 43210 USA*
[2] *Department of Chemistry and Biochemistry, The Ohio State University, Columbus, Ohio 43210 USA*

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*herbert@chemistry.ohio-state.edu

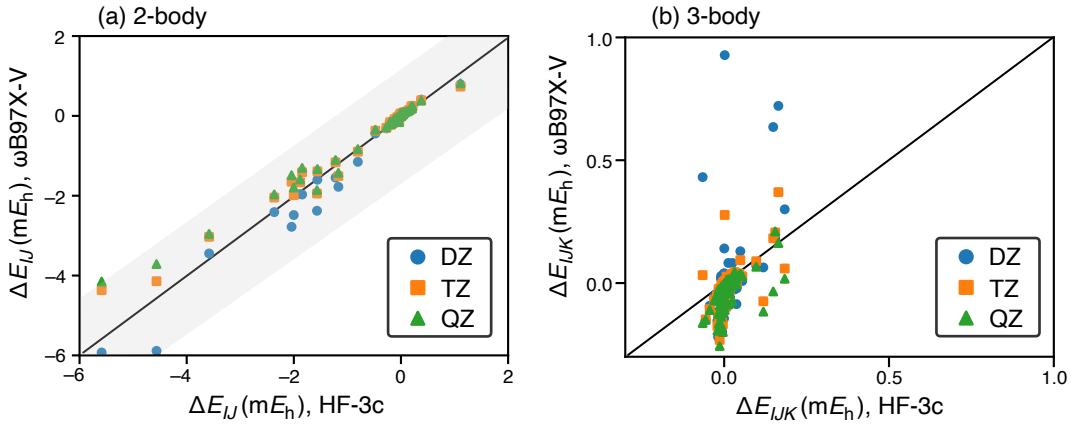

Figure S1: Correlations between HF-3c and ωB97X-V for (a) two-body and (b) three-body corrections, for 1LI2. This plot is analogous to the one in Fig. 2.

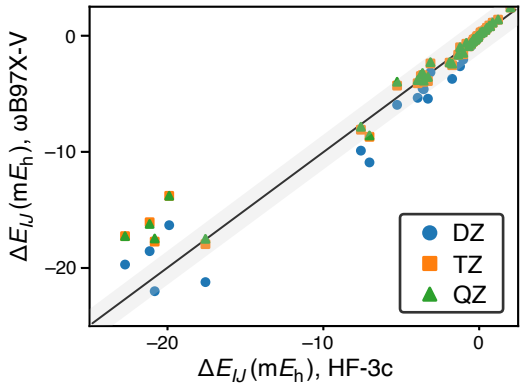

Figure S2: Correlations between HF-3c and ωB97X-V for two-body corrections in 1O48. This plot is analogous to the one in Fig. 2 except that only the two-body terms are plotted here.

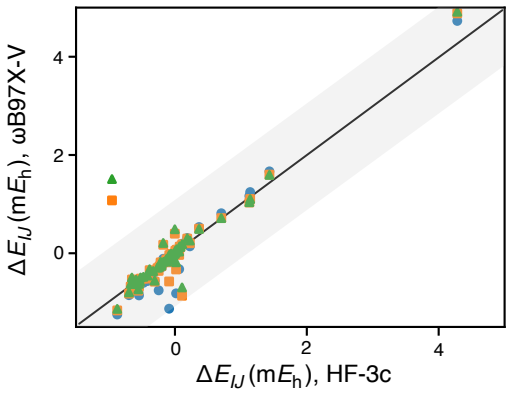

Figure S3: Correlations between HF-3c and ωB97X-V for two-body corrections in 1BOZ. This plot is analogous to the one in Fig. 2 except that only the two-body terms are plotted here.

Table S1: Linear fit parameters for the $\Delta E_{I,\text{ligand}}$ data.

Basis	181L		1LI2		1O48		1BOZ	
Set	slope	R^2	slope	R^2	slope	R^2	slope	R^2
DZ	1.12	0.963	1.14	0.980	0.97	0.959	1.24	0.946
TZ	0.85	0.928	0.86	0.983	0.82	0.969	0.84	0.877
QZ	0.81	0.919	0.80	0.981	0.81	0.973	0.79	0.853

Table S2: Results for distance-based models of 181L.

d	No.	Error (kcal/mol)	
(Å)	Atoms	MBE(2)	MBE(3)
2.5	120	−10.4	−10.5
3.0	204	−5.7	−5.8
4.0	243	−4.2	−4.1
5.0	284	−2.2	−2.4
6.0	452	−1.3	−1.6
7.0	665	−0.4	−0.7
8.0	744	−0.4	−0.7
9.0	927	−0.3	−0.6
10.0	1,050	−0.3	−0.6

Table S3: Results for distance-based models of 1LI2.

d (Å)	No. Atoms	Error (kcal/mol) MBE(2)	MBE(3)
2.5	124	−7.3	−7.4
3.0	205	−2.1	−2.1
4.0	244	−2.3	−2.3
5.0	302	−0.6	−0.7
6.0	475	0.3	0.0
7.0	619	0.6	0.4
8.0	758	0.9	0.6
9.0	903	0.9	0.6
10.0	1,064	0.9	0.6

Table S4: Results for distance-based models of 1O48.

d (Å)	No. Atoms	Error (kcal/mol) MBE(2)	MBE(3)
2.5	226	−29.2	−34.4
3.0	381	2.5	−1.7
4.0	418	3.3	−0.8
5.0	502	1.8	−1.9
6.0	619	2.4	−1.2
7.0	797	2.3	−1.5
8.0	928	3.5	−0.2
9.0	1,004	3.6	−0.2
10.0	1,154	3.8	0.0

Table S5: Results for distance-based models of 1BOZ.

d (Å)	No. Atoms	Error (kcal/mol) MBE(2)	MBE(3)
2.5	305	−3.2	−3.5
3.0	340	−0.5	−1.0
4.0	467	3.3	1.5
5.0	474	4.0	2.4
6.0	658	3.9	2.5
7.0	947	5.8	4.3
8.0	1,292	5.6	4.2
9.0	1,471	5.7	4.3
10.0	1,726	5.5	4.1