Electronic Supplementary Information for

A Physics-Aware Neural Network for Protein-Ligand Interactions with Quantum Chemical Accuracy

Zachary L. Glick,[1] Derek P. Metcalf,[1] Caroline S. Glick,[1] Steven A. Spronk,[2] Alexios Koutsoukas,[2] Daniel L. Cheney,[2] and C. David Sherrill[1]

[1)]*Center for Computational Molecular Science and Technology, School of Chemistry and Biochemistry, and School of Computational Science and Engineering, Georgia Institute of Technology, Atlanta, Georgia 30332-0400, USA*

[2)]*Molecular Structure and Design, Bristol Myers Squibb Company, P. O. Box 5400, Princeton, NJ 08543*

TABLE S1. Difference in interaction energies (kcal mol^{-1}) for alchemical substitutions in nine protein-ligand complexes. The PDB entry of the crystallographic structures from which each dimer pair was derived is given. The interaction energies are decomposed into the four SAPT components.

	Electrostatics $\Delta\Delta E$		Exchange $\Delta\Delta E$		Induction $\Delta\Delta E$		Dispersion $\Delta\Delta E$	
PDB Entry	SAPT0	AP-Net	SAPT0	AP-Net	SAPT0	AP-Net	SAPT0	AP-Net
2CJI	-2.32	-2.43	+2.38	+2.77	-0.34	-0.26	-1.78	-1.75
2O7N	+1.36	+0.80	+4.66	+5.40	+0.54	+0.44	-2.39	-2.37
2PR3	-0.63	-0.85	+0.43	+0.63	-0.01	-0.13	-0.82	-1.06
2UZT	-0.14	+0.05	+1.04	+1.33	-0.40	-0.25	-0.33	-0.21
2W26	-2.37	-3.37	+2.47	+4.91	-0.09	-0.68	-2.01	-1.86
2Y5(G/H)	-3.69	-4.35	+1.24	+1.65	-0.06	+0.09	-0.96	-1.04
3ENS	-5.89	-4.39	+8.12	+8.43	-1.90	-1.73	-5.29	-5.26
4YFF	+0.86	+0.48	-0.14	-0.16	+0.11	+0.04	+0.03	+0.02
4YHT	-2.32	-3.01	+0.84	+0.90	+0.07	+0.01	-0.82	-0.87

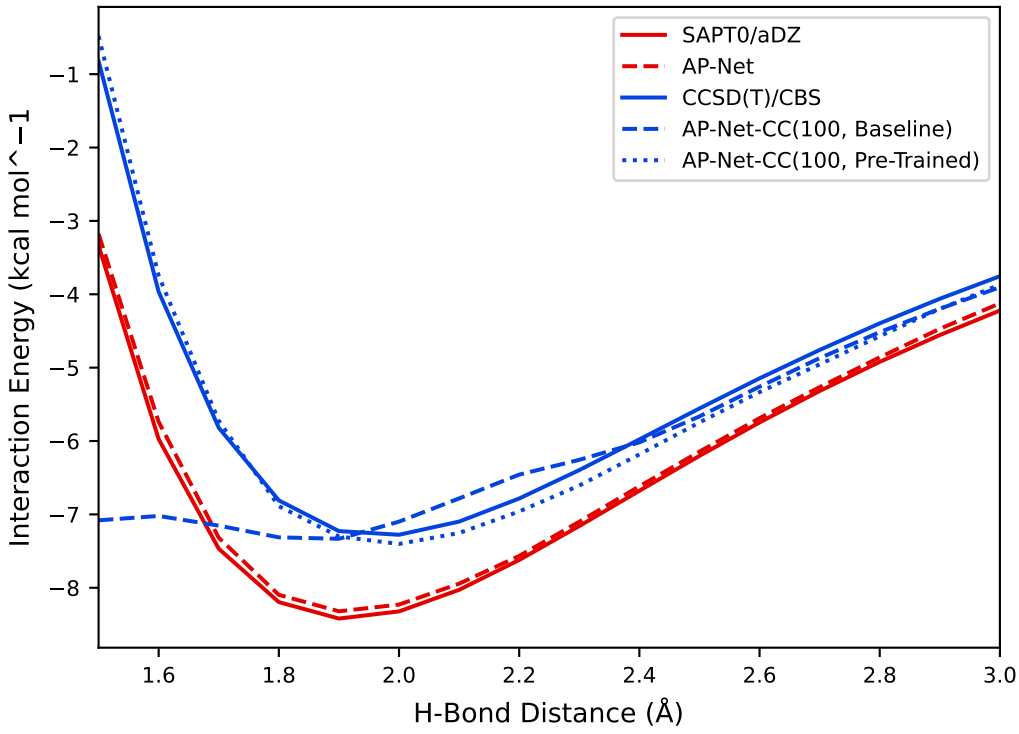

FIG. S1. A one-dimensional slice of the two-dimensional NMA dimer interaction energy scan. In this figure, the hydrogen bond angle is fixed at 0° and the hydrogen bond distance is varied.