Effective Fragment Potentials for Flexible Molecules: Transferability of Parameters and Amino Acid Database
Supporting Information

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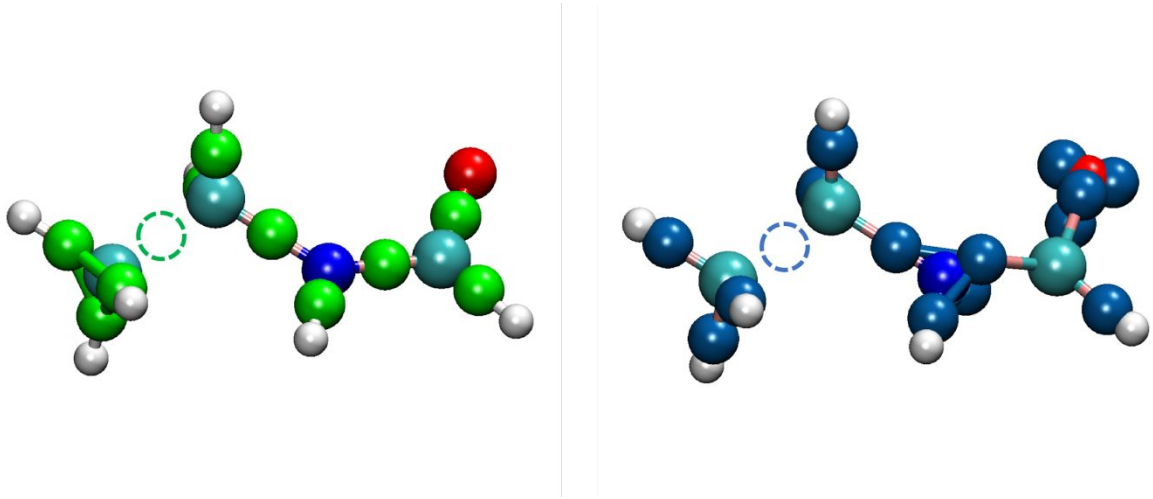

Fig. S1. Fragmentation into the backbone and side-chain groups on an example of the alanine residue. (Left) positions of bond mid-points (shown in green) and (right) positions of LMO centroids (shown in sapphire). Empty circles denote excluded parameters.

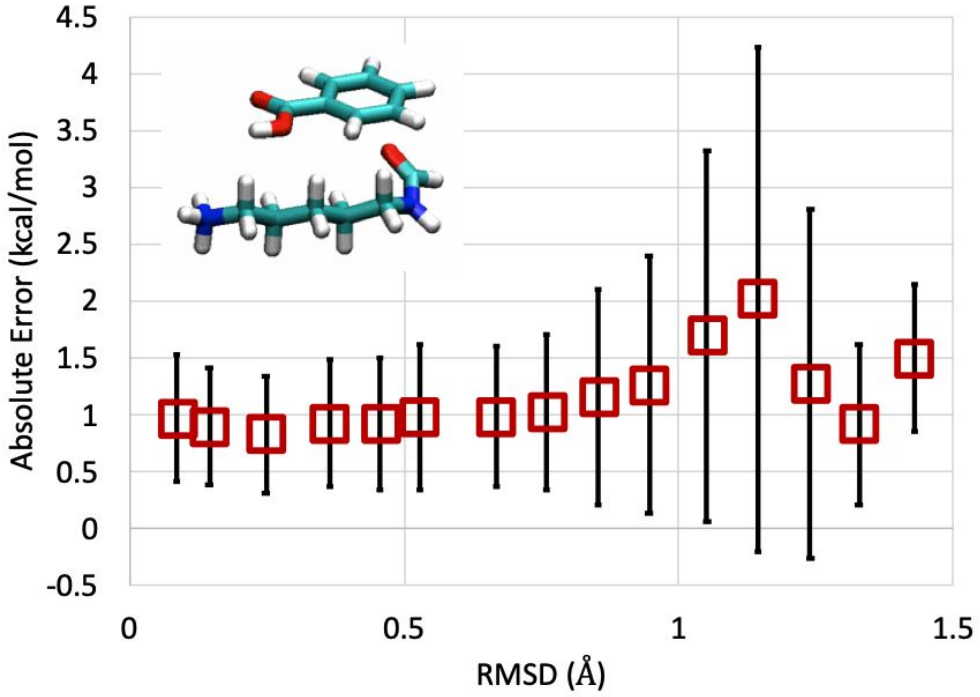

Fig. S2. Lysine-benzoic acid dimer at a separation 4 Å between monomer centers of masses. Average absolute errors (red squares) and their standard deviations (black vertical lines), in kcal/mol, of the Flexible EFP scheme versus standard EFP, as a function of RMSD between lysine geometry in the dimer and lysine geometry in the EFPDB database. The data are averaged for 1000 geometries of lysine-benzoic acid dimer, each using one of the 54 database lysine EFP potentials (the total set contains 54000 data points). Benzoic acid monomer is kept rigid in all calculations; lysine geometries are extracted from the MD trajectory of cryptochrome. Absolute errors are averaged for RMSDs within 0.1 Å, i.e., for RMSD bins 0-0.1 Å, 0.1-0.2 Å, etc. The graph suggests that the accuracy of the Flexible EFP scheme is preserved for RMSD values below 0.7 Å. Interaction energies in the considered lysine-benzoic acid dimers vary between -10 and +30 kcal/mol, such that the observed average errors < 1kcal/mol are consistent within a typical accuracy of EFP calculations.

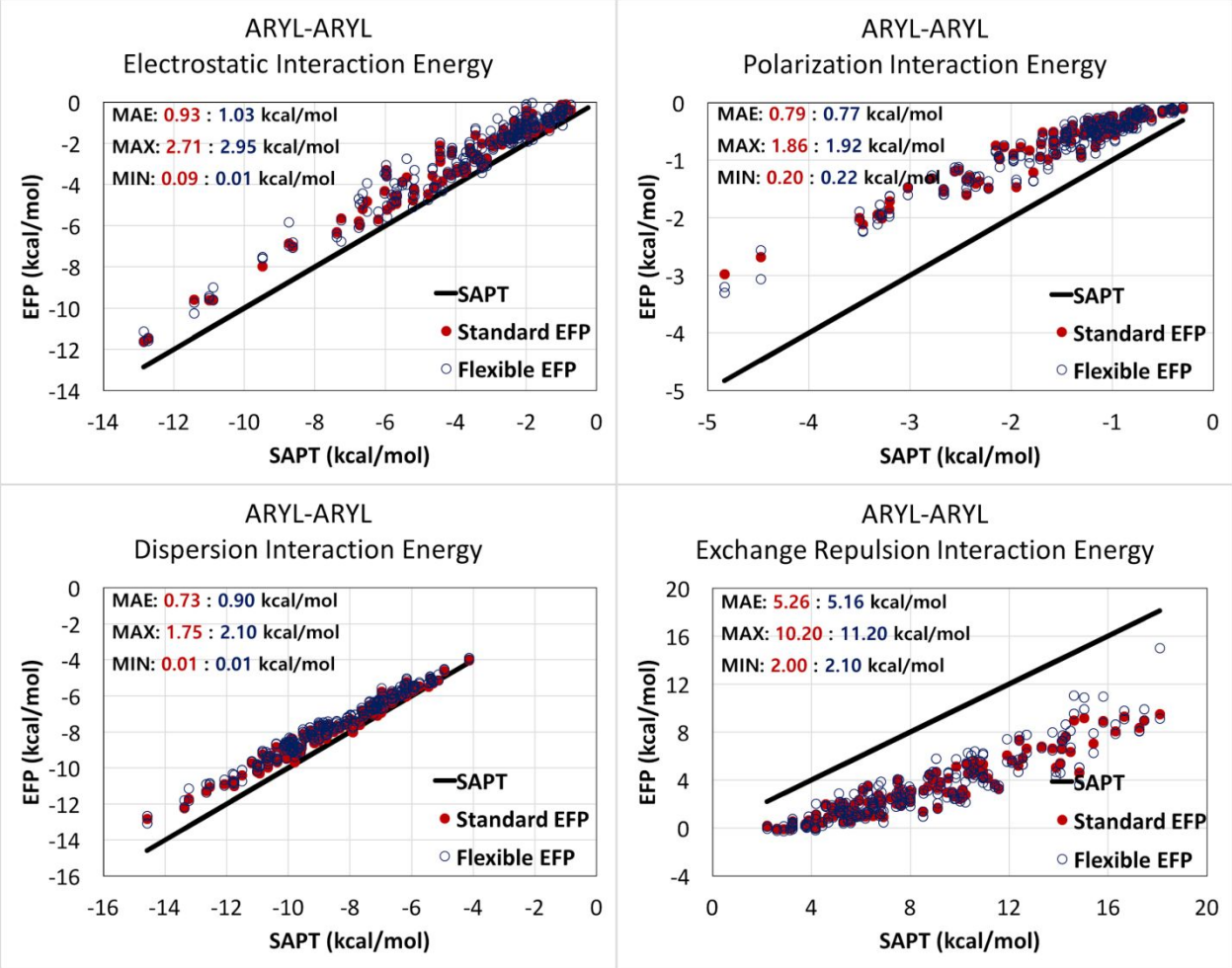

Fig. S3. Interaction energy components in aryl-aryl complexes computed with Standard EFP (red circles) and Flexible EFP (blue circles) against sSAPT0/jun-cc-pVDZ.

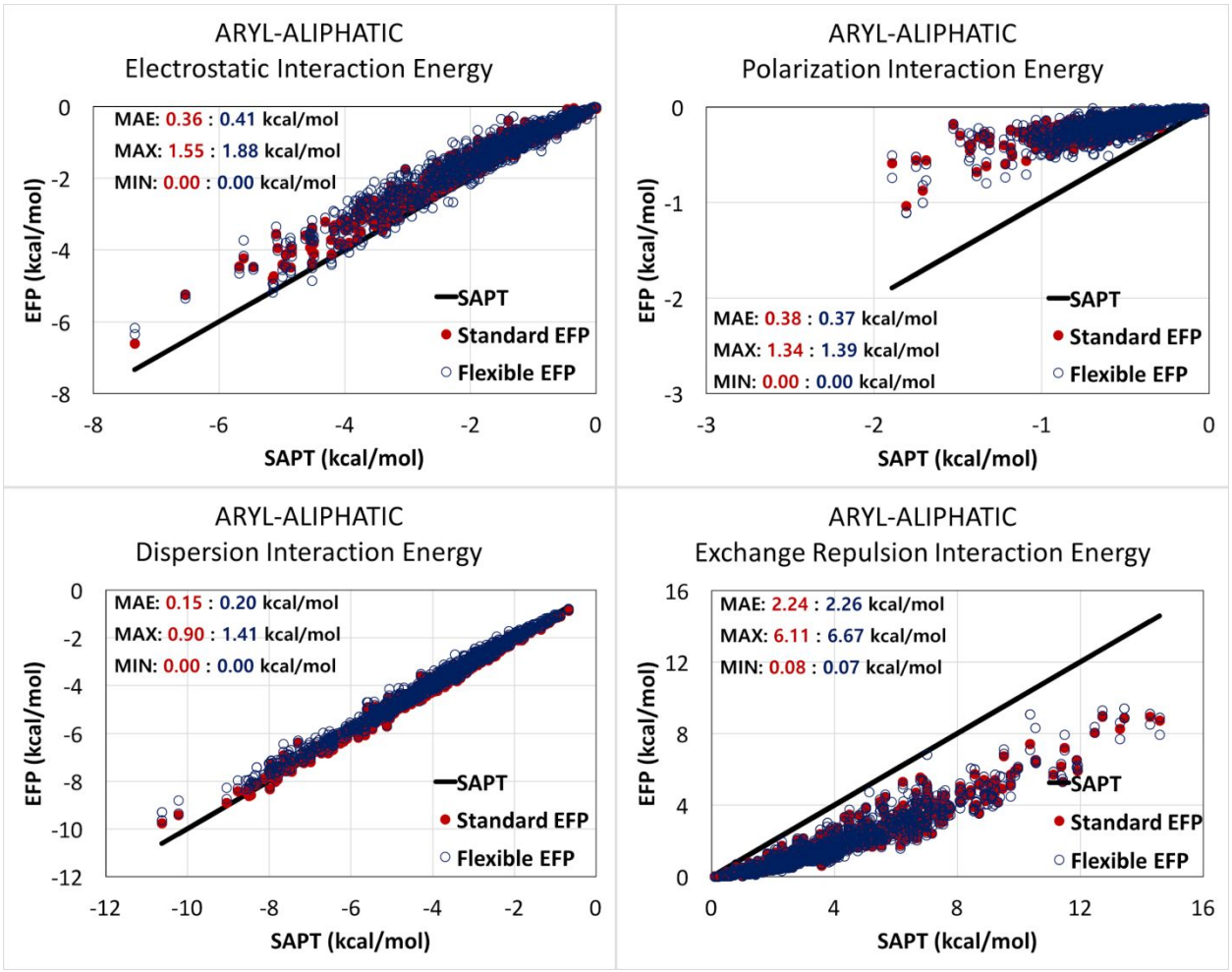

Fig. S4. Interaction energy components in aryl-aliphatic complexes computed with Standard EFP (red circles) and Flexible EFP (blue circles) against sSAPT0/jun-cc-pVDZ.

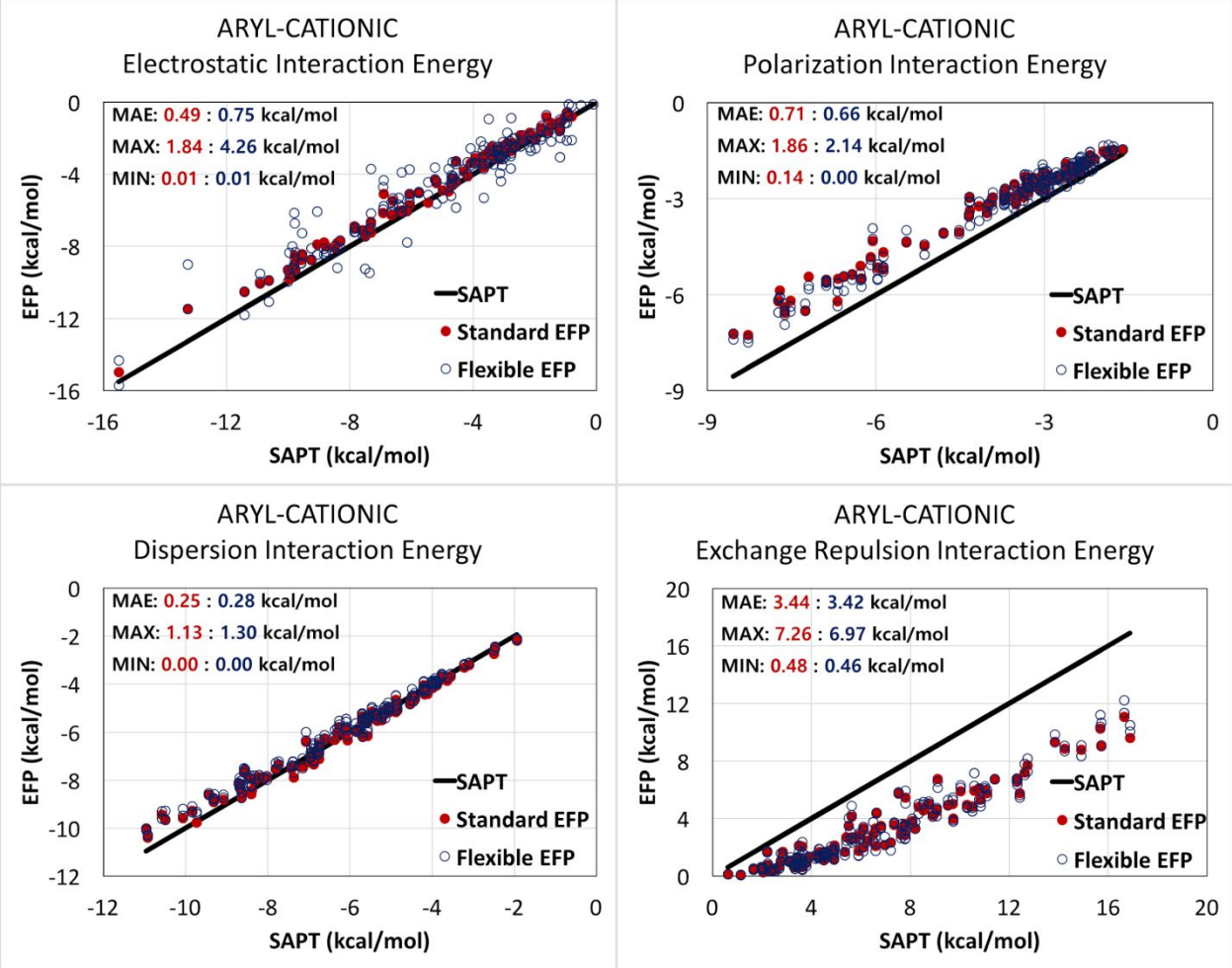

Fig. S5. Interaction energy components in aryl-cationic complexes computed with Standard EFP (red circles) and Flexible EFP (blue circles) against sSAPT0/jun-cc-pVDZ.

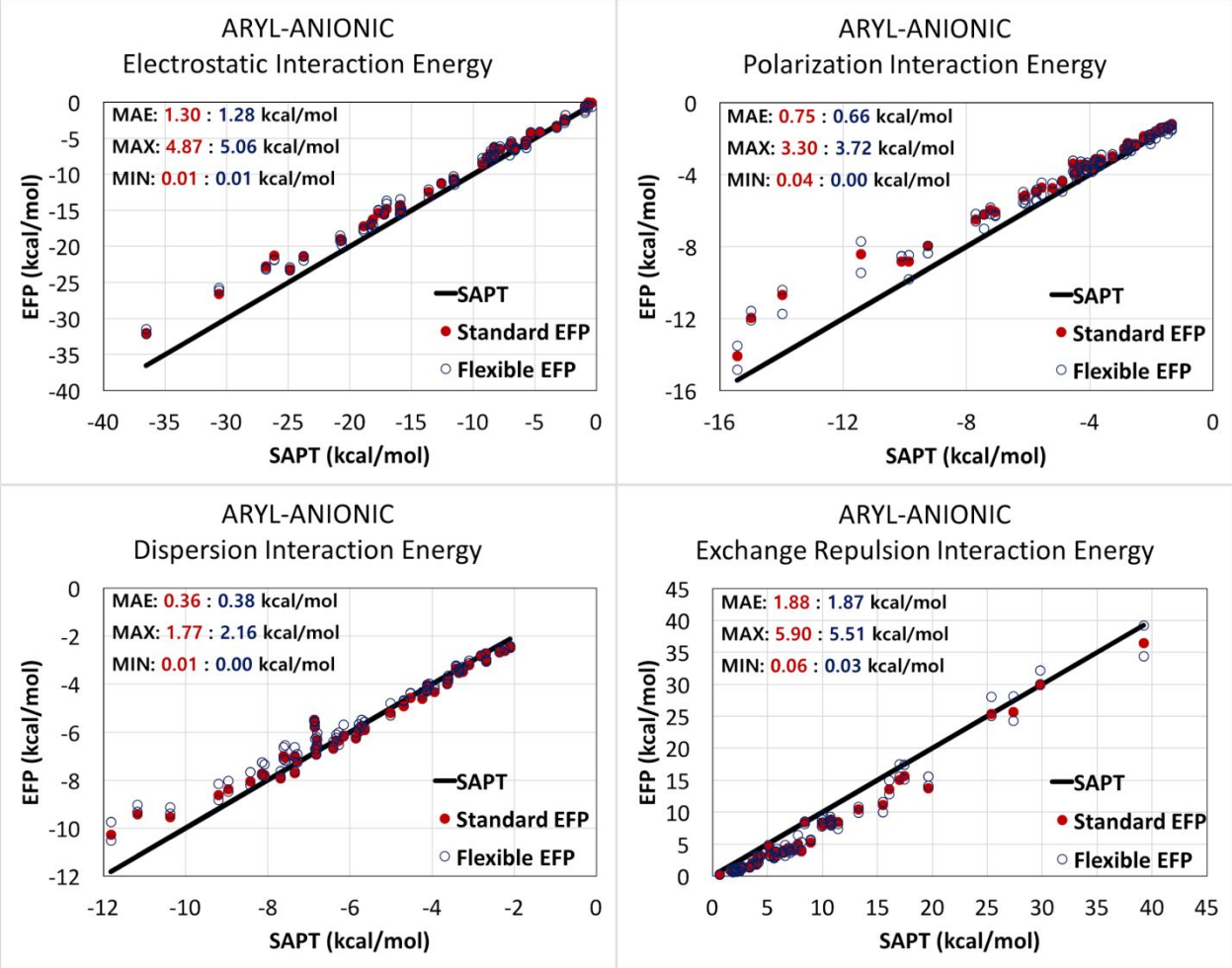

Fig. S6. Interaction energy components in aryl-anionic complexes computed with Standard EFP (red circles) and Flexible EFP (blue circles) against sSAPT0/jun-cc-pVDZ.

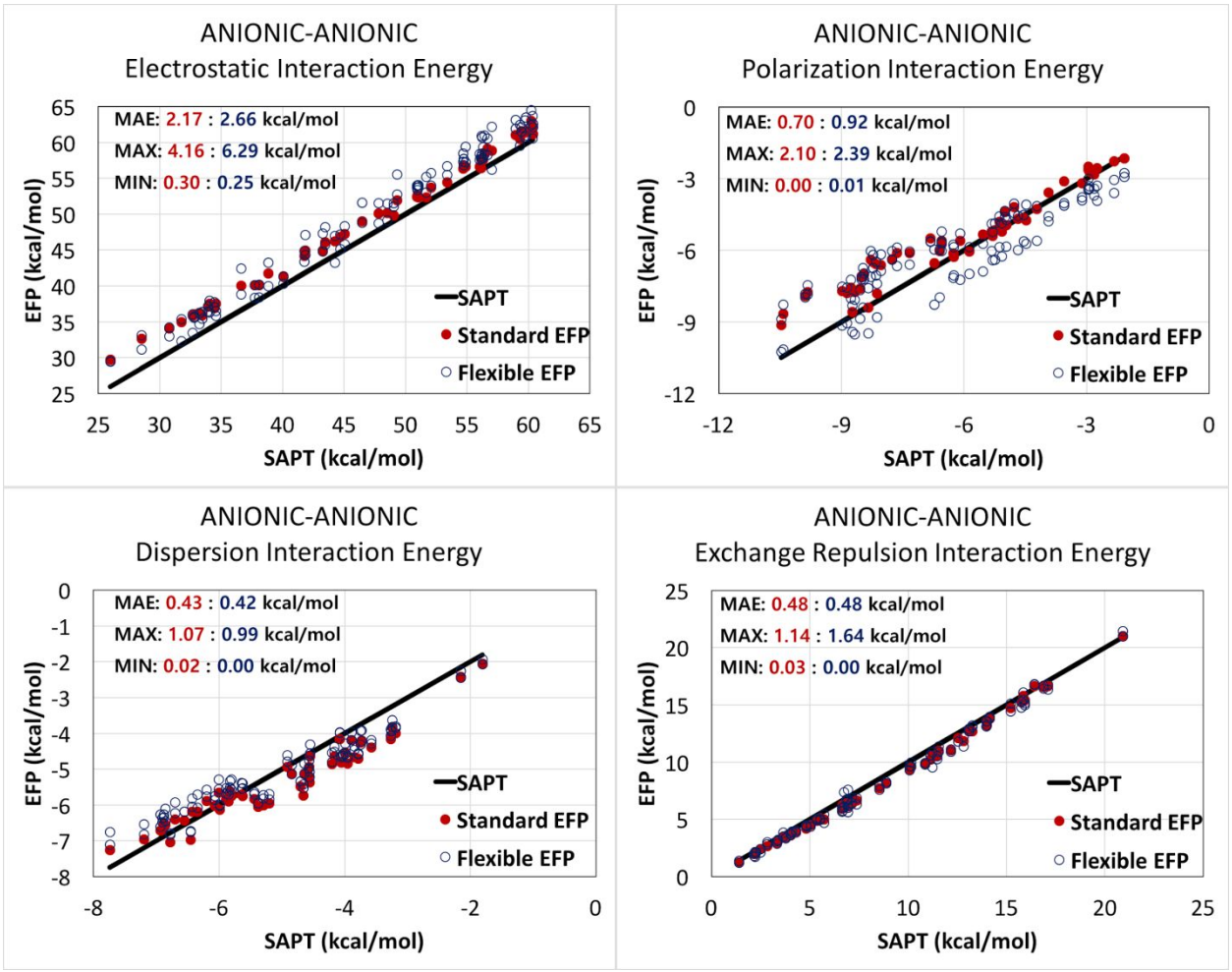

Fig. S7. Interaction energy components in anionic-anionic complexes computed with Standard EFP (red circles) and Flexible EFP (blue circles) against sSAPT0/jun-cc-pVDZ.

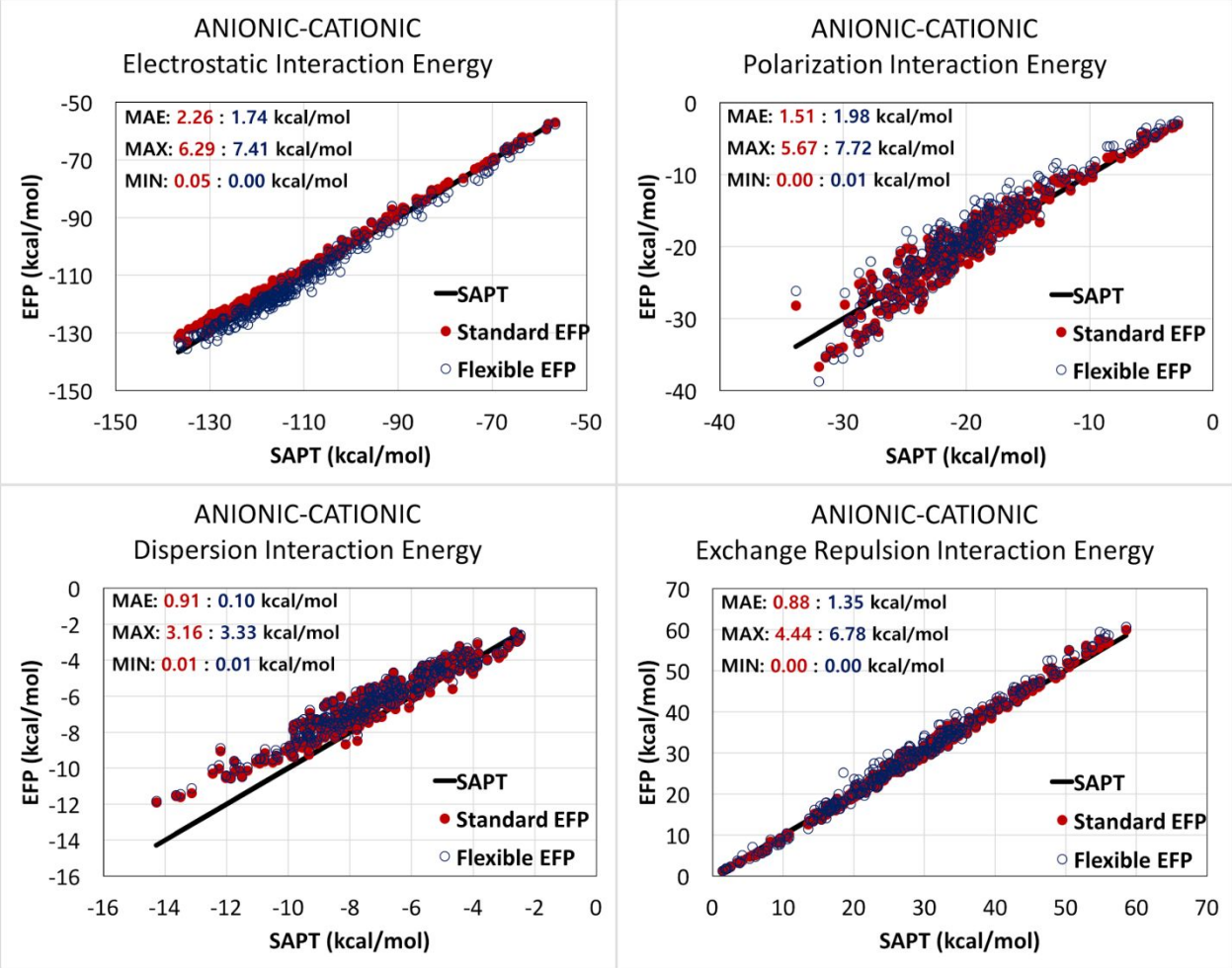

Fig. S8. Interaction energy components in anionic-cationic complexes computed with Standard EFP (red circles) and Flexible EFP (blue circles) against sSAPT0/jun-cc-pVDZ.

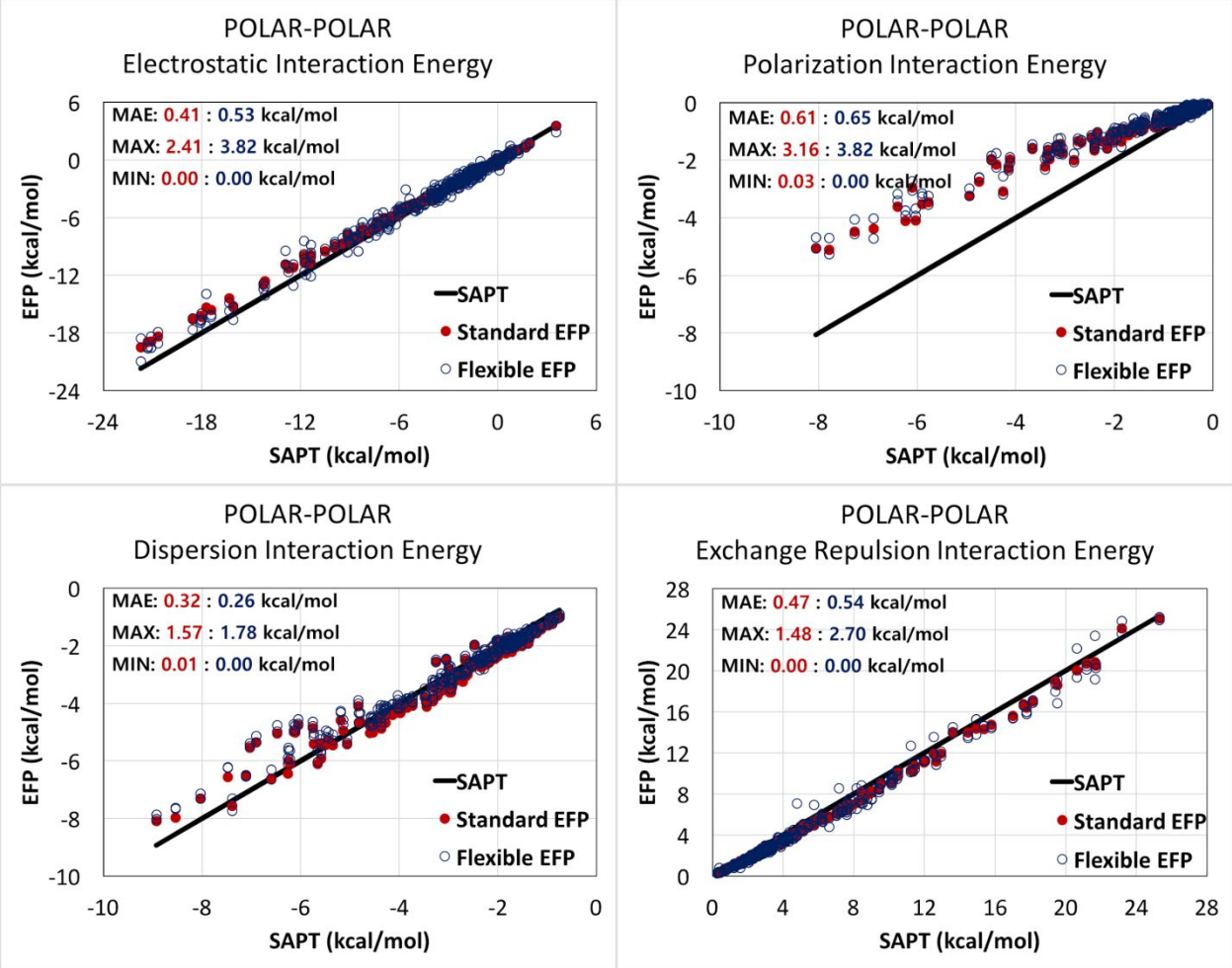

Fig. S9. Interaction energy components in polar-polar complexes computed with Standard EFP (red circles) and Flexible EFP (blue circles) against sSAPT0/jun-cc-pVDZ.

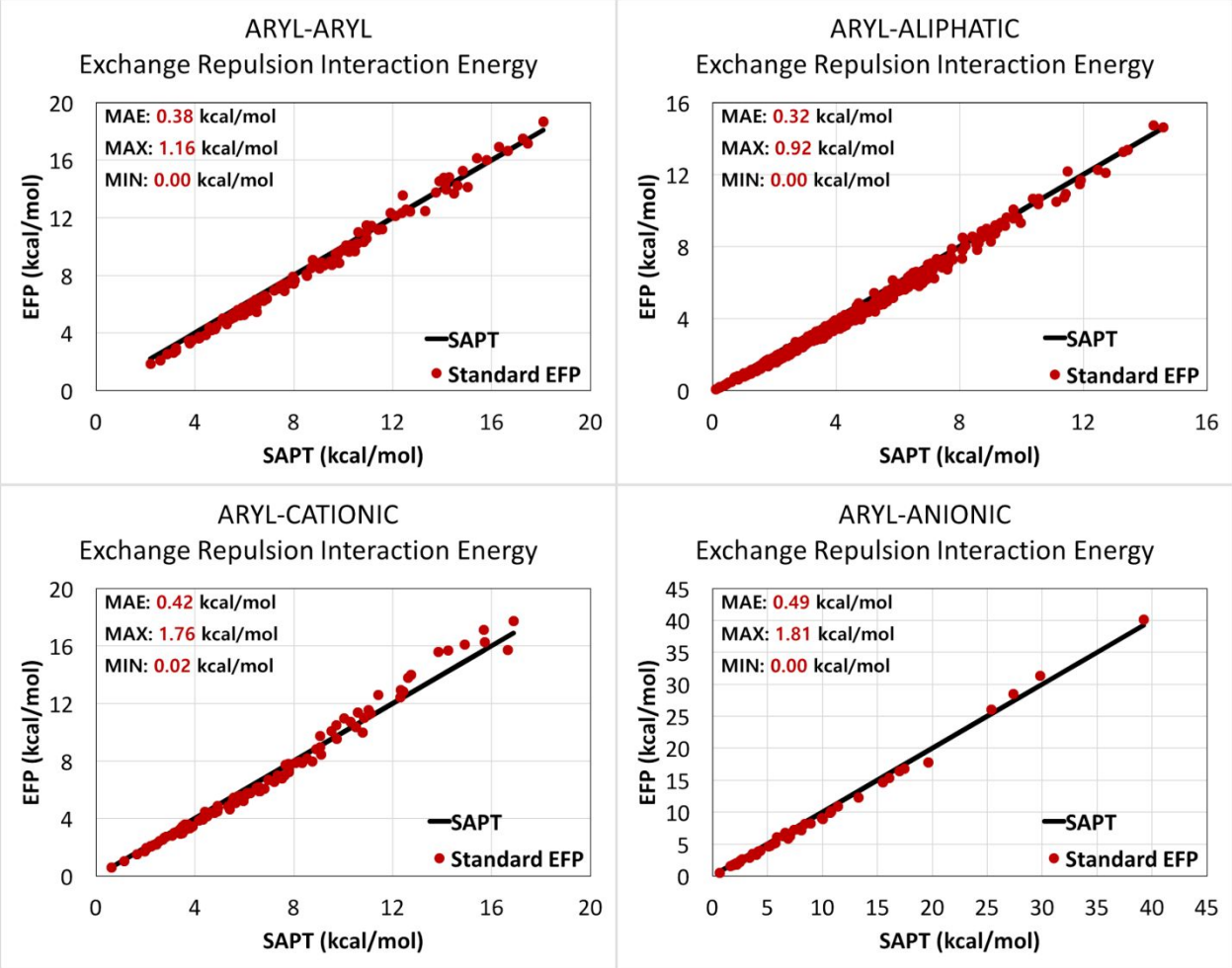

Fig. S10. Exchange-repulsion energies in aryl-containing complexes computed with Standard EFP (red circles) against sSAPT0/jun-cc-pVDZ.

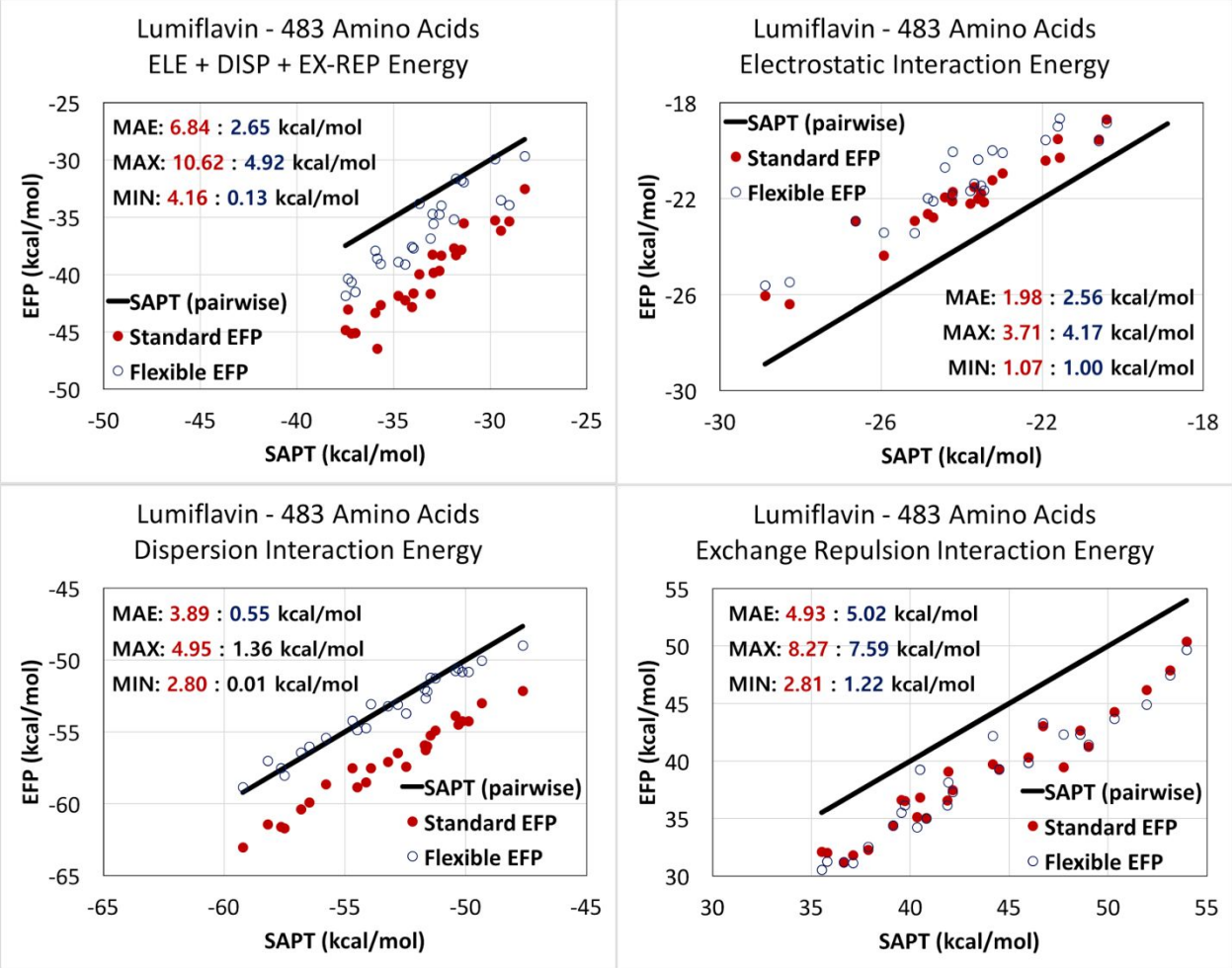

Fig. S11. Comparison of pairwise interaction energy components in the lumiflavin-protein system. Red circles: Standard EFP; blue circles: Flexible EFP. Comparison is done against sSAPT/jun-cc-pVDZ.

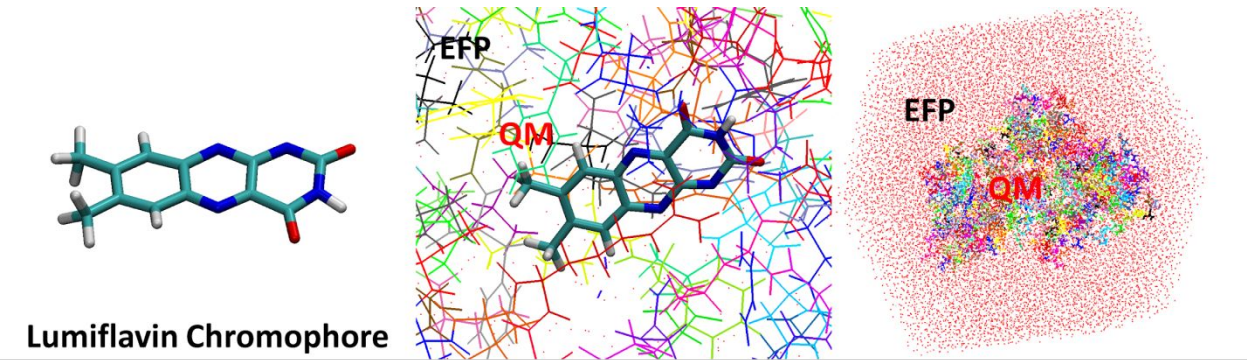

Fig. S12. Scheme of QM/EFP calculations of Cry1At protein.

Table S1. VEA and VIE at each MD structure computed with the Standard and Flexible EFP schemes. OX and SEMI correspond to MD simulations for oxidized and semireduced forms of lumiflavin, respectively.

Ensemble	**VEA, eV**		**Ensemble**	**VIE, eV**	
OX	**Standard EFP**	**Flexible EFP**	**SEMI**	**Standard EFP**	**Flexible EFP**
snap_01	2.324	2.280	snap_01	4.993	4.907
snap_02	2.703	2.642	snap_02	4.766	4.764
snap_03	2.768	2.772	snap_03	4.577	4.467
snap_04	2.390	2.383	snap_04	4.882	4.835
snap_05	2.658	2.655	snap_05	4.978	4.896
snap_06	2.431	2.372	snap_06	4.861	4.840
snap_07	2.547	2.503	snap_07	4.893	4.892
snap_08	2.573	2.568	snap_08	5.083	5.036
snap_09	2.056	2.053	snap_09	5.080	5.080
snap_10	2.630	2.603	snap_10	4.858	4.784
snap_11	2.694	2.664	snap_11	5.221	5.208
snap_12	2.480	2.426	snap_12	4.752	4.750
snap_13	2.035	2.008	snap_13	4.651	4.657
snap_14	2.876	2.902	snap_14	5.189	5.171
snap_15	2.125	2.099	snap_15	5.080	5.038
snap_16	2.359	2.365	snap_16	5.112	5.030
snap_17	2.449	2.383	snap_17	5.279	5.271
snap_18	2.702	2.573	snap_18	5.261	5.148
snap_19	2.407	2.342	snap_19	4.965	4.880
snap_20	2.297	2.220	snap_20	4.771	4.744
snap_21	1.890	1.913	snap_21	4.468	4.436
snap_22	2.337	2.379	snap_22	4.925	4.929
snap_23	2.207	2.156	snap_23	4.982	4.916
snap_24	1.991	1.935	snap_24	4.892	4.802
snap_25	2.253	2.251	snap_25	4.637	4.577