Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.
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Supplementary information

SI 1. SCF iterations and energy convergence

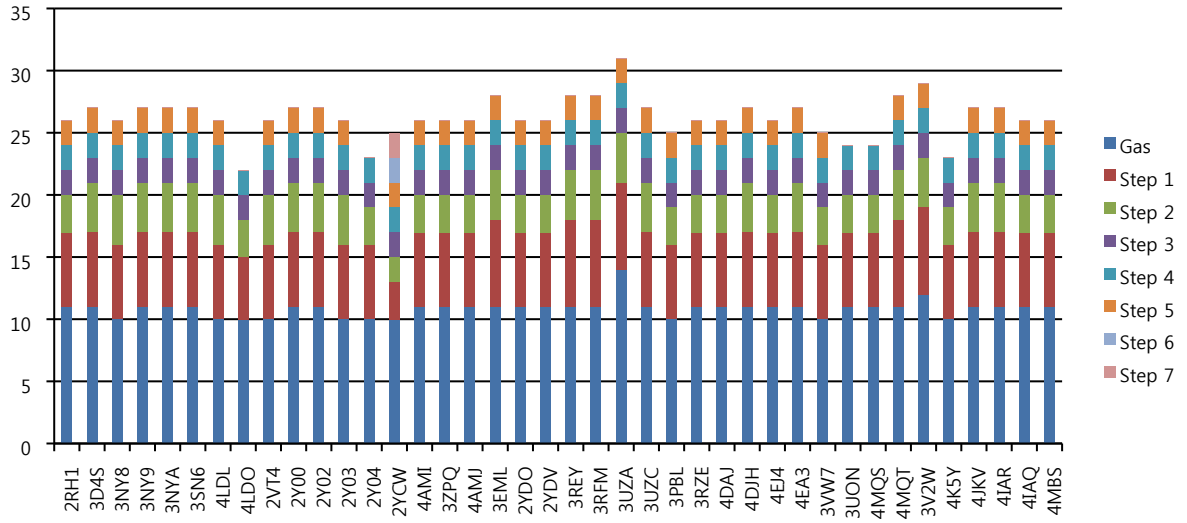


Figure 1. Number of iterations for each step of solvation QM/MM charge calculations. After gas phase QM/MM calculations, in all cases except for 2YCW, which took 7 steps, the calculations were terminated in 5 steps.

Energy convergence plot of XAC (ligand for 3REY)

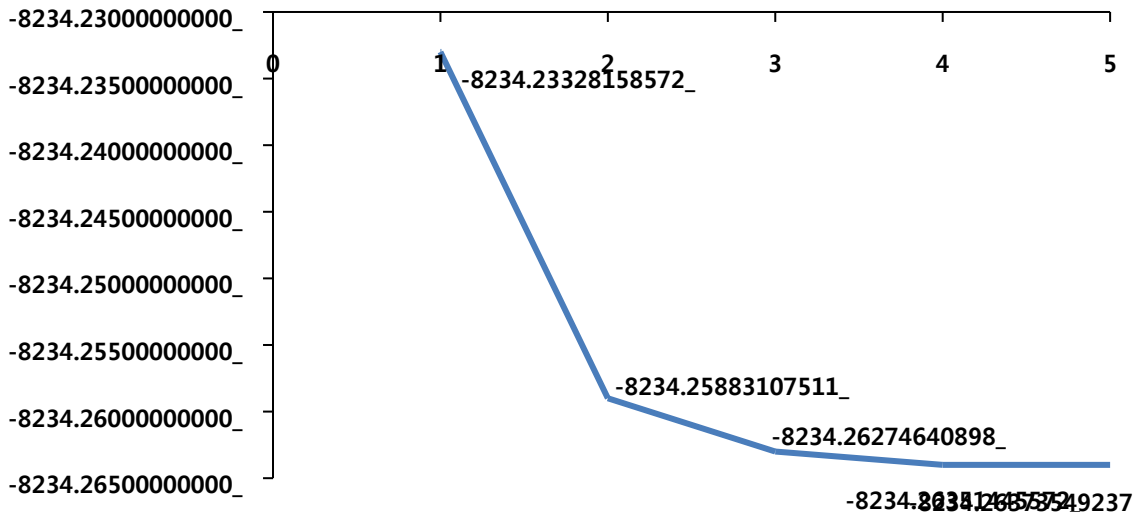


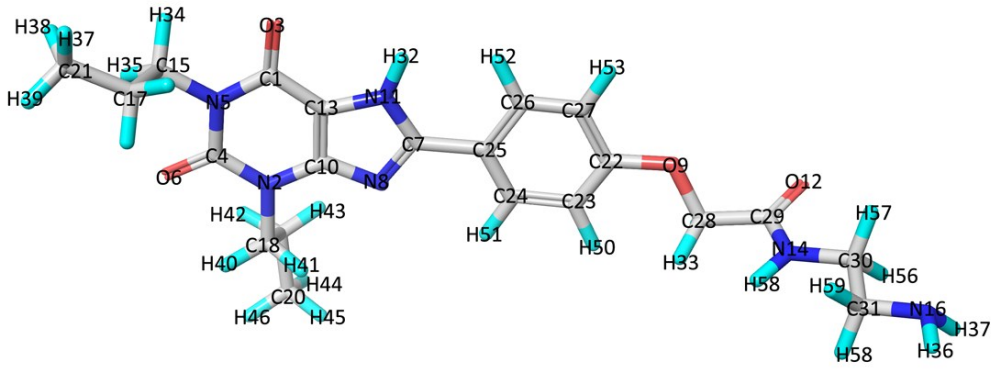
Figure 2. Plot of energy vs. iteration step for 3REY charge calculations. The criterion of convergence was set to 5e-05 hartree.

SI2. Intermediate values of SolvQMDock calculation for 3REY

Table 1. Initial poses generated by SolvQMDock

	Pose 1	Pose 2	Pose 3	Pose 4	Pose 5	Pose 6	Pose 7	Pose 8	Pose 9	Pose 10
Initial docking RMSD	4.012	3.748	8.569	4.093	6.799	8.341	9.608	1.249	10.957	12.125
The number of iterations in Gas (SCF)	11	11	12	11	11	11	12	11	11	11
The number of iterations in solvation (Step 1)	7	7	7	7	7	7	7	7	7	7
Step 2	4	4	4	4	4	4	4	4	4	4
Step 3	2	2	2	2	2	2	3	3	3	3
Step 4	2	2	2	2	2	2	2	2	2	2
Step 5	2	2	2	2	2	2	2	2	2	2
Ecvdw energy	-39.5	-32.1	-39.8	-37.9	- 42.4	-36.1	-43.8	-45.3	-42.4	-43.7
RMSD of subsequent docking	8.320	8.385	8.371	4.200	4.990	9.070	8.450	1.243	9.565	9.070

Table 2. Charge values on atoms of XAC (ligand for 3REY)



	Force Field	Pose 1	Pose 2	Pose 3	Pose 4	Pose 5	Pose 6	Pose 7	Pose 8	Pose 9	Pose 10
C1	0.746	0.806	1.542	0.665	1.442	0.753	0.458	1.146	1.309	0.526	1.004
N2	-0.257	-0.839	-0.921	-0.355	-0.793	-0.971	-0.488	-0.220	-1.178	-0.244	0.128
O3	-0.508	-0.584	-0.776	-0.639	-0.810	-0.573	-0.507	-0.696	-0.766	-0.578	-0.673
C4	0.753	1.073	1.670	0.307	1.331	0.903	0.743	0.773	1.471	0.767	0.758
N5	-0.295	-0.606	-1.440	-0.344	-1.352	-0.328	-0.406	-1.214	-1.290	-0.464	-0.683
O6	-0.508	-0.647	-0.738	-0.469	-0.703	-0.618	-0.576	-0.581	-0.745	-0.616	-0.523
C7	0.353	0.187	0.004	0.164	0.682	0.760	0.715	0.649	0.310	0.719	0.664
N8	-0.563	-0.695	-0.621	-0.486	-0.695	-0.950	-0.765	-0.765	-0.740	-0.497	-0.042
O9	-0.285	-0.651	-0.797	-0.480	-0.360	-0.280	-0.412	-0.369	-0.499	-0.454	-0.758
C10	0.345	1.082	1.258	0.215	0.767	0.944	0.519	0.859	1.051	0.108	-0.120

N11	-0.257	0.163	0.498	-0.613	-0.282	-0.502	-0.831	-0.487	0.065	-0.795	-0.563
O12	-0.500	-0.530	-0.513	-0.614	-0.718	-0.619	-0.669	-0.602	-0.763	-0.646	-0.631
C13	-0.214	-0.742	-1.195	0.160	-0.595	-0.393	0.214	-0.498	-0.706	0.215	-0.178
N14	-0.500	0.030	-0.250	-0.688	-0.450	-0.987	-0.192	-0.402	-1.165	-0.701	0.739
C15	-0.070	0.404	0.717	0.277	1.221	-1.009	0.092	1.123	1.169	0.090	-0.287
N16	-0.900	-1.293	-1.115	-1.239	-1.004	-1.115	-1.250	-1.146	-0.862	-1.214	-1.099
C17	-0.120	-0.829	-0.453	-0.368	-0.540	0.772	-0.341	0.291	-0.717	0.018	0.659
C18	-0.070	-0.108	-0.228	0.648	0.149	0.612	0.051	-0.366	0.878	-0.061	-0.757
C19	-0.120	0.555	-0.521	0.433	-0.639	-0.156	-0.319	0.296	-0.765	0.086	0.395
C20	-0.180	-1.068	0.013	-1.157	0.457	-0.138	0.020	0.419	-0.170	-0.208	0.155
C21	-0.180	0.302	0.427	-0.374	-0.230	-0.699	0.037	0.447	0.292	-0.175	-0.082
C22	0.085	0.600	0.642	0.554	0.204	-0.060	0.511	0.173	0.270	0.509	0.756
C23	-0.115	-0.233	-0.308	-0.320	0.110	0.118	-0.270	0.032	-0.156	-0.303	-0.596
C24	-0.115	-0.375	-0.426	-0.241	-0.429	-0.647	0.168	0.114	-0.041	-0.099	0.057
C25	0.000	-0.054	0.198	0.064	-0.211	0.219	-0.585	-0.760	0.082	-0.216	-0.360
C26	-0.115	0.351	0.100	0.038	0.010	-0.602	0.298	0.294	-0.482	-0.009	0.037
C27	-0.115	-0.559	-0.525	-0.213	-0.220	0.492	-0.341	-0.331	-0.041	-0.371	-0.486
C28	0.140	0.512	0.985	0.017	-0.064	-0.280	-0.068	0.114	0.439	0.032	0.309
C29	0.500	0.200	0.072	0.568	0.767	0.781	0.618	0.537	0.852	0.733	0.272
C30	0.080	-0.274	-0.002	0.413	-0.206	0.656	-0.840	-0.087	0.343	0.216	-1.071
C31	0.060	0.622	0.504	0.416	0.755	0.207	0.832	0.480	0.373	0.352	0.075
H32	0.306	0.260	-0.004	0.421	0.239	0.464	0.499	0.432	0.098	0.395	0.121
H33	0.300	0.051	0.164	0.389	0.253	0.429	0.275	0.060	0.538	0.349	-0.527
H34	0.060	-0.060	-0.075	0.013	-0.171	0.413	0.120	-0.331	-0.149	0.093	0.122
H35	0.060	0.228	-0.066	0.059	-0.244	0.345	0.029	-0.425	-0.213	0.049	0.169
H36	0.060	0.444	0.524	0.526	0.546	0.424	0.421	0.424	0.340	0.453	0.403
H37	0.060	0.460	0.287	0.445	0.328	0.399	0.506	0.399	0.294	0.440	0.490
H38	0.060	0.352	0.033	0.078	0.136	-0.135	0.097	-0.113	0.098	0.023	-0.063
H39	0.060	0.167	-0.065	0.204	-0.114	-0.137	0.024	-0.163	-0.040	0.033	-0.569
H40	0.060	0.106	0.119	-0.106	0.128	0.046	0.169	0.192	-0.005	0.078	0.241
H41	0.060	-0.059	0.203	-0.099	0.039	-0.135	0.185	0.105	-0.217	0.145	0.164
H42	0.060	-0.097	0.138	-0.161	0.155	0.019	0.043	-0.052	0.251	0.018	-0.140
H43	0.060	-0.122	0.153	-0.011	0.163	0.061	0.106	-0.122	0.249	0.020	-0.136
H44	0.060	0.200	-0.003	0.578	-0.129	0.028	-0.056	-0.045	0.033	0.069	-0.054
H45	0.060	0.279	0.074	0.345	0.092	-0.119	-0.097	-0.100	-0.062	0.059	-0.057
H46	0.060	0.289	-0.009	0.135	-0.204	0.029	-0.012	-0.258	0.132	0.047	-0.024
H47	0.060	0.020	0.097	0.055	0.179	0.134	-0.057	-0.193	0.113	0.045	-0.040
H48	0.060	-0.074	-0.194	0.064	0.063	0.068	0.053	-0.234	-0.135	0.043	-0.071
H49	0.060	-0.198	0.169	0.186	0.485	0.256	0.012	-0.167	0.260	0.056	-0.004
H50	0.115	0.086	0.247	0.173	0.132	0.115	0.159	0.096	-0.012	0.168	0.577
H51	0.115	0.338	0.211	0.181	0.218	0.188	0.000	0.092	0.090	0.147	0.035

H52	0.115	-0.349	0.059	0.122	0.076	0.286	0.047	0.060	0.244	0.120	0.107
H53	0.115	0.244	0.142	0.106	0.051	-0.162	-0.045	0.202	0.167	0.184	0.245
H54	0.030	0.033	-0.312	0.057	0.034	0.196	0.136	-0.059	-0.225	0.071	0.019
H55	0.030	-0.120	-0.054	0.135	0.078	0.267	0.097	0.029	0.038	0.092	-0.063
H56	0.060	0.161	0.130	-0.125	0.204	-0.104	0.374	0.101	0.163	0.032	0.337
H57	0.060	-0.025	-0.057	0.007	0.049	-0.094	0.253	0.138	-0.012	0.054	0.225
H58	0.060	-0.076	-0.082	-0.061	-0.363	0.008	-0.219	-0.067	-0.043	0.035	0.351
H59	0.060	-0.030	-0.013	-0.036	-0.113	0.021	-0.045	0.042	-0.025	-0.039	-0.007