Table Suppl_2. Interaction Energies (kJ/mol). R is the distance between molecular centroids (mean atomic position) in Å.

1						
Type	R (Å)	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
AB NH···N	6.70	-59.1	-13.8	-31.1	75.6	-53.2
BA NH···N	8.44	-47.0	-12.5	-17.1	51.5	-42.0
AB CH···N	6.26	-8.8	-1.7	-17.6	11.6	-18.8
AA π···π	4.25	-6.1	-1.6	-50.1	25.1	-35.8
BB π···π	5.01	-5.3	-1.4	-50.4	26.6	-34.0
BA CH···N	6.61	-5.6	-1.3	-22.7	11.8	-19.3
AB π···π	8.51	-1.7	-0.6	-21.9	11.6	-14.2
AB CH···π	7.97	-5.5	-0.7	-20.2	12.4	-16.2
BA CH···π	10.20	-11.5	-2.6	-11.4	13.0	-16.0
2						
A···H_2O	2.92	-65.9	-15.1	-11.2	63.8	-51.3
B···H_2O	2.81	-81.6	-22.2	-12.5	78.0	-65.5
H_2O···H_2O	2.83	-36.0	-7.6	-4.2	36.6	-24.8
AB	6.47	-5.3	-1.5	-16.7	7.8	-16.4
AA π···π	4.22	-17.6	-4.3	-71.8	38.8	-60.4
H_2O···A	4.99	-48.3	-11.2	-10.2	58.6	-32.0
CH(A)···π (B)	9.23	-0.7	-2.7	-22.2	14.1	-13.4
BB π···π	4.70	-18.1	-6.8	-70.6	47.1	-56.5
BB π···π	4.22	-21.6	-9.0	-79.1	43.5	-71.6
BA NH···N	10.81	-51.5	-15.4	-18.0	59.8	-44.6
BA CH···π	7.19	-9.0	-2.2	-17.7	11.7	-19.3
H_2O···B	5.13	-55.4	-12.8	-10.5	65.7	-36.6
3						

AB π···π	3.38	-35.4	-10.1	-101.4	74.4	-87.3
BB π···π	5.09	-22.7	-7.0	-82.4	48.7	-70.9
AA π···π	7.18	-29.7	-7.0	-61.7	38.8	-66.4
CC π···π	7.27	-34.4	-8.0	-67.0	49.9	-69.8
CD π···π	3.38	-33.3	-10.0	-99.9	68.4	-87.4
DD π···π	4.89	-18.8	-6.9	-83.6	47.8	-68.3
LA···H_2O	2.86	-79.8	-22.3	-11.9	74.7	-65.0
LB···H_2O	2.79	-90.8	-25.3	-13.5	92.4	-69.3
LC···H_2O	2.73	-103.1	-28.7	-14.6	113.6	-72.7
LD···H_2O	2.91	-75.4	-20.9	-11.9	69.5	-62.6
H_2OA·H_2OB	2.87	-27.3	-5.6	-3.6	25.9	-20.2
H_2OC·H_2OD	2.89	-32.5	-6.6	-3.7	29.0	-24.5
H_2O···LA	5.10	-38.1	-8.7	-9.9	42.6	-29.0
H_2O···LC	5.41	-43.1	-10.3	-9.3	42.6	-35.0
H_2O···N	5.37	-44.3	-10.1	-9.7	46.3	-34.1
4						
L···MeOH	4.91	-15.8	-7.4	-14.1	13.2	-26.3
π···π	3.36	-127.0	-33.2	-87.7	105.3	-170.2
π··· π	4.13	-109.3	-39.5	-77.8	50.5	-181.4
CH···N	10.13	-38.8	-14.3	-13.0	22.1	-49.3
5						
L·H_2O	8.31	-81.0	-24.7	-5.1	67.7	-66.5
L·trifl	4.28	-20.6	-69.9	-21.7	55.6	-58.0
L L π···π	4.03	-220.4	-52.6	-70.9	45.4	-305.7
L·trifl	6.99	-10.6	-39.1	-13.4	22.2	-38.2
H_2O·L	4.62	-63.5	-8.8	-11.2	70.7	-39.7
H_2O·L	6.45	-9.1	-6.6	-5.5	8.4	-14.2
H_2O·trifl	4.29	-17.4	-16.8	-4.5	30.2	-16.1

L·trifl	7.46	-2.1	-13.1	-11.4	5.3	-18.6
						6
L···L π···π	5.89	-94.6	-74.5	-24.3	9.2	-170.6
L···L π···π	8.97	-7.0	-50.5	-15.9	4.5	-55.9
L·trifl1	4.19	-30.6	-97.1	-26.3	102.7	-63.8
L·trifl2	5.68	-41.3	-76.4	-19.5	57.7	-81.5
L·trifl2	7.50	-69.0	-14.1	-6.0	14.0	-79.9
L···triflA CH···O	8.93	-2.6	-20.6	-5.5	3.5	-20.6
L·triflA	6.62	-15.2	-47.8	-17.8	28.3	-49.5
L···triflA CH···O	4.91	23.9	-53.7	-19.5	13.4	-23.1
L···trifl N···O	4.56	14.0	-56.2	-20.3	12.6	-36.7
L···triflA CH···O	4.91	2.5	-53.7	-19.5	14.1	-45.4
L···triflA CH···O	8.39	-11.1	-34.6	-12.5	14.7	-39.2
L···triflA CH···O	6.06	-20.4	-11.1	-3.9	0.8	-32.8
L···triflA CH···O	4.19	-18.2	-97.1	-26.3	111.0	-45.4
L···triflB	4.56	11.9	-56.2	-20.3	13.0	-38.6
L···triflB	5.68	-52.2	-76.4	-19.5	58.3	-92.7
L···triflA CH···O	6.62	-14.0	-47.8	-17.8	25.1	-50.2