Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Table S1. Binding free energy contributions of key binding-site residues calculated by the binding energy decomposition for three representative compounds(kcal/mol).

	cmp 17j					cmp 20				
	ΔE_{vdw}	ΔE_{ele}	ΔG_{GB}	ΔG_{SA}	ΔG_{bind}	ΔE_{vdw}	ΔE_{ele}	ΔG_{GB}	ΔG_{SA}	ΔG_{bind}
Tyr612	-2.10	-1.32	1.50	-0.40	-2.32	-1.50	-1.16	1.32	-0.30	-1.64
Ile768	-1.68	-0.10	0.08	-0.14	-1.82	-2.26	-0.14	0.08	-0.14	-2.46
Val782	-4.06	-0.02	0.02	-0.32	-4.38	-5.18	-0.01	0.20	-0.50	-5.58
Phe786	-4.92	-0.50	1.46	-1.00	-4.96	-5.50	-0.86	1.64	-0.98	-5.70
Phe787	-2.12	-0.08	0.16	-0.02	-2.38	-0.92	-0.20	0.58	-0.06	-0.60
Ile813	-1.86	-0.50	0.68	-0.18	-1.86	-1.46	-0.18	0.28	-0.20	-1.58
Met816	-3.80	-0.48	0.70	-0.54	-4.12	-4.22	-0.10	0.48	-0.62	-4.44
Gln817	-3.02	-5.64	4.78	-0.24	-4.14	-2.32	-2.36	2.76	-0.24	-2.18
Phe820	-7.74	-0.74	0.58	-0.78	-7.20	-5.78	-0.48	0.82	-0.78	-5.30

	cmp 57					cmp 59				
	ΔE_{vdw}	ΔE_{ele}	ΔG_{GB}	ΔG_{SA}	ΔG_{bind}	ΔE_{vdw}	ΔE_{ele}	ΔG_{GB}	ΔG_{SA}	ΔG_{bind}
Tyr612	-1.98	-1.20	1.44	-0.26	-2.00	-1.44	-0.24	0.88	-0.22	-1.00
Ile768	-3.18	-0.46	0.30	-0.30	-3.62	-3.32	-0.08	0.02	-0.32	-3.64
Val782	-5.12	-0.20	0.06	-0.54	-5.52	-3.58	-0.20	0.12	-0.50	-4.18
Phe786	-5.66	-0.18	1.14	-0.54	-5.26	-3.64	-0.38	1.10	-0.88	-3.80
Phe787	-1.40	-0.02	0.46	-0.14	-1.06	-1.34	-0.02	0.14	-0.08	-1.32
Ile813	-2.40	-0.20	0.24	-0.18	-2.50	-1.50	-0.32	0.40	-0.24	-1.66
Met816	-2.08	-0.12	0.40	-0.12	-1.94	-3.56	-0.32	0.74	-0.56	-3.70
Gln817	-3.98	-4.30	4.30	-0.48	-4.46	-3.38	-3.94	4.32	-0.52	-3.50
Phe820	-7.18	-0.58	0.90	-0.58	-6.30	-5.82	-0.42	0.76	-0.90	-5.54