

Host	Host conc	Guest conc (mM)	Run number	K (M ⁻¹)	ΔG (KJ/mol)	ΔH (KJ/mol)	ΔS (J/mol/K)
bCD	2.5	37.5	bCDRrim1	36491.91 ± 1737.70	-26.22 ± 0.12	-43.26 ± 1.75	-56.80 ± 5.83
	2.5	37.5	bCDRrim2	33572.61 ± 1563.02	-26.01 ± 0.12	-43.85 ± 1.76	-59.44 ± 5.88
MGLab34	5	37.5	MGLab34Rrim1	19532.83 ± 733.92	-24.66 ± 0.09	-43.67 ± 1.57	-63.36 ± 5.25
	2.5	19	MGLab34Rrim2	5690.03 ± 192.09	-21.58 ± 0.08	-30.51 ± 0.93	-29.75 ± 3.12
MGLab35	2	19	MGLab35Rrim2	27807.38 ± 1045.27	-25.54 ± 0.09	-31.59 ± 1.30	-20.16 ± 4.33
	2	19	MGLab35Rrim3	25648.94 ± 1023.43	-25.34 ± 0.1	-29.36 ± 1.28	-13.41 ± 4.27
MGLab8	4	37.5	MGLab8Rrim1	780.56 ± 31.98	-16.62 ± 0.1	-27.40 ± 1.18	-35.91 ± 3.96
	2	37.5	MGLab8Rrim2	874.24 ± 32.42	-16.90 ± 0.1	-30.46 ± 1.47	-45.18 ± 4.91
	2	37.5	MGLab8Rrim3	839.11 ± 31.63	-16.80 ± 0.09	-31.37 ± 1.34	-48.53 ± 4.48
MGLab24	4	75	MGLab24Rrim3	1161.66 ± 44.16	-17.61 ± 0.09	-35.46 ± 1.52	-59.47 ± 5.09
	4	75	MGLab24Rrim4	1038.92 ± 35.79	-17.33 ± 0.09	-36.92 ± 1.56	-65.27 ± 5.20
MGLab9	1.25	45	MGLab9Rrim7	683.17 ± 21.71	-16.29 ± 0.08	-38.12 ± 1.73	-72.72 ± 5.76
	4	75	MGLab9Rrim6	713.79 ± 20.94	-16.40 ± 0.07	-37.61 ± 1.75	-70.68 ± 19.10
MGLab23	4	75	MGLab23Rrim1	1427.70 ± 56.95	-18.13 ± 0.10	-32.09 ± 1.38	-46.51 ± 1.60
	4	75	MGLab23Rrim3	1588.79 ± 59.25	-18.39 ± 0.09	-31.54 ± 1.33	-43.79 ± 4.45
MGLab19	2.5	37.5	MGLab19Rrim1	315.83 ± 17.83	-14.36 ± 0.14	-47.55 ± 3.40	-110.57 ± 11.34
	4	80	MGLab19Rrim4	318.33 ± 9.41	-14.38 ± 0.07	-48.60 ± 2.75	-114.00 ± 9.17
MGLab36	2	37.5	MGLab36Rrim1	372.79 ± 15.55	-14.78 ± 0.10	-45.52 ± 3.70	-102.43 ± 12.34
	2	37.5	MGLab36Rrim2	335.42 ± 14.34	-14.51 ± 0.11	-45.37 ± 3.93	-102.82 ± 13.11

ΔS (J/mol/K)	Unc. In ΔS (J/mol/	$T\Delta S$ (kJ/mol)	Unc in $T\Delta S$ (J/mol)	N	T (K)=	300.15
-56.8	5.83	-17.04852	1.7498745	1.00 ±0.03		
-59.44	5.88	-17.840916	1.764882	1.00 ±0.03		
-63.36	5.25	-19.017504	1.5757875	0.95 ±0.02		
-29.75	3.12	-8.9294625	0.936468	1.04 ±0.02		
-20.16	4.33	-6.051024	1.2996495	0.75 ±0.02		
-13.41	4.27	-4.0250115	1.2816405	0.81 ±0.03		
-35.91	3.96	-10.7783865	1.188594	0.96 ±0.03		
-45.18	4.91	-13.560777	1.4737365	1.10 ±0.04		
-48.53	4.48	-14.5662795	1.344672	1.18 ±0.04		
-59.47	5.09	-17.8499205	1.5277635	1.05 ±0.03		
-65.27	5.2	-19.5907905	1.56078	1.01 ±0.03		
-72.72	5.76	-21.826908	1.728864	0.98 ±0.03		
-70.68	19.1	-21.214602	5.732865	1.02 ±0.03		
-46.51	1.6	-13.9599765	0.48024	0.88 ±0.03		
-43.79	4.45	-13.1435685	1.3356675	0.83 ±0.03		
-110.57	11.34	-33.1875855	3.403701	1.09 ±0.06		
-114	9.17	-34.2171	2.7523755	0.79 ±0.04		
-102.43	12.34	-30.7443645	3.703851	0.83 ±0.05		
-102.82	13.11	-30.861423	3.9349665	0.85 ±0.06		