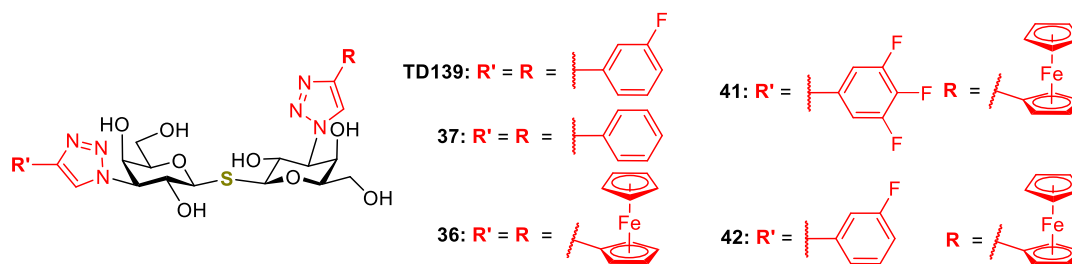


Table 4. Thermodynamic parameters for binding to *hgal-1* and *hgal-3*-CRD obtained by ITC at T = 298 K.



Entry	Compound	K_d (μM)	ΔG (kcal/mol)	ΔH (kcal/mol)	$-T\Delta S$ (kcal/mol)	n	Selectivity to <i>hgal-1</i> ^a
<i>hgal-1</i>							
1	TD139 ^b	0.220 ± 0.05	-9.1 ± 0.2	-16.7 ± 0.4	7.6 ± 0.4	0.96 ± 0.04	0.31
2	TD139	0.279 ± 0.001	-8.9 ± 0.1	-16.9 ± 0.4	8.0 ± 0.4	1.03 ± 0.04	0.07
3	37	0.288 ± 0.006	-8.9 ± 0.1	-9.6 ± 0.4	0.7 ± 0.4	1.04 ± 0.02	0.33
4	36	0.258 ± 0.004	-9.0 ± 0.1	-12.8 ± 1.4	3.8 ± 1.5	1.06 ± 0.07	3.6
5	41	0.340 ± 0.019	-8.9 ± 0.1	-10.2 ± 0.1	1.3 ± 0.1	1.03 ± 0.00	0.07
6	42	0.366 ± 0.031	-8.8 ± 0.1	-9.5 ± 0.1	0.6 ± 0.1	1.03 ± 0.02	0.18
<i>hgal-3</i> -CRD							
7	TD139 ^b	0.068 ± 0.01	-9.9 ± 0.4	-18.2 ± 0.8	8.3 ± 0.9	0.96 ± 0.01	-
8	TD139	0.019 ± 0.003	-10.6 ± 0.1	-16.4 ± 0.4	5.8 ± 0.3	1.08 ± 0.01	-
9	37	0.096 ± 0.005	-9.6 ± 0.1	-11.2 ± 0.3	1.7 ± 0.2	1.03 ± 0.03	-
10	36	0.923 ± 0.04	-8.3 ± 0.1	-12.7 ± 0.2	4.4 ± 0.1	1.08 ± 0.02	-
11	41	0.023 ± 0.006	-10.5 ± 0.2	-14.0 ± 1.3	3.6 ± 1.5	1.03 ± 0.04	-
12	42	0.066 ± 0.010	-9.8 ± 0.1	-12.0 ± 0.2	2.3 ± 0.4	1.01 ± 0.00	-

^a Defined as the ratio $K_d(\textit{hgal-3})/K_d(\textit{hgal-1})$. ^b Taken from ref.^{12b}