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Supporting information for article:

Jacalin–carbohydrate interactions: distortion of the ligand molecule as a determinant of affinity

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Table S1 Isothermal calorimetric data for Gal and its derivatives at all temperatures

Complex	T (in K)	$K_b \times 10^{-3} (M^{-1})$	$-\Delta H_b (kJ mol^{-1})$	$-\Delta G_b (kJ mol^{-1})$	$-T\Delta S (kJ mol^{-1})$	$\Delta C_p (kJ mol^{-1} K^{-1})$
D-Gal (Gal)	278	1.21 (± 0.04)	22.56 (± 0.09)	16.41	6.11	0.029
	283	1.09 (± 0.03)	22.70 (± 0.13)	16.45	6.23	
	288	0.97 (± 0.04)	22.81 (± 0.18)	16.47	6.31	
	293	0.85 (± 0.04)	22.96 (± 0.15)	16.43	6.50	
	298	0.80 (± 0.03)	23.17 (± 0.09)	16.56	6.57	
Methyl α -D-Gal (Me- α -Gal)	278	45.8 (± 2.44)	41.58 (± 0.18)	24.81	15.82	0.267
	283	40.1 (± 0.70)	42.69 (± 0.09)	24.94	17.74	
	288	32.6 (± 0.41)	43.95 (± 0.09)	24.89	19.05	
	293	22.3 (± 0.54)	45.45 (± 0.34)	24.39	21.83	
	298	20.0 (± 0.21)	46.88 (± 0.08)	24.53	22.33	
Methyl β -D-Gal (Me- β -Gal)	278	0.31 (± 0.010)	7.63 (± 0.09)	13.27	-5.71	0.199
	283	0.28 (± 0.031)	8.30 (± 0.16)	13.21	-4.92	
	288	0.23 (± 0.011)	9.71 (± 0.20)	12.99	-3.29	
	293	0.17 (± 0.004)	10.48 (± 0.12)	12.48	-1.99	
	298	0.15 (± 0.003)	11.51 (± 0.14)	12.41	-0.92	
<i>p</i> -Nitrophenyl α -D-Gal (PNP- α -Gal)	278	479 (± 5.85)	39.92 (± 0.29)	30.23	9.65	0.481
	283	164 (± 2.99)	42.44 (± 0.06)	28.25	14.09	
	288	157 (± 1.95)	46.46 (± 0.05)	28.65	17.73	
	293	94.5 (± 1.86)	47.55 (± 0.09)	27.90	19.63	
	298	77.9 (± 1.10)	49.39 (± 0.07)	27.91	21.46	
<i>p</i> -Nitrophenyl β -D-Gal (PNP- β -Gal)	278	6.52 (± 0.06)	28.55 (± 0.12)	20.29	8.23	0.515
	283	4.58 (± 0.05)	31.07 (± 0.19)	19.83	11.21	

	288	3.67 (\pm 0.09)	33.93 (\pm 0.37)	19.65	14.22	
	293	2.62 (\pm 0.04)	36.38 (\pm 0.40)	19.17	17.17	
	298	2.37 (\pm 0.08)	38.76 (\pm 1.12)	19.23	19.46	
UMB α -D-Gal (MUF- α -Gal)	278	1290 (\pm 63.50)	53.99 (\pm 0.17)	32.52	21.41	0.785
	283	929 (\pm 23.6)	57.59 (\pm 0.10)	32.33	25.21	
	288	703 (\pm 28.10)	60.48 (\pm 0.18)	32.24	28.20	
	293	473 (\pm 31.4)	64.46 (\pm 0.37)	31.83	33.11	
	298	335 (\pm 15.10)	70.19 (\pm 0.25)	31.52	38.67	
UMB β -D-Gal (MUF- β -Gal)	278	77.6 (\pm 6.25)	21.62 (\pm 0.25)	26.02	-4.42	0.542
	283	35.8 (\pm 0.66)	27.06 (\pm 0.09)	24.67	2.37	
	288	23.8 (\pm 1.23)	30.34 (\pm 0.35)	24.13	6.18	
	293	14.7 (\pm 0.61)	31.34 (\pm 0.27)	23.37	7.94	
	298	12.9 (\pm 0.86)	33.04 (\pm 0.78)	23.45	9.57	