

Table 4: Comparison of Experimental to Calculated Binding Enthalpies for Binding of the Disaccharides to Galectin

disaccharide	no. of close contacts at distances <4.0 Å	–exptl $\Delta H_b$ (kJ mol <sup>-1</sup> )	–calcd $\Delta H_b^a$ (kJ mol <sup>-1</sup> )
Gal $\beta$ 1,3GlcNAc	5	24.5 $\pm$ 0.5	27.6
Gal $\beta$ 1,4Glc	7	25.4 $\pm$ 3.2	24.6
Gal $\beta$ 1,4Fruc	11	30.3 $\pm$ 4.1	24.6
Gal $\beta$ 1,4GlcNAc	6	30.9 $\pm$ 1.4	27.4
Gal $\beta$ 1,4Man	7	36.0 $\pm$ 2.4	24.4
Gal $\beta$ 1,3Ara	7	40.3 $\pm$ 3.3	23.5
Gal $\beta$ 1S1 $\beta$ Gal	7	42.2 $\pm$ 3.3	25.2

<sup>a</sup> Calculated using differences in the solvent-accessible surface area as described in ref 15.