Electronic Supplementary Material for PCCP

Electronic Supplementary Material

Controlled aggregation of adenine by sugars : physicochemical studies, molecular modelling simulations of sugar-aromatic CH-π stacking interactions, and biological significance

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Figure 1: Effects of disaccharides and corresponding monosaccharides mixtures on the self-aggregation of adenine.

Adenine (152 mM) was solubilised in water alone or in the presence of D-lactose (panel A), D-maltose (panel B) and D-sucrose (panel C) at concentrations close to their respective IC_{50} (i.e. 0.1M for D-lactose, 0.5M for D-maltose, and 0.4M for D-sucrose). For each disaccharide tested, the effects of the relevant monosaccharides (alone or in combination at the indicated concentration) on adenine stacking were also investigated. Each bar represents the mean of three independent experiments ± S.D. (n = 3). Statistical significances were addressed by the Student's T test. In each panel, bars without a common letter differ with at least $p < 0.05$.

Figure 2: Energy minimization models of disaccharides

Molecular models of β-D-lactose, β-D-maltose, and β-D-sucrose are shown in two distinct orientations. The models were obtained with the Polak-Ribiere algorithm (RMS gradient < 0.1 kcal/mole). Total energy values were respectively of -11.44, -12.32, and -3.47 kcal/mole for the β anomers of lactose, maltose and sucrose, respectively. The apolar surfaces of the sugars are indicated in yellow.

Figure 3: Thin layer chromatography of synthetic GalCer and GlcCer.

Synthetic C12-GalCer (lanes 1, 3, 5) and C12-GlcCer (lanes 2, 4, 6) were separated by HPTLC with two distinct solvent systems: (A) chloroform : methanol : water, 60 : 35 :8 (vol :

vol : vol) or (B) chloroform : methanol : water, 65 : 35 : 4 (vol : vol : vol). The plates were stained with orcinol. In (A) the quantities of glycolipid were 1.25 (lanes 1-2), 2.50 (lanes 3-4) or 5.00 μg (lanes 5-6). In (B), 5.00 μg of each glycolipid were deposited on the HPTLC plate.

Figure 1

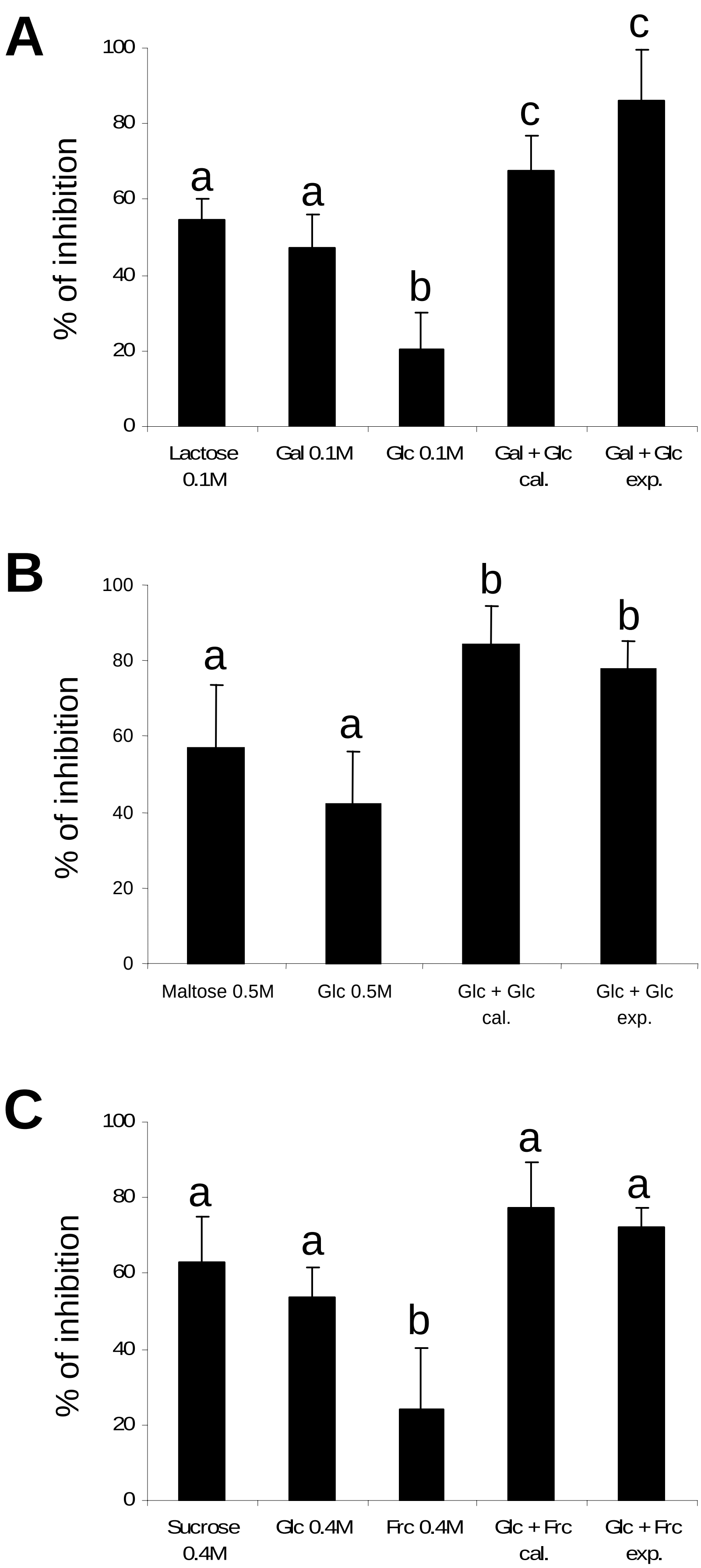
A
% of inhibition
100
80
60
40
20
0
a
a
b
c
c
Lactose 0.1M
Gal 0.1M
Glc 0.1M
Gal + Glc cal.
Gal + Glc exp.
B
% of inhibition
100
80
60
40
20
0
a
a
b
b
Maltose 0.5M
Glc 0.5M
Glc + Glc cal.
Glc + Glc exp.
C
% of inhibition
100
80
60
40
20
0
a
a
b
a
a
Sucrose 0.4M
Glc 0.4M
Frc 0.4M
Glc + Frc cal.
Glc + Frc exp.

Figure 2

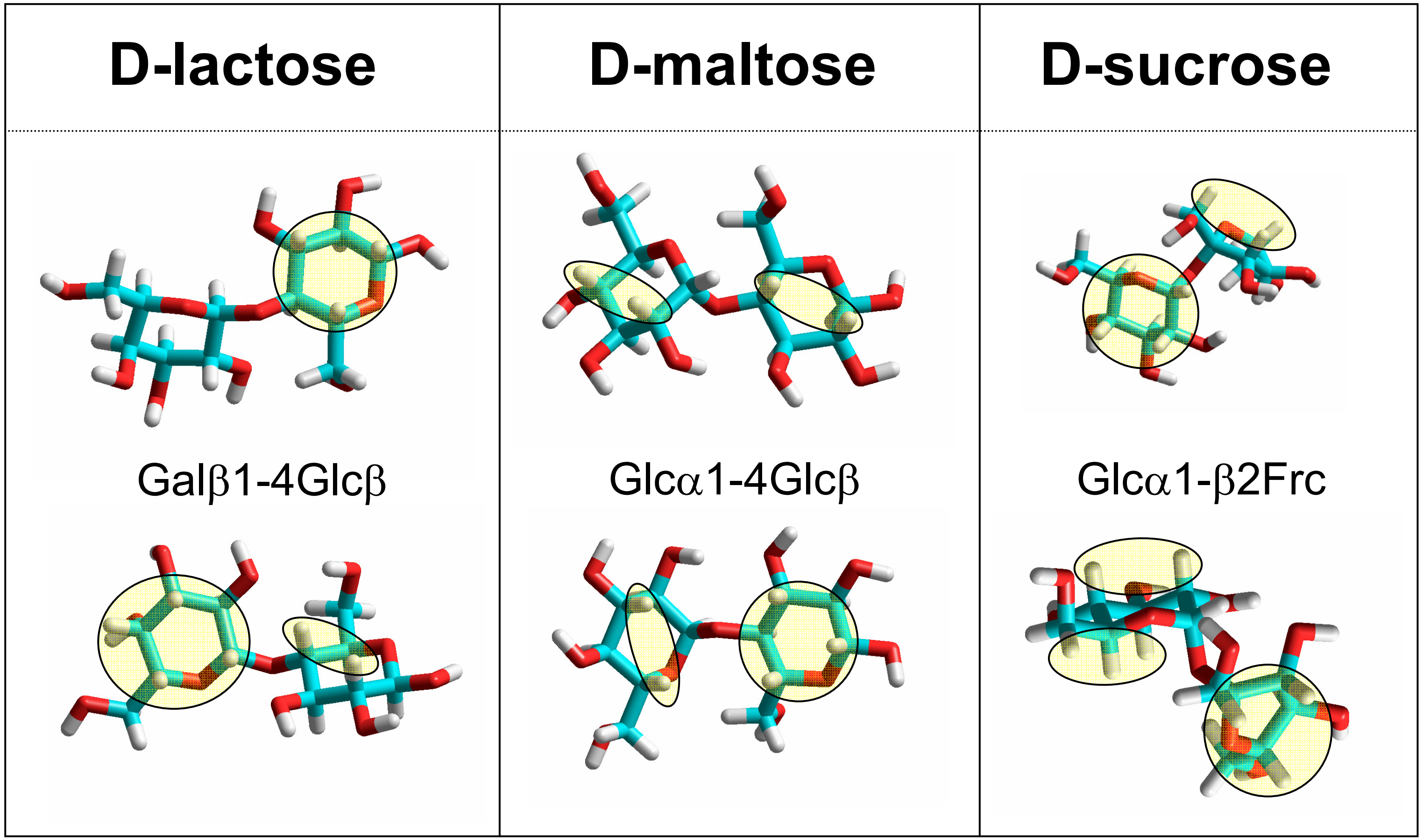
D-lactose
D-maltose
D-sucrose
Galβ1-4Glcβ
Glcα1-4Glcβ
Glcα1-β2Frc

Figure 3