# Steroid-porphyrin conjugate for saccharide sensing in protic media

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# UV-vis titration data

Binding isotherms, absorbance changes in the Soret region of **6** and corresponding Job plots indicating the stoichiometry of the complexes are presented for all studied saccharides (Figures 1-15). Binding of octyl  $\beta$ -D-glucopyranoside in a CHCl<sub>3</sub> - CH<sub>3</sub>OH mixture (9:1) measured using UV-vis (Figures 16,17). Blank experiment documenting absorbance changes after addition of saccharide (Figure 18).

### Maltose

Figure 1. Absorbance changes of 5.6  $\mu$ M **6** upon addition of maltose in 50 % 2-propanol. Solid line is the theoretical isotherm obtained by the least-squares fit to the experimental data.



Figure 2. Job plot for binding maltose calculated from absorbance changes at 416 nm. The sum of total concentrations of interacting components is constant (5.6  $\mu$ M), x is the molar fraction of saccharide.



Figure 3. UV-vis titration of 5.6  $\mu$ M **6** with maltose in 50 % 2-propanol. The arrow shows changes due to increasing concentration of maltose.



#### **D**-glucose

Figure 4. Absorbance changes of 5.6  $\mu$ M **6** upon addition of D-glucose in 50 % 2-propanol. Solid line is the theoretical isotherm obtained by the least-squares fit to the experimental data.



Figure 5. Job plot for binding D-glucose calculated from absorbance changes at 416 nm. The sum of total concentrations of interacting components is constant (5.6  $\mu$ M), x is the molar fraction of saccharide.



Figure 6. UV-vis titration of 5.6  $\mu$ M **6** with D-glucose in 50 % 2-propanol. The arrow shows changes due to increasing concentration of D-glucose.



#### *Maltotrios*e

Figure 7. Absorbance changes of 5.6  $\mu$ M **6** upon addition of maltotriose in 50 % 2-propanol. Solid line is the theoretical isotherm obtained by the least-squares fit to the experimental data.



Figure 8. Job plot for binding maltotriose calculated from absorbance changes at 416 nm. The sum of total concentrations of interacting components is constant (5.6  $\mu$ M), x is the molar fraction of saccharide.



Figure 9. UV-vis titration of 5.6  $\mu$ M **6** with maltotriose in 50 % 2-propanol. The arrow shows changes due to increasing concentration of maltotriose.



#### Maltotetraose

Figure 10. Absorbance changes of 5.6  $\mu$ M **6** upon addition of maltotetraose in 50 % 2propanol. Solid line is the theoretical isotherm obtained by the least-squares fit to the experimental data.



Figure 11. Job plot for binding maltotetraose calculated from absorbance changes at 416 nm. The sum of total concentrations of interacting components is constant (5.6  $\mu$ M), x is the molar fraction of saccharide.



Figure 12. UV-vis titration of 5.6  $\mu$ M **6** with maltotetraose in 50 % 2-propanol. The arrow shows changes due to increasing concentration of maltotetraose.



#### Maltopentaose

Figure 13. Absorbance changes of 5.6  $\mu$ M **6** upon addition of maltopentaose in 50 % 2propanol. Solid line is the theoretical isotherm obtained by the least-squares fit to the experimental data.



Figure 14. Job plot for binding maltopentaose calculated from absorbance changes at 416 nm. The sum of total concentrations of interacting components is constant (5.6  $\mu$ M), x is the molar fraction of saccharide.



Figure 15. UV-vis titration of 5.6  $\mu$ M **6** with maltopentaose in 50 % 2-propanol. The arrow shows changes due to increasing concentration of maltopentaose.



# Octyl β-D-glucopyranoside

Figure 16. Absorbance changes of 5.6  $\mu$ M **6** upon addition of octyl  $\beta$ -D-glucopyranoside in a CHCl<sub>3</sub> - CH<sub>3</sub>OH mixture (9:1). Solid line is the theoretical isotherm obtained by the least-squares fit to the experimental data.



Figure 17. UV-vis titration of 5.6  $\mu$ M **6** with octyl  $\beta$ -D-glucopyranoside in a CHCl<sub>3</sub> - CH<sub>3</sub>OH mixture (9:1). The arrow shows changes due to increasing concentration of octyl  $\beta$ -D-glucopyranoside.



Figure 18. Blank experiment.

All titration experiments shown above were performed in a 1 cm square quartz cell filled with 5.6  $\mu$ M **6** in a water - 2-propanol (1:1 v/v) or CHCl<sub>3</sub> - CH<sub>3</sub>OH (9:1 v/v) mixture at room temperature. A stock saccharide solution in 5.6  $\mu$ M **6** was added stepwise in small increments.

In the blank experiment the stock solution <u>without</u> saccharide was added in the same increments as in binding experiments. In the absence of saccharides <u>no changes</u> to the absorption spectra occurred. After addition of approximately 1 mg maltotriose into the cell immediately the described absorbance changes were observed indicating the formation of the maltotriose-**6** complex (see green line).

