Supplementary Material

Synthesis of cyclodextrin derivatives with monosacharides and their binding with ampicillin and selected lectins

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Dedicated to Professor Michael Orfanopoulos on the occasion of his 67th birthday

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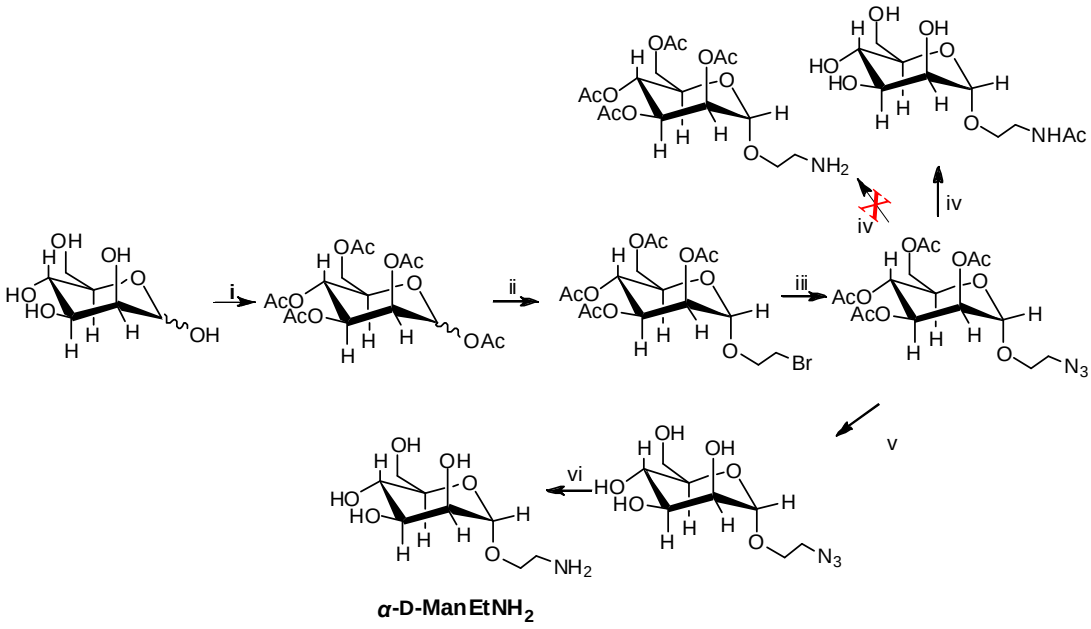
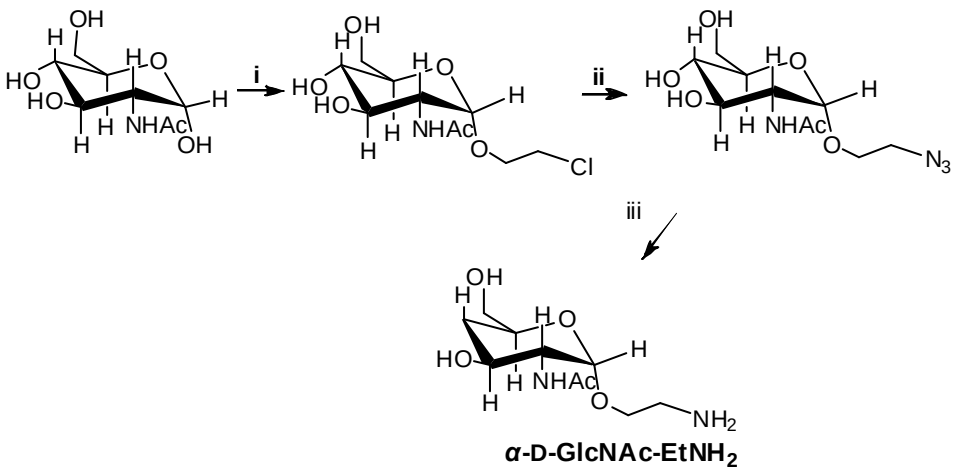


Figure S1. Preparation and NMR spectra of ***α*-D-Man-EtNH$_2$:**[1] i) Acetic anhydride, pyridine, DMAP, rt, 100%; ii) 1-bromoethanol, $BF_3 \cdot OEt_2$, CH_2Cl_2, rt, 67%; iii) NaN_3, DMF, 60 ^oC, 91%; iv) Pd/C 10%, H_2, MeOH, rt, 25%; v) MeONa, MeOH, rt, 100%; vi) Pd/C 10%, H_2, MeOH, rt, 98%, and ^1H and ^{13}C NMR spectra (500 and 125.8 MHz, respectively, D_2O).



***α*-D-GlcNAc-EtNH$_2$**

Figure S2: Preparation and NMR spectra of ***α*-D-GlcNAc-EtNH$_2$:**[2,3] i) 2-Chloroethanol, AcCl, 70 ^{o}C, 61-69%; ii) NaN_3, DMF, 60 ^{o}C, 100%; iii) Pd/C 10%, H_2, MeOH, rt, 100%, and ^{1}H and ^{13}C NMR spectra (500 and 125.8 MHz, respectively, D_2O).

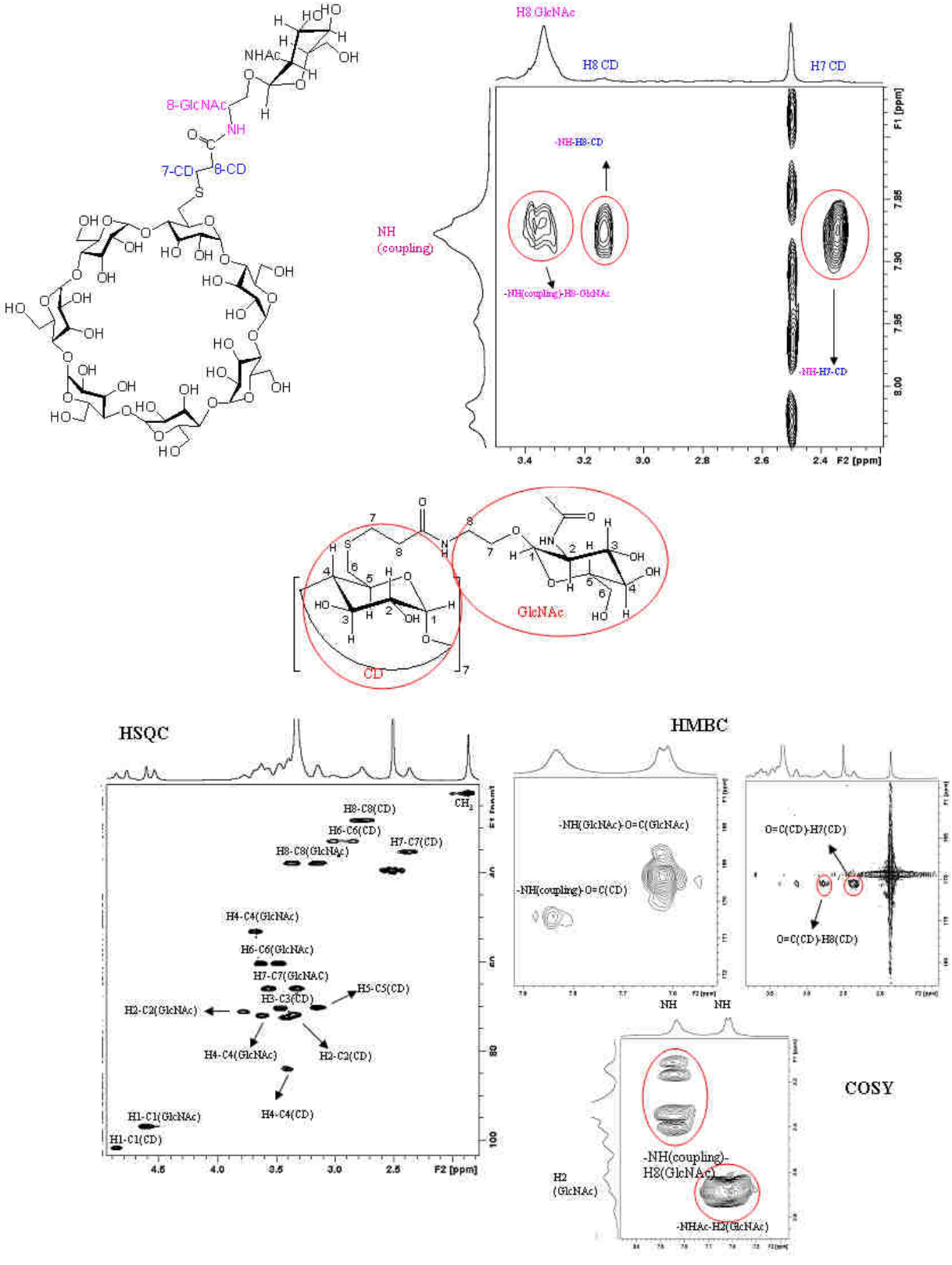


Figure S3. Top: 2D ROESY NMR spectrum of **9**; bottom: HSQC, HMBC and COSY spectra of **5** (500 MHz, DMSO-d_6, 298 K) sowing the connectivity of the cyclodextrin core with the mono-saccharide.

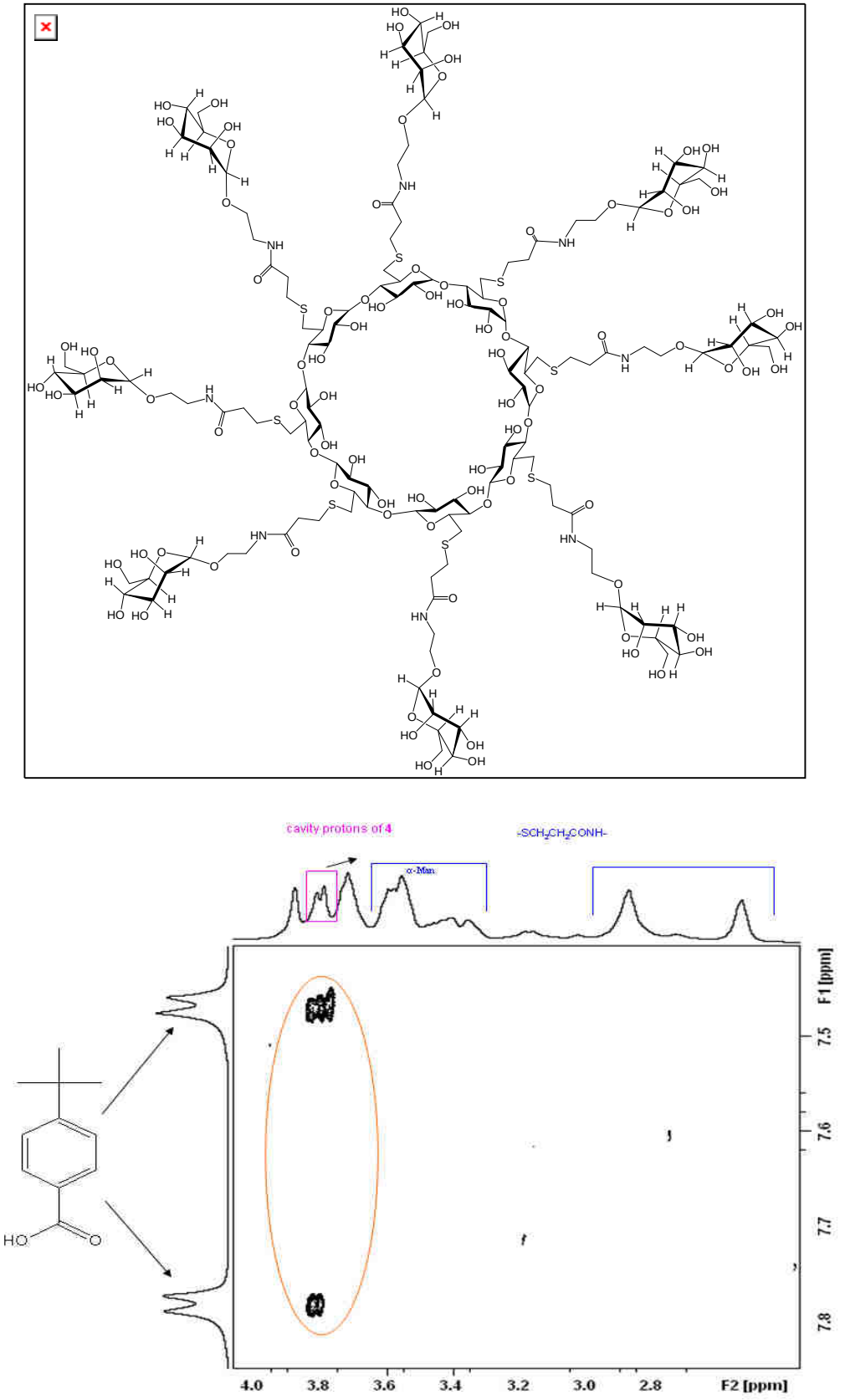


Figure S4. Partial ROESY spectrum of **4** in the presence of excess *p-tert*-butylbenzoic acid (500 MHz, D_2O, 298 K, pH ~8).

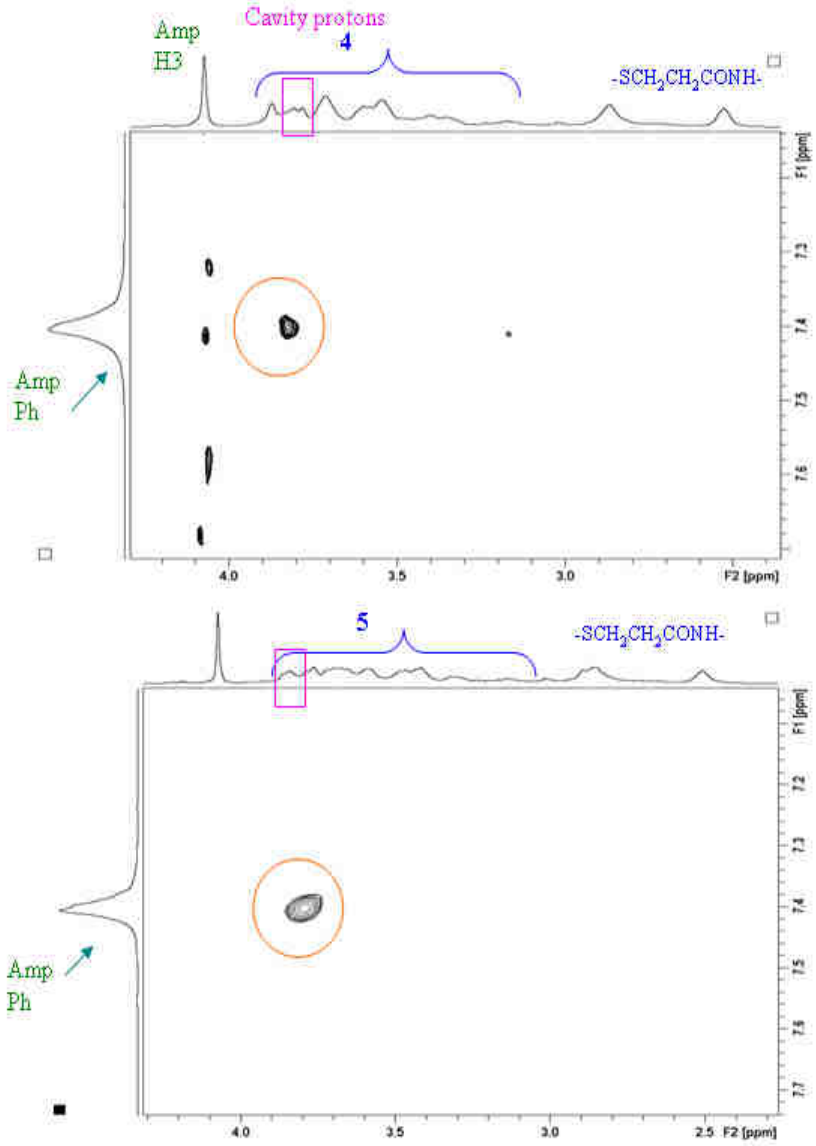


Figure S5. Partial ROESY spectrum of **4** (top) and **5** (bottom) with excess ampicillin (500 MHz, D_2O, 298 K, pH ~8). The dipolar interactions of ampicillin's phenyl group with the cavity protons of the hosts are shown.

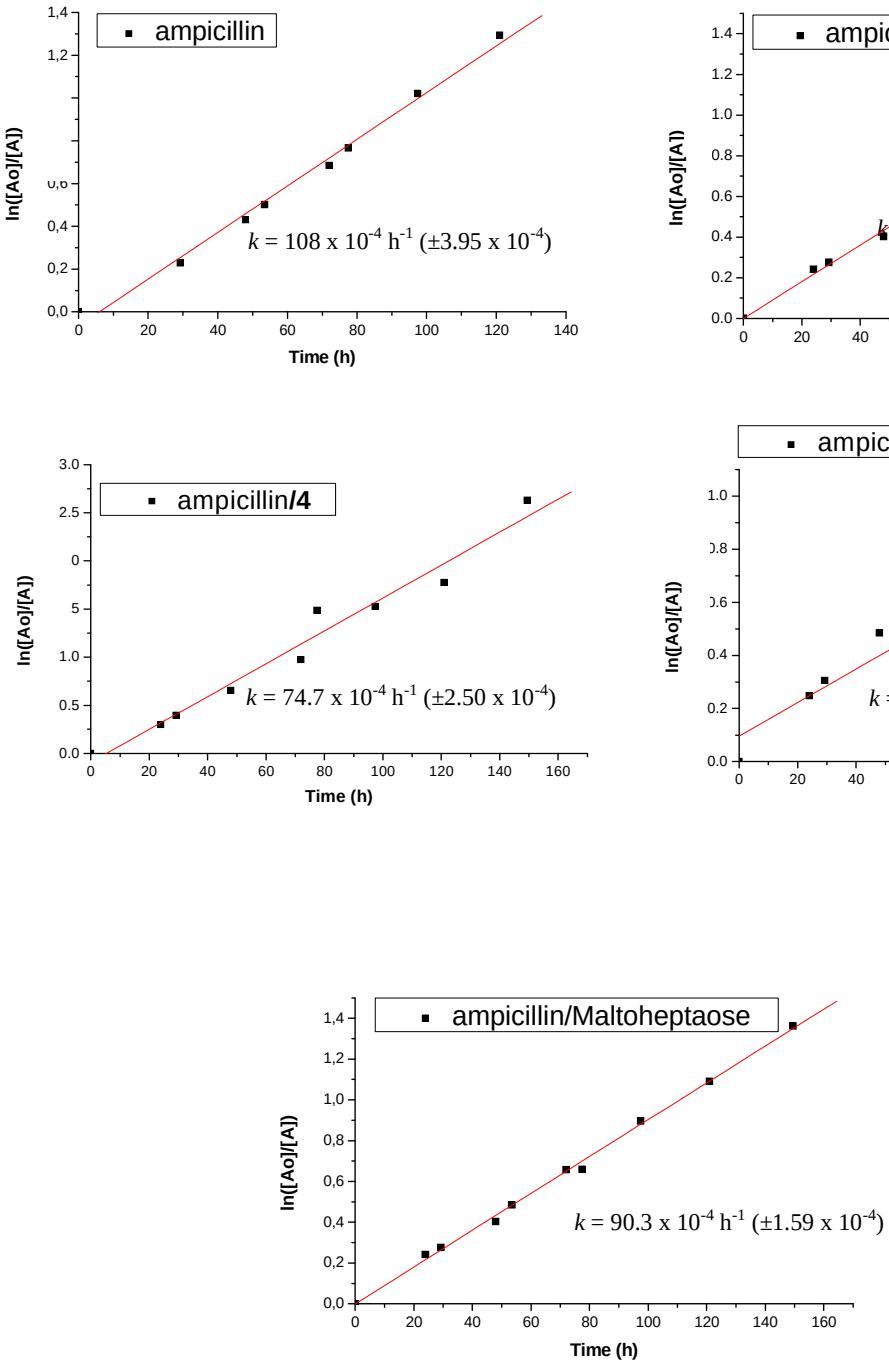


Figure S6. Linear fitting of experimental data from the enzymatic hydrolysis of ampicillin by *β*-lactamase in the presence either of glycoclusters or linear maltoheptaose according to the equation $\ln([A_0]/[A]) = kt$, where $[A_0]$ is the initial ampicillin concentration and [A] is the concentration at time t.

Analysis of WLRS Curves

From the binding curves the *on* (layer build-up) and *off* (wash off) parts were analysed separately.

The binding of the compounds with the immobilized proteins were processed assuming a first order reaction and a mono-exponential growth equation:

$y = a(1-e^{-bt})$, where

$y = \Delta\lambda_{max}$,

t = *time (s)*

$b(s^{-1}) = k_{on}.[compound] \Rightarrow k_{on} = (b/[compound])\ (s^{-1}.M^{-1}) \Rightarrow k_{on} = b.[compound]^{-1}(s^{-1}.M^{-1})$

Therefore, the association rate constant k_{on} depends only on the concentration of the compound introduced in the WLRS setup. For the dissociation process the following mono-exponential decay equation was used:

$y = A_1e^{-x/t_1,}$ where

$y = \Delta\lambda_{max}$,

t = *time (s)*

$t_1 = 1/k_{off}$

$k_{off} = 1/t_1\ (s^{-1})$

The results of the exponential fittings are presented in Table 2 (main text).

References

1. Izumi, M.; Okumura, S.; Yuasa, H.; Hashimoto, H. *J. Carbohydr. Chem.* **2003**, *22*, 317.
2. Disney, M. D.; Seeberger, P. H. *Chem. Biol.* **2004**, *11*, 1701.
3. Roy, R.; Kim, J. M. *Tetrahedron* **2003**, *59*, 3881.

