

Supporting information for:

**Characterising polar compounds using
supercritical fluid chromatography - nuclear
magnetic resonance spectroscopy (SFC-NMR)**

F. H. M. van Zelst,^{†,‡} S. G. J. van Meerten,^{†,‡} and A. P. M. Kentgens^{*,†}

[†]*Institute for Molecules and Materials (IMM), Radboud University, 6525 AJ Nijmegen, The
Netherlands*

[‡]*TI-COAST, Science Park 904, Amsterdam, The Netherlands*

E-mail: A.Kentgens@nmr.ru.nl

S1: SFC UV chromatogram of tocopherol mixture

Before NMR analysis, samples of ManNAc (0.78 M) and GlcNAc (0.73 M) in ultra pure water were separated by SFC on a Waters 2-PIC column at 120 bar, 60 °C and a flow rate of 1.5 ml/min. An isocratic elution was performed with 30 % methanol in CO₂. The UV chromatogram of these separation were recorded at a wavelength of 210 nm and are depicted in Figure S1.

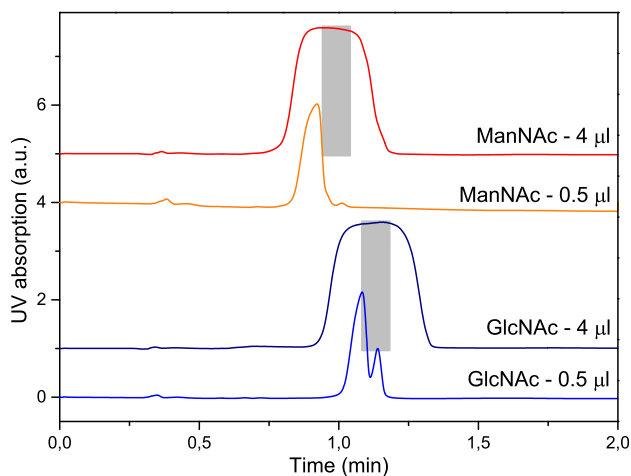


Figure S1: SFC UV chromatograms of ManNAc and GlcNAc in water, separated with a mobile phase of 30 % MeOH/CO₂ on a Waters 2-PIC SFC column. Injection volumes of 0.5 μ L and 4 μ L are compared. An injection volume of 4 μ L was used for SFC-NMR analysis. The fraction of the peaks that were selected for SFC-NMR analysis are indicated in gray.

At injection volumes of 0.5 μ L it can nicely be seen, especially for GlcNAc, that there is a partial separation between the α - and β -stereoisomer. At 4 μ L injection volume, a strange peak shape is observed, which is due to overloading of the UV detector. This does not mean by definition that the SFC column is also overloaded. However, the two stereoisomers can not be distinguished any more. An injection volume of 4 μ L was used for the SFC-NMR analyses, to have enough sample to detect by NMR. The whole peak could not be selected for NMR, therefore the most intense part of the peak was selected, indicated by the gray rectangles.