Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Exploration of conformational flexibility and hydrogen bonding of xylosides in different solvents, as a model system for enzyme active site interactions

Jerk Rönnols,[a] Sophie Manner,[b] Anna Siegbahn,[b] Ulf Ellervik,[b] and Göran Widmalm*[a]

[a]*Department of Organic Chemistry, Arrhenius Laboratory, Stockholm University, SE-106 91, Stockholm, Sweden*
[b]*Center for Analysis and Synthesis, Chemical Center, Lund University, PO Box 124, SE-221 00 Lund, Sweden*

**Corresponding author. E-mail: gw@organ.su.se*

Supporting information

Contents **Page**

$^{3}J_{HH}$ coupling constants for compound **1** (Table S1) S1

δ_H and δ_C references (Table S2) S2

^{1}H and ^{13}C NMR spectra of compounds **1** – **5** and **10** – **11** S3 – S9

Table S1. $^{3}J_{HH}$ coupling constants for compound **1** in different solvents, given in Hz.

Solvent	$J_{1,2}$	$J_{2,3}$	$J_{3,4}$	$J_{4,5pro\text{-}R}$	$J_{4,5pro\text{-}S}$	$J_{5pro\text{-}R,5pro\text{-}S}$
Dimethyl sulfoxide-d_6	7.325	8.906	8.661	5.343	10.243	–11.208
Methanol-d_4	7.492	9.104	8.803	5.355	10.125	–11.454
N,*N*-Dimethylformamide-d_7	7.406	8.885	8.723	5.294	10.068	–11.257
Pyridine-d_5	7.449	8.897	8.525	5.284	10.06	–11.254
Acetone-d_6	7.094	8.941	8.272	5.127	9.670	–11.369
Nitromethane-d_3	7.146	8.679	8.682	5.102	9.648	–11.475
Tetrahydrofurane-d_8	7.169	8.620	8.276	5.161	9.639	–11.300
Aniline-d_7	7.133	8.687	8.468	5.078	9.580	–11.484
Phenol-d_6	7.080	8.797	8.483	5.057	9.504	–11.745
Dichloromethane-d_2	6.576	8.172	7.945	4.718	8.787	–11.716
Chloroform-*d*	6.224	7.786	7.634	4.501	8.268	–11.880
Toluene-d_8	5.736	7.514	7.290	3.973	7.850	–11.859
Chlorobenzene-d_5	6.135	7.665	7.522	4.474	8.092	–11.745
Benzene-d_6	5.803	7.354	7.191	4.163	7.716	–11.786

Table S2. δ_H and δ_C references of intrinsic solvent signals.[a]

Solvent	^{1}H	^{13}C
Dimethyl sulfoxide-d_6	2.50	39.52
Methanol-d_4	3.31	49.00
N,*N*-Dimethylformamide-d_7	2.91	30.10
Pyridine-d_5	8.71	123.50
Acetone-d_6	2.05	29.84
Nitromethane-d_3	4.33	
Tetrahydrofurane-d_8	3.58	67.40
Aniline-d_7	6.64	115.07
Phenol-d_6	7.24	
Dichloromethane-d_2	5.32	53.80
Chloroform-*d*	7.26	77.16
Toluene-d_8	7.09	
Chlorobenzene-d_5	7.14	
Benzene-d_6	7.16	128.06

[a]Data obtained from three sources:
- Fulmer, G.R.; Miller, A.J.M.; Sherden, N.H.; Gottlieb, H.E.; Nudelman, A.; Stoltz, B.M.; Bercaw, J.E.; Goldberg, K.I. *Organometallics*, **2010**, *29*, 2176 – 2179.
- Isotec Inc.
- http://riodb01.ibase.aist.go.jp/sdbs/cgi-bin/direct_frame_top.cgi, accessed February 2012.