Electronic Supplementary Material (ESI) for Analyst.

Supporting Information

Solvent-independent Determination of Heteroatom Protonation States from NMR Spectra by Differential Deuterium Isotope Shifts

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Table S1. DIS-values (given in ppm) of various compounds measured in three representative deuterated solvents (methanol, pyridine and chloroform).

Compound Name	Solvent	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-11	C-12
butane-2,3-diol	methanol-d_4	0.05	0.09										
	chloroform-d	0.06	0.12										
	pyridine-d_5	0.06	0.11										
butane-1-ol	methanol-d_4	0.10	0.02	-0.01	0.00								
	chloroform-d	0.16	0.05	-0.03	-0.01								
	pyridine-d_5	0.12	-0.02	-0.03	-0.01								
iso-butanol	methanol-d_4	0.13	0.05	0.00									
	chloroform-d	0.15	0.04	-0.01									
	pyridine-d_5	0.13	0.05	0.01									
2-(2-ethoxyethoxy)ethanol	methanol-d_4	0.12	0.03	0.00	0.00	0.00	0.01						
	chloroform-d	0.12	0.01	0.00	0.00	0.00	0.00						
	pyridine-d_5	0.12	0.04	0.01	0.01	0.00	0.01						
2-phenoxyethanol	methanol-d_4	0.06	-0.01	-0.05	-0.03	-0.02	-0.02						
	chloroform-d	0.14	0.02	0.01	0.00	0.00	0.00						
	pyridine-d_5	0.11	0.04	0.00	0.00	0.00	0.00						
dimethoxyethane	methanol-d_4	0.00	0.00										
	chloroform-d	0.00	0.00										
	pyridine-d_5	0.00	0.00										
1,4-benzodioxane-6-amine	methanol-d_4	-0.01	0.00	-0.01	0.00	0.09	0.01	-0.01	-0.04				
	chloroform-d	-0.01	0.00	0.00	0.00	0.11	0.02	0.00	-0.02				
	pyridine-d_5	0.01	0.01	0.01	0.00	0.13	0.02	0.01	-0.03				
1-adamantylamine	methanol-d_4	0.13	0.09	-0.01	0.02								
	chloroform-d	0.22	0.06	-0.01	0.01								
	pyridine-d_5	0.21	0.08	-0.01	0.01								
benzylamine	methanol-d_4	0.13	-0.09	-0.06	-0.06	-0.08							
	chloroform-d	0.15	-0.03	-0.02	-0.02	-0.02							
	pyridine-d_5	0.21	0.03	0.05	0.03	0.04							
1-aminoindane	methanol-d_4	0.18	0.04	-0.01	-0.02	0.00	0.02	0.01	0.00	-0.03			
	chloroform-d	0.15	0.02	-0.03	0.00	-0.01	-0.01	-0.02	-0.02	-0.01			
	pyridine-d_5	0.18	0.08	-0.01	-0.02	0.00	0.00	0.00	-0.01	0.02			
dimethylamine	methanol-d_4	0.06	0.00										
	chloroform-d	0.19	0.07										
	pyridine-d_5	0.10	0.03										
cyclohexylamine	methanol-d_4	0.18	0.06	0.01	0.02								
	chloroform-d	0.22	0.10	0.01	0.03								
	pyridine-d_5	0.18	0.07	-0.01	0.01								
2-(methylamino)ethanol	methanol-d_4	0.06	0.06	0.05									
	chloroform-d	0.03	0.10	0.07									
	pyridine-d_5	0.11	0.12	0.09									
2-(methoxyethyl)methylamine	methanol-d_4	0.04	-0.02	0.08	0.00								
	chloroform-d	0.07	-0.01	0.09	0.01								
	pyridine-d_5	0.10	0.01	0.10	0.00								

Table S2. DIS-values (given in ppm) of 1,2;5,6-di-*O*-isopropylglucofuranose measured in a range of deuterated solvents. Note that C-3 is the α-carbon of the hydroxy-group. A total of five ethers are present.

Compound Name	Solvent	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-11	C-12
1,2;5,6-di-*O*-isopropylglucofuranose	methanol-d_4	-0.02	0.00	0.06	0.01	-0.02	-0.01	-0.01	0.00	0.00	0.00	-0.01	-0.01
	chloroform-d	-0.01	0.03	0.10	0.01	-0.04	-0.01	0.01	-0.01	0.00	0.00	0.00	-0.10
	pyridine-d_5	-0.01	0.01	0.09	0.02	-0.01	-0.02	0.01	0.00	-0.01	0.00	0.00	-0.01
	DCM-d_2	0.00	0.03	0.10	0.02	-0.04	-0.01	0.01	0.00	0.01	-0.01	0.00	0.01
	ACN-d_3	0.01	0.04	0.12	0.03	0.01	0.01	-0.01	0.01	0.01	-0.01	0.01	0.01
	THF-d_8	-0.01	0.02	0.11	0.01	-0.01	0.00	0.01	0.00	0.00	0.01	0.01	0.00
	acetone-d_6	-0.02	-0.02	0.08	0.00	-0.03	-0.03	0.01	-0.03	-0.03	0.01	-0.02	-0.02
	DMSO-d_6	0.01	0.04	0.10	0.03	0.00	0.00	0.00	0.01	0.01	-0.01	0.01	0.01
	toluene-d_8	-0.01	0.02	0.10	0.02	-0.02	0.00	0.01	0.00	0.01	-0.01	0.01	0.01