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Supporting Information

Conformational properties of alkyl glucosyl sulfones in solution

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A) Experimental Spectra



Figure S1. ¹H NMR of **4a** (600 MHz. CDCl₃)



Figure S2. ¹H NMR of **4b** (500 MHz. CDCl₃)



Figure S3. ¹H NMR of **4c** (400 MHz. CDCl₃)



Figure S4. ¹H NMR 4d (600 MHz. CDCl₃)



Figure S5. ¹H NMR of **4e** (400 MHz. CDCl₃)



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Figure S7. ¹H NMR of **9a** (500 MHz. CDCl₃)



Figure S8. ¹H NMR of **9b** (500 MHz. CDCl₃)



Figure S9. ¹H NMR of **9c** (400 MHz. CDCl₃)



Figure S10. ¹H NMR of **9d** (400 MHz. CDCl₃)



Figure S11. ¹H NMR of **9e** (400 MHz. CDCl₃)





Figure S12. ¹H NMR of **9f** (500 MHz. CDCl₃)



Figure S13. ¹H NMR of **4d** (600 MHz. C₆D₆)



Figure S14. ¹H NMR of 4d (600 MHz. CD₃CN)



Figure S15. ¹H NMR of **4d** (600 MHz. CD₃OD)



Figure S16. ¹³C NMR of **4a** (top) and **4b** (bottom) (100 MHz. CDCl₃)



Figure S17. 13 C NMR of **4c** (top) and **4d** (bottom) (100 MHz. CDCl₃)



Figure S18. ^{13}C NMR of 4e (top) and 4f (bottom) (100 MHz. CDCl₃)



Figure S19. ¹³C NMR of **9a** (top) and **9b** (bottom) (100 MHz. CDCl₃)



Figure S20. ¹³C NMR of **9c** (top) and **9d** (bottom) (100 MHz. CDCl₃)



Figure S21. ¹³C NMR of **9e** (top) and **9f** (bottom) (100 MHz. CDCl₃)





Figure S22. ¹H NMR (top) and 1D-NOESY (bottom) of **4a** (600 MHz. CD₃CN)





Figure S23. ¹H NMR (top) and 1D-NOESY (bottom) of **4b** (600 MHz. CD₃CN)



Figure S24. ¹H NMR (top) and 1D-NOESY (bottom) of **4d** (600 MHz. CD₃CN)





Figure S25. ¹H NMR (top) and 1D-NOESY (bottom) of **4f** (600 MHz. CD₃CN)

B) Spectral simulation

Table S1. Analysis of ABX Spin System in CDCl₃ to Determine the Order Coupling.

Cmpd	Spectrometer (MHz)	δ H6R (ppm)	δ H6S (ppm)	δ H5 (ppm)	J _{5,6R} (Hz)	J _{5,6S} (Hz)	J _{6R,6S} (Hz)	Δδ _{5,6R} (Hz)	Δδ _{5,65} (Hz)	Δδ _{6R,6S} (Hz)	Δδ _{5,6} /J 5,6	Δδ _{5,65} /J _{5,65}	$\Delta \delta_{6R,6S}/J_{6R,6S}$
4a	500	4.30	4.21	3.85	4.7	1.5	12.6	225	180	45	48	120	3.6
4b	500	4.27	4.21	3.82	4.5	2.0	12.5	225	195	30	50	98	2.4
4c	500	4.26	4.21	3.82	4.7	2.1	12.5	220	195	25	47	93	2.0
4d	600	4.20	4.23	3.8	4.8	2.4	12.6	240	258	18	50	108	1.4
4e	500	4.17	4.23	3.79	5.5	2.3	12.4	190	220	30	35	96	2.4
4f	500	4.14	4.24	3.81	6.6	1.9	12.4	165	215	50	25	113	4.0
9a	500	4.44	4.61	4.12	5.0	2.0	12.0	160	245	85	32	123	7.1
9b	500	4.43	4.58	4.10	5.5	3.0	12.5	165	240	75	30	80	6.0
9c	500	4.44	4.60	4.11	5.0	2.2	12.2	165	245	80	33	111	6.6
9d	500	4.36	4.50	4.02	5.8	2.4	12.3	170	240	70	29	100	5.7
9e	500	4.42	4.56	4.09	5.8	2.1	12.4	165	235	70	28	112	5.6
9f	500	4.40	4.57	4.12	6.5	2.5	12.5	140	225	85	22	90	6.8

Formulas used: 1. $\Delta\delta$ (ppm) × spectrometer frequency= $\Delta\delta$ (Hz); 2. $\Delta\delta/J = \Delta\delta$ (Hz) / J (Hz); the system is considered second order if $\Delta\delta/J \le 10$

¹H NMR spectra simulation:

Spectra simulations were carried out using Bruker's simulation and iteration tool (Daisy), available in TopSpin 4.0.7. The three spin systems of interest (H5, H6*R*, and H6*S*) were entered in the "Frequencies" and "Scalars" tabs. Subsequently, both the simulation and iteration of the δ H5, δ H6R, δ H6S, ${}^{3}J_{H5.6R}$ and ${}^{3}J_{H5.H6S}$ values were performed using the standard iteration algorithm, with a linewidth of 0.3 Hz, medium signal broadening, and a medium number of cycles. The resulting simulated spectra were peak-picked and plotted. The simulated data presented in **Tables S2** and **S3** correspond to the chemical shifts and coupling constants obtained from these spectra.

Table S2. δ H5, δ H6*R*, δ H6*S*, ${}^{3}J_{H5.6R}$ and ${}^{3}J_{H5.H6S}$ data from experimental and simulated spectra of acetates **4a–4g** and dibenzoates **9a–9g** in CDCl₃.

	Exp	erimenta	al data				Si	mulated	data			
Cmpd.	δ H6 <i>R</i> (ppm)	δ H6 <i>S</i> (ppm)	δ H5 (ppm)	J _{5.6R} (Hz)	J _{5.6S} (Hz)	J _{6R.6S} (Hz)	δ H6 <i>R</i> (ppm)	δ H6 <i>S</i> (ppm)	δ H5 (ppm)	J _{5.6R} (Hz)	J _{5.6S} (Hz)	J _{6R.6S} (Hz)
4a	4.32	4.20	3.85	4.8	2.2	12.7	4.32	4.20	3.85	5.1	2.3	12.8
4b	4.26	4.21	3.83	4.7	2.1	12.7	4.27	4.21	3.82	4.6	2.2	12.7
4c	4.26	4.20	3.82	4.8	2.3	12.6	4.26	4.20	3.81	4.9	2.3	12.5
4d	4.20	4.23	3.80	4.8	2.4	12.6	4.19	4.23	3.79	5.1	2.2	12.6
4e	4.16	4.22	3.78	5.6	2.3	12.5	4.11	4.18	3.72	5.2	2.3	11.9
4f	4.13	4.24	3.80	6.5	2.4	12.5	4.13	4.23	3.80	6.3	1.9	12.2
9a	4.44	4.61	4.13	4.9	3.0	12.7	4.44	4.61	4.11	5.3	2.8	12.7
9b	4.43	4.60	4.11	5.3	3.0	12.5	4.43	4.59	4.09	5.5	2.6	12.5
9c	4.44	4.60	4.11	5.4	3.0	12.5	4.44	4.60	4.11	5.1	2.6	12.2
9d	4.43	4.56	4.09	5.8	2.7	12.3	4.44	4.57	4.09	5.7	2.4	12.2
9e	4.42	4.55	4.08	5.9	2.4	12.5	4.41	4.56	4.08	6.0	2.4	12.7
9f	4.39	4.58	4.12	6.8	2.6	12.2	4.39	4.57	4.11	6.3	2.3	12.2

Experimental data									Simulated data				
Cmpd.	δ H6 <i>R</i> (ppm)	δ H6 <i>S</i> (ppm)	δ H5 (ppm)	J _{5.6R} (Hz)	J _{5.6S} (Hz)	J _{6R.6S} (Hz)	Δδ _{6R.6S} /J _{6R.6S}	δ H6 <i>R</i> (ppm)	δ H6 <i>S</i> (ppm)	δ H5 (ppm)	J _{5.6R} (Hz)	J _{5.6S} (Hz)	J _{6R.6S} (Hz)
4a	4.25	4.18	4.00	5.1	2.4	12.6	2.8	4.25	4.18	4.00	5.5	2.2	12.5
4b	4.24	4.17	4.00	5.4	2.4	12.6	2.8	4.24	4.16	3.99	5.3	1.7	12.5
4c	4.34	4.44	4.22	5.4	2.4	12.5	4.4	4.34	4.44	4.21	5.1	2.7	12.5
4d	4.23	4.15	4.02	6.0	2.4	12.6	3.2	4.23	4.15	4.02	5.9	2.1	12.6
4e	4.19	4.16	3.99	5.3	3.0	12.6	1.2	4.19	4.16	3.99	5.9	2.5	12.6
4f	4.13	4.17	4.03	6.1	2.9	12.6	1.6	4.13	4.17	4.03	6.3	2.0	12.6

Table S3. δ H5, δ H6*R*, δ H6*S*, ${}^{3}J_{H5.6R}$ and ${}^{3}J_{H5.H6S}$ data from experimental and simulated spectra of acetates **4a-4g** in CD₃CN.

Table S4. δ H5, δ H6*R*, δ H6*S*, ${}^{3}J_{H5,6R}$ and ${}^{3}J_{H5,H6S}$ data from experimental and simulated spectra of sulfone **4d** in C₆D₆ and CD₃OD.

		E	kperimen	tal data	1		Simulated data						
Cmpd.	δ H6 <i>R</i> (ppm)	δ H6 <i>S</i> (ppm)	δ H5 (ppm)	J _{5.6R} (Hz)	J _{5.6S} (Hz)	J _{6R.6S} (Hz)	Δδ _{6R.6S} /J _{6R.6S}	δ H6 <i>R</i> (ppm)	δ H6 <i>S</i> (ppm)	δ H5 (ppm)	J _{5.6R} (Hz)	J _{5.6S} (Hz)	J _{6R.6S} (Hz)
C ₆ D ₆													
4d	3.95	3.94	2.90	4.4	3.0	12.6	0.5	3.95	3.94	2.90	5.2	2.1	12.7
CD₃OD													
4d	4.28	4.25	4.11	5.4	2.4	12.6	1.4	4.28	4.25	4.11	5.6	2.0	12.5



Overlaid regions of experimental and simulated ¹H NMR spectra of 4a–4f and 9a–9f

Figure S26. Overlaid regions of experimental (blue) and simulated (red) ¹H NMR spectra showing H5, H6*R*, and H6*S* for 2,3,4,6–tetra–O–acetyl-1-(methylsulfonyl)- β -D-glucopyranoside **(4a)** in CDCl₃.



Figure S27. Overlaid regions of experimental (blue) and simulated (red) NMR spectra showing H5, H6*R*, and H6*S* for 2,3,4,6–tetra–O–acetyl-1-(ethylsulfonyl)- β -D-glucopyranoside **(4b)** in CDCl₃.



Figure S28. Overlaid regions of experimental (blue) and simulated (red) ¹H NMR spectra showing H5, H6*R*, and H6*S* for 2,3,4,6–tetra–O–acetyl-1-(*n*-propylsulfonyl)- β -D-glucopyranoside (4c) in CDCl₃.



Figure S29. Overlaid regions of experimental (blue) and simulated (red) ¹H NMR spectra showing H5, H6*R*, and H6*S* for 2,3,4,6–tetra–O–acetyl-1-(*iso*-propylsulfonyl)- β -D-glucopyranoside (4d) in CDCl₃.



Figure S30. Overlaid regions of experimental (blue) and simulated (red) ¹H NMR spectra showing H5, H6*R*, and H6*S* for 2,3,4,6–tetra–O–acetyl-1-(cyclohexylsulfonyl)- β -D-glucopyranoside **(4e)** in CDCl₃



Figure S31. Overlaid regions of experimental (blue) and simulated (red) ¹H NMR spectra showing H5, H6*R*, and H6*S* for 2,3,4,6–tetra–O–acetyl-1-(*tert*-butylsulfonyl)- β -D-glucopyranoside **(4f)** in CDCl₃



Figure 32. Overlaid regions of experimental (blue) and simulated (red) ¹H NMR spectra showing H5, H6*R*, and H6*S* for 2,3,4,6–tetra–O–acetyl-1-(methylsulfonyl)- β -D-glucopyranoside **(4a)** in CD₃CN



Figure S33. Overlaid regions of experimental (blue) and simulated (red) ¹H NMR spectra showing H5, H6*R*, and H6*S* for 2,3,4,6–tetra–O–acetyl-1-(ethylsulfonyl)- β -D-glucopyranoside **(4b)** in CD₃CN



Figure 34. Overlaid regions of experimental (blue) and simulated (red) ¹H NMR spectra showing H5, H6*R*, and H6*S* for 2,3,4,6–tetra–O–acetyl-1-(*n*-propylsulfonyl)- β -D-glucopyranoside (4c) in CD₃CN



Figure 35. Overlaid regions of experimental (blue) and simulated (red) NMR spectra showing H5, H6*R*, and H6*S* for 2,3,4,6–tetra–O–acetyl-1-(*iso*-propylsulfonyl)- β -D-glucopyranoside (4d) in CD₃CN



Figure S36. Overlaid regions of experimental (blue) and simulated (red) ¹H NMR spectra showing H5, H6*R*, and H6*S* for 2,3,4,6–tetra–O–acetyl-1-(cyclohexylsulfonyl)- β -D-glucopyranoside **(4e)** in CD₃CN



Figure S37. Overlaid regions of experimental (blue) and simulated (red) ¹H NMR spectra showing H5, H6*R*, and H6*S* for 2,3,4,6–tetra–O–acetyl-1-(*tert*-butylsulfonyl)- β -D-glucopyranoside **(4f)** in CD₃CN



Figure S38. Overlaid regions of experimental (blue) and simulated (red) ¹H NMR spectra showing H5, H6*R*, and H6*S* for 2,3–di–*O*–acetyl-4,6-bis-*O*-(4-bromobenzoyl)-1-(methylsulfonyl)-β-D-glucopyranoside **(9a)** in CDCl₃



Figure S39. Overlaid regions of experimental (blue) and simulated (red) ¹H NMR spectra showing H5, H6*R*, and H6*S* for 2,3–di–*O*–acetyl-4,6-bis-*O*-(4-bromobenzoyl)-1-(ethylsulfonyl)-β-D-glucopyranoside **(9b)** in CDCl₃



Figure S40. Overlaid regions of experimental (blue) and simulated (red) ¹H NMR spectra showing H5, H6*R*, and H6*S* for 2,3–di–O–acetyl-4,6-bis-O-(4-bromobenzoyl)-1-(n-propylsulfonyl)- β -D-glucopyranoside (9c) in CDCl₃

Figure S41. Overlaid regions of experimental (blue) and simulated (red) ¹H NMR spectra showing H5, H6*R*, and H6*S* for 2,3–di–*O*–acetyl-4,6-bis-*O*-(4-bromobenzoyl)-1-(*iso*-propylsulfonyl)-β-D-glucopyranoside **(9d)** in CDCl₃

Figure S42. Overlaid regions of experimental (blue) and simulated (red) ¹H NMR spectra showing H5, H6*R*, and H6*S* for 2,3–di–O–acetyl-4,6-bis-O-(4-bromobenzoyl)-1-(cyclohexylsulfonyl)- β -D-glucopyranoside (**9e**) in CDCl₃

Figure S43. Overlaid regions of experimental (blue) and simulated (red) ¹H NMR spectra showing H5, H6*R*, and H6*S* for 2,3–di–*O*–acetyl-4,6-bis-*O*-(4-bromobenzoyl)-1-(*tert*-butylsulfonyl)-β-D-glucopyranoside **(9f)** in CDCl₃

Figure S44. Overlaid regions of experimental (blue) and simulated (red) NMR spectra showing H5, H6*R*, and H6*S* for 2,3,4,6–tetra–O–acetyl-1-(*iso*-propylsulfonyl)- β -D-glucopyranoside (4d) in C₆D₆

Figure S45. Overlaid regions of experimental (blue) and simulated (red) NMR spectra showing H5, H6*R*, and H6*S* for 2,3,4,6–tetra–O–acetyl-1-(*iso*-propylsulfonyl)- β -D-glucopyranoside (4d) in CD₃OD.

C) Hydroxymethyl rotamer populations from simulated coupling constants

Table S5. Hydroxymethyl rotamer populations of *per*-acetylated alkyl sulfones **4a**–**4f** (CDCl₃ and CD₃CN) and dibenzoates **9a**–**9f** (CDCl₃) calculated from the simulated ${}^{3}J_{H5,H6R}$ and ${}^{3}J_{H5,H6S}$ coupling constants (Tables S2 and S3).

		CDCI ₃		CD₃CN						
Cmpd.	P_{gg}	P_{gt}	P_{tg}	P_{gg}	P_{gt}	P_{tg}				
4a	59	41	0	55	45	0				
4b	64	36	0	57	43	0				
4c	61	39	0	56	39	5				
4d	59	41	0	51	49	0				
4e	58	42	0	50	48	2				
4f	48	52	0	48	52	0				
9a	53	41	6							
9b	53	44	3							
9c	57	40	0							
9d	53	47	0							
9e	50	50	0							
9f	47	53	0							

Figure S46. P_{gg} (red color),¹ and P_{gt} (blue color)² (calculated from simulated ³J_{H5,H6R} and ³J_{H5,H6S} coupling constants) versus alkyl's Charton values for alkyl sulfones 4a-4f in CDCl3

¹ $P_{gg} = -18.7v + 72.7 (R^2 = 0.82)$ ² $P_{gt} = 18.7v + 27.3 (R^2 = 0.82)$

Figure S47. Pgg (red color),³ and Pgt (blue color)⁴ (calculated from simulated ³JH5,H6R and ³JH5,H6S coupling constants) versus alkyl's Charton values for alkyl sulfones 4a-4f in CD₃CN

³ $P_{gg} = -12.4 v + 62.5 (R^2 = 0.80)$ ⁴ $P_{gt} = 13.3 v + 35.7 (R^2 = 0.56)$

Figure S48. P_{gg} (red color),⁵ and P_{gt} (blue color)⁶ (calculated from simulated ³J_{H5,H6R} and ³J_{H5,H6S} coupling constants) versus alkyl's Charton values for alkyl sulfones **9a–9f** in CDCl₃

 $^{^{5}}P_{gg} = -9.9 v + 59.9 (R^{2} = 0.61)$

 $^{^{6}}P_{gt} = 17.1 v + 32.5 (R^{2} = 0.78)$