SUPPLEMENTARY DATA

Glucosinolates in *Reseda lutea* L.: distribution in plant tissues during flowering time

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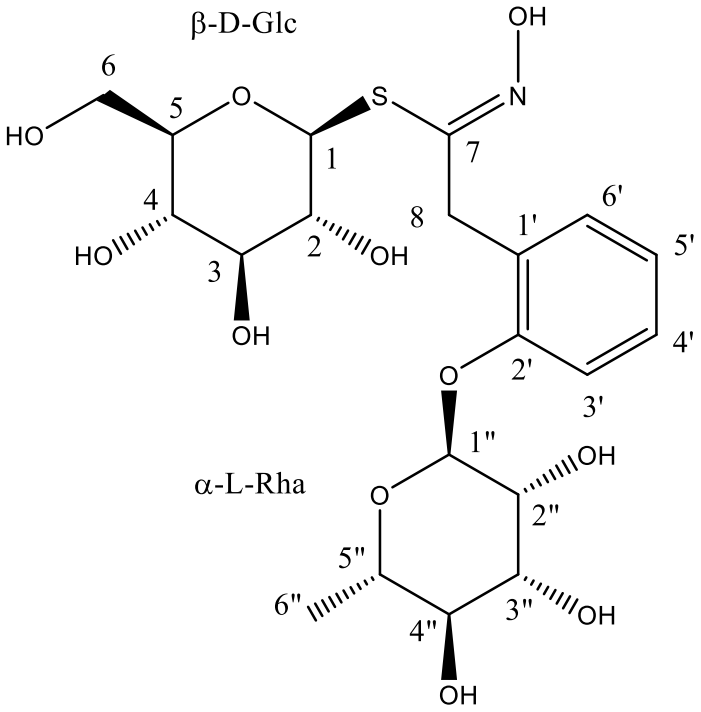

Figure S1. Structure of desulfated compound **2** (DS-isoGMG).

Table S1. Description and assignment of ^{1}H (600 MHz) and ^{13}C (151 MHz) NMR spectra of desulfated compound **2** in D_2O (298 K).

Position	δ ^{13}C	δ ^{1}H	multiplicity, J(Hz)
1	84.1	4.85	d (9.7)*
2	74.9	3.38	dd (9.7, 8.9)*
3	80	3.4	dd (9.7, 8.9)*
4	71.7	3.46	t (9.7)*
5	82.6	3.33	ddd (9.7, 4.7, 2.3)
6	63.2	3.75	dd (12.5, 2.3)*
		3.71	dd (12.5, 4.7)*
7	157.7		
8	36.4	4.02	AB (17)
		4.01	AB (17)
1'	127.7		
2'	156.1		
3'	117	7.21	d (8.3)
4'	131.8	7.36	ddd (8.3, 7.4, 1.6)
5'	125.6	7.1	t (7.4)
6'	133.4	7.31	dd (7.4, 1.6)
1"	100.1	5.6	d (1.8)
2"	73	4.15	dd (3.4, 1.8)
3"	73.1	4	dd (9.8, 3.4)
4"	74.9	3.52	t (9.8)
5"	72.4	3.71	dq (9.8, 6.2)*
6"	19.5	1.24	d (6.2)

* strong coupling effect and/or superimposition

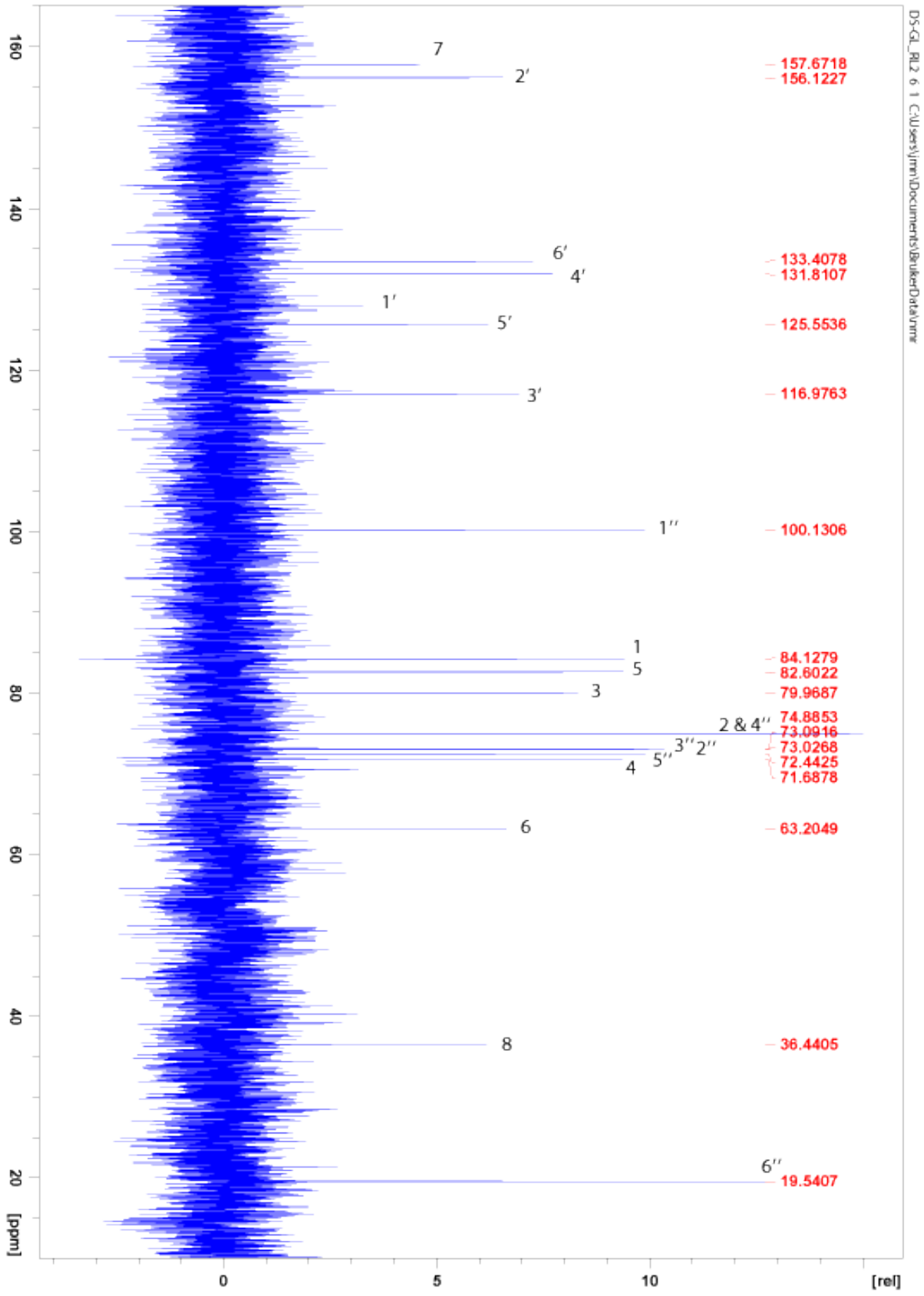

Figure S2. ^{13}C NMR spectrum of desulfated compound **2** in D_2O, 151 MHz, 298 K.

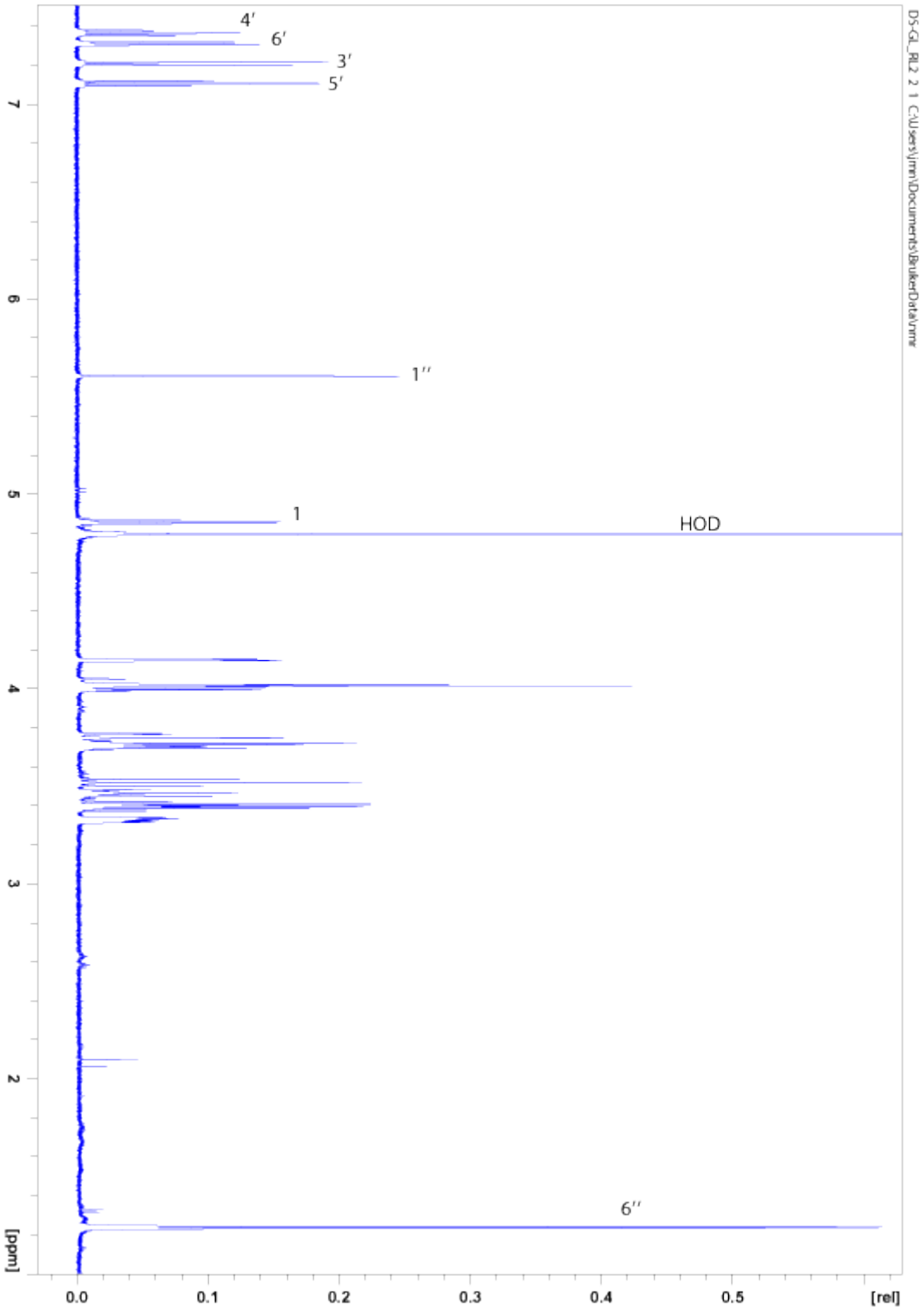

Figure S3. ^{1}H NMR spectrum of desulfated compound **2** in D_2O, 600 MHz, 298 K (part 1).

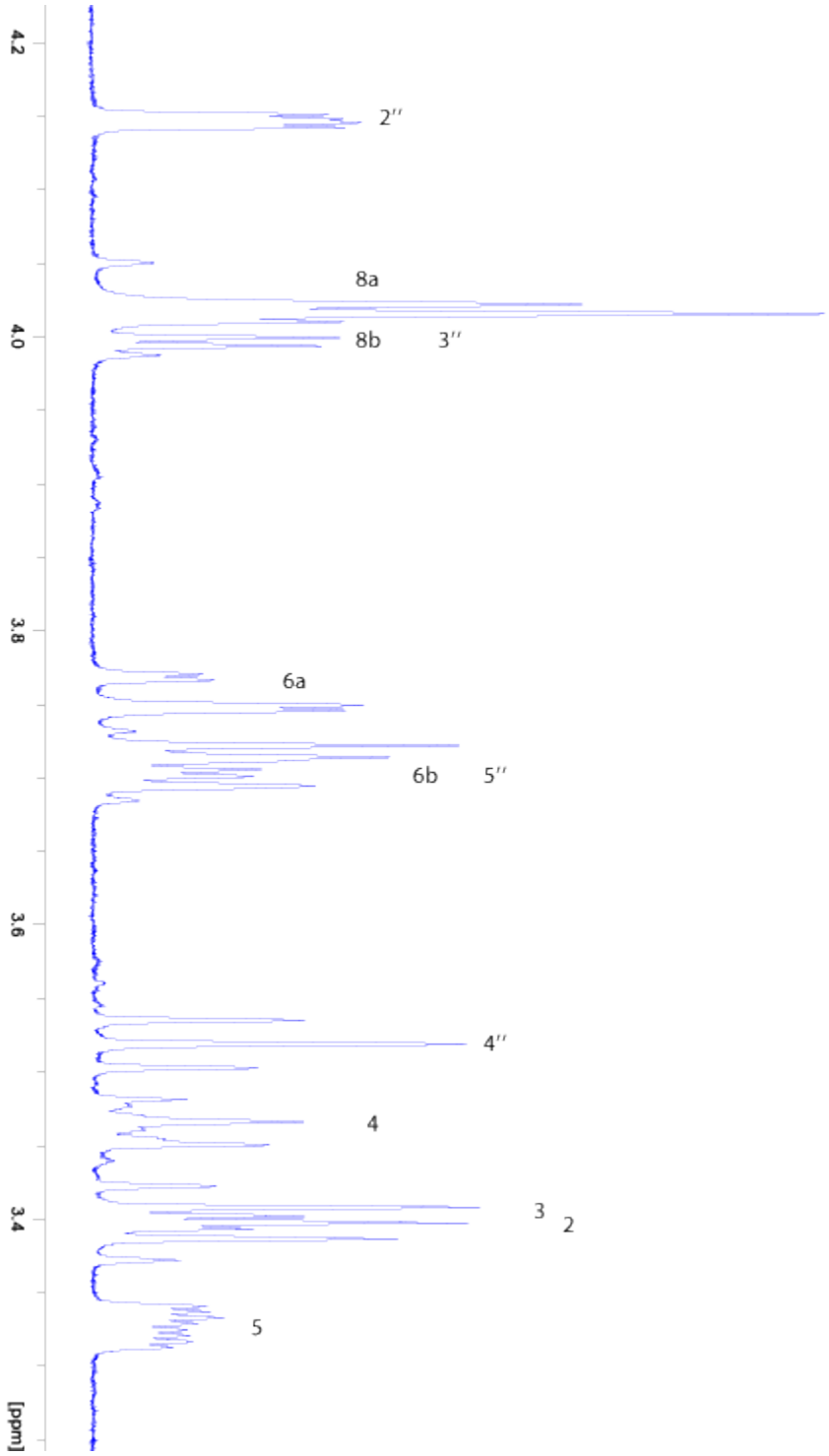

Figure S3. ^{1}H NMR spectrum of desulfated compound **2** in D_2O, 600 MHz, 298 K (part 2).

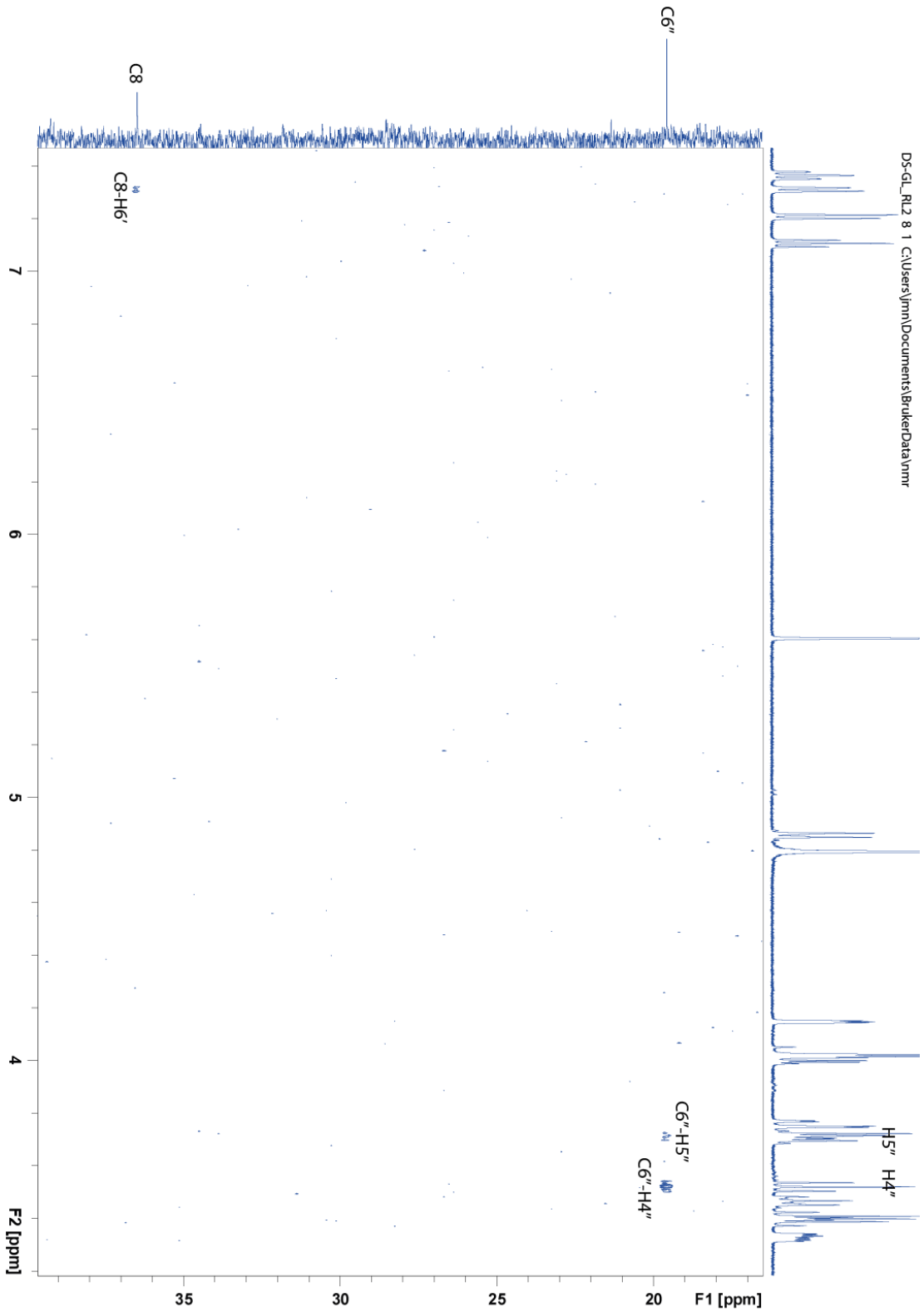

Figure S4. ^{1}H-^{13}C HMBC NMR spectrum of desulfated compound **2** in D_2O, 600 MHz, 298 K (part 1).

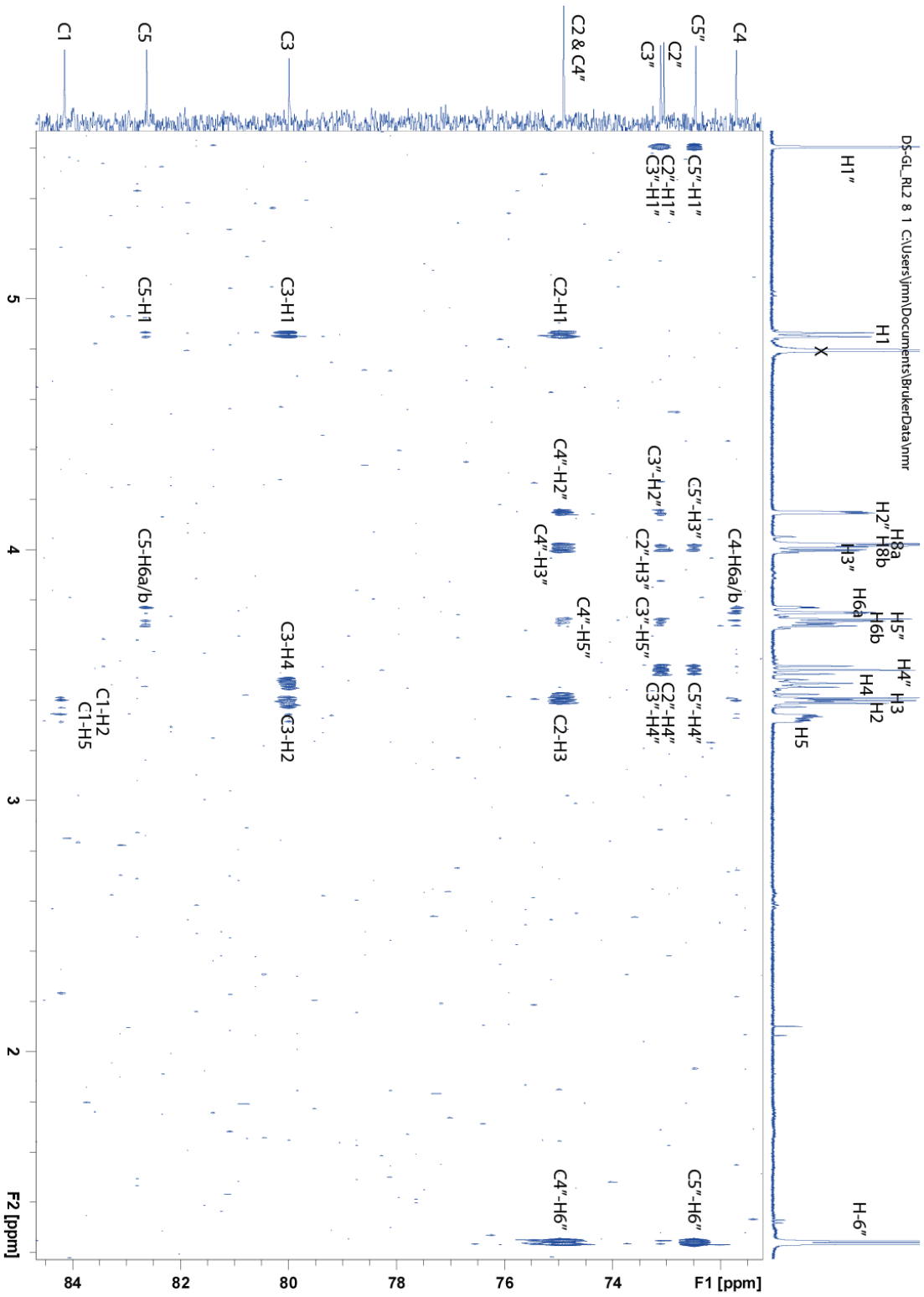

Figure S4. ^{1}H-^{13}C HMBC NMR spectrum of desulfated compound **2** in D_2O, 600 MHz, 298 K (part 2).

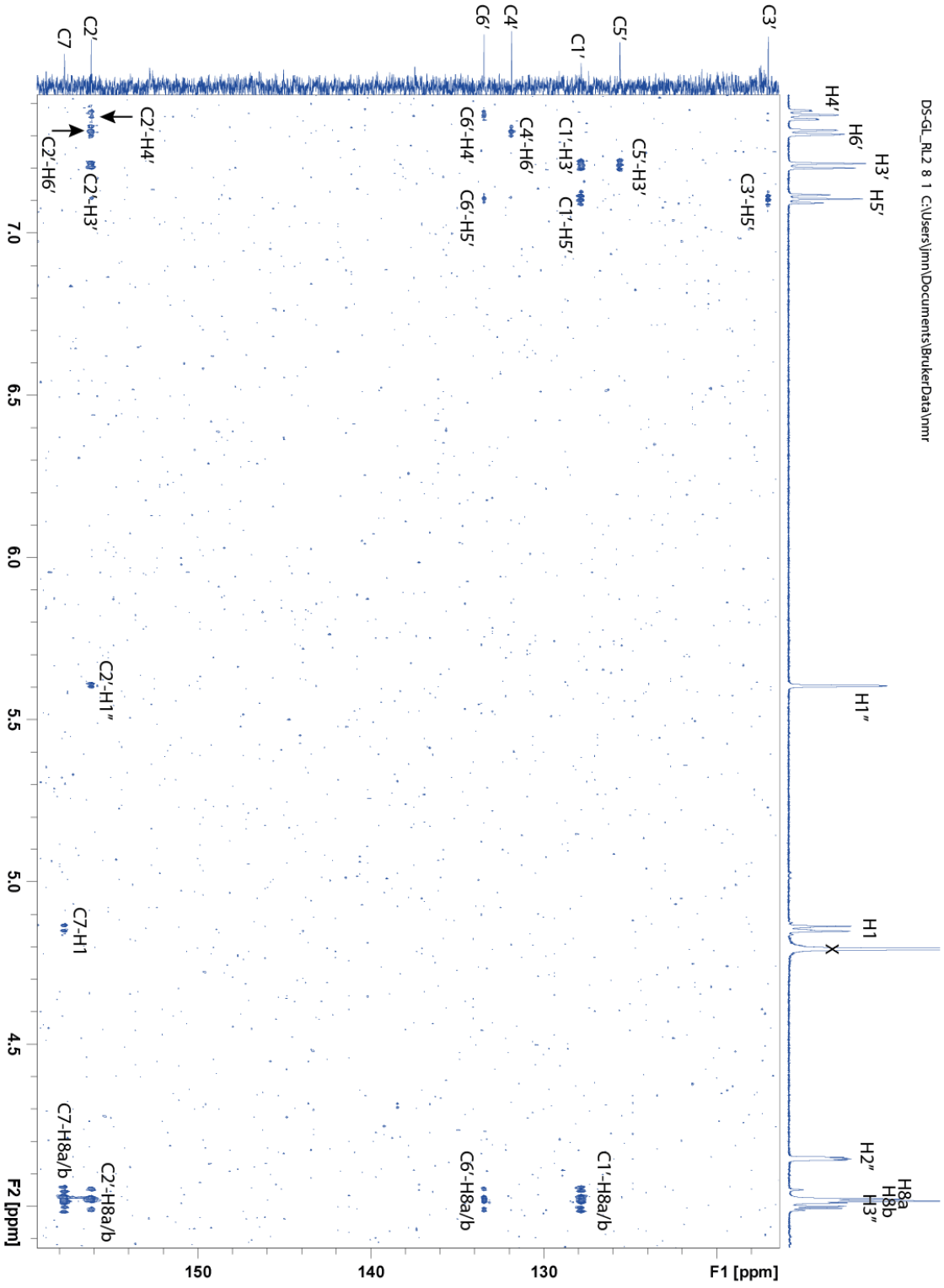

Figure S4. ^{1}H-^{13}C HMBC NMR spectrum of desulfated compound **2** in D_2O, 600 MHz, 298 K (part 3).

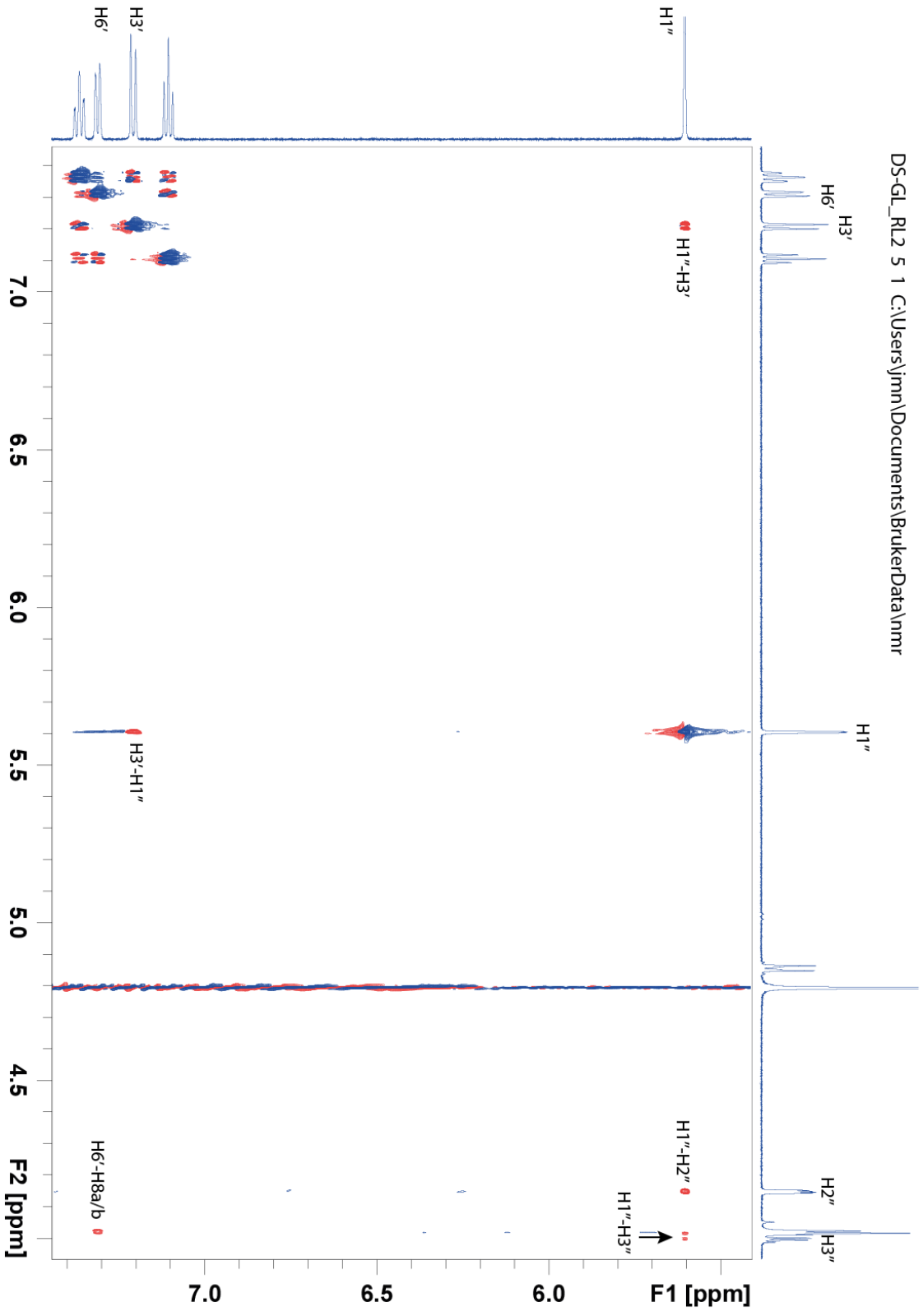

Figure S5. ^{1}H-^{1}H ROESY NMR spectrum of desulfated compound **2** in D_2O, 600 MHz, 298 K (part 1).

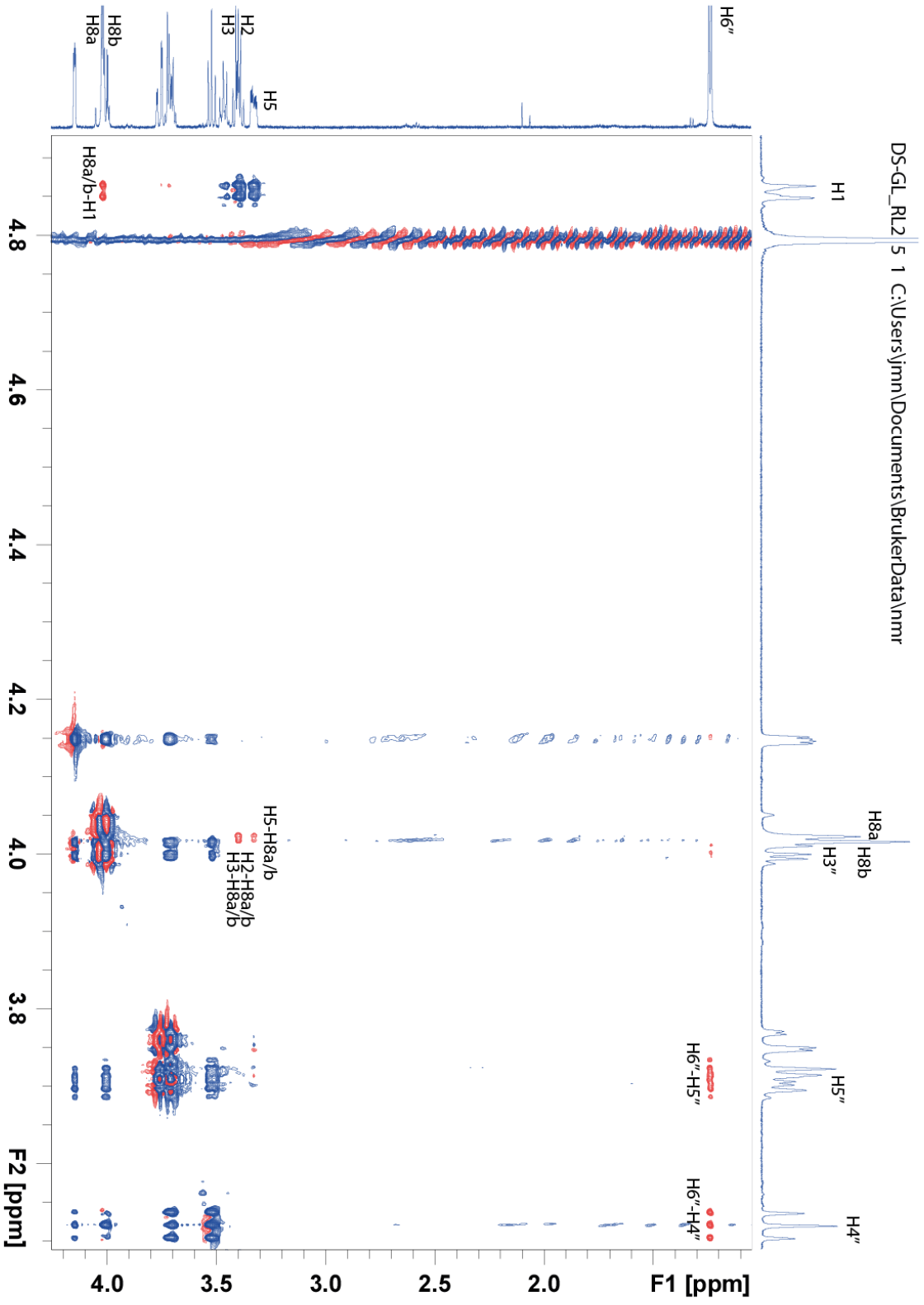

Figure S5. ^{1}H-^{1}H ROESY NMR spectrum of desulfated compound **2** in D_2O, 600 MHz, 298 K (part 2).

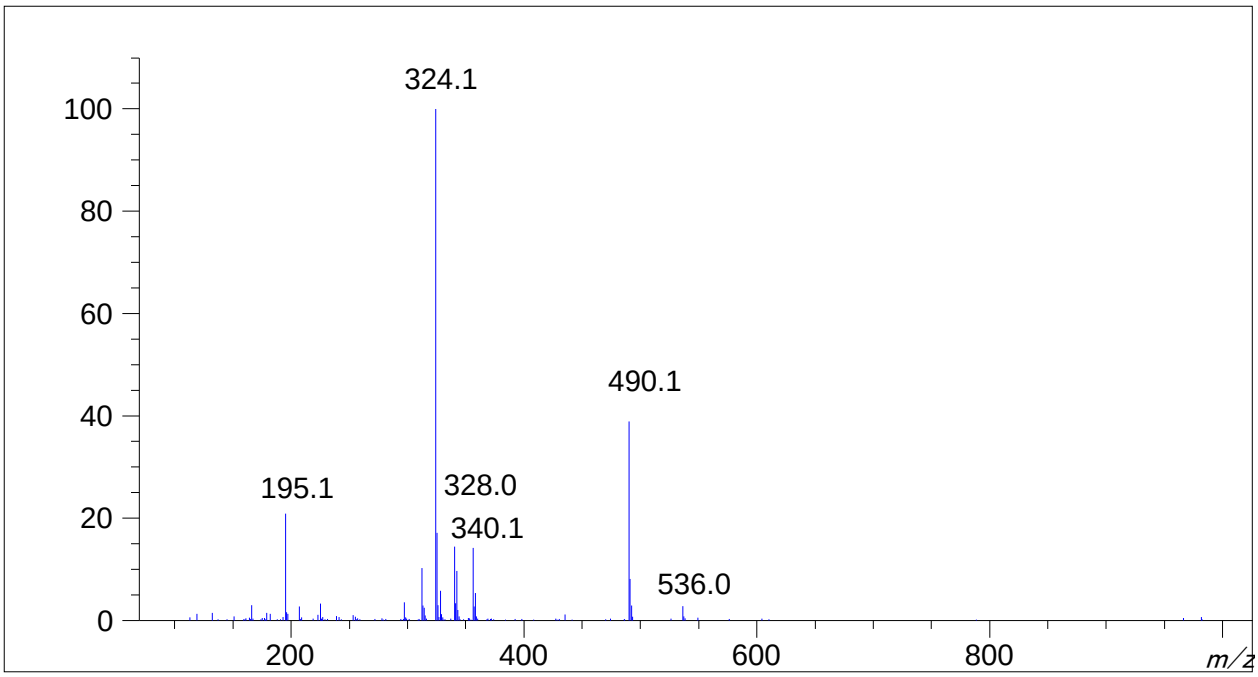

Figure S6. APCI$^-$-MS spectrum of desulfated compound **2** (DS-isoGMG).

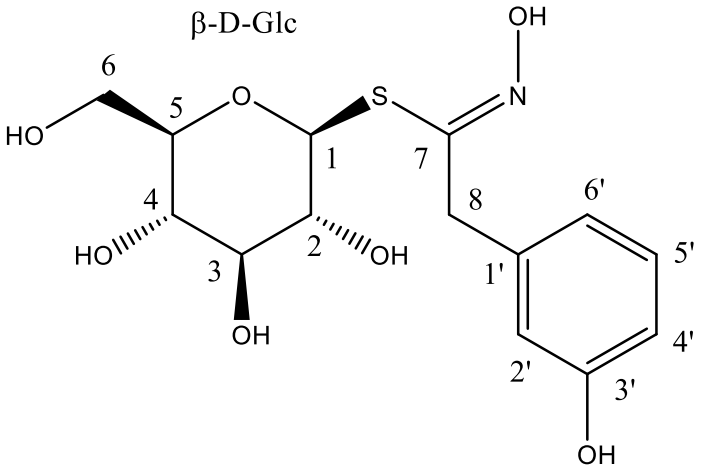

Figure S7. Structure of desulfated compound **4** (DS-glucolepigramine).

Table S2. Description and assignment of ^{1}H (600 MHz) and ^{13}C (151 MHz) NMR spectra of desulfated compound **4** in D_2O (298 K).

Position	δ ^{13}C	δ ^{1}H	multiplicity, *J*(Hz)
1	83.9	4.695	m
2	74.8	3.26	m
3	79.9	3.284	m
4	71.6	3.352	m
5	82.4	3.166	ddd (9.8, 4.6, 2.7)
6	63.1	3.61	dd (12.6, 2.7)
		3.59	dd (12.6, 4.6)
7	157.3		
8	40.7	3.94	AB (17)
		3.92	AB (17)
1'	140.7		
2'	117.6	6.773	s
3'	158.8		
4'	117	6.779	d (7.6)
5'	133.3	7.238	t (7.6)
6'	122.9	6.846	d (7.6)

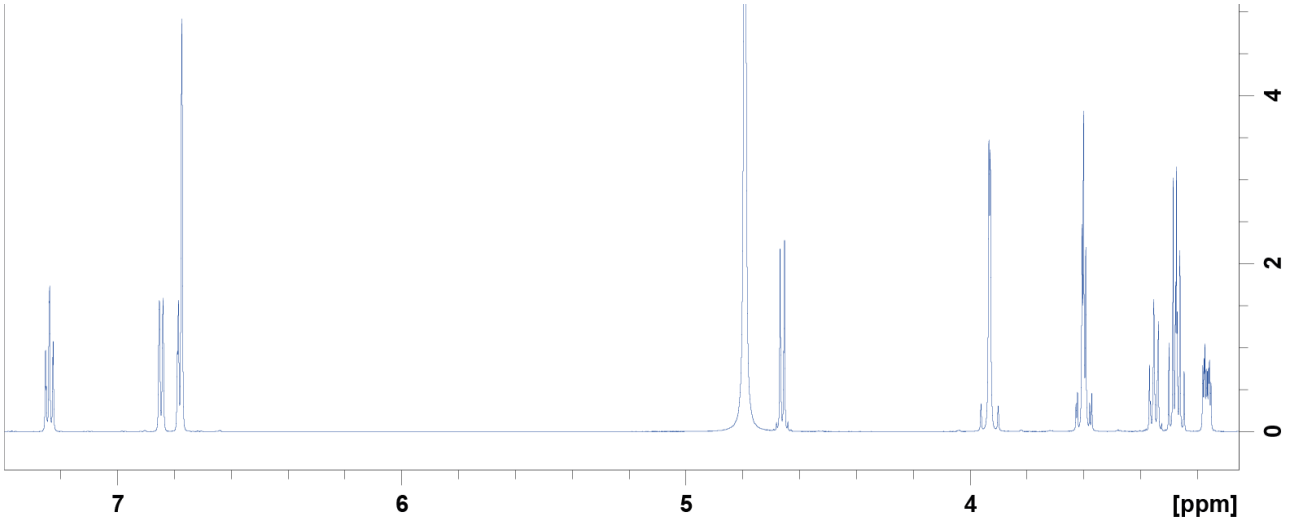

Figure S8. ^{1}H NMR spectrum of desulfated compound **4** in D_2O, 600 MHz, 298 K. (part 1)

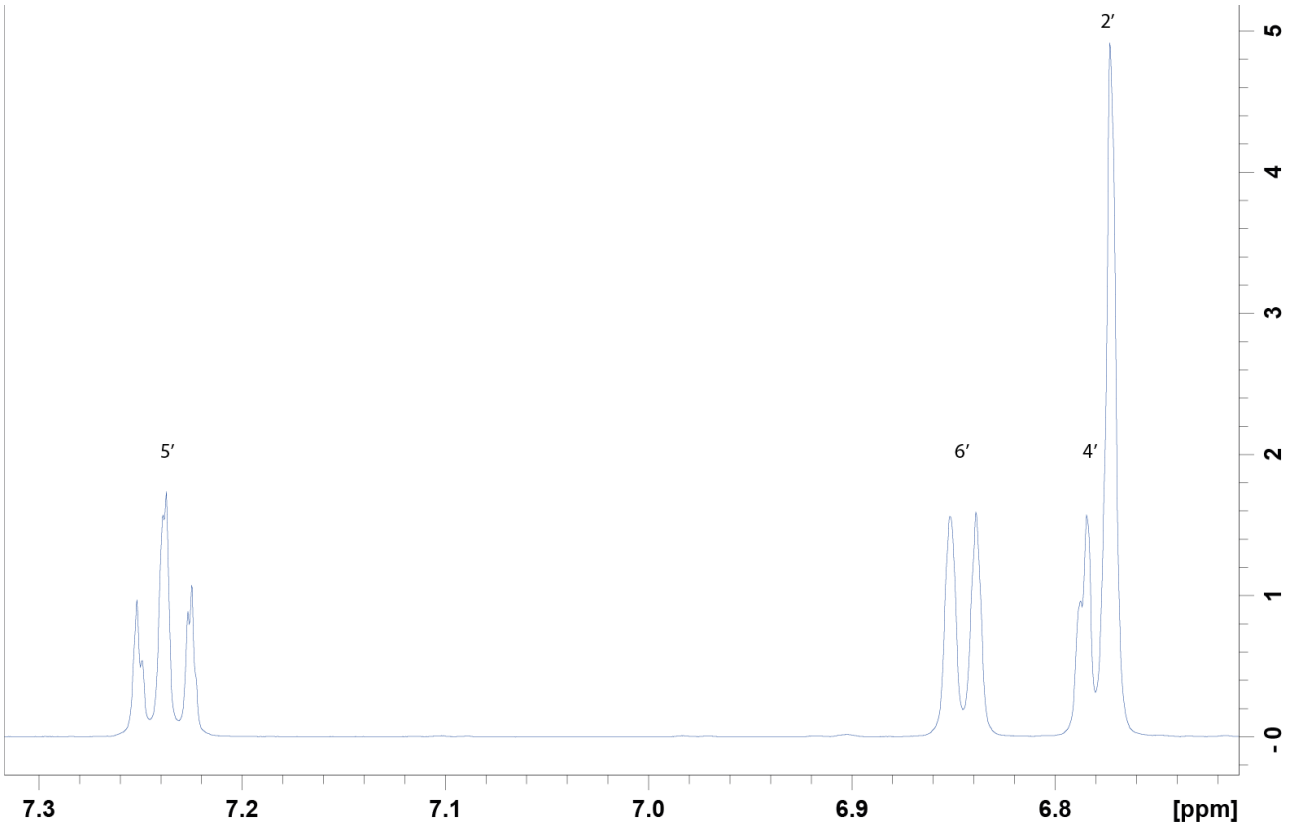

Figure S8. ^{1}H NMR spectrum of desulfated compound **4** in D_2O, 600 MHz, 298 K. (part 2)

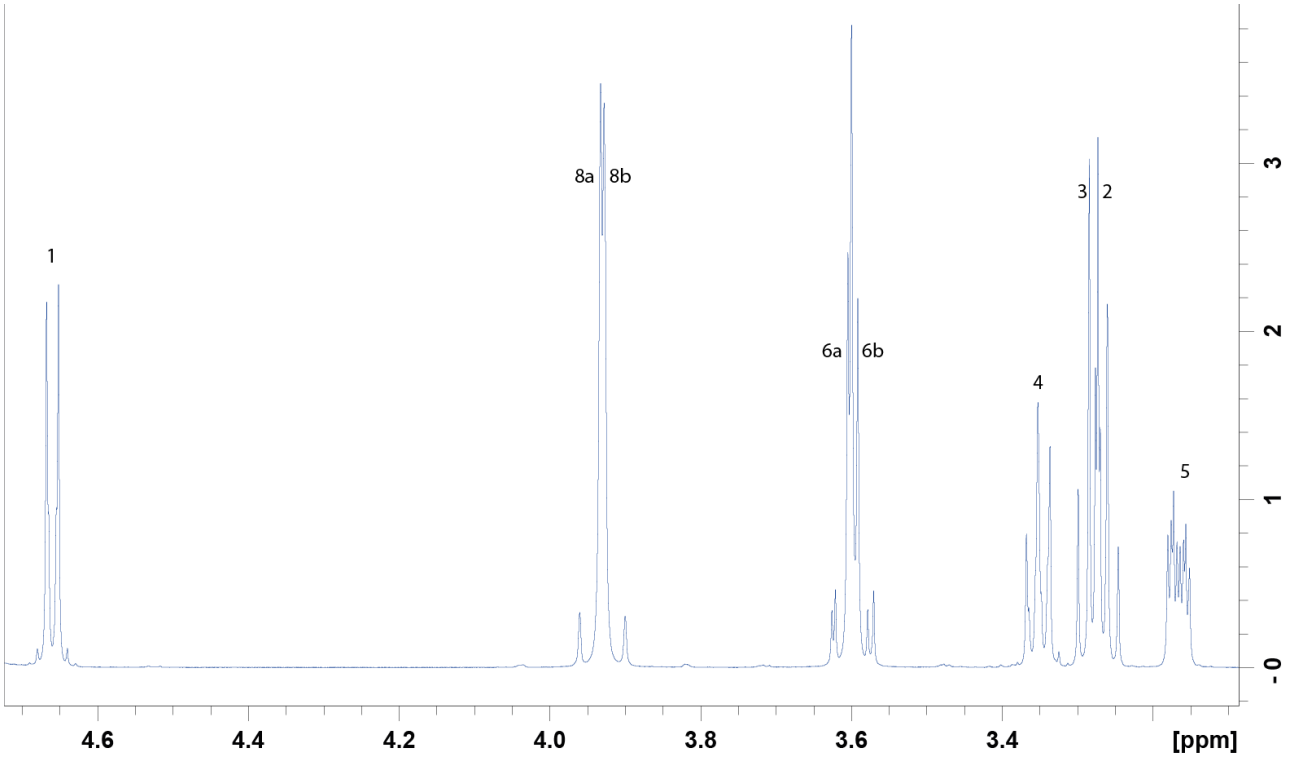

Figure S8. ^{1}H NMR spectrum of desulfated compound **4** in D_2O, 600 MHz, 298 K. (part 3)

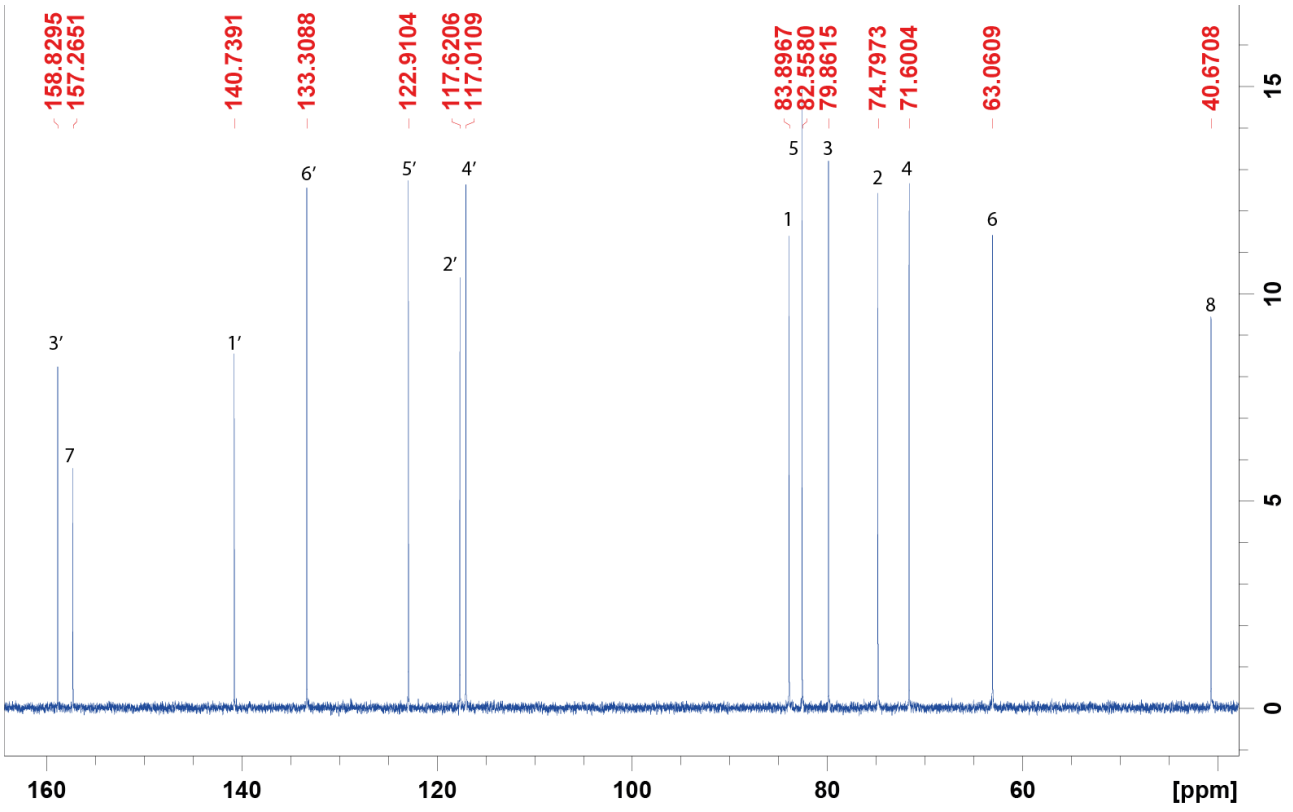

Figure S9. ^{13}C NMR spectrum of desulfated compound **4** in D_2O, 151 MHz, 298 K.

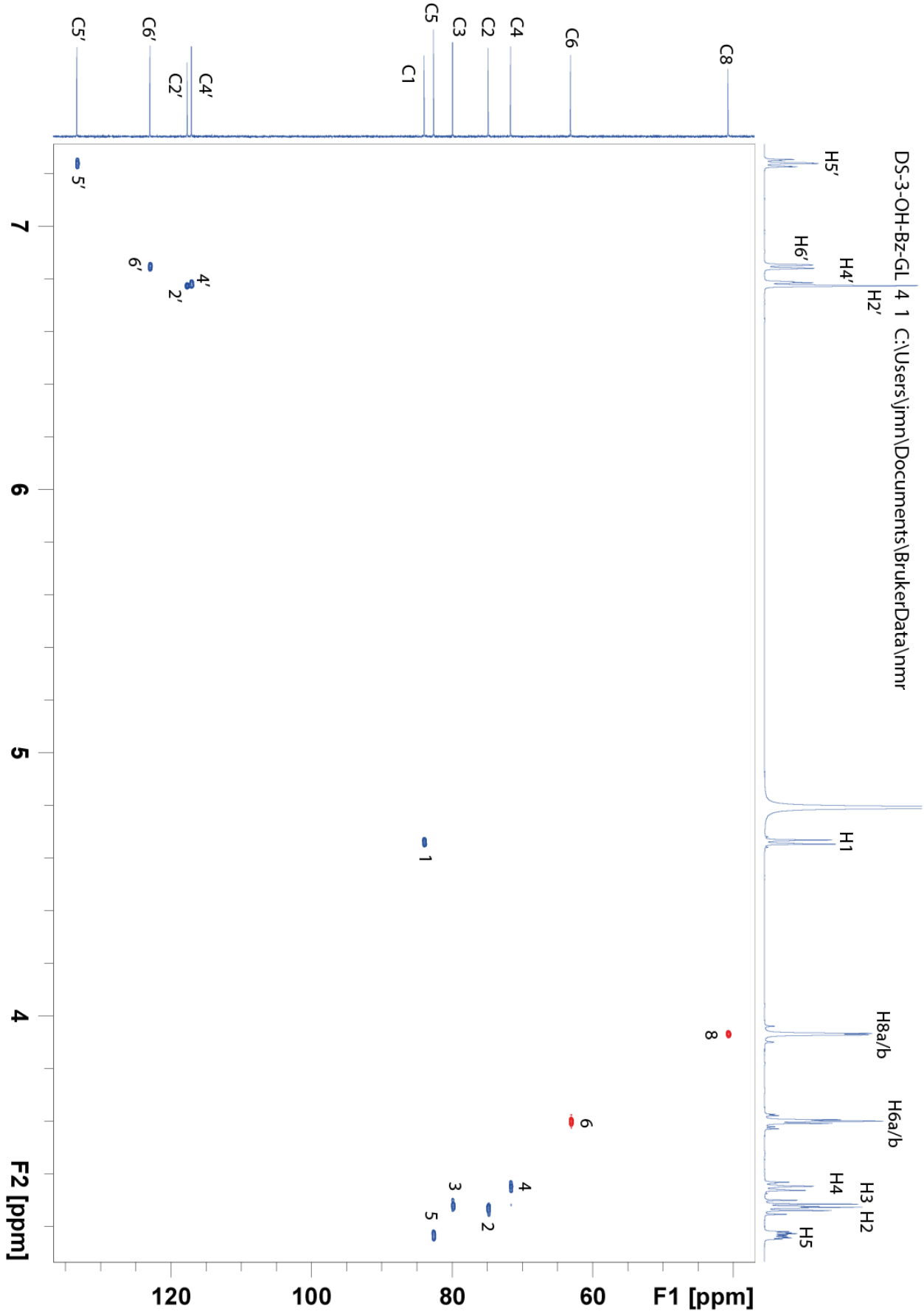

Figure S10. ^{1}H-^{13}C HSQC NMR spectrum of desulfated compound **4** in D_2O, 600 MHz, 298 K.

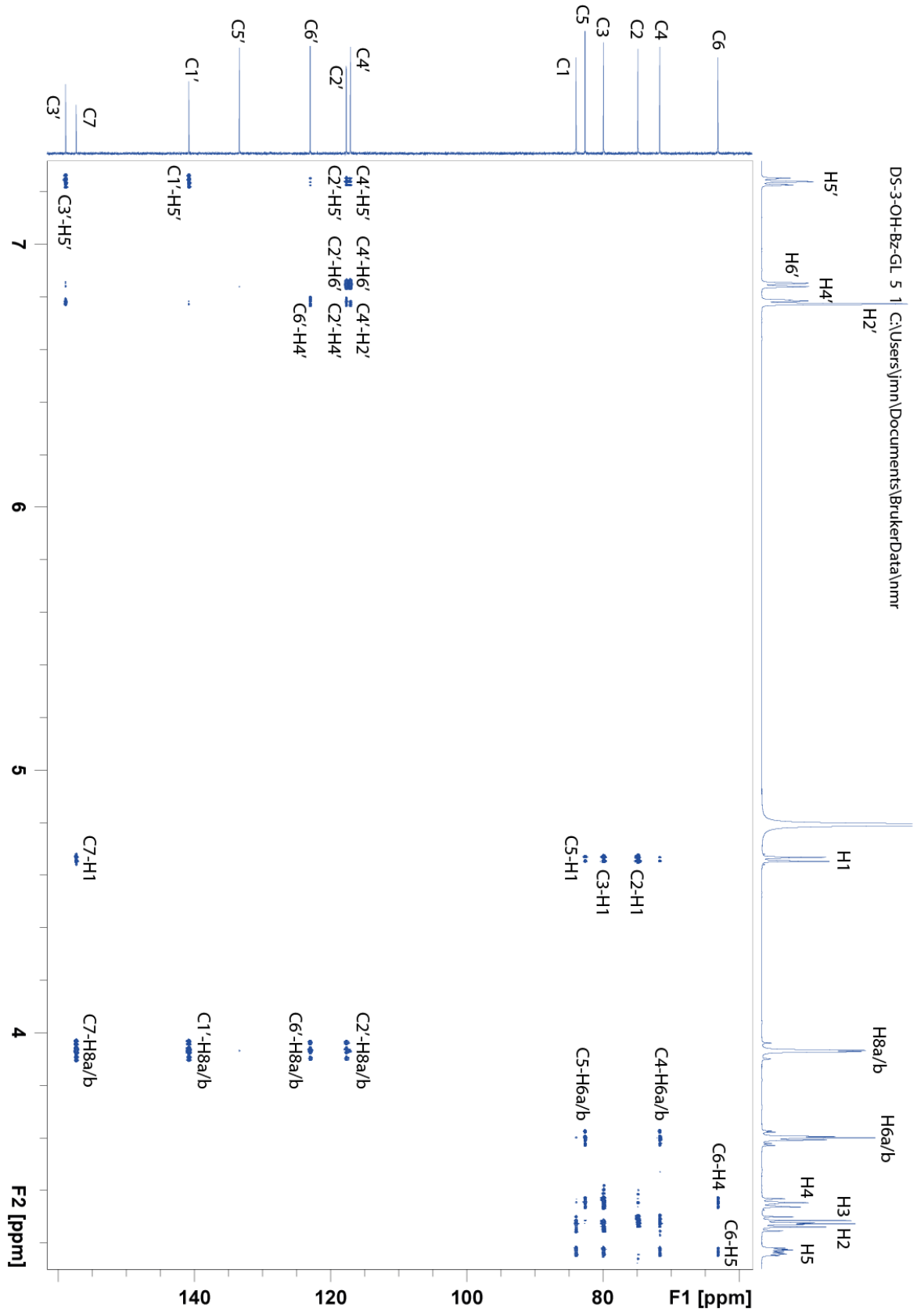

Figure S11. ^{1}H-^{13}C HMBC NMR spectrum of desulfated compound **4** in D_2O, 600 MHz, 298 K.

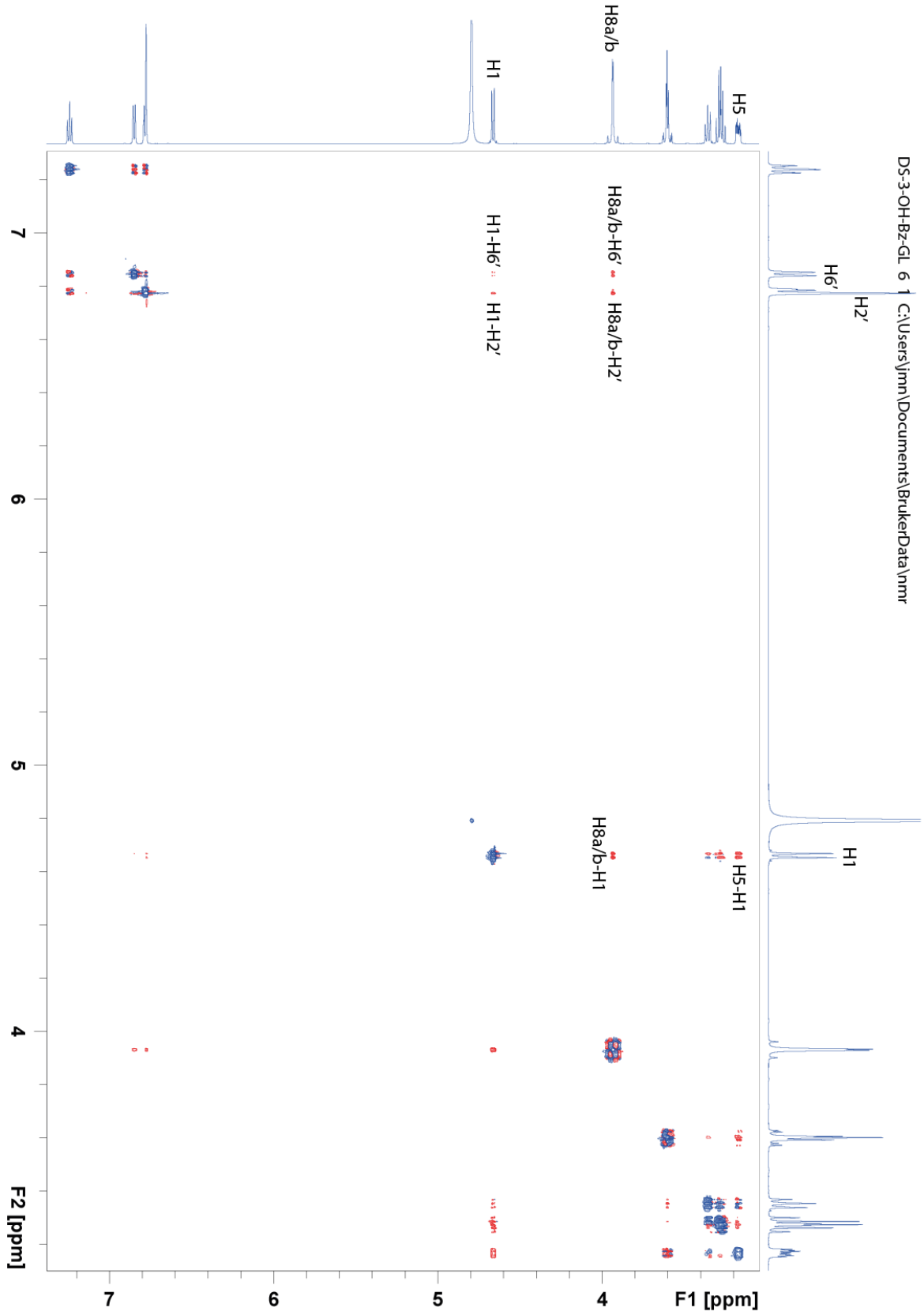

Figure S12. ^{1}H-^{1}H ROESY NMR spectrum of desulfated compound **4** in D_2O, 600 MHz, 298 K.

Availability of raw NMR data

DS-isoGMG and DS-glucolepigramin 1D and 2D NMR raw data and spectra (desulfated compounds **2** and **4**) are stored in an archive file named Reseda_lutea_flowers_NMR.zip in Bruker format. This file can be temporarily accessed from https://www.dropbox.com/s/o0gyhy036t37eme/Reseda_lutea_flowers_SI.zip?dl=0 and permanently from https://doi.org/10.5281/zenodo.3262193. NMR files can be opened with the TopSpin software, which is free for academics.