Supporting Information for: Indolo[3,2-*a*]carbazoles from a Deep-water Sponge of the Genus *Asteropus*

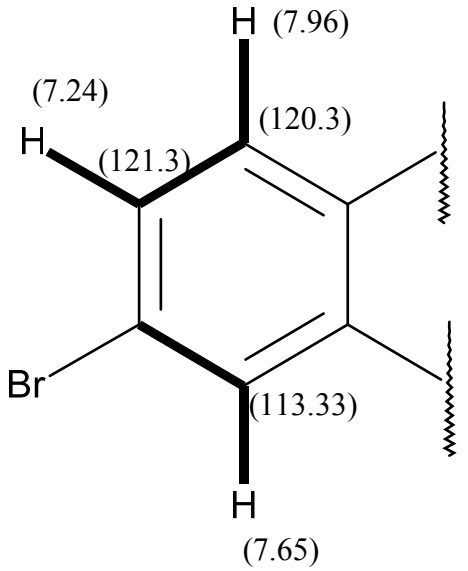
Floyd Russell, Dedra Harmody, Peter J. McCarthy, Shirley A. Pomponi and Amy E. Wright*

Marine Biomedical and Biotechnology Program, Harbor Branch Oceanographic Institute, Florida Atlantic University. 5600 US 1 North, Ft. Pierce, Florida 34946

Corresponding Author:
Wright: Tel: 772-242-2459 x 459; E-mail: awrigh33@hboi.fau.edu

Fig S1. A: Partial structure showing the 1,2,4 substituted aromatic ring spin system based upon the 2D DQF-gCOSY spectrum B: Key long range ^{1}H-^{13}C couplings seen in the ^{1}H-^{13}C HMBC and Band selective ^{1}H-^{13}C HMBC spectra which support the first indole ring.

A



B

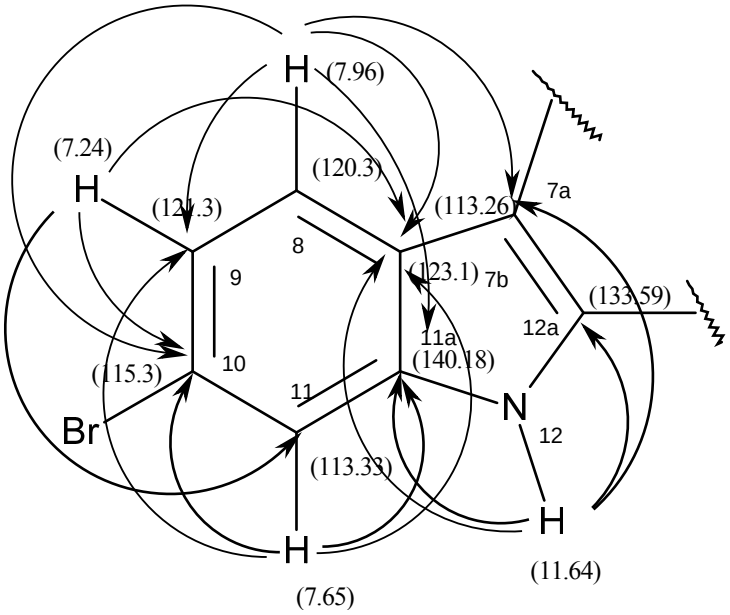


Fig S2. Partial structure showing key ^{1}H-^{13}C long range couplings observed in the ^{1}H-^{13}C g-HMBC spectrum and Band Selective ^{1}H-^{13}C g-HMBC spectrum which support the second indole ring

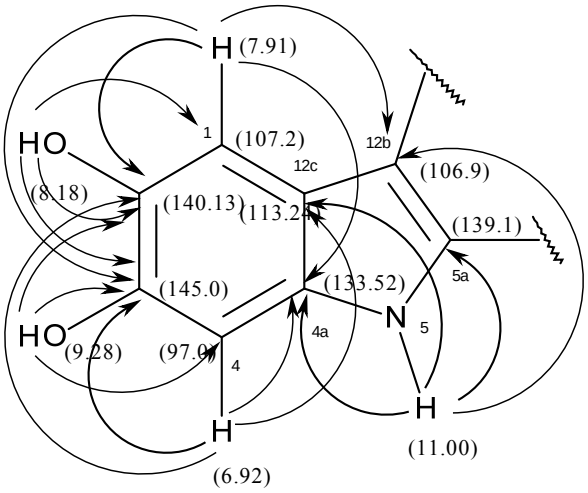


Fig S3. Key HMBC Correlations that support the linking of the two indole rings with the C-6/C-7 spin system.

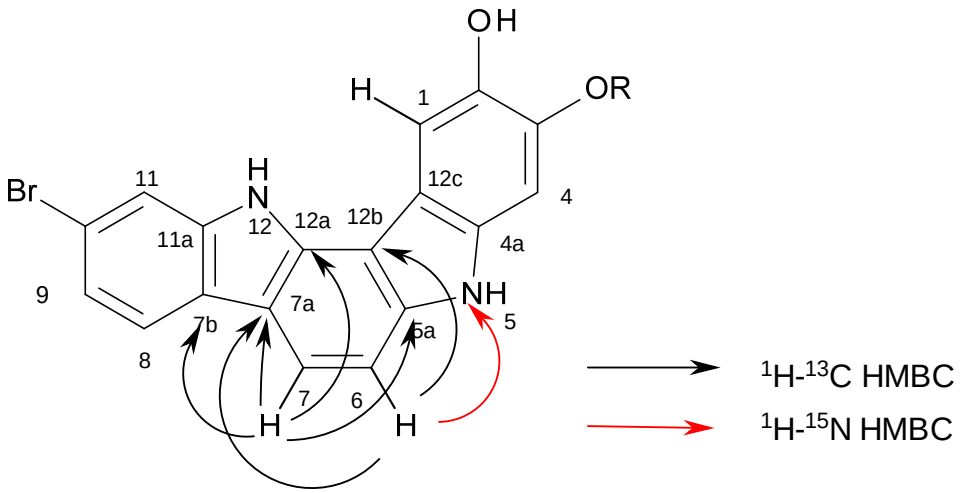
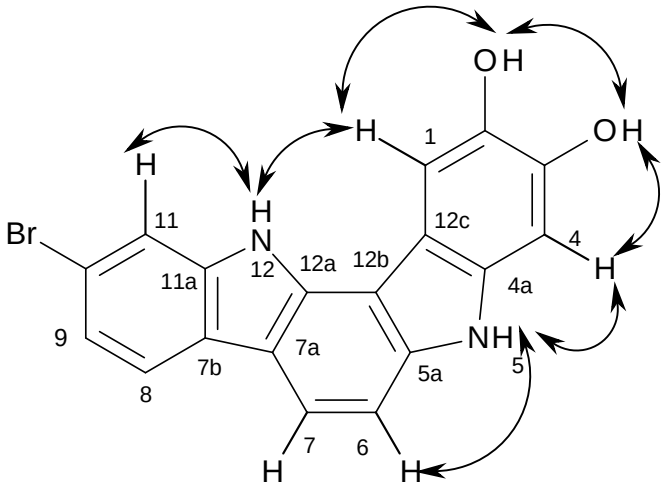


Fig S4 Structure of **1** with key NOESY correlations

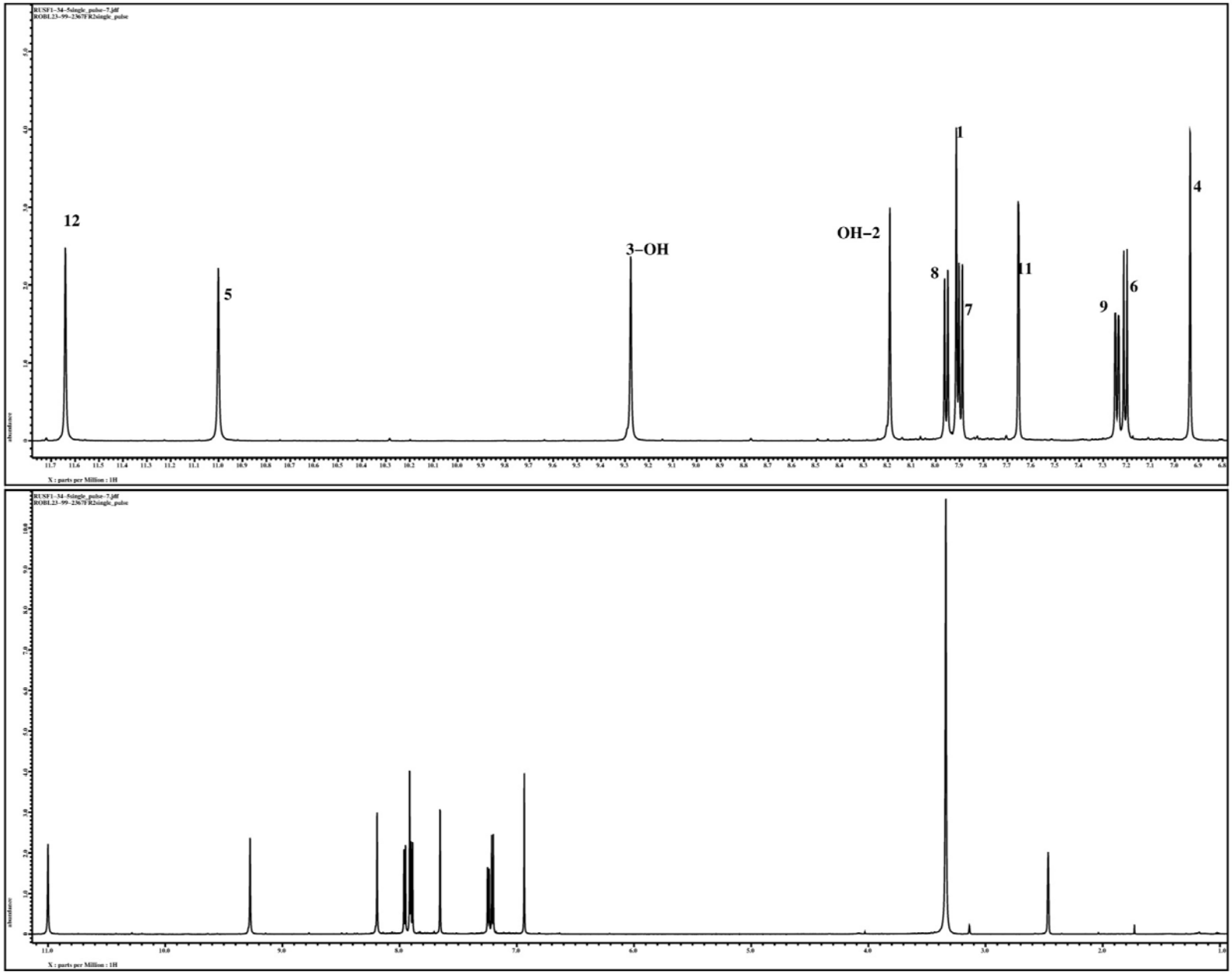


S5. Table of ^{1}H and ^{13}C NMR Data for 1 (DMSO-*d6*, 600 MHz)

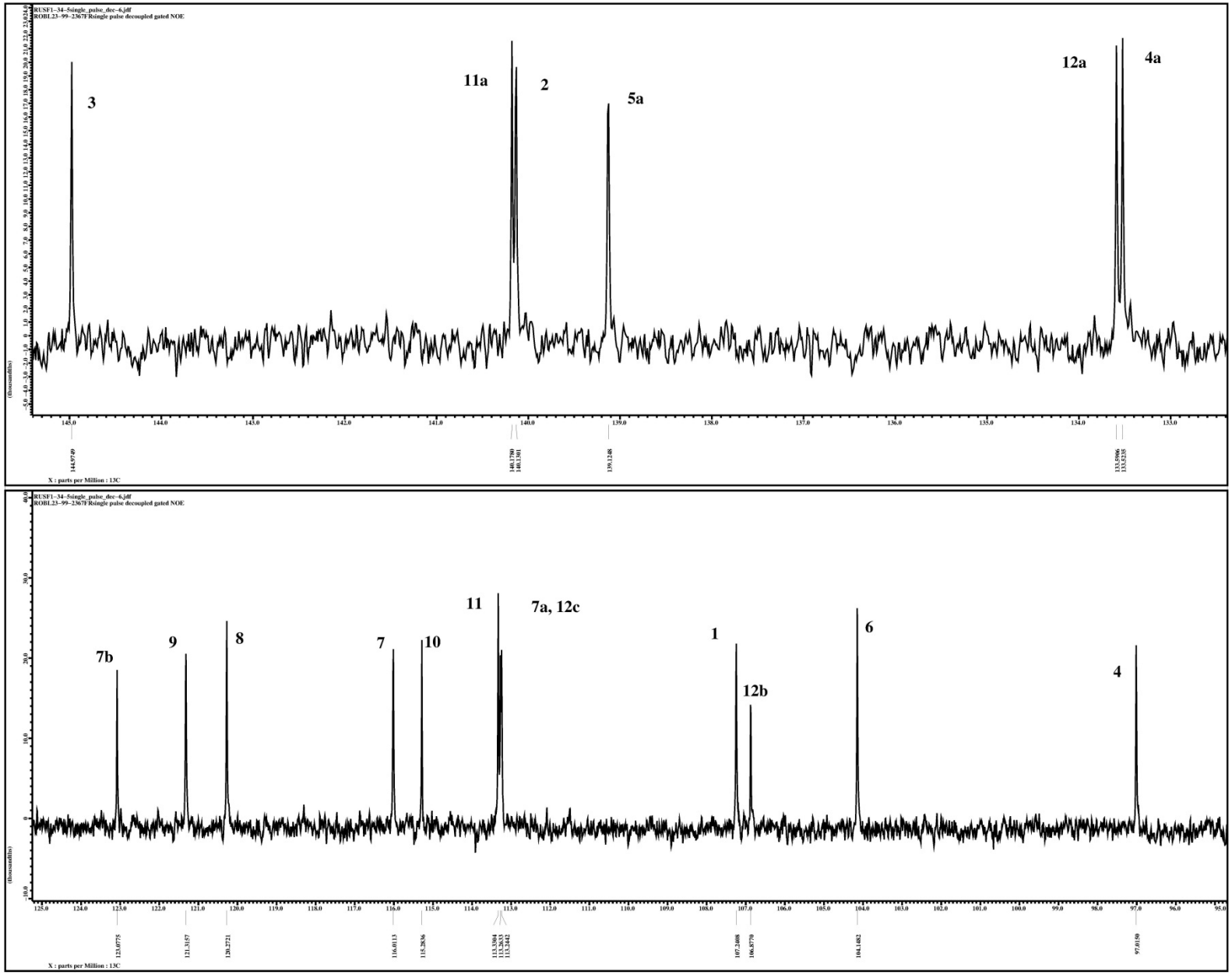
Position	δ_C, mult	δ_N	δ_H (*J* in Hz)	COSY	HMBC	NOESY
1	107.2, CH		7.91, s		2, 3, 4a, 12b, 12c	NH-12
2	140.13, C[b]					
OH-2			8.18, s		1, 2, 3	OH-3
3	145.0, C					
OH-3			9.28, s		2, 3, 4	OH-2, 4
4	97.0, CH		6.92, s		2, 3, 4a, 12c, N-5	NH-5, OH-3
4a	133.52, C					
5		113	11.00, bs		4a, 5a, 12b, 12c	4, 6
5a	139.1, C					
6	104.1, CH		7.20, d (8.2)	8’	7a, 12b, N-5	NH-5
7	116.0, CH		7.89, d (8.2)	8	5a, 7a, 7b, 12a	
7a	113.26, C[b]					
7b	123.1, C					
8	120.3, CH		7.96, d (8.0)	5’	7a, 7b, 10, 11a	
9	121.3, CH		7.24, dd (8.0, 1.4)	4’, 7’	7b, 10, 11	
10	115.3, C					
11	113.33, CH[b]		7.65, d (1.4)		7b, 9, 10, 11a, N-12	NH-12
11a	140.18, C[b]					
12		112	11.64, bs		12a, 7a, 7b, 11a	1, 11
12a	133.59, C					
12b	106.9, C					
12c	113.24, C[b]					

[a]HMBC correlations, optimized for 8 Hz, are from proton(s) stated to the indicated atom; ^{1}H and ^{13}C NMR data were measured at 600.2 and 150.9 respectively. [b]Congested areas of the spectrum; assignments were made on the basis of a band selective ^{1}H-^{13}C *g*-HMBC experiment. Two decimal places are shown to distinguish resonances of very similar chemical shifts, but which could be clearly resolved in the band selective experiment.

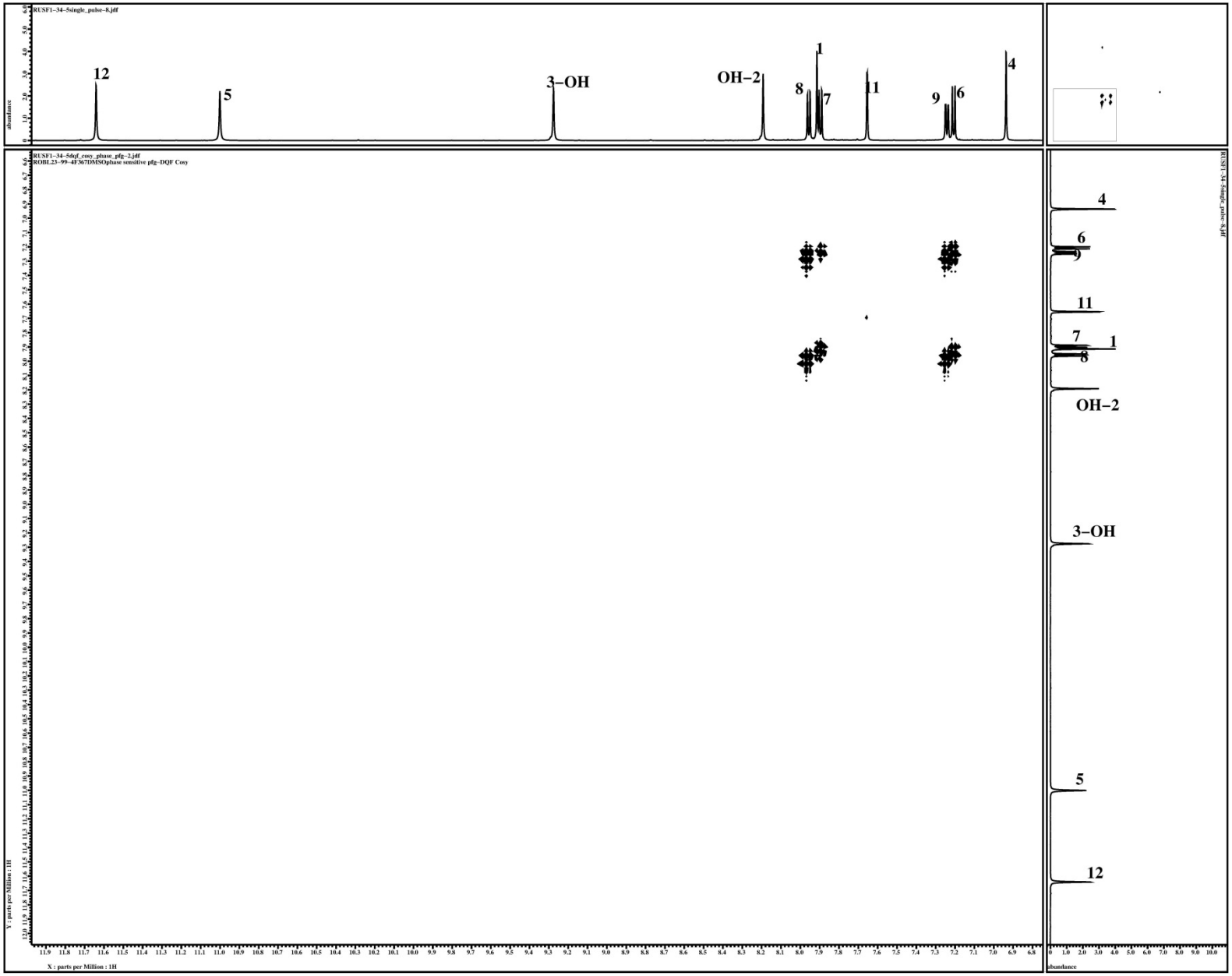
S6. ^{1}H NMR spectrum of **1** (600 MHz d_6-DMSO).



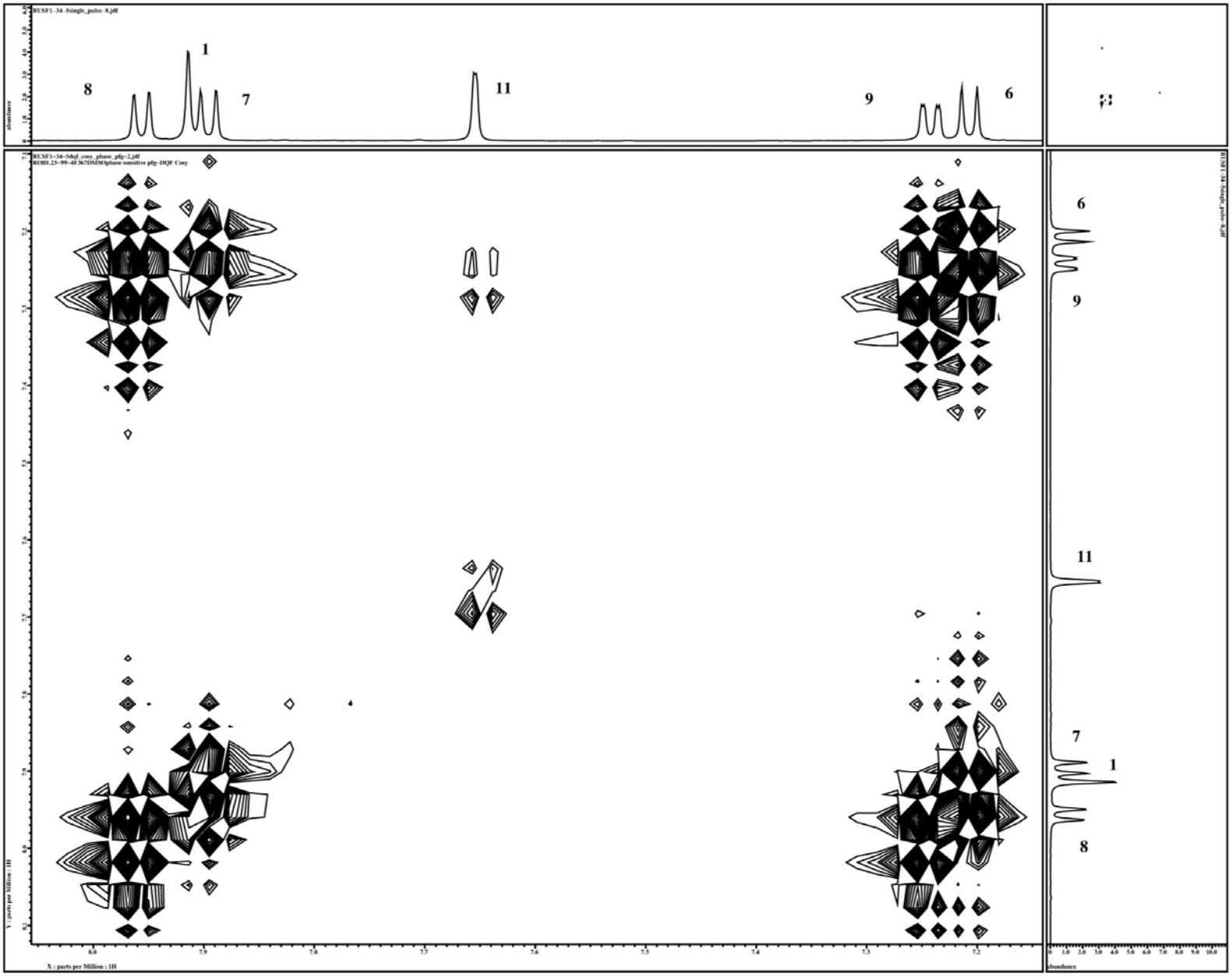
S7. ^{13}C NMR Spectrum of **1** (150.9 MHz d_6-DMSO).



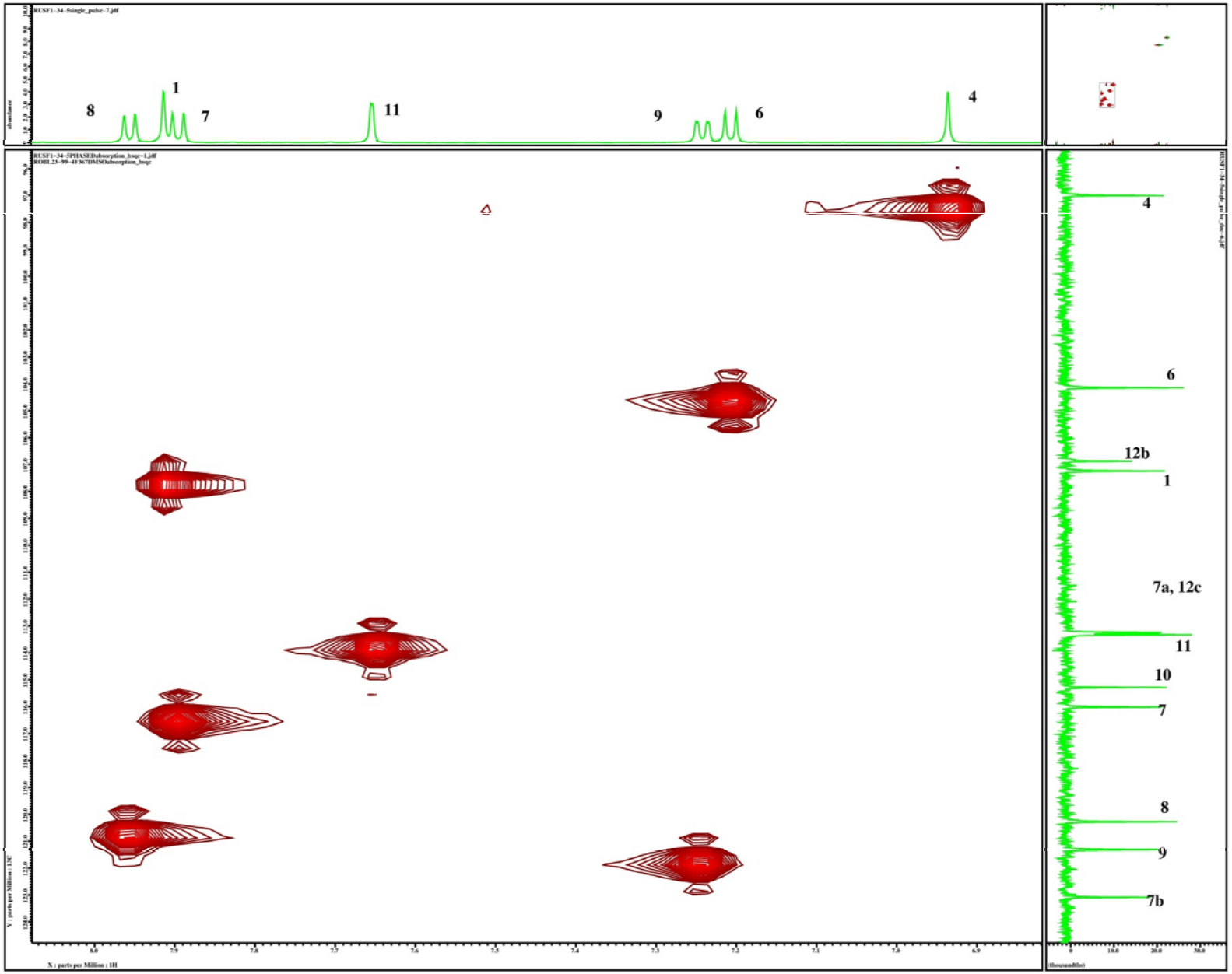
S8. g-DQF-COSY spectrum of **1** (600 MHz d_6-DMSO).



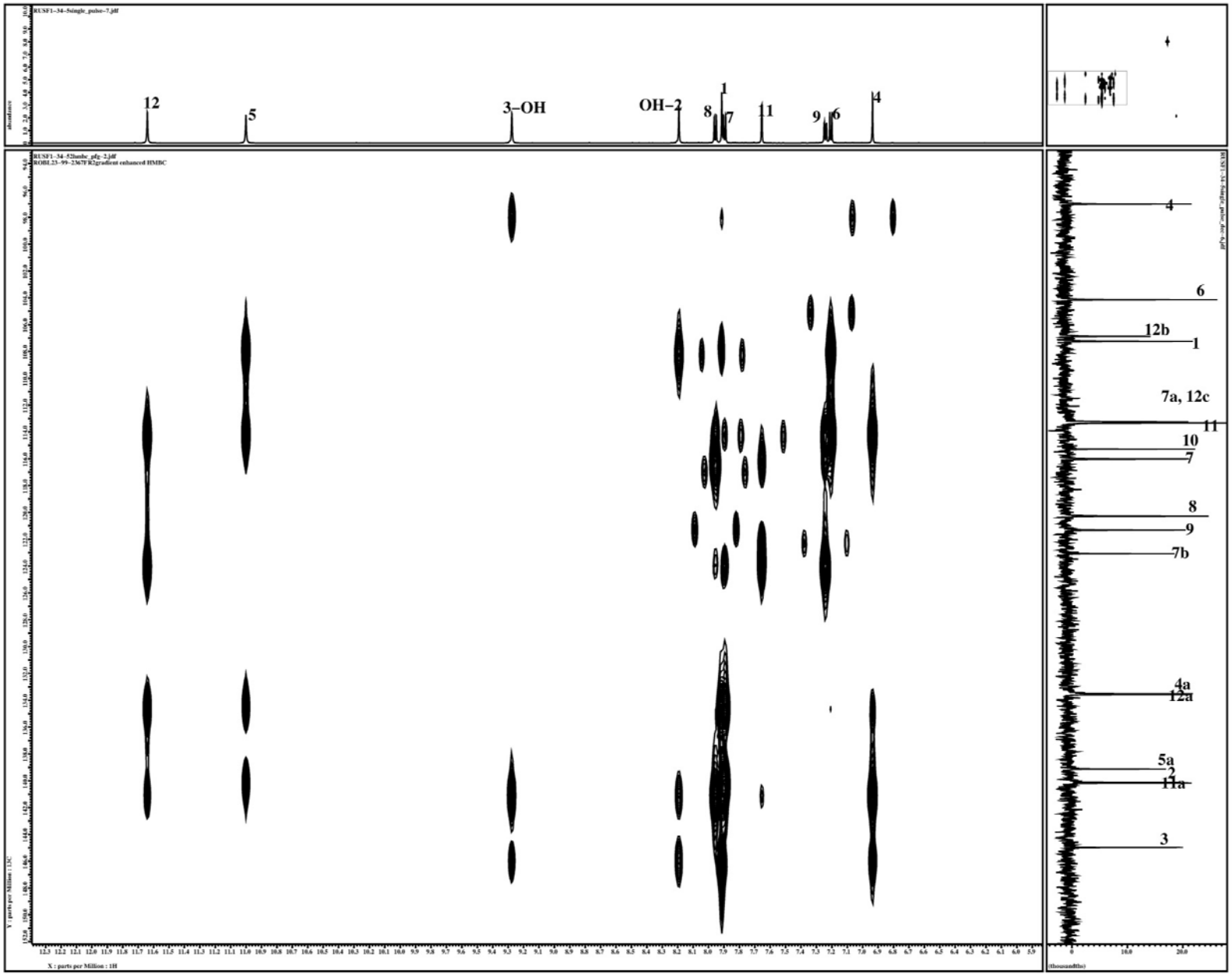
S9. Expansion of g-DQF-COSY spectrum of **1** (600 MHz d_6-DMSO).



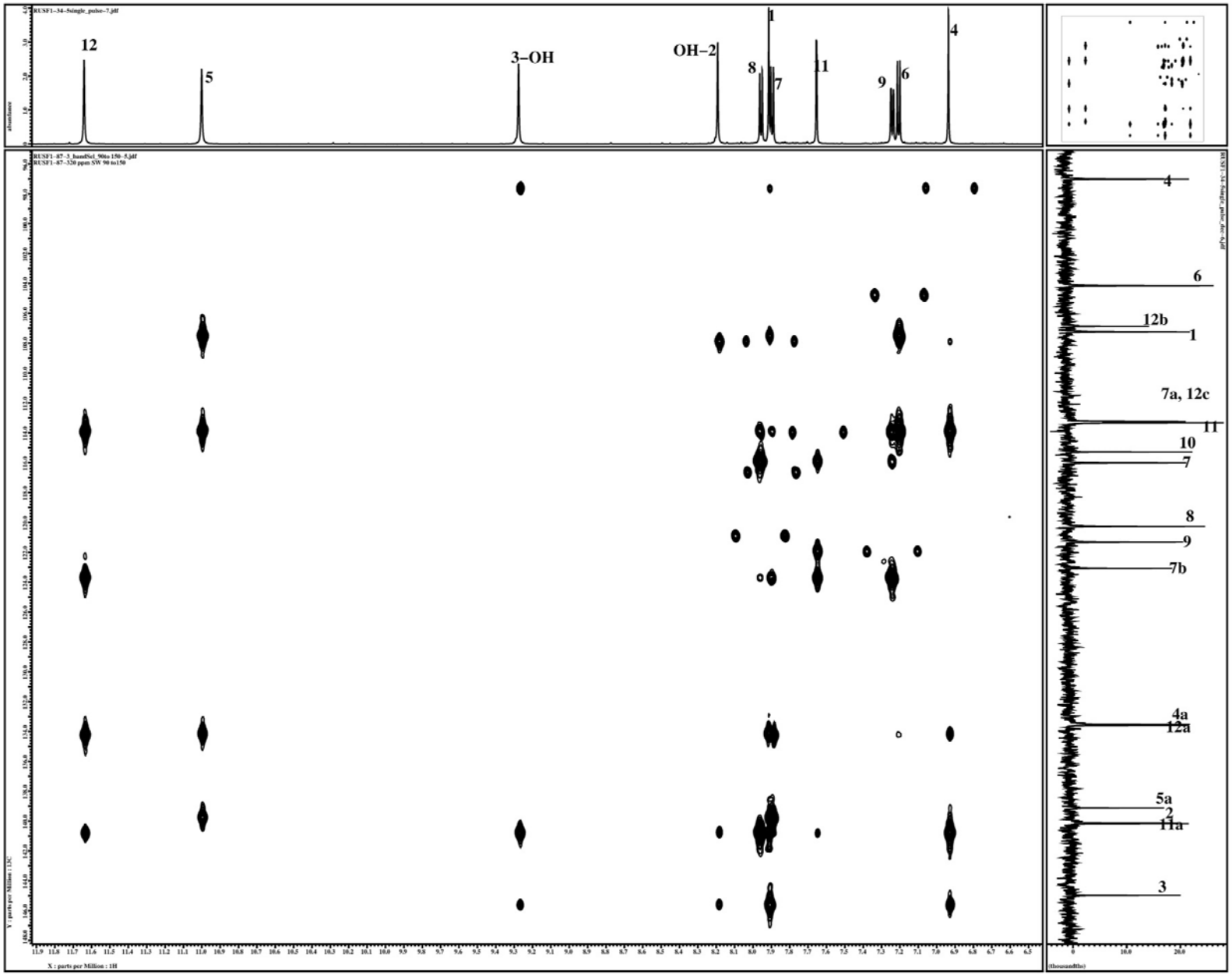
S10. Edited g-HSQC spectrum of **1** (600 MHz d_6-DMSO).



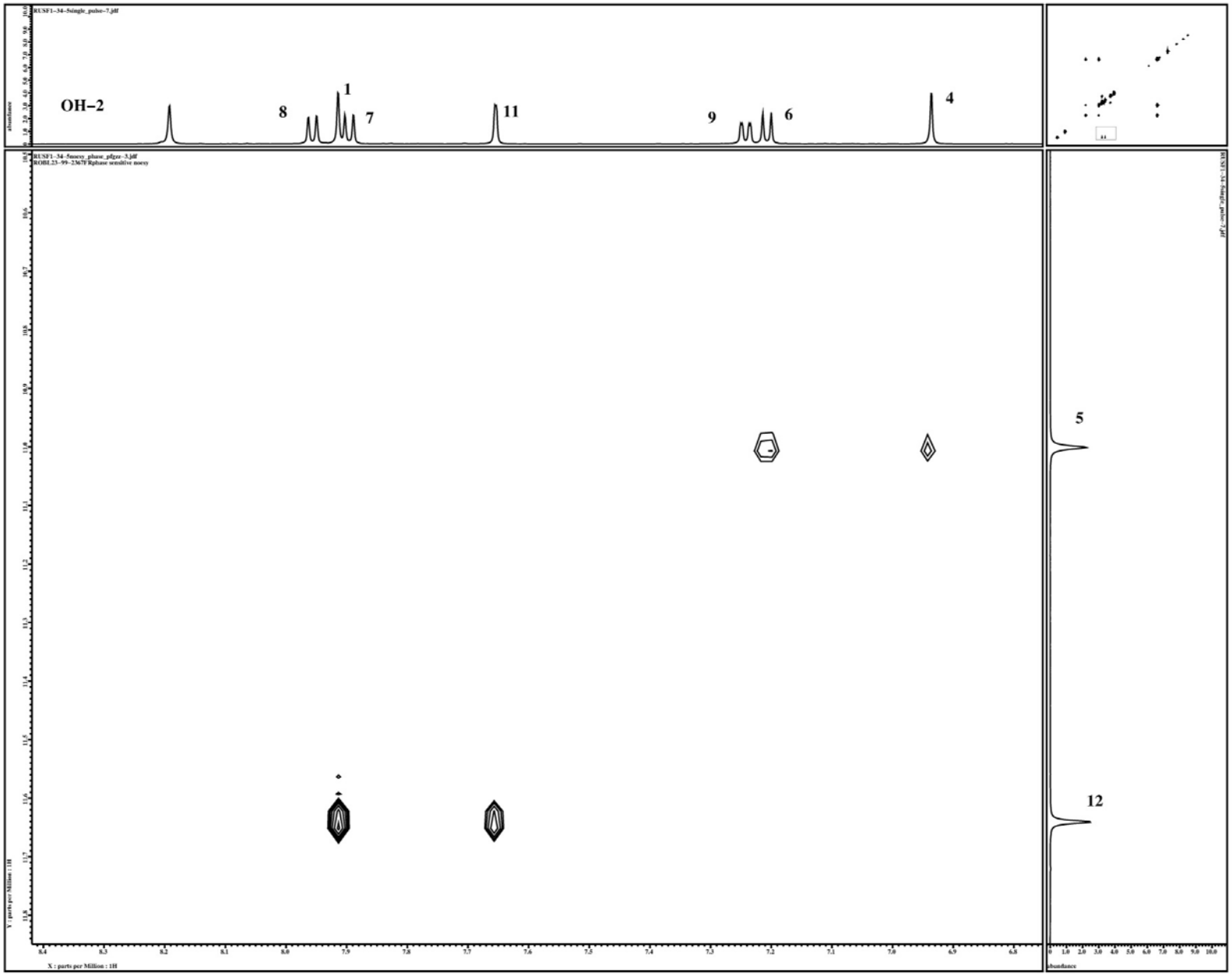
S11. ^{1}H-^{13}C-HMBC Spectrum of **1** (600 MHz d_6-DMSO).



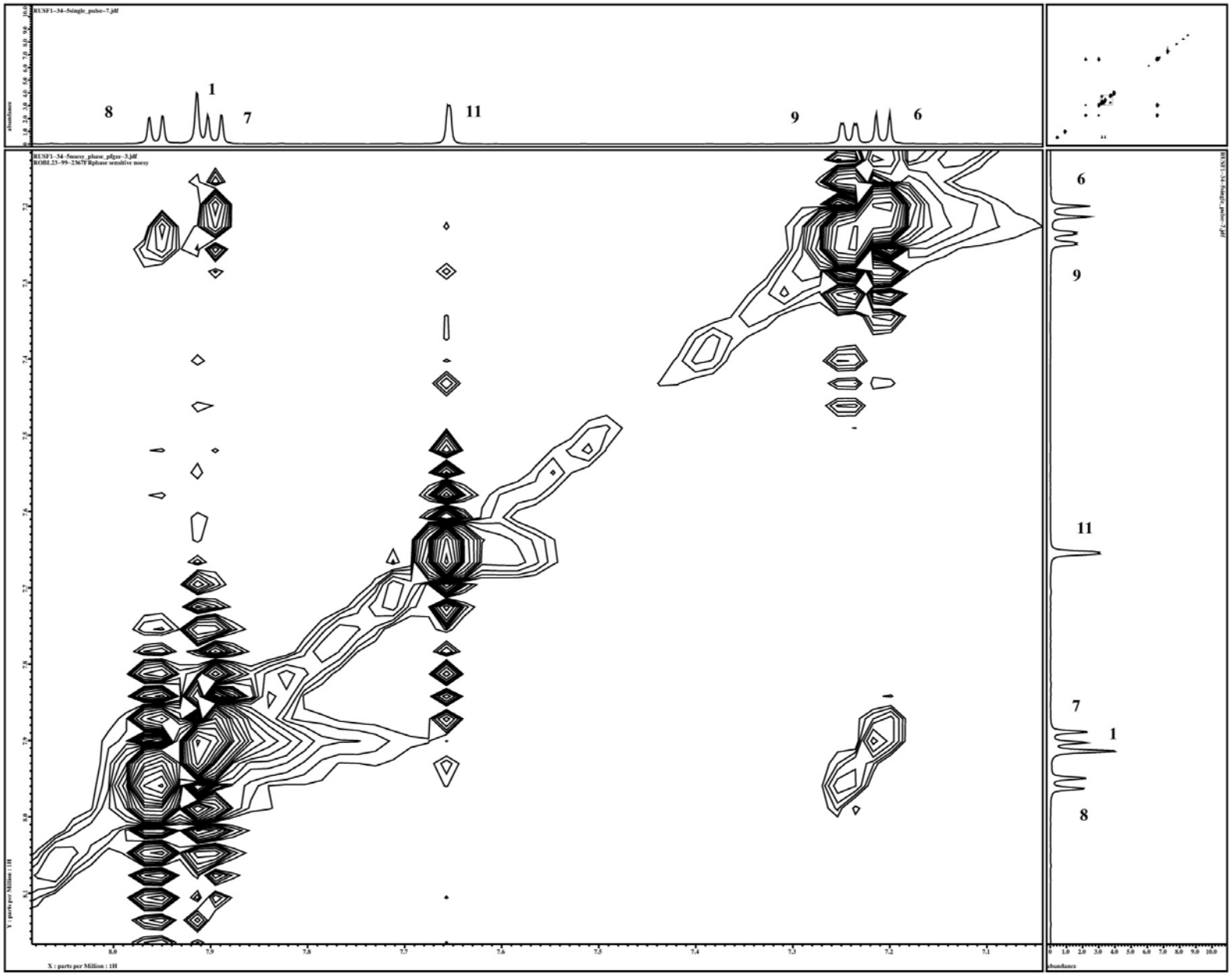
S12. Band Selective ^{1}H-^{13}C-HMBC Spectrum of **1** (600 MHz d_6-DMSO).



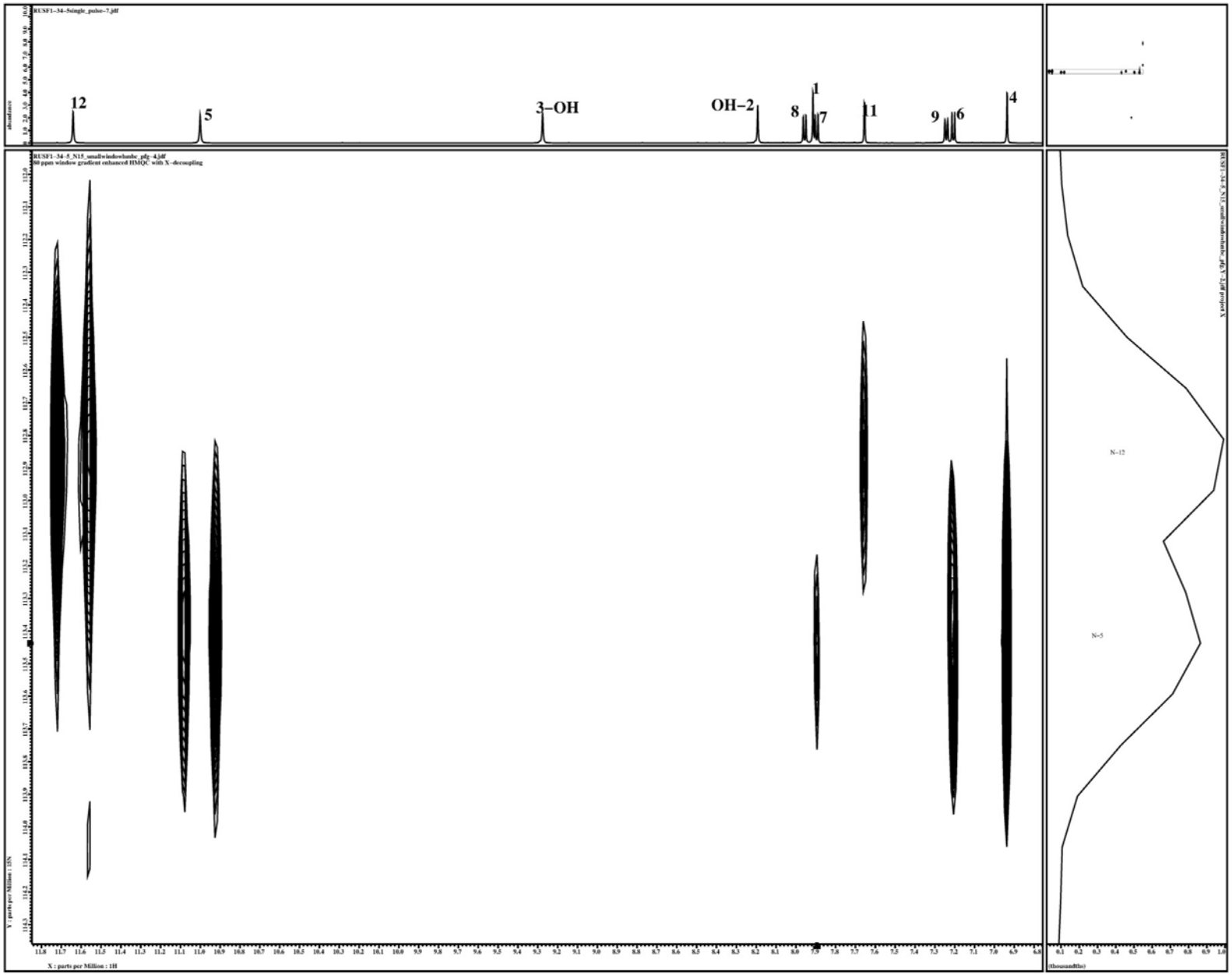
S13. Expansion of 2D-NOESY Spectrum of **1** (600 MHz d_6-DMSO).



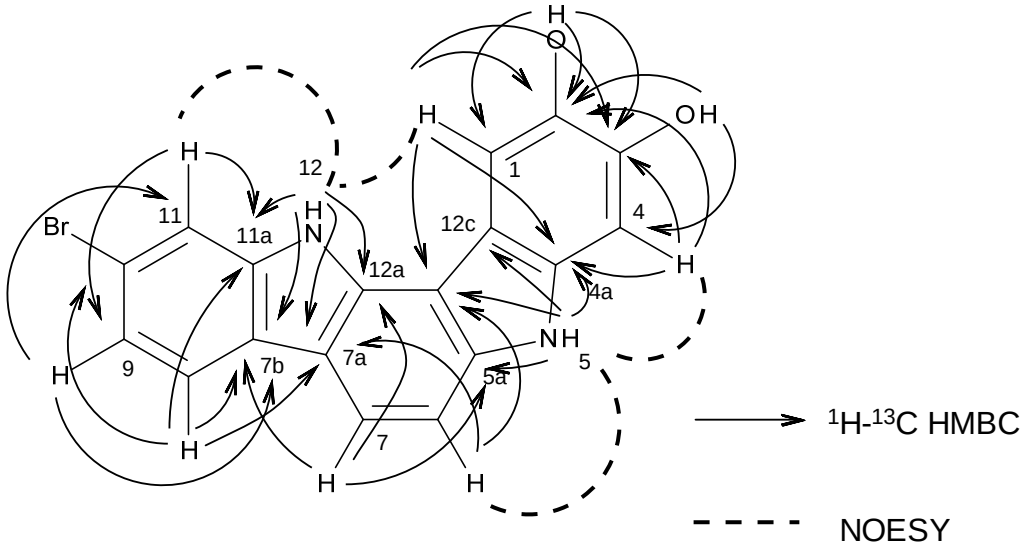
S14. Expansion of 2D-NOESY Spectrum of **1** (600 MHz d_6-DMSO).



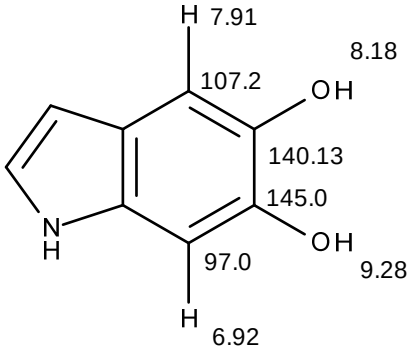
S15. ^{1}H-^{15}N-HMBC Spectrum of **1** (600 MHz d_6-DMSO).

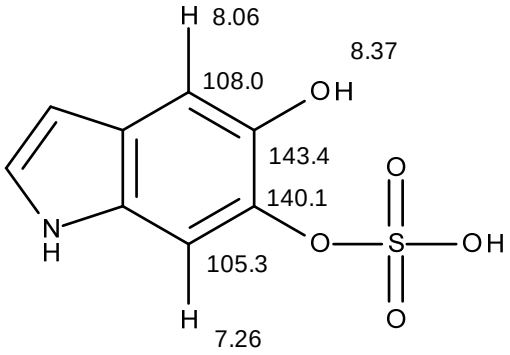


S16 Key HMBC Correlations that support the structure assignment for **2**.

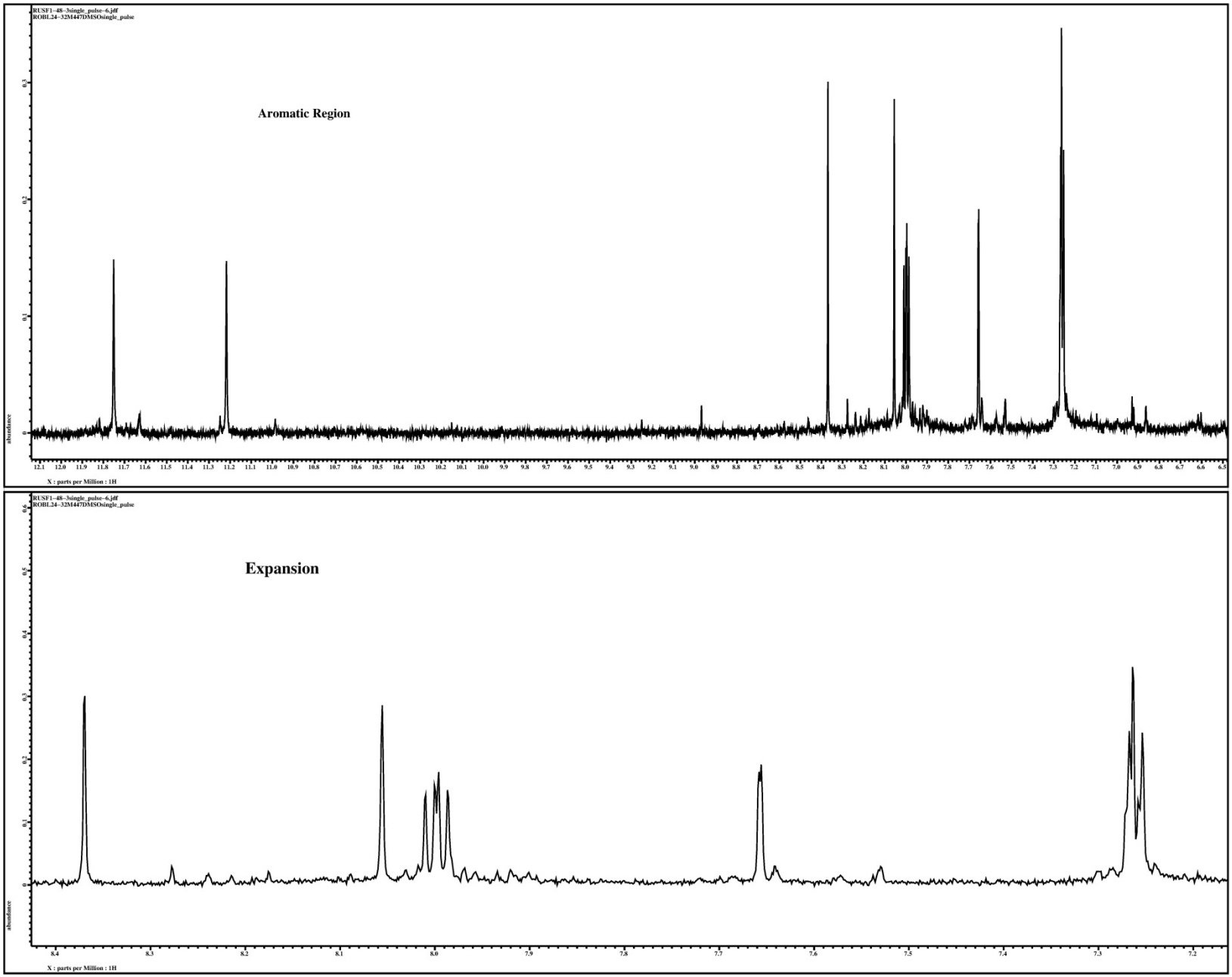


S17. Comparison of chemical shifts for molecules **1** and **2** for atoms 1 to 4 resulting from sulfate substitution at C-3 **.**

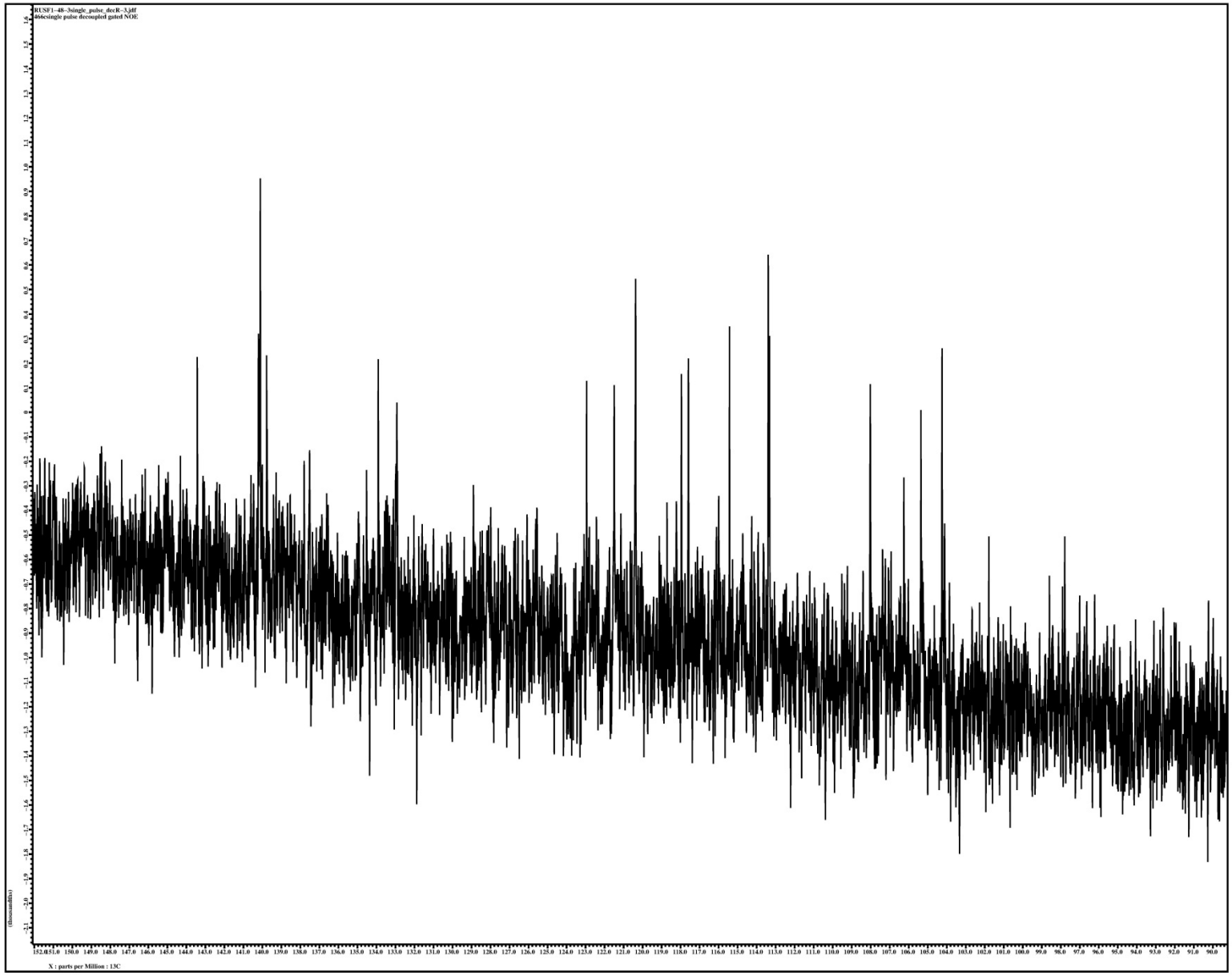




S18. ^{1}H NMR Spectrum of **2** (600 MHz d_6-DMSO).



S.19 ^{13}C NMR Spectrum of **2** (150.9 MHz d_6-DMSO).

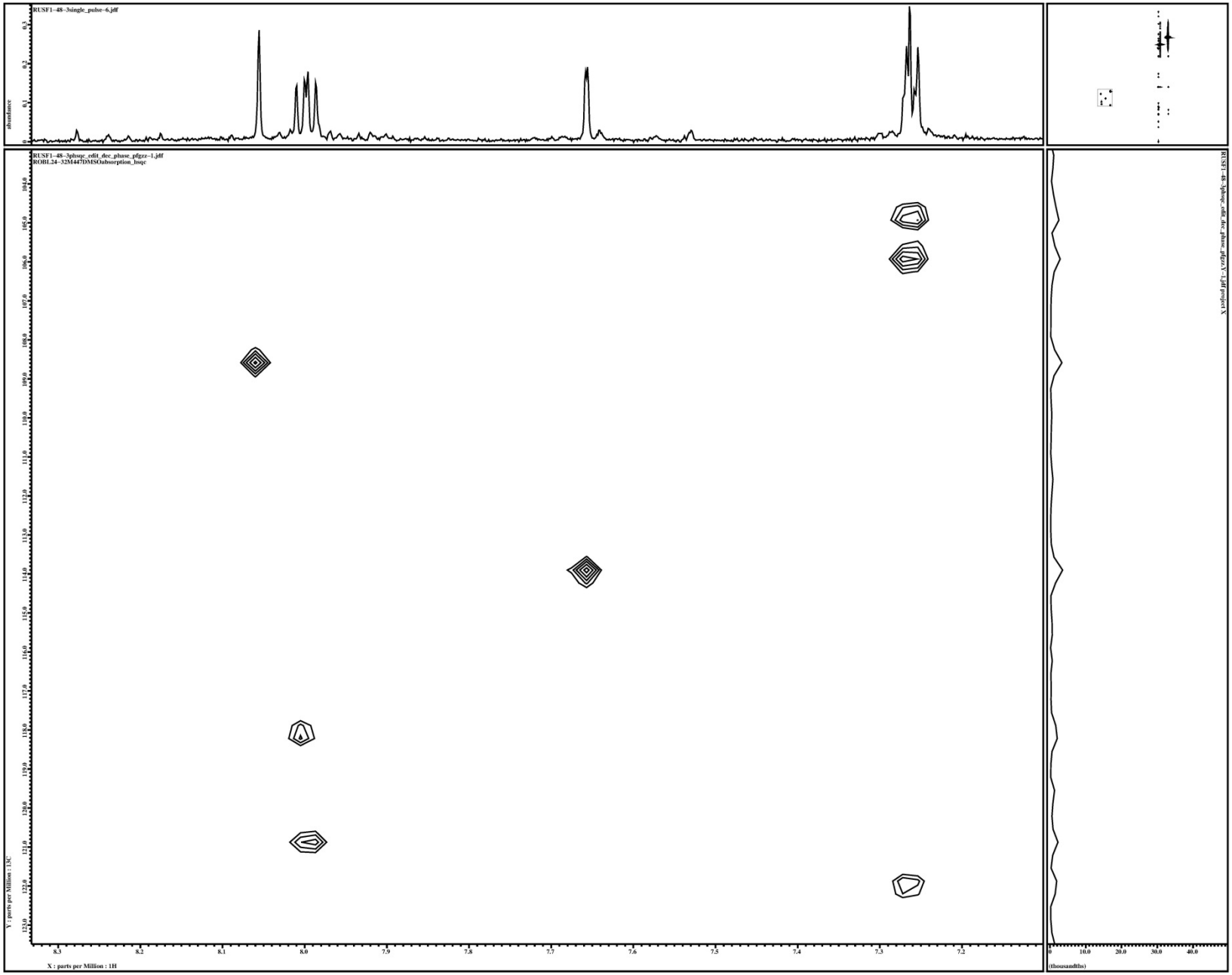


S20. Table of ^{1}H and ^{13}C NMR Data for **2** (DMSO-d_6, 600 MHz)

Position	δC, mult.	δN	δH (*J* in Hz)	COSY	HMBC	NOESY
1	108.0, CH		8.06, s		12b,2,3, 4a	
2	143.4, C					
OH-2			8.37, s		1,2, 3	
3	140.1, C					
4	105.3, CH		7.26, m		2, 3, 4a	
4a	132.9, C					
5		114	11.22, s		5a, 12b, 12c, 4a	4, 6
5a	140.2 [c], C					
6	104.3, CH		7.26, m	7	7a, 12b	
7	117.6, CH		8.00, d (8.2)	6	12a, 7b	
7a	113.4[b], C					
7b	122.9, C					
8	120.4, CH		7.99, d (8.2)	9	7a, 7b, 10, 11a	
9	121.5, CH		7.26, m	8, 11	7b, 11	
10	115.4, C					
11	113.3[b], CH		7.65, d (1.4)	9	10, 11a	12
11a	140.3[c], C					
12		113	11.75, s		12a, 7a, 7b, 11a	1, 11
12a	134.1, C					
12b	106.2, C					
12c	118.0, C					

[a]HMBC correlations, optimized for 8 Hz, are from proton(s) stated to the indicated atom; ^{1}H and ^{13}C NMR data were measured at 600.2 and 150.9 respectively. [b,c] Assignments are interchangeable.

S.21 Edited *g*-HSQC Spectrum of **2** (600 MHz d_6-DMSO).



S.22 ^{1}H-^{13}C *g*-HMBC Spectrum of **2** (600 MHz d_6-DMSO).