

Supplementary Materials

New Hybrid Phenalenone Dimer, Highly Conjugated Dihydroxylated C₂₈ Steroid and Azaphilone from the Culture Extract of a Marine Sponge-Associated Fungus, *Talaromyces pinophilus* KUFA 1767

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Figure S1. ^1H NMR spectrum of **1** (DMSO-d_6 , 300 MHz).

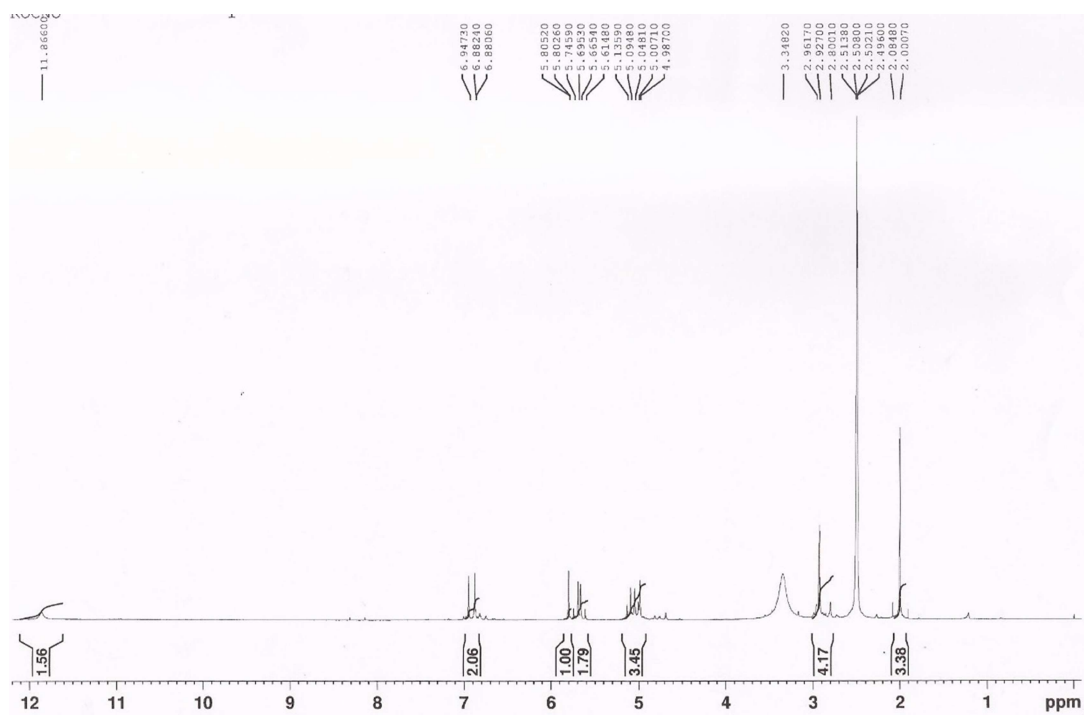


Figure S2. ^{13}C NMR spectrum of **1** (DMSO-d_6 , 75 MHz).

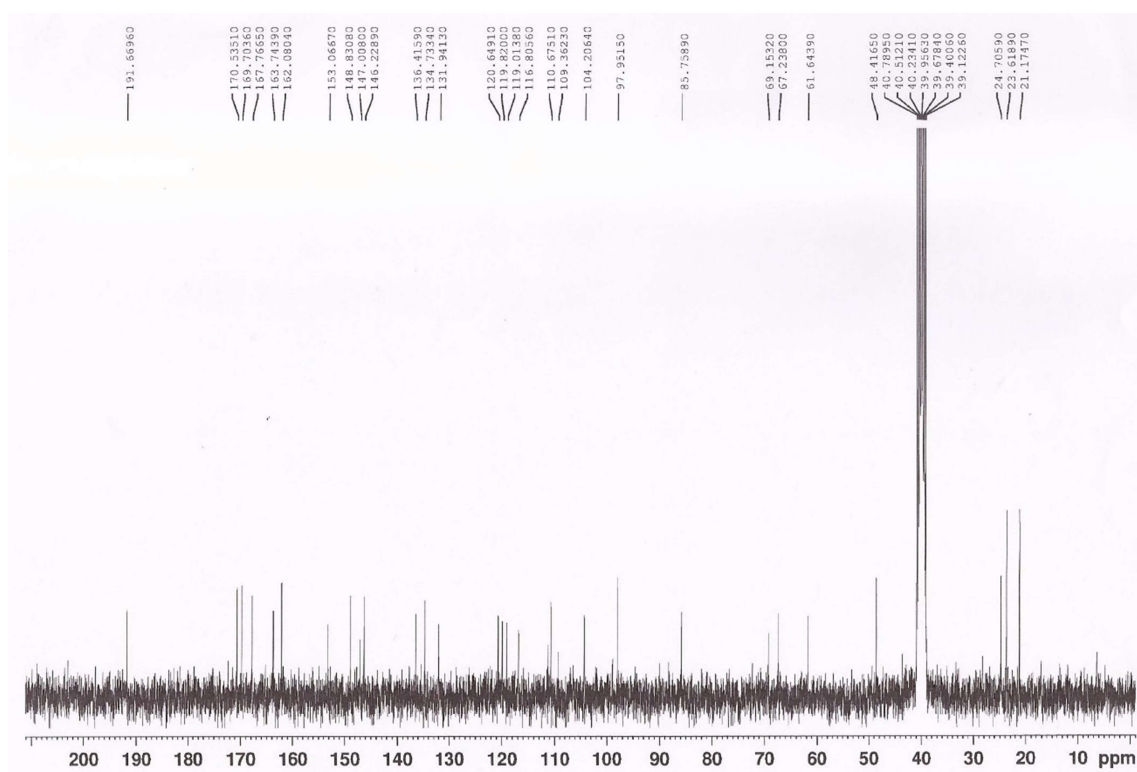


Figure S3. ^1H NMR spectrum of **2** (DMSO-d_6 , 300 MHz).

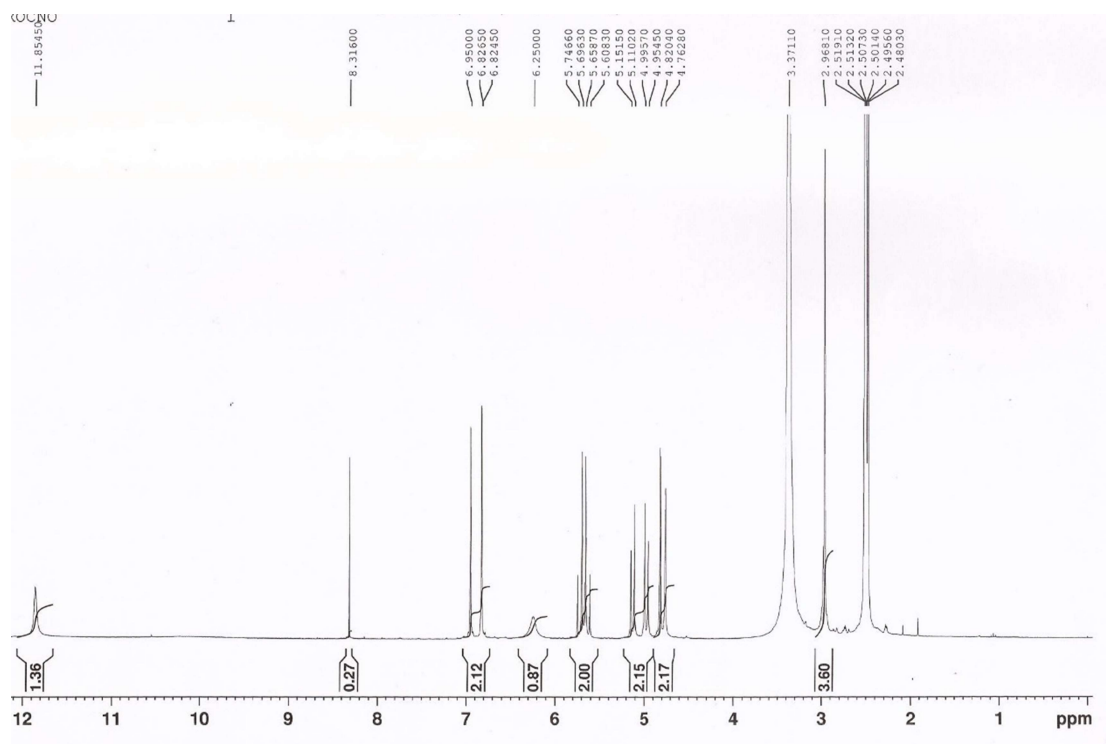


Figure S4. ^{13}C NMR spectrum of **2** (DMSO-d_6 , 75 MHz).

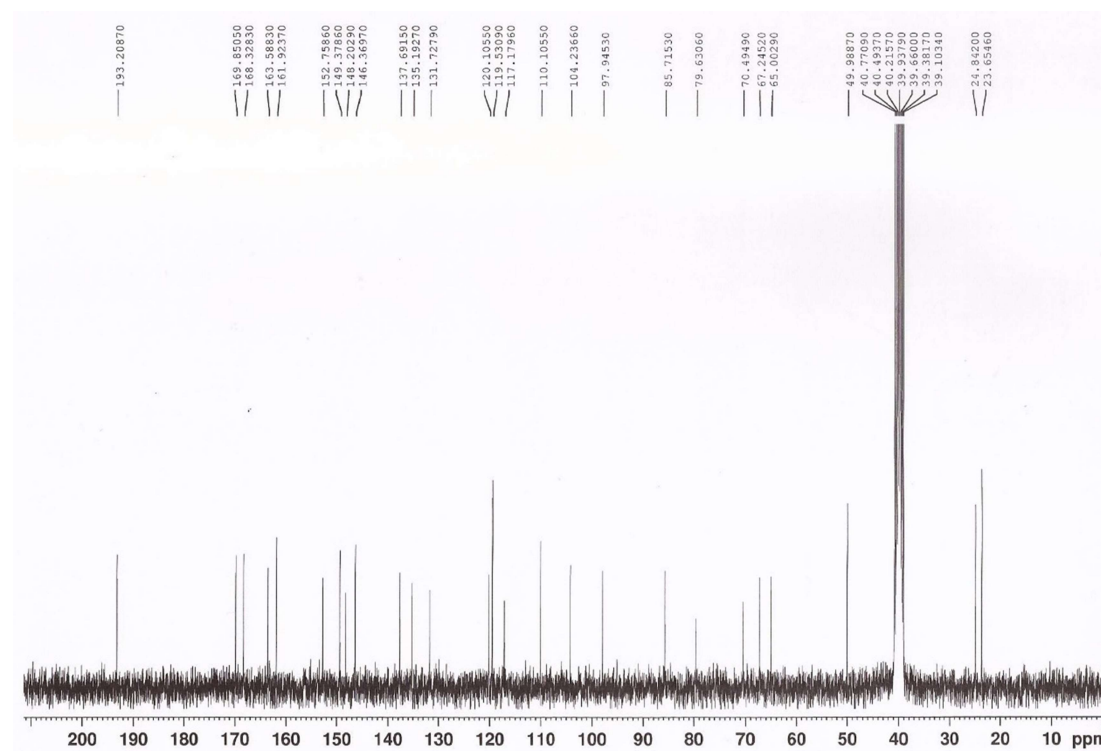


Figure 5 ROESY spectrum of **2** (DMSO_d6, 300 MHz).

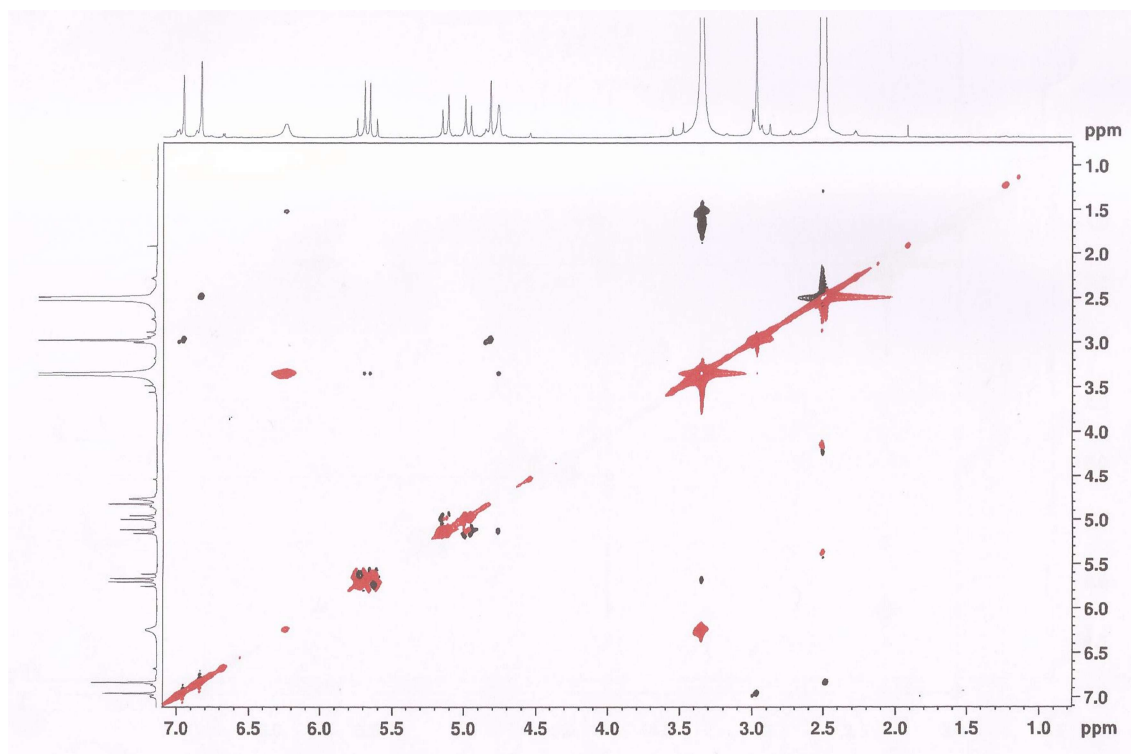


Figure S6. ¹H NMR spectrum of **3** (DMSO_d6, 300 MHz).

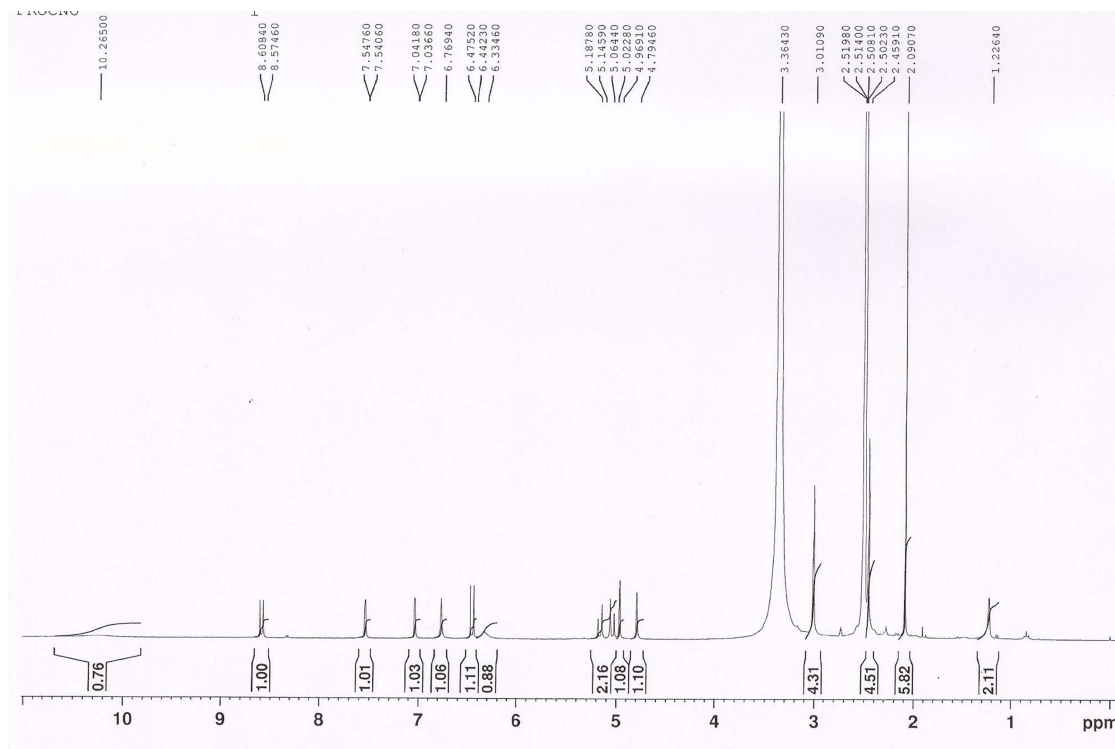


Figure S7. ^{13}C NMR spectrum of **3** (DMSO-d_6 , 75 MHz).

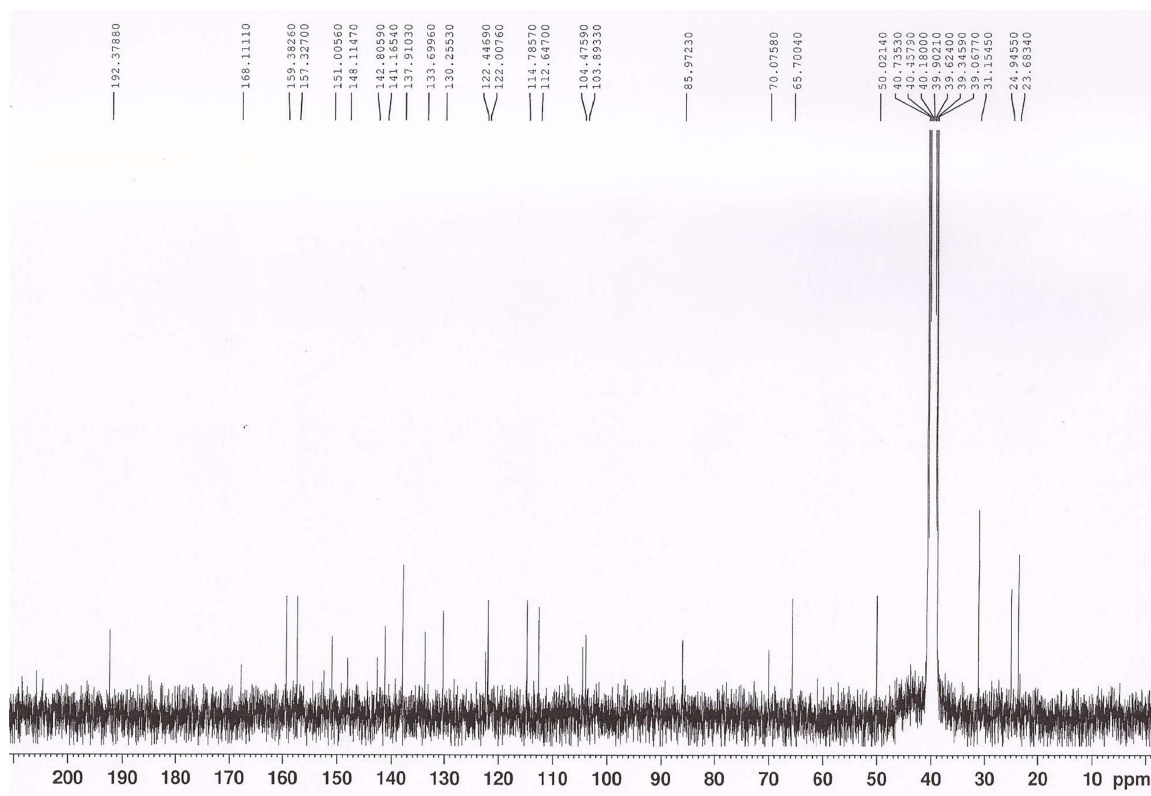


Figure S8. COSY spectrum of **3** (DMSO-d_6 , 300 MHz).

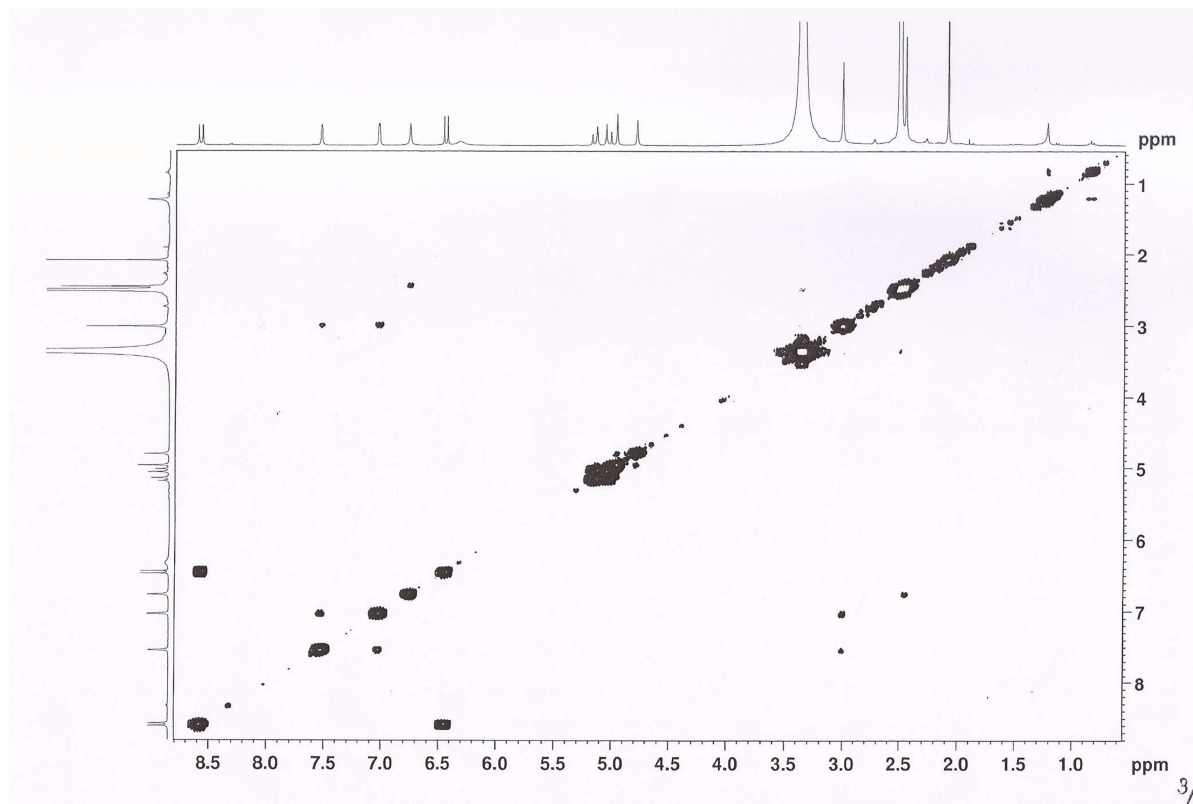


Figure S9. HSQC spectrum of **3** (DMSO_{d6}, 300 MHz).

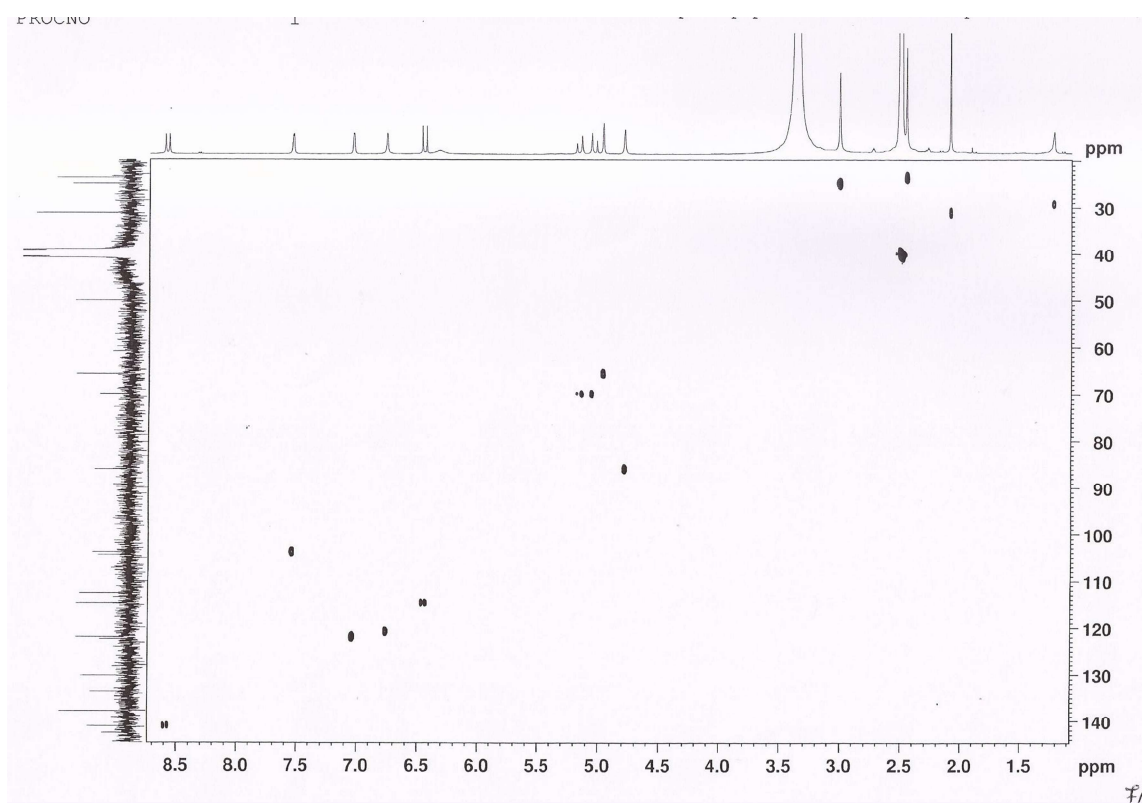


Figure S10. HMBC spectrum of **3** (DMSO_{d6}, 300 MHz).

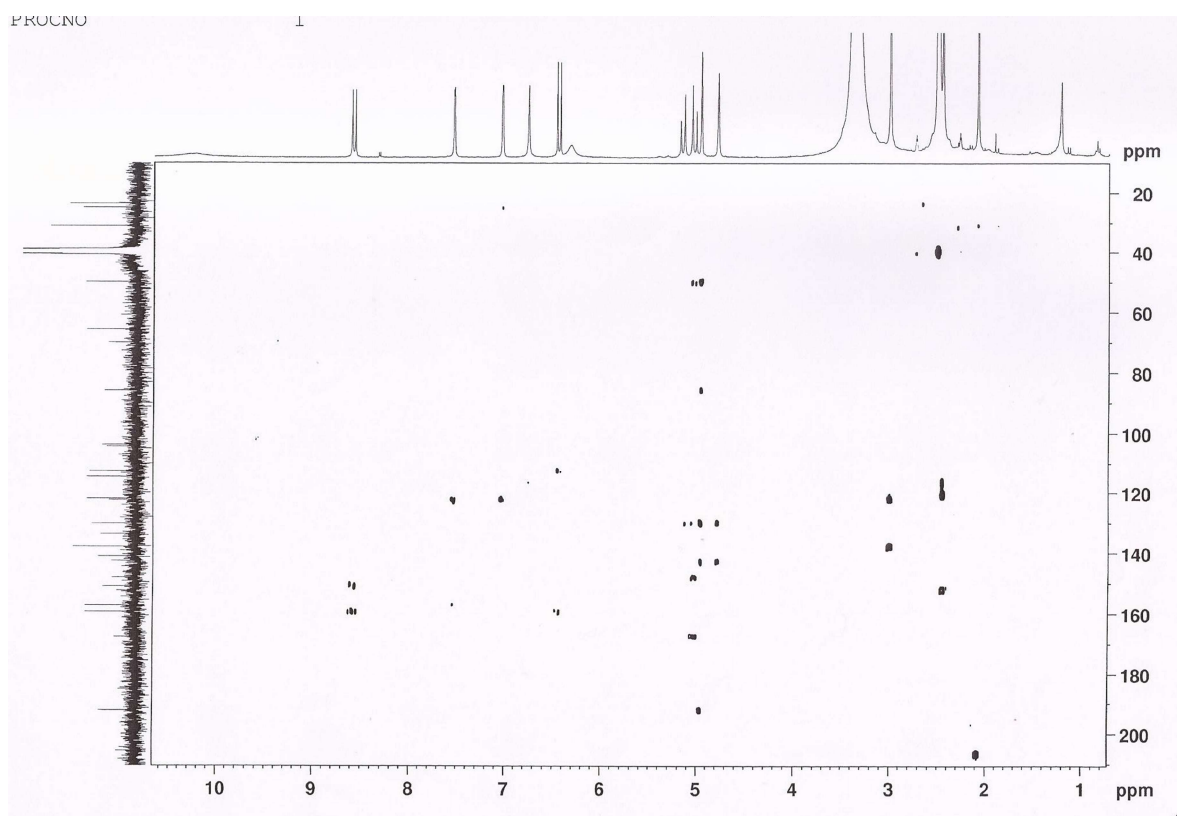


Figure S11. ROESY spectrum of **3** (DMSO_{d6}, 300 MHz).

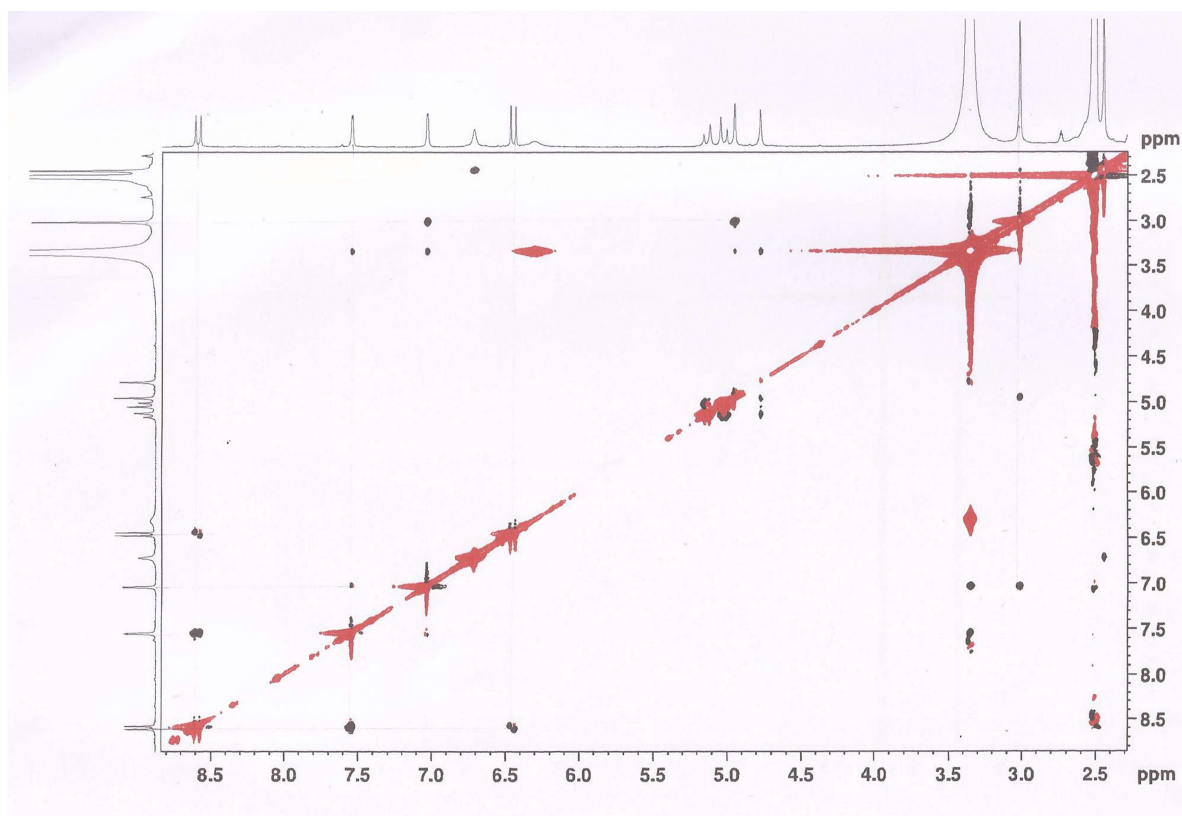


Figure S12. ¹H NMR spectrum of **4** (DMSO_{d6}, 300 MHz).

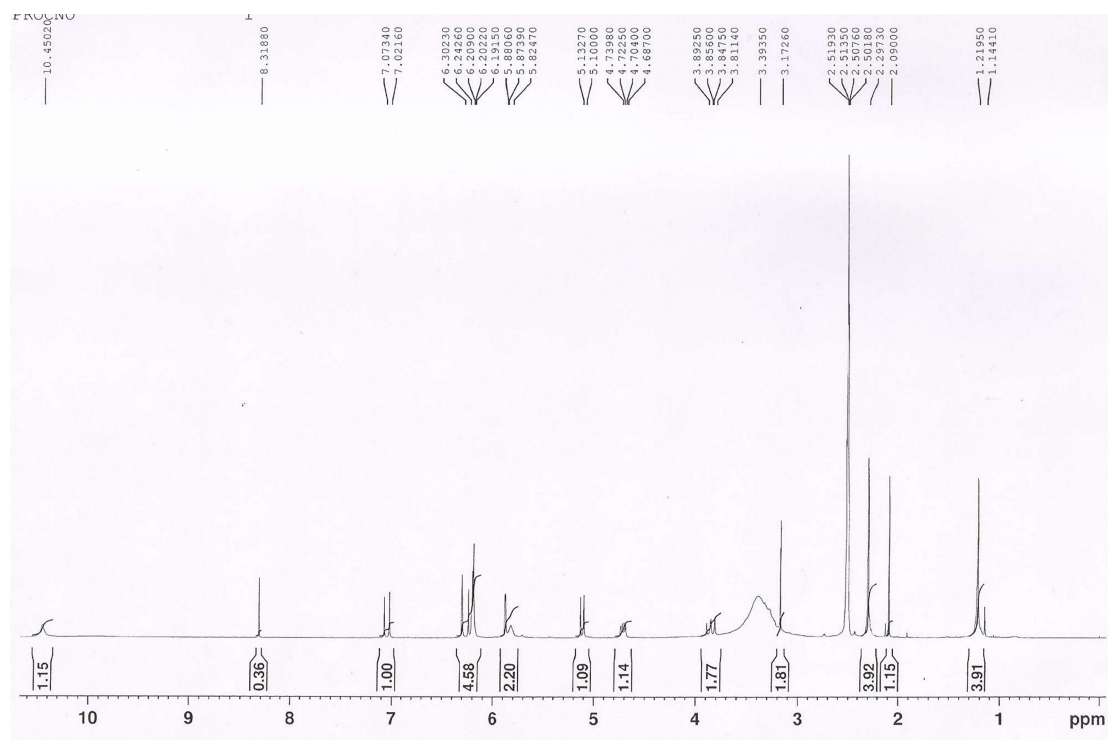


Figure S13. ^{13}C NMR spectrum of **4** (DMSO-d_6 , 75 MHz).

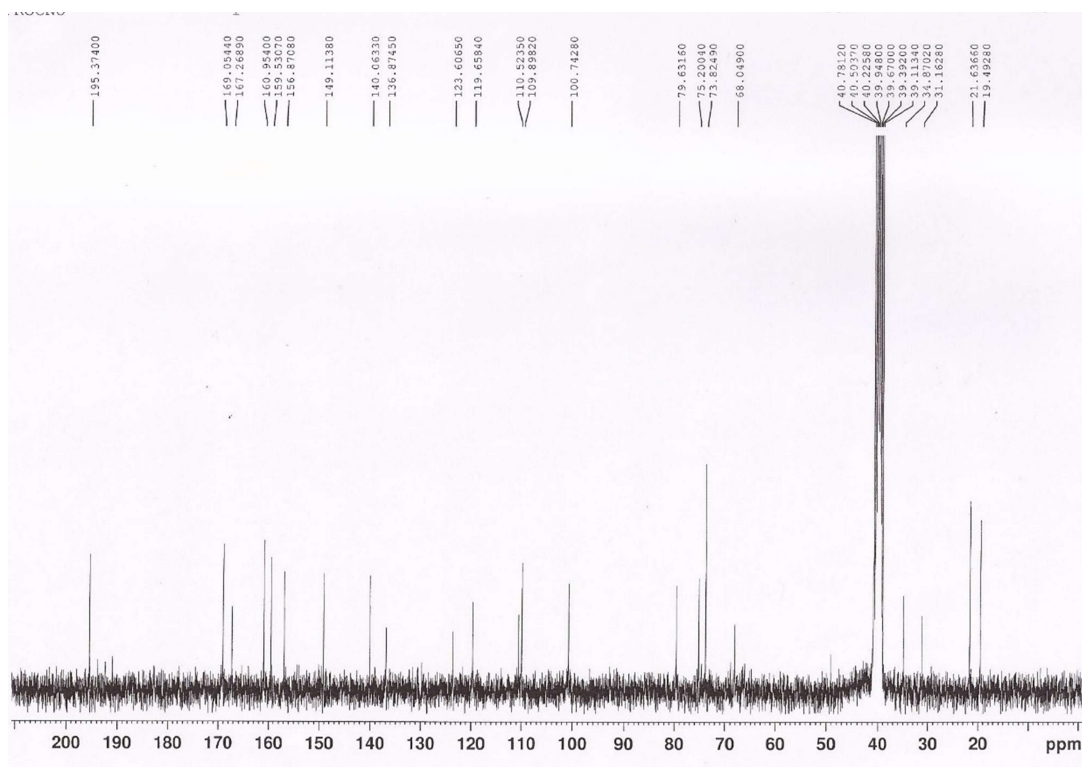


Figure S14. COSY spectrum of **4** (DMSO-d_6 , 300 MHz).

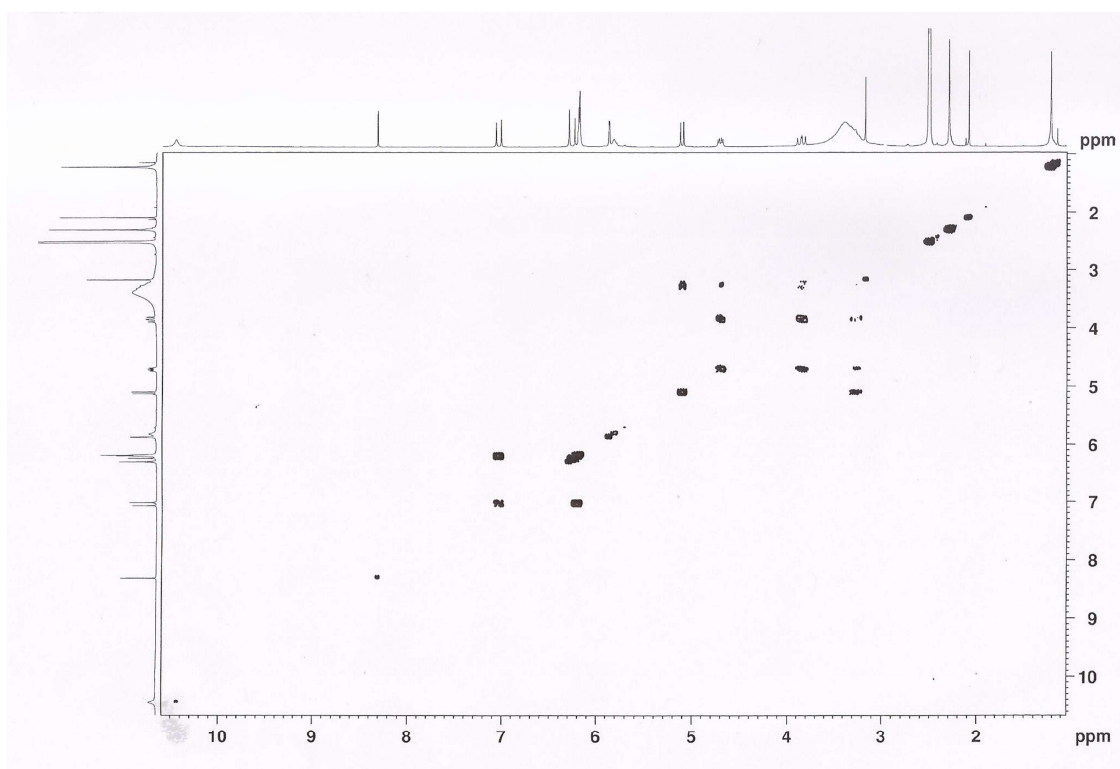


Figure S15. HSQC spectrum of **4** (DMSO-d_6 , 300 MHz).

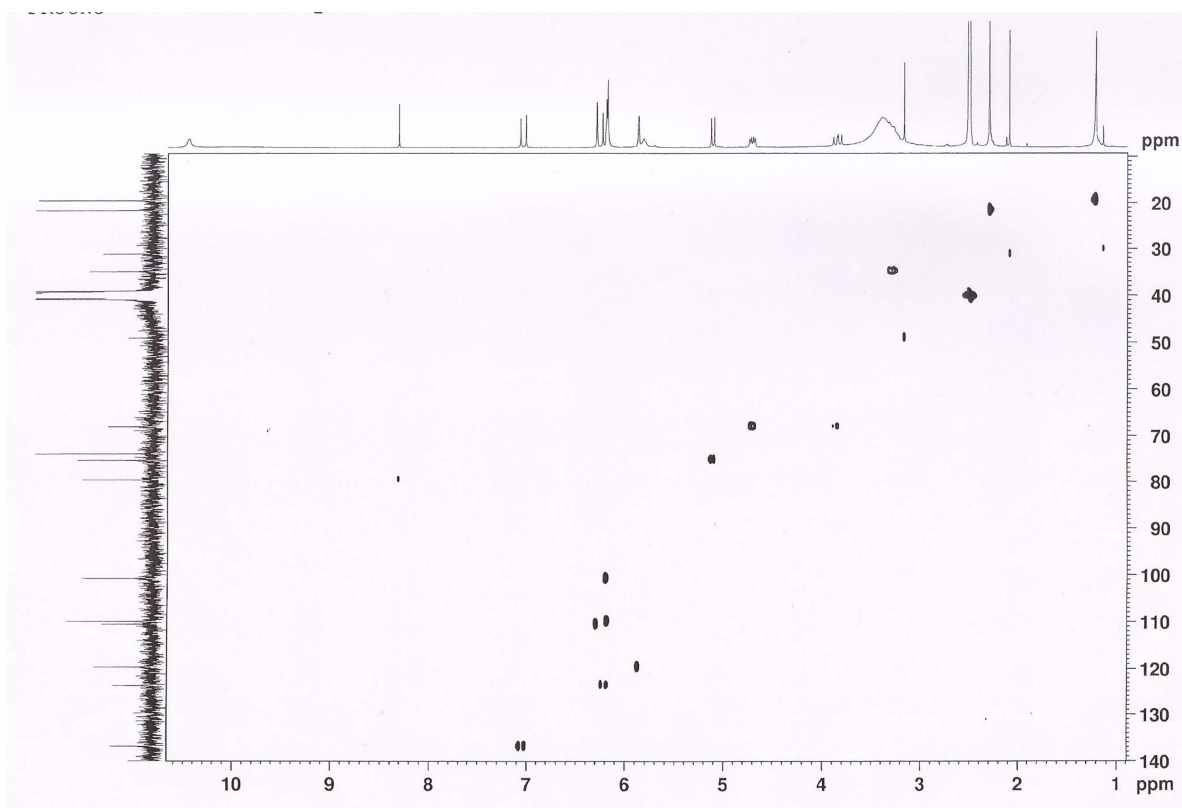


Figure S16. HMBC spectrum of **4** (DMSO-d_6 , 300 MHz).

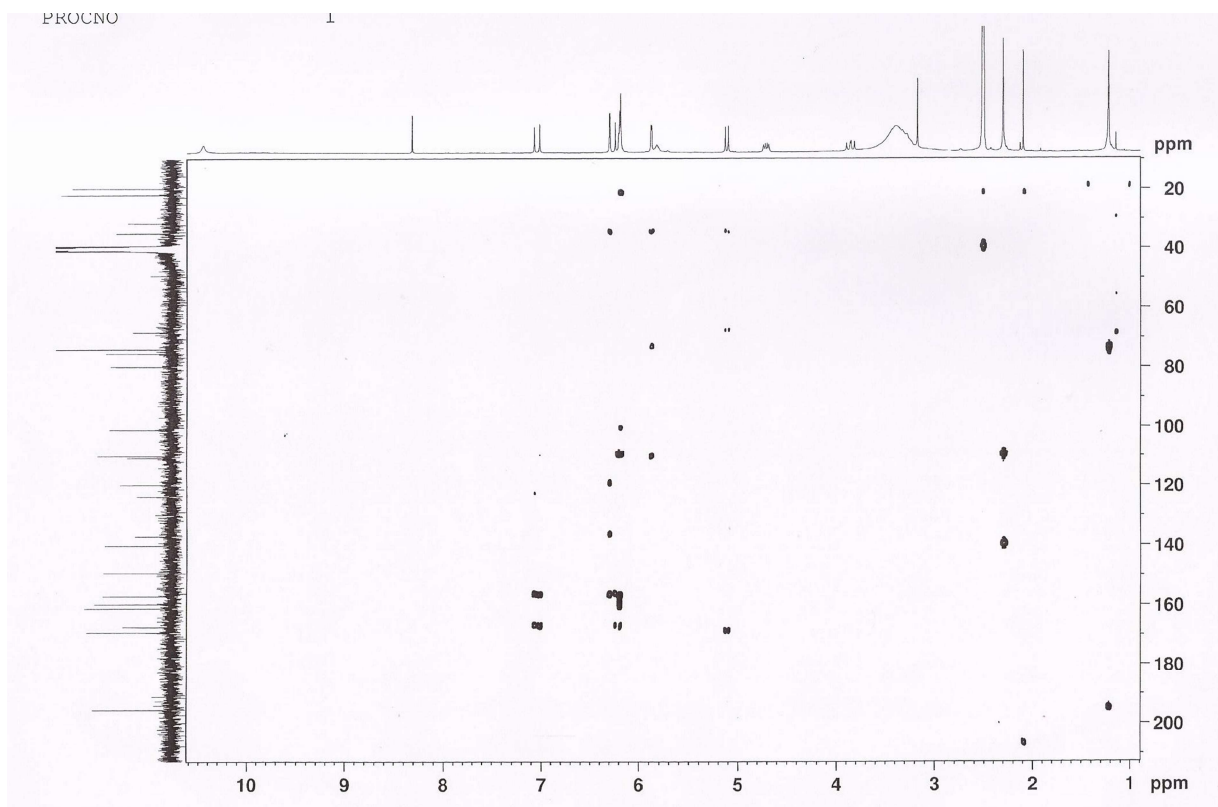


Figure S17. ROESY spectrum of **4** (DMSO_{d6}, 300 MHz).

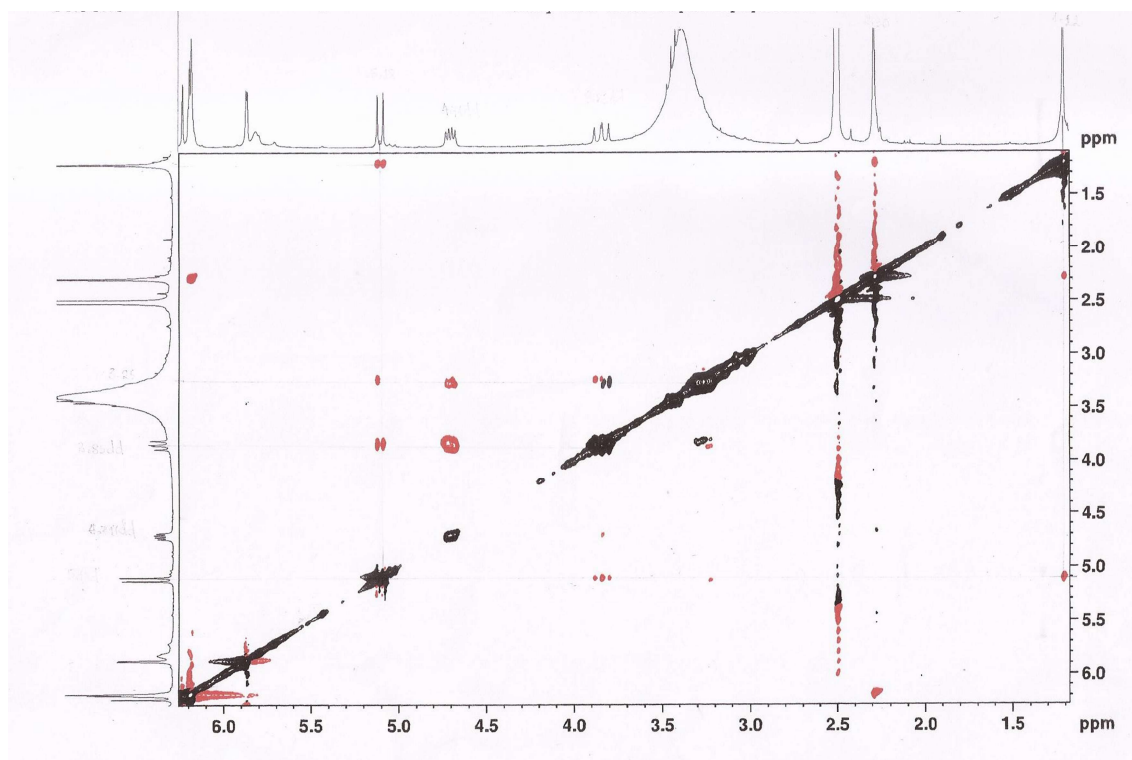


Figure S18. ¹H spectrum of **5** (DMSO_{d6}, 300 MHz).

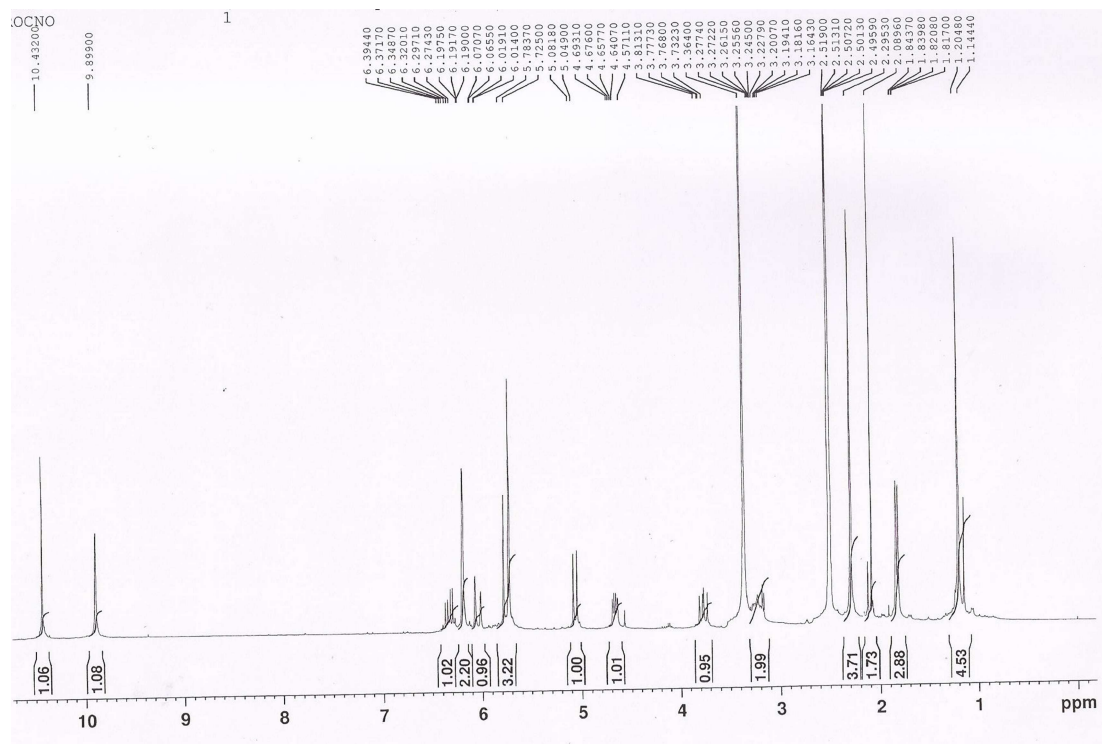


Figure S19. ^{13}C spectrum of **5** (DMSO-d_6 , 75 MHz).

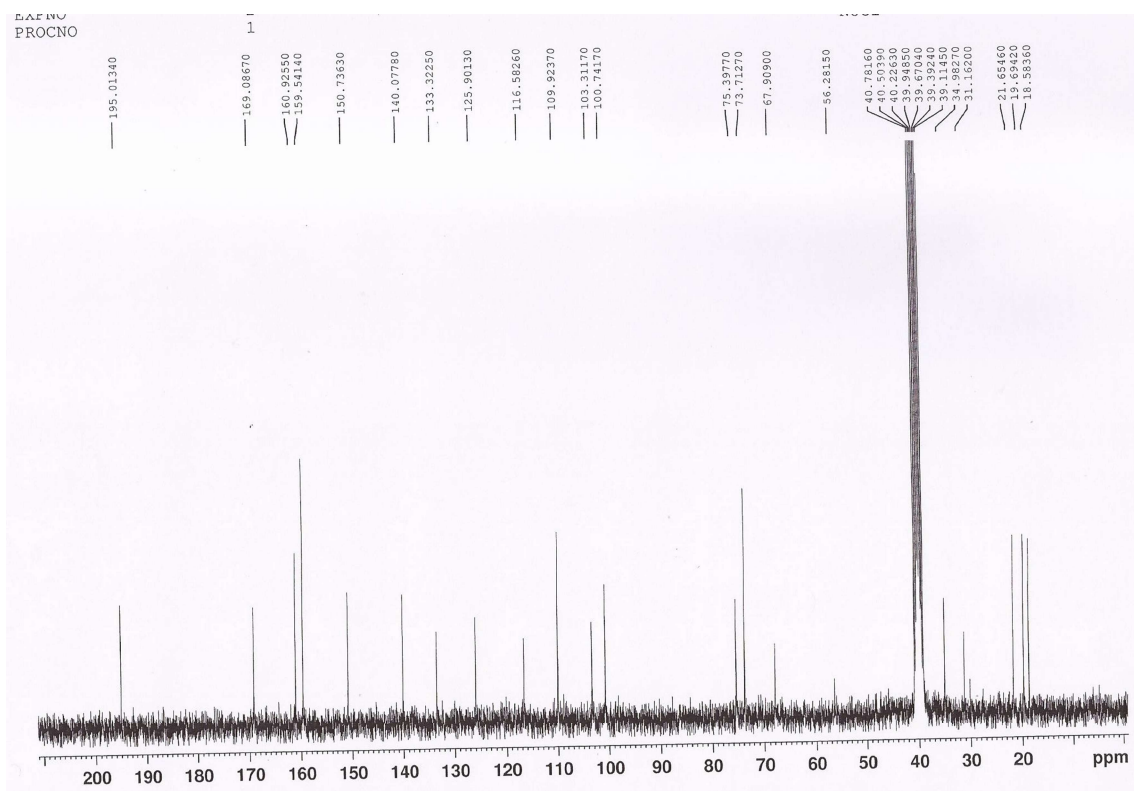


Figure S20. ROESY spectrum of **5** (DMSO-d_6 , 300 MHz).

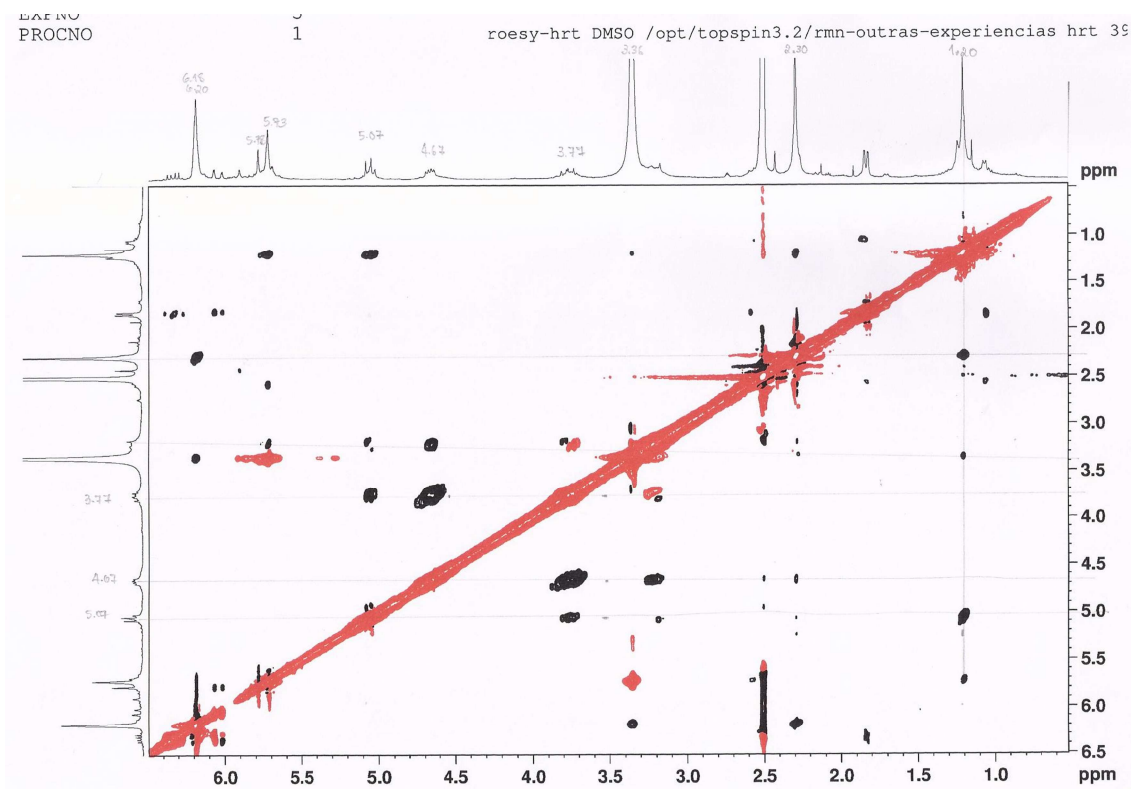


Figure S21. ^1H spectrum of **6** (DMSO-d_6 , 300 MHz).

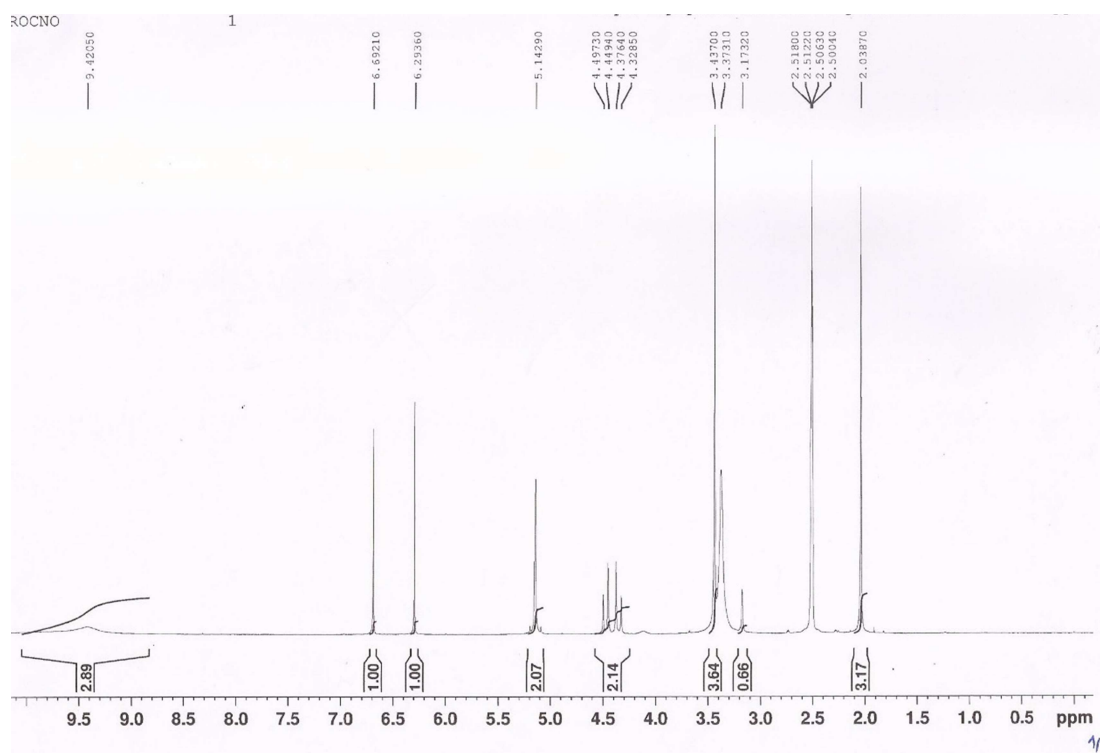


Figure S22. ^{13}C spectrum of **6** (DMSO-d_6 , 300 MHz).

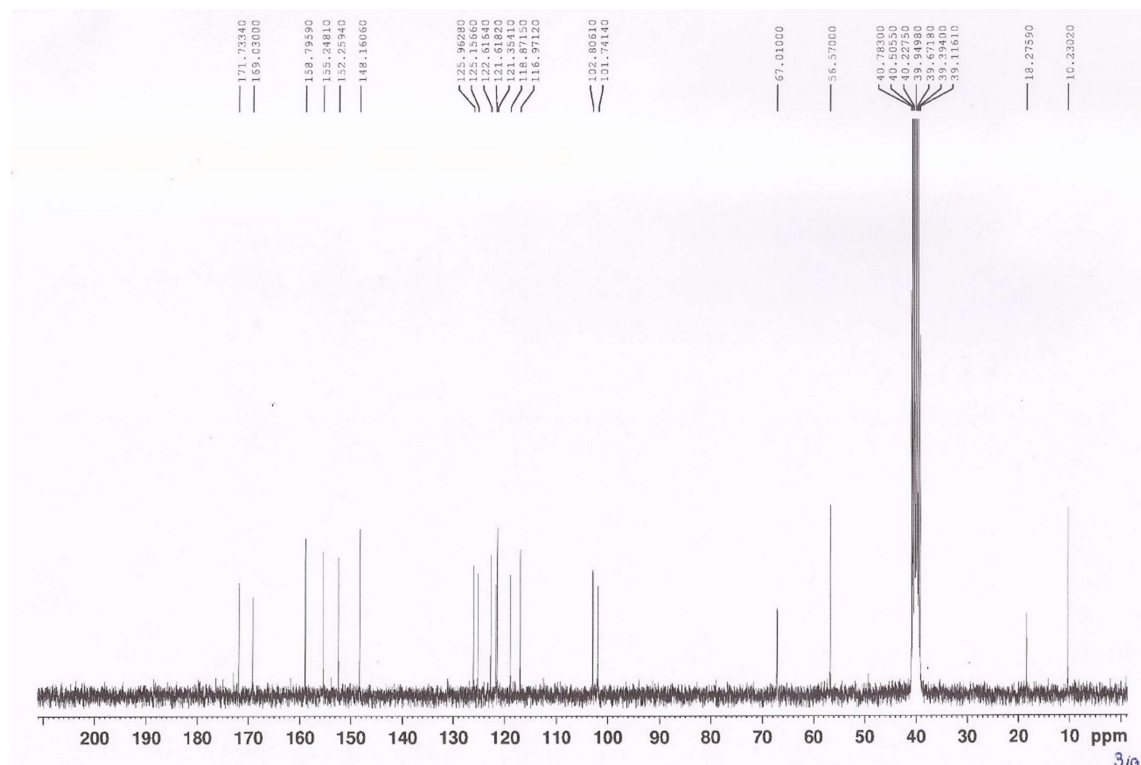


Figure S23. COSY spectrum of **6** (DMSO_{d6}, 300 MHz).

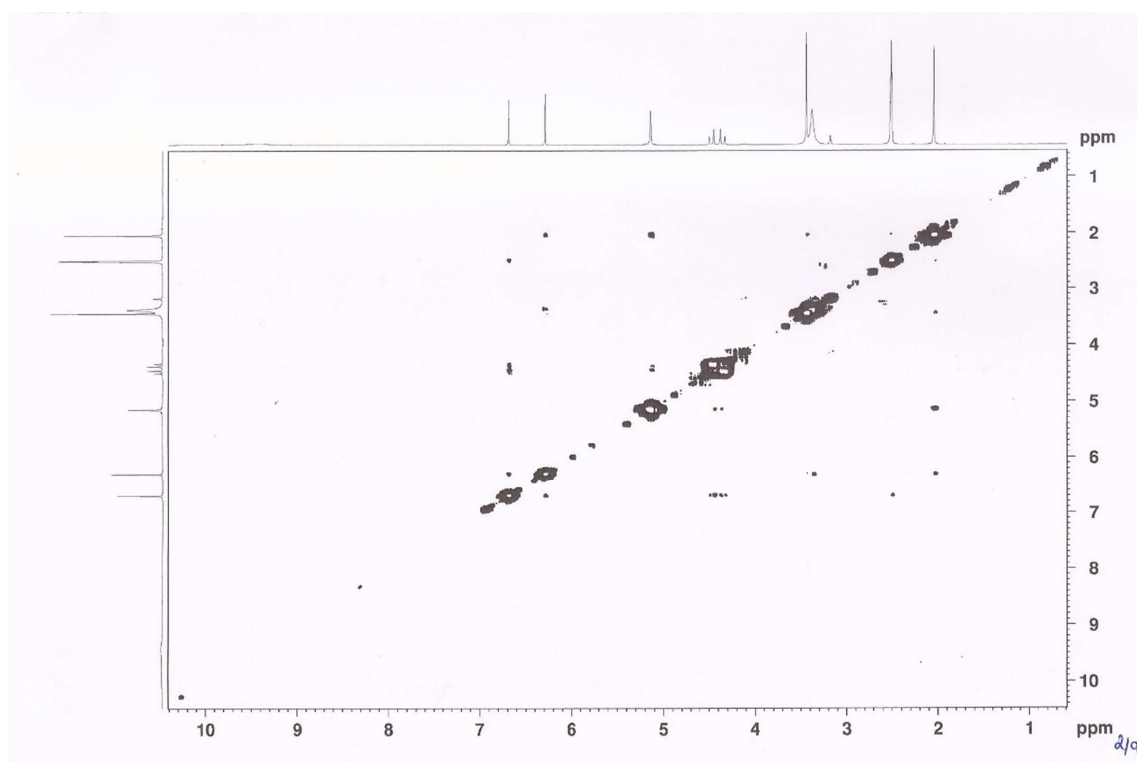


Figure S24. HSQC spectrum of **6** (DMSO_{d6}, 300 MHz).

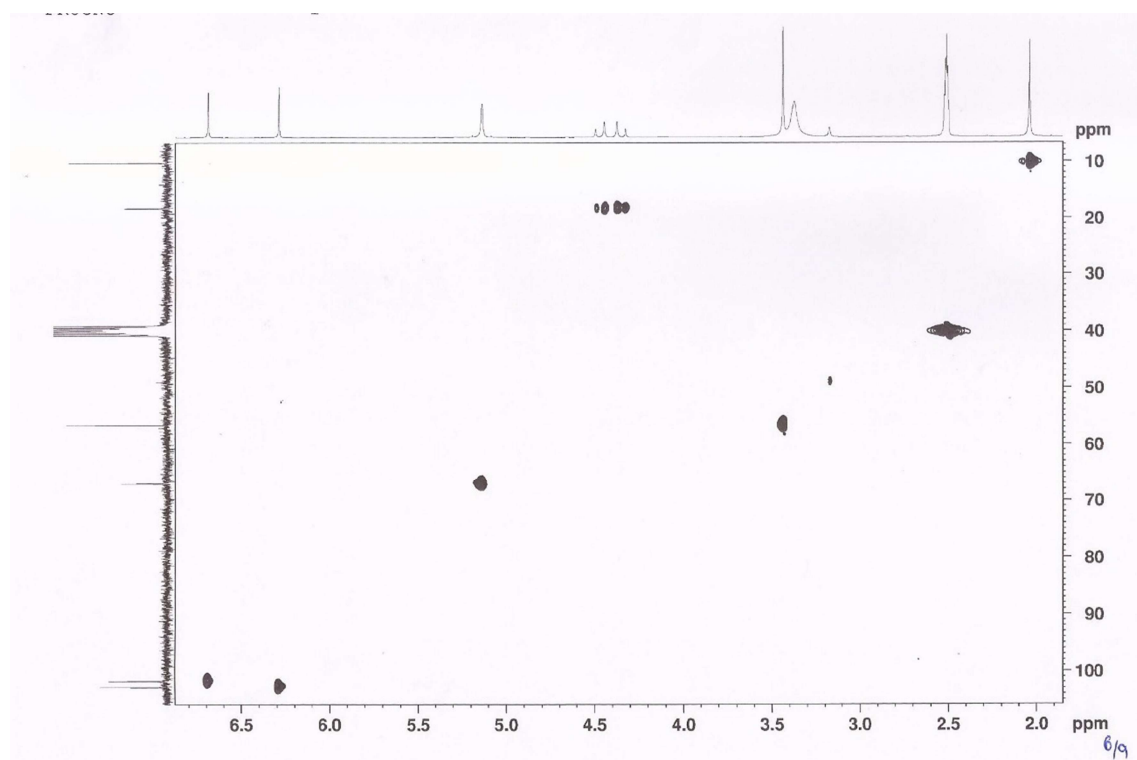


Figure S25. HMBC spectrum of **6** (DMSO_d₆, 300 MHz).

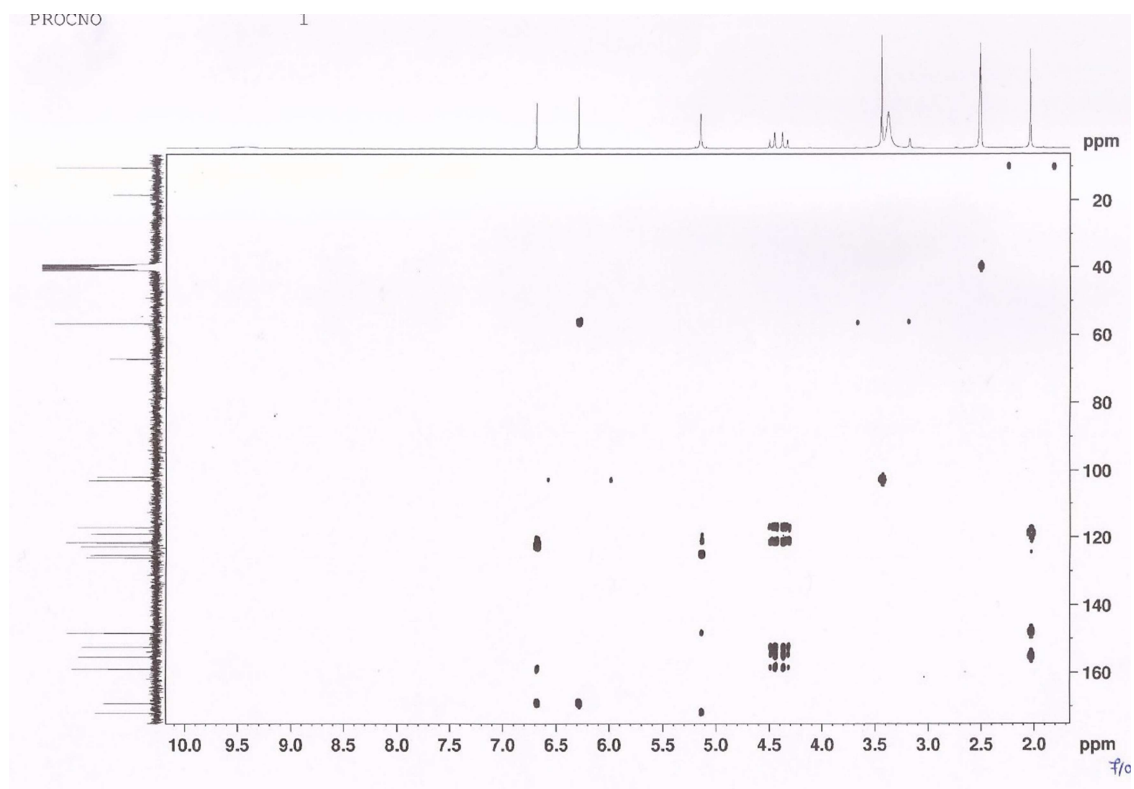


Figure S26. ¹H spectrum of **7** (DMSO_d₆, 300 MHz).

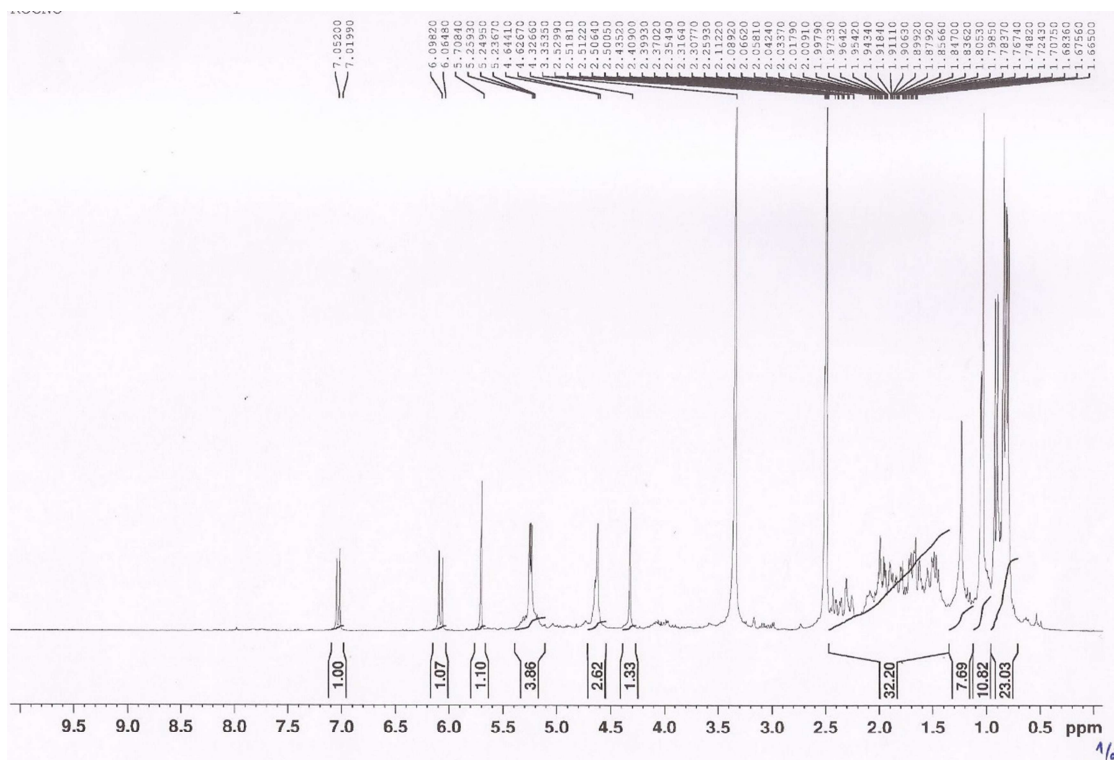


Figure S27. ¹³C spectrum of **7** (DMSO_d₆, 75 MHz).

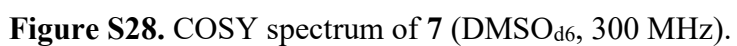


Figure S29. HSQC spectrum of **7** (DMSO_{d6}, 300 MHz).

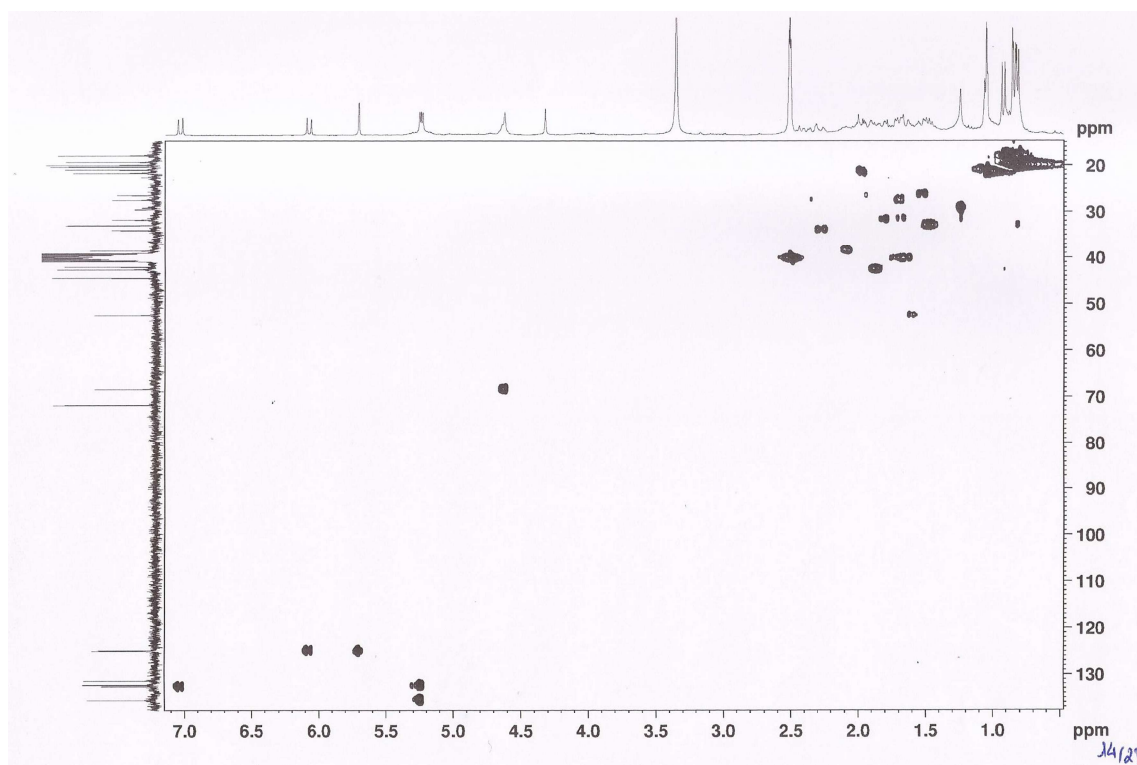
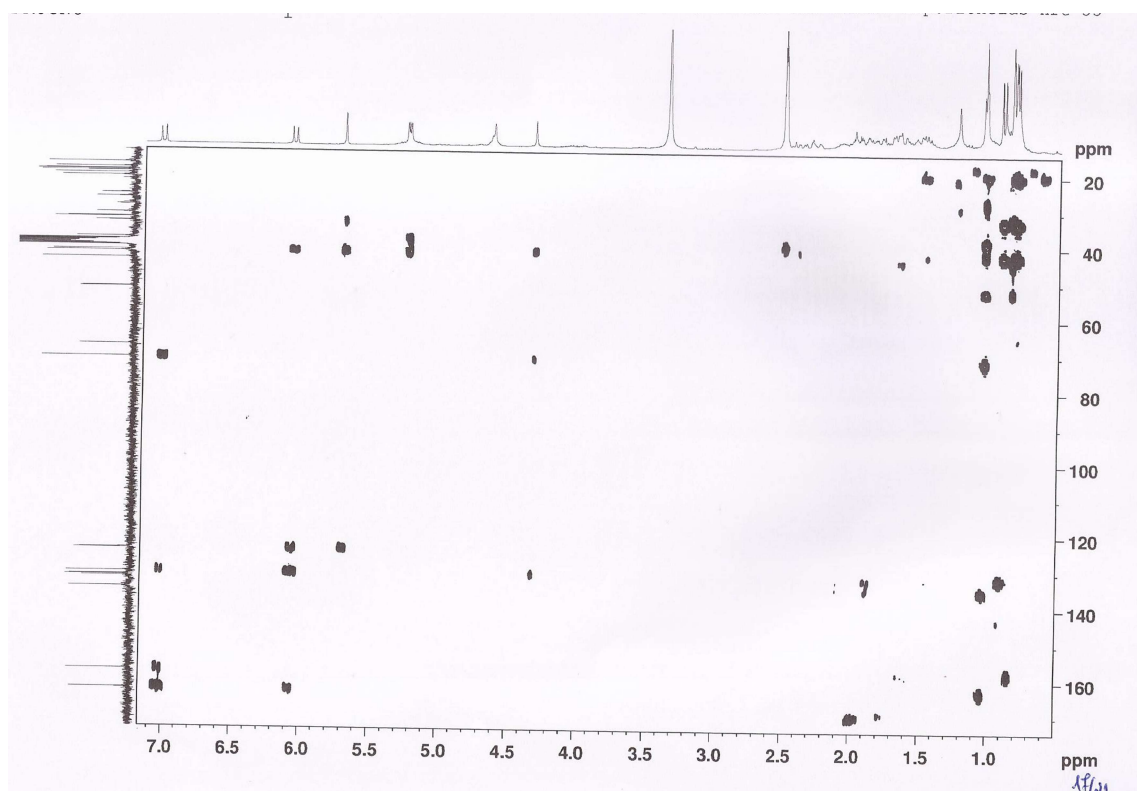


Figure S30. HMBC spectrum of **7** (DMSO_{d6}, 300 MHz).



¹H NMR spectrum (CDCl₃) of compound 1. The x-axis represents chemical shift in ppm, ranging from 0 to 12. The spectrum shows several peaks with corresponding integration values and chemical shift labels.

Chemical Shift (ppm)	Integration
~11.33450	1.00
~6.70050, 6.69200, 6.69030, 6.68230	2.12
~3.47960, 3.45990, 3.45660, 3.45330, 3.43410, 3.41460, 3.41200, 3.41200, 3.38820, 2.99360, 2.97180, 2.96930, 2.96830, 2.34380, 2.34000, 2.33620, 2.27650	3.27
~1.58380, 1.47340, 1.45010, 1.45010, 1.10550	1.14, 1.13, 1.14, 1.59, 3.48
0.00020	-

13C NMR spectrum (CDCl₃) of compound 10. The x-axis represents chemical shift in ppm, ranging from 20 to 200. The spectrum shows several sharp peaks, with the most intense at 77.4940 ppm (CDCl₃ solvent). Other labeled peaks include 195.28200, 166.81640, 165.27120, 164.91480, 148.117650, 144.65060, 134.51220, 103.23590, 103.05420, 100.80350, 77.4940, 77.2850, 77.0610, 76.60260, 56.04490, 42.79770, 28.38430, and 21.00780.

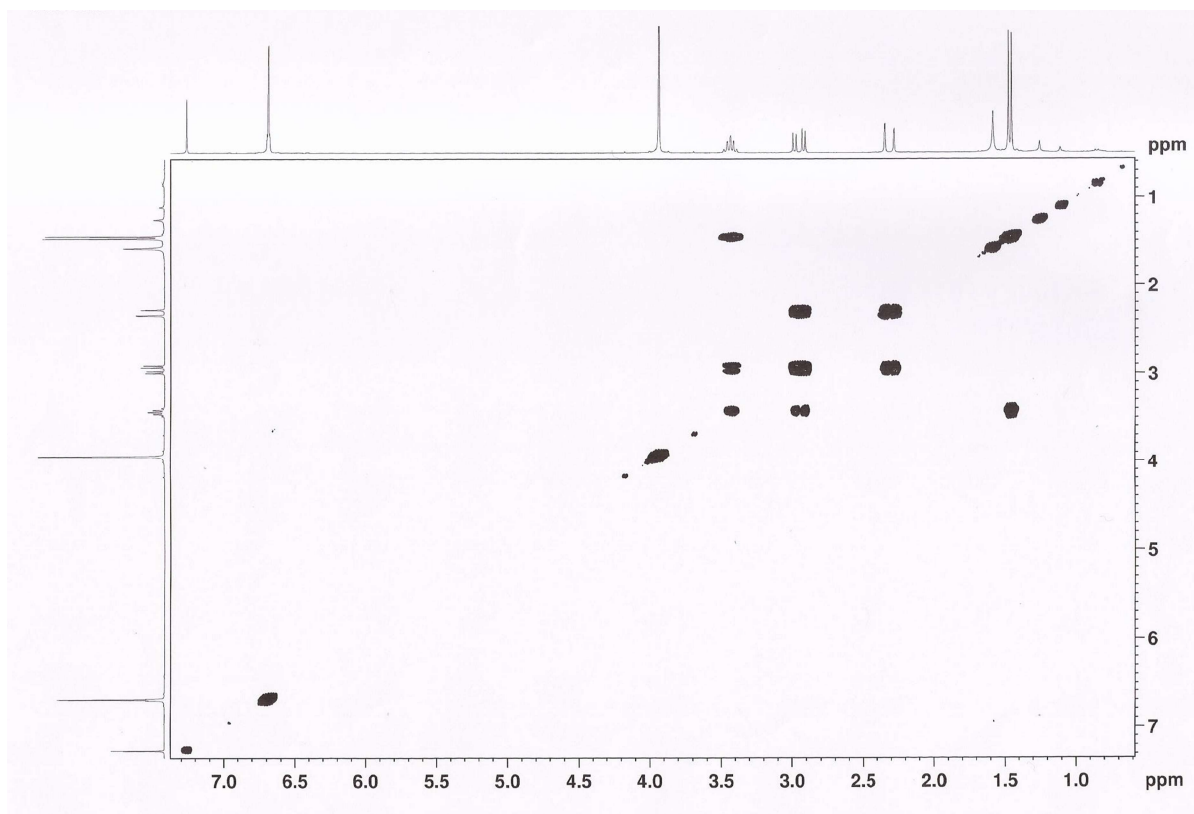


Figure S34. HSQC spectrum of **8** (CDCl₃, 300 MHz).

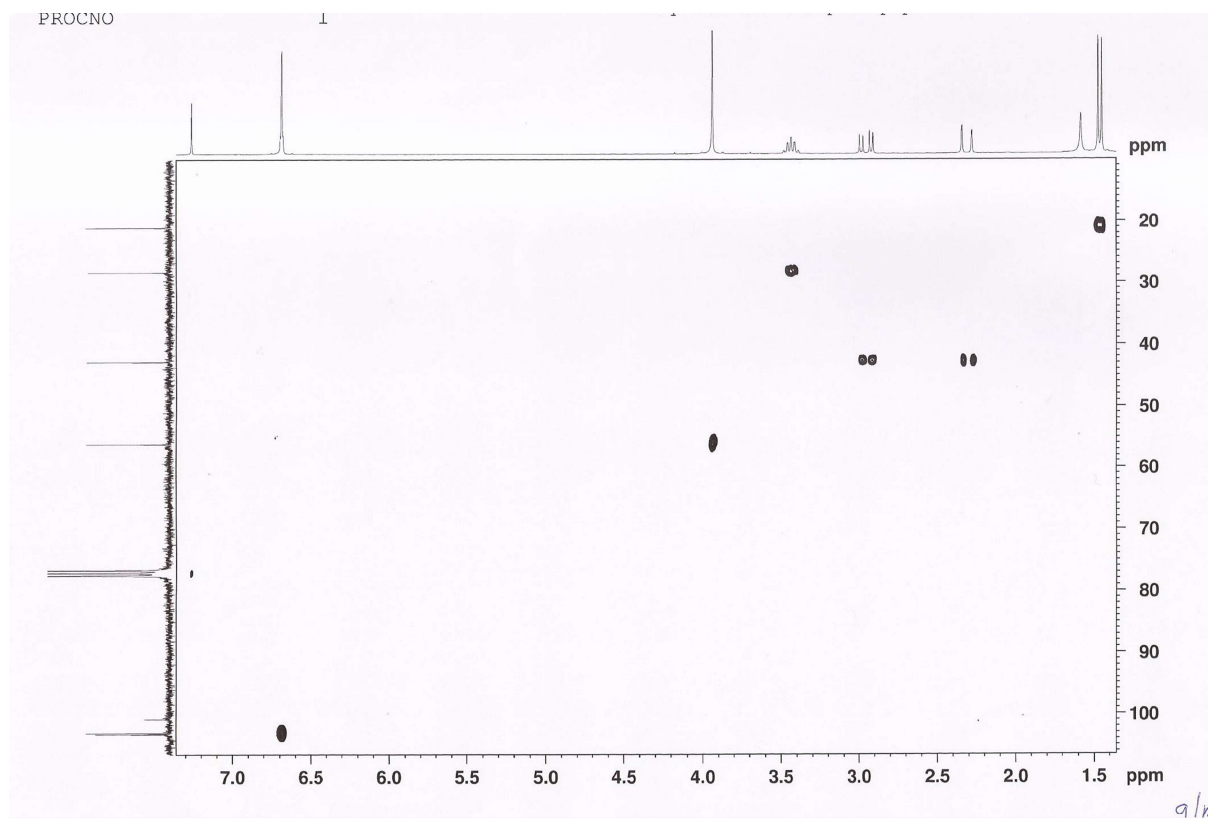


Figure S35. HMBC spectrum of **8** (CDCl₃, 300 MHz).

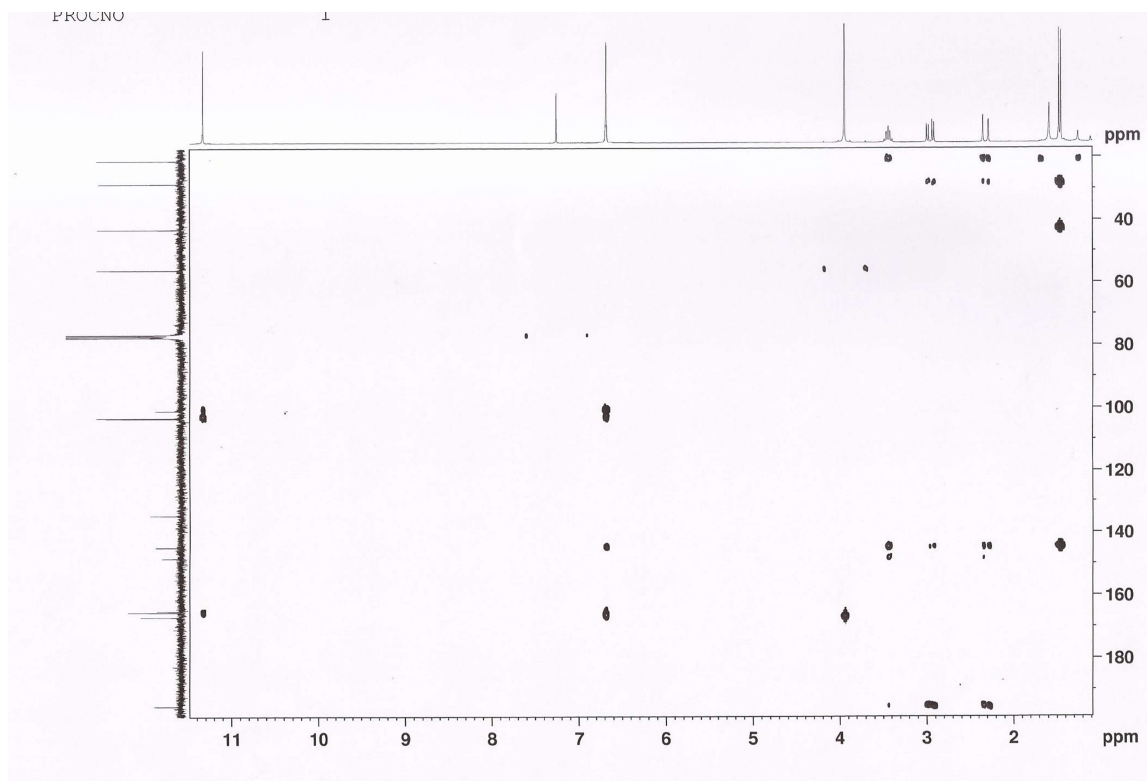


Figure S36. ^1H spectrum of **9** (DMSO-d_6 , 500 MHz).

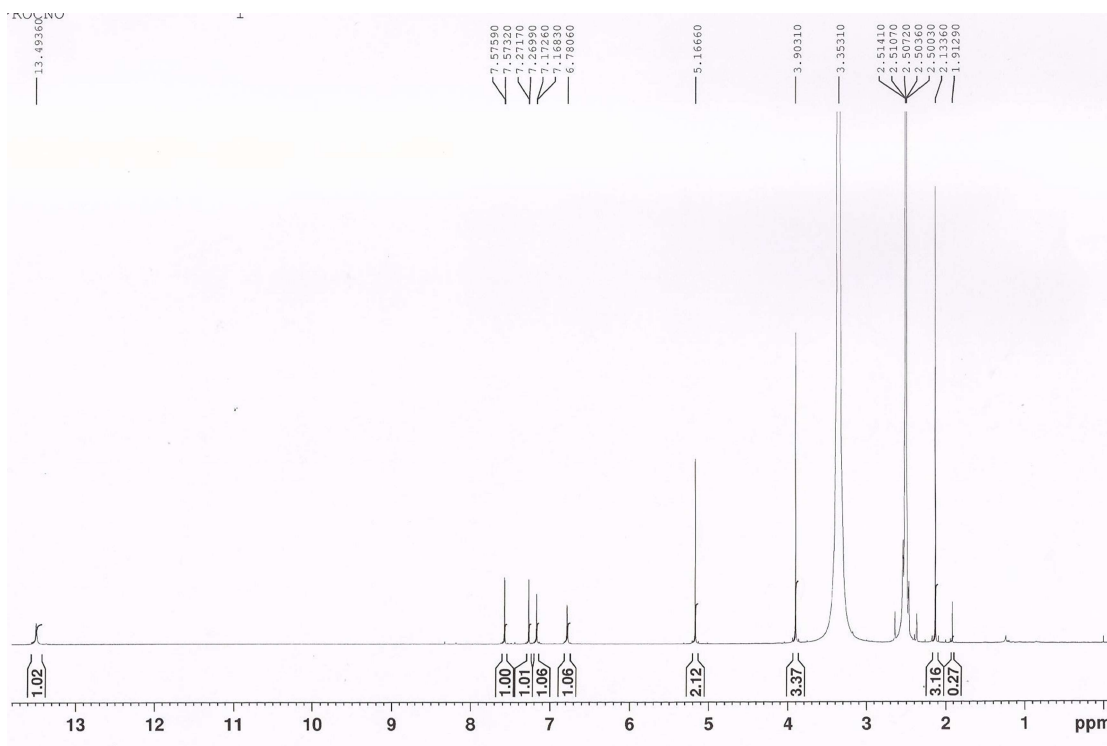


Figure S37. ^{13}C spectrum of **9** (DMSO-d_6 , 125MHz).

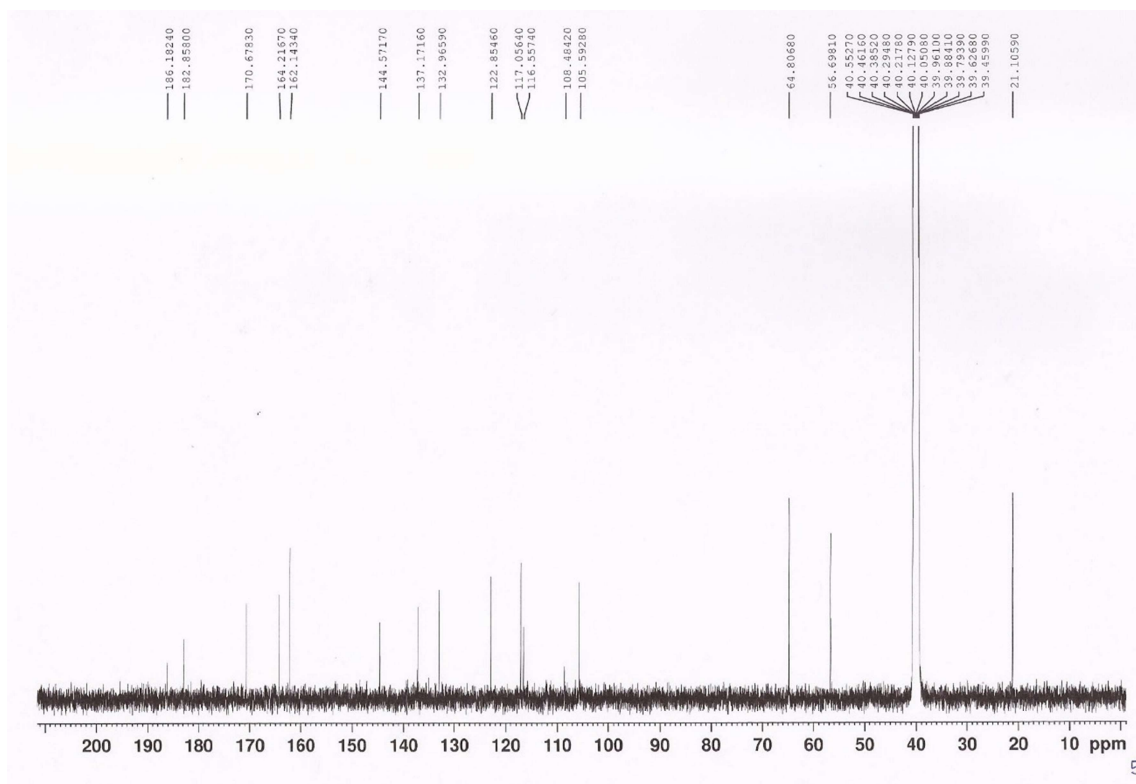


Figure S38. ^1H spectrum of **10** (DMSO-d_6 , 300 MHz).

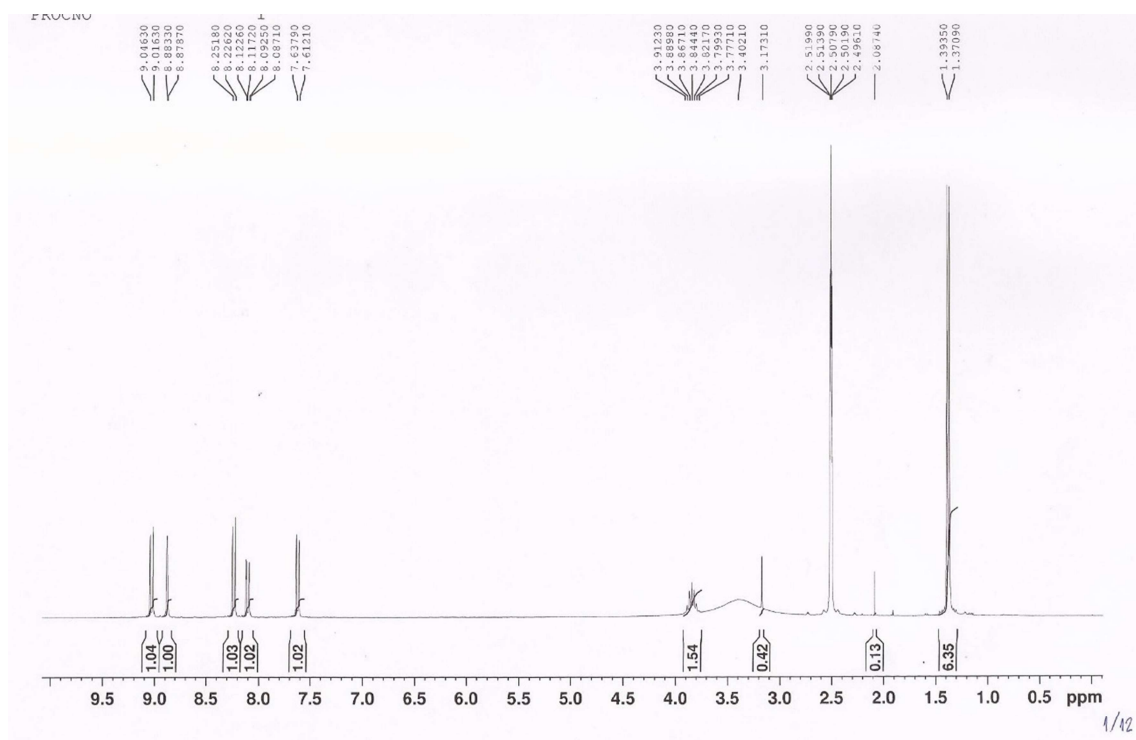


Figure S39. ^{13}C spectrum of **10** (DMSO-d_6 , 75 MHz).

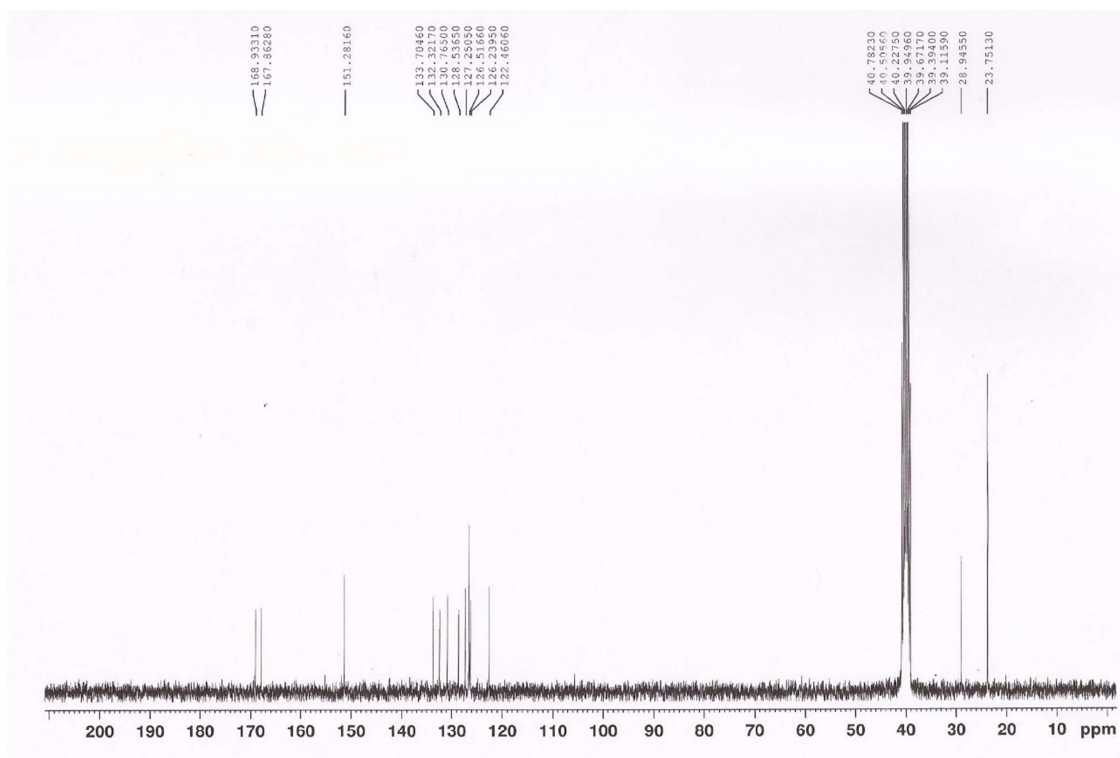


Figure S40. ¹H spectrum of **11** (DMSO-d₆, 300 MHz).

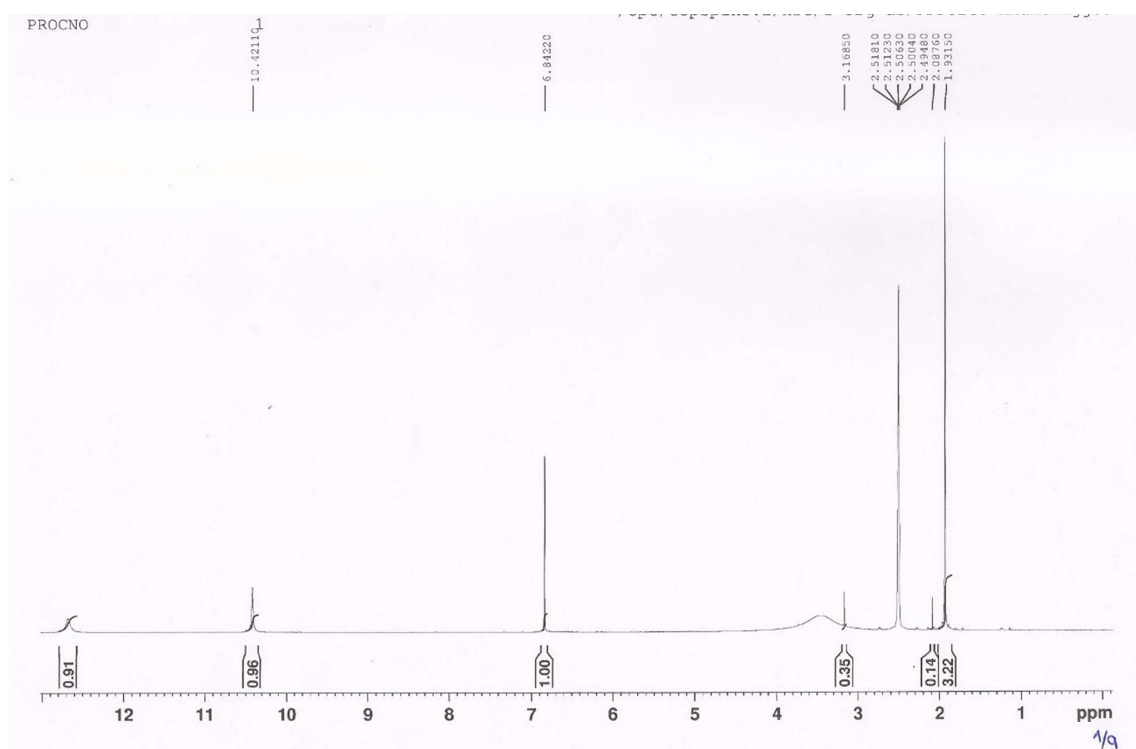


Figure S41. ^{13}C spectrum of **11** (DMSO-d_6 , 75 MHz).

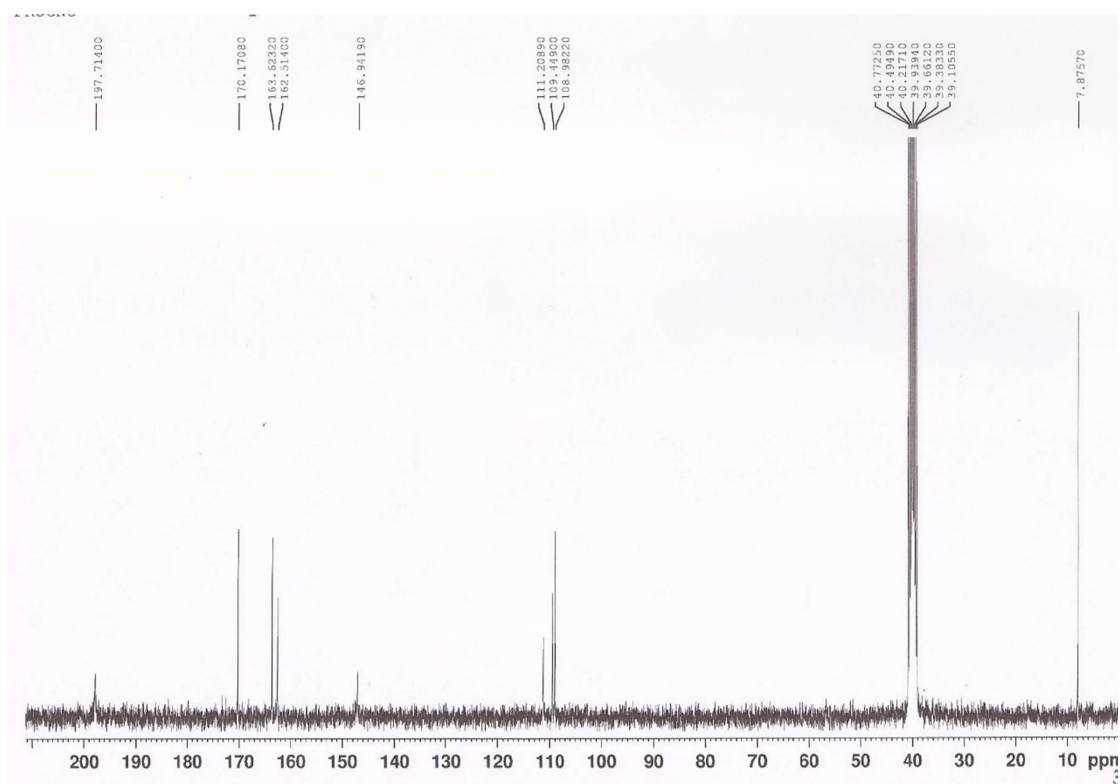


Figure S42. (+)-HRESIMS of 3

Elemental Composition Report [MH]⁺

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

30 formula(e) evaluated with 1 results within limits (up to 100 closest results for each mass)

Elements Used:

C: 27-27 H: 0-150 O: 0-30

Minimum: -1.5

Maximum: 5.0 5.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
471.1075	471.1080	-0.5	-1.1	18.5	778.2	n/a	n/a	C27 H19 O8

Elemental Composition Report [MNa]⁺

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

61 formula(e) evaluated with 1 results within limits (up to 100 closest results for each mass)

Elements Used:

C: 27-27 H: 0-150 O: 0-30 Na: 0-1

Minimum: -1.5

Maximum: 5.0 5.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
493.0895	493.0899	-0.4	-0.8	18.5	752.8	n/a	n/a	C27 H18 O8 Na

AKTP-294-336/215-248
ANAKH-G2-224 22.1 (1.955)

1: TOF MS ES+
1.21e+006

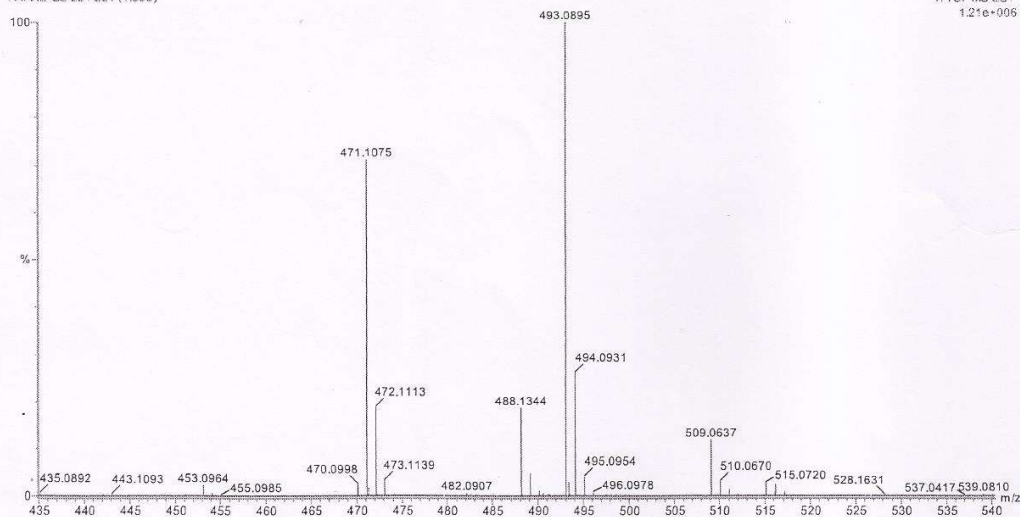


Figure S43. (+)-HRESIMS of 4

Elemental Composition Report [MH]⁺

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

27 formula(e) evaluated with 1 results within limits (up to 100 closest results for each mass)

Elements Used:

C: 21-21 H: 0-150 O: 0-30

Minimum: -1.5

Maximum: 5.0 5.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
417.1186	417.1186	0.0	0.0	11.5	514.2	n/a	n/a	C21 H21 O9

AKTP 440-456 Sep 9-11
ANAKE-G2-236 202 (1.698)

1: TOF MS ES+
7.78e+006

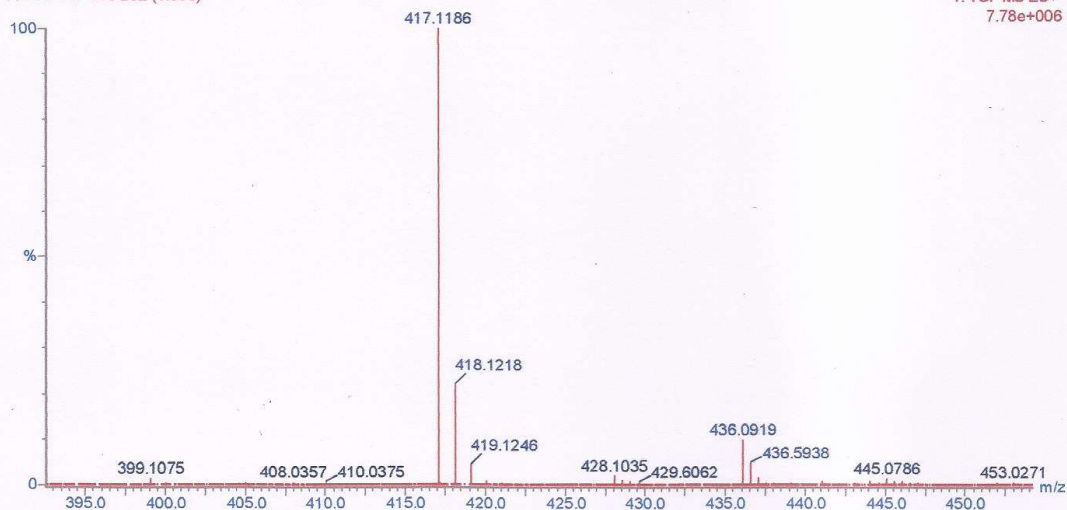


Figure S44. (+)-HRESIMS of 6

Elemental Composition Report [MH]⁺

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

25 formula(e) evaluated with 1 results within limits (up to 100 closest results for each mass)

Elements Used:

C: 19-19 H: 0-150 O: 0-30

Minimum: -1.5

Maximum: 5.0 5.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
389.0870	389.0873	-0.3	-0.8	11.5	410.3	n/a	n/a	C ₁₉ H ₁₇ O ₉

AKTP-457-500 Sep 10-12
ANAKE-G2-228 210 (1.730)

1: TOF MS ES+
5.24e+006

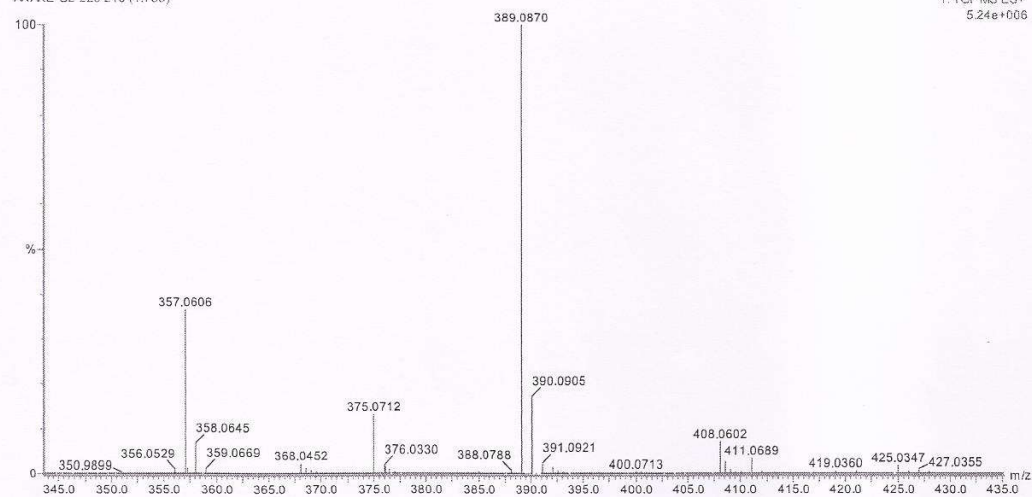


Figure S45. (+)-HRESIMS of 7.

Elemental Composition Report [MH]⁺

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

27 formula(e) evaluated with 1 results within limits (up to 100 closest results for each mass)

Elements Used:

C: 28-28 H: 0-150 O: 0-30

Minimum:

-1.5

Maximum:

5.0

5.0

100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
425.3053	425.3056	-0.3	-0.7	8.5	810.3	n/a	n/a	C28 H41 O3

Elemental Composition Report [MNa]⁺

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

55 formula(e) evaluated with 1 results within limits (up to 100 closest results for each mass)

Elements Used:

C: 28-28 H: 0-150 O: 0-30 Na: 0-1

Minimum:

-1.5

Maximum:

5.0

5.0

100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
447.2870	447.2875	-0.5	-1.1	8.5	576.6	n/a	n/a	C28 H40 O3 Na

AKTP 280-286

ANAKG-G2-223 321 (2.769)

1: TOF MS ES+
8.01e+007

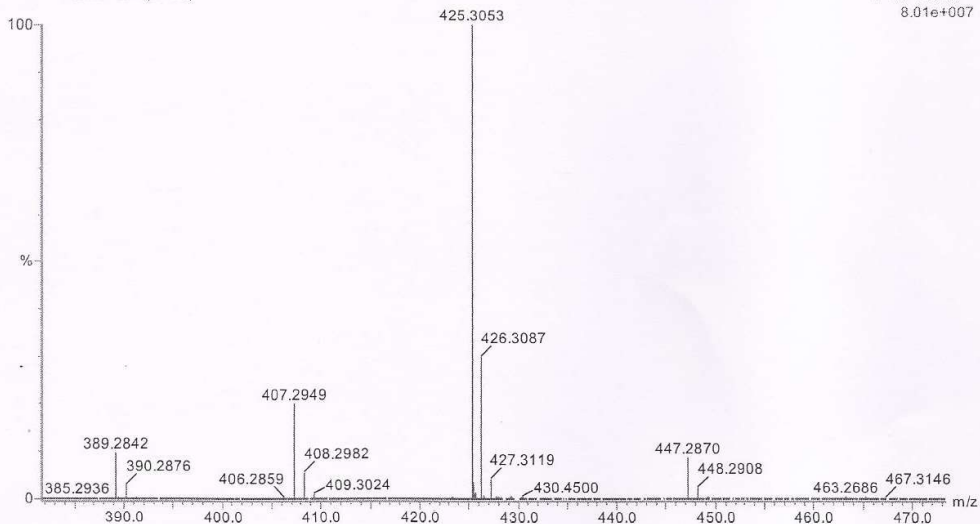


Table S1. ^1H and ^{13}C NMR data (CDCl_3 , 300 and 75 MHz), COSY and HMBC for **AKTP 93-102P** (8).

Position	δ_{C} , type	δ_{H} , (J in Hz)	COSY	HMBC
1	164.9, CO	-		
3	148.2, C	-		
4	144.7, C	-		
4a	134.5, C	-		
5	103.1, CH	6.68, d (2.3)		C-4, 6, 7, 8a
6	166.8, C	-		
7	103.2, CH	6.69, d (2.3)		C-5, 6, 8a,
8	165.3, C	-		
8a	100.8, C	-		
9	195.3, CO	-		
10a b	42.8, CH_2	2.95, dd (19.0, 6.5) 2.31, dd (19.0, 1.4)	H-10b H-10a	C-1, 4 C-1, 4
11	28.4, CH	3.44, dq (6.5, 1.4)	H-10a, 10b, 12	C-3, 4, 9
12	21.0, CH_3	1.46, d (6.9)	H-11	C-4, 10, 11
OMe-6	56.0, CH_3	3.94, s		C-6
OH-8	-	11.33, s		C-7, 8, 8a