Supporting Information

Antimicrobial sesterterpenoids with a unique 5/8/6/5 tetracyclic carbon-ring-system and diepoxide polyketides from a deep sea-sediment-sourced fungus *Chaetomium globosum* SD-347

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Table S1. Crystal Data for compound **1**

Identification code	a_a		
Empirical formula	$C_{25}H_{42}O_3$		
Formula weight	390.58		
Temperature	293(2) K		
Wavelength	1.54178 Å		
Crystal system	Orthorhombic		
Space group	$P2_12_12_1$		
Unit cell dimensions	a = 8.005 Å	□	α = 90°.
	b = 10.685 Å	□	β = 90°.
	c = 26.893 Å	□	γ = 90°.
Volume	2300.3 $Å^3$		
Z	4		
Density (calculated)	1.128 Mg/m^3		
Absorption coefficient	0.554 mm^{-1}		
F(000)	864		
Crystal size	0.180 x 0.150 x 0.120 mm^3		
Theta range for data collection	5.287 to 68.440°.		
Index ranges	-9<=h<=9, -12<=k<=12, -32<=l<=32		
Reflections collected	28454		
Independent reflections	4211 [$R(int)$ = 0.0360]		
Completeness to theta = 67.679°	99.7 %		
Refinement method	Full-matrix least-squares on F^2		
Data / restraints / parameters	4221 / 2 / 260		
Goodness-of-fit on F^2	1.066		
Final R indices [I>2$sigma$(I)]	R_1 = 0.0867, wR_2 = 0.2500		
R indices (all data)	R_1 = 0.0900, wR_2 = 0.2563		
Absolute structure parameter	0.1(5)		
Extinction coefficient	n/a		
Largest diff. peak and hole	1.061 and -0.577 $e.Å^{-3}$		

Table S2. Crystal Data for compound **2**

Identification code	a	
Empirical formula	$C_{25}H_{42}O_3$	
Formula weight	390.58	
Temperature	295(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P1	
Unit cell dimensions	a = 7.9393(3) Å □	α = 86.790(2)°.
	b = 12.0041(5) Å □	β = 89.802(2)°.
	c = 12.3904(5) Å □	γ = 73.896(2)°.
Volume	1132.65(8) $Å^3$	
Z	2	
Density (calculated)	1.145 Mg/m^3	
Absorption coefficient	0.563 mm^{-1}	
F(000)	432	
Crystal size	0.200 x 0.180 x 0.140 mm^3	
Theta range for data collection	3.839 to 68.364°.	
Index ranges	-9<=h<=9, -14<=k<=14, -14<=l<=14	
Reflections collected	14451	
Independent reflections	7466 [$R(int)$ = 0.0534]	
Completeness to theta = 67.679°	97.6 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7466 / 3 / 521	
Goodness-of-fit on F^2	1.087	
Final R indices [I>2$sigma$(I)]	R_1 = 0.0701, wR_2 = 0.2320	
R indices (all data)	R_1 = 0.0830, wR_2 = 0.2412	
Absolute structure parameter	0.05(12)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.321 and -0.214 $e.Å^{-3}$	

Table S3. Crystal Data for compounds **3** and **4**

Identification code	190225b	
Empirical formula	$C_9H_{12}O_4$	
Formula weight	184.19	
Temperature	295(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P1	
Unit cell dimensions	a = 5.5136(4) Å □	α = 78.4590(10)°.
	b = 7.5778(6) Å □	β = 82.801(2)°.
	c = 11.5822(9) Å □	γ = 77.4670(10)°.
Volume	461.13(6) $Å^3$	
Z	2	
Density (calculated)	1.327 Mg/m^3	
Absorption coefficient	0.882 mm^{-1}	
F(000)	196	
Crystal size	0.36 x 0.18 x 0.10 mm^3	
Theta range for data collection	6.08 to 65.96°.	
Index ranges	-6<=h<=5, -8<=k<=7, -13<=l<=12	
Reflections collected	2488	
Independent reflections	1855 [$R(int)$ = 0.0525]	
Completeness to theta = 67.679°	98.1 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1855 / 3 / 240	
Goodness-of-fit on F^2	1.052	
Final R indices [I>2$sigma$(I)]	R_1 = 0.0688, wR_2 = 0.1576	
R indices (all data)	R_1 = 0.1001, wR_2 = 0.1778	
Absolute structure parameter	0.0(9)	
Extinction coefficient	0.035(4)	
Largest diff. peak and hole	0.274 and -0.300 $e.Å^{-3}$	

Figure S1. ^{1}H NMR Spectrum (500 MHz) of compound **1** in $CDCl_3$

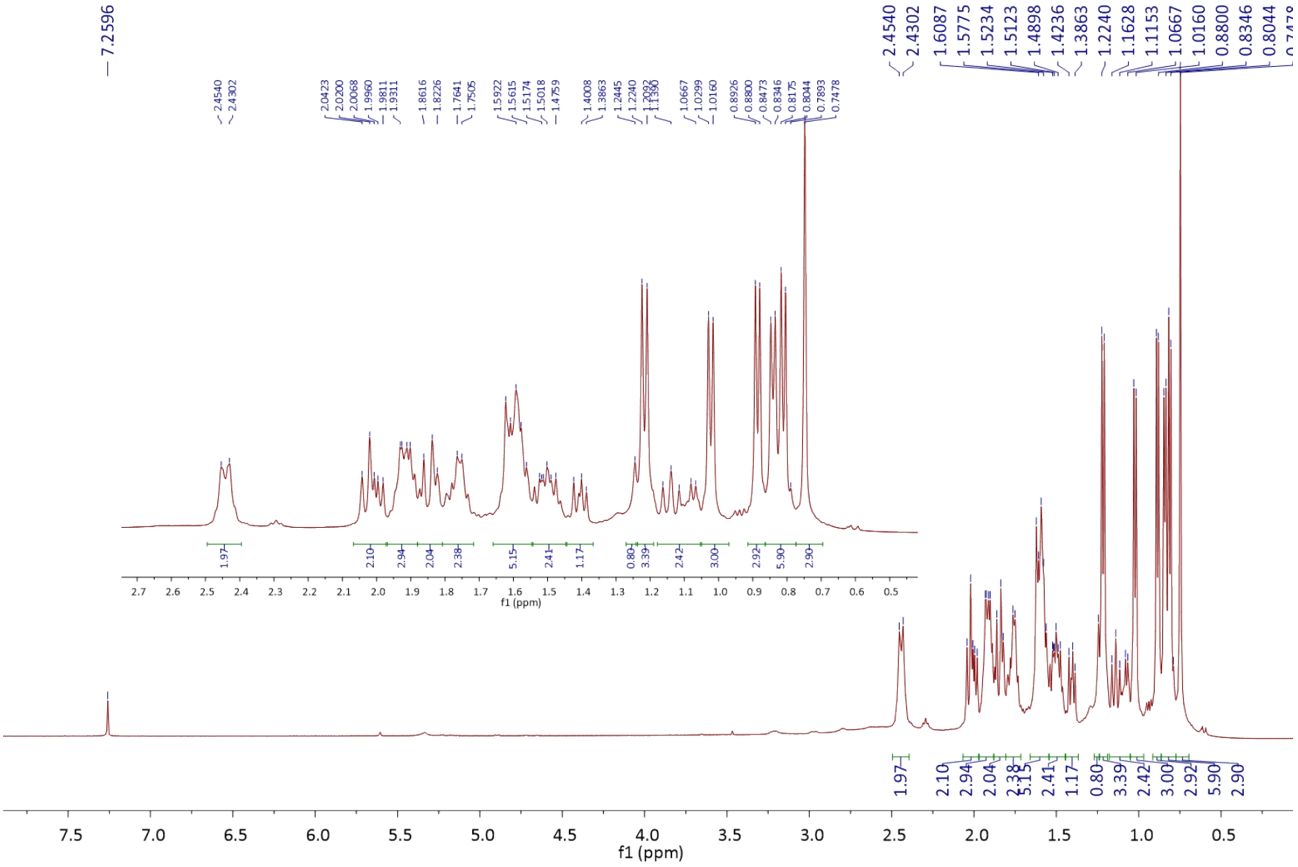

Figure S2. ^{13}C NMR Spectrum (125 MHz) of compound **1** in $CDCl_3$

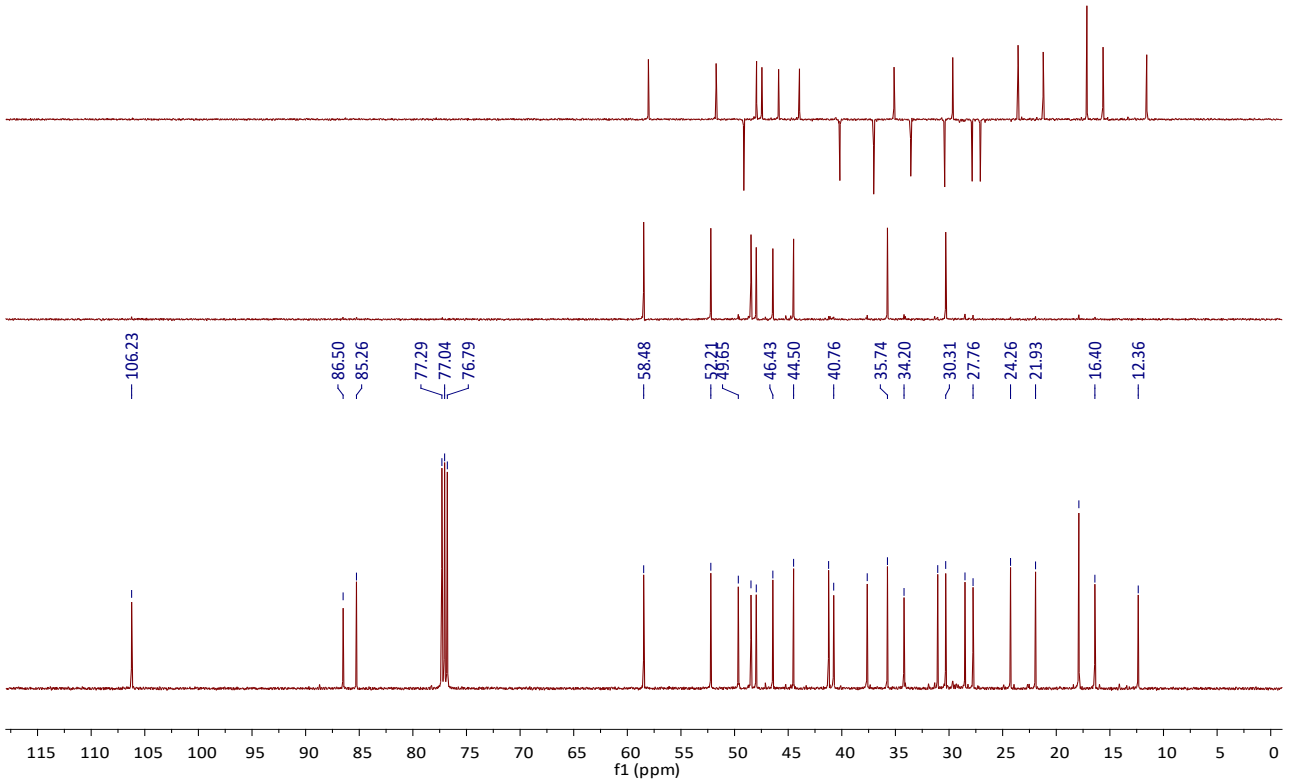

Figure S3. COSY Spectrum of compound **1** in $CDCl_3$

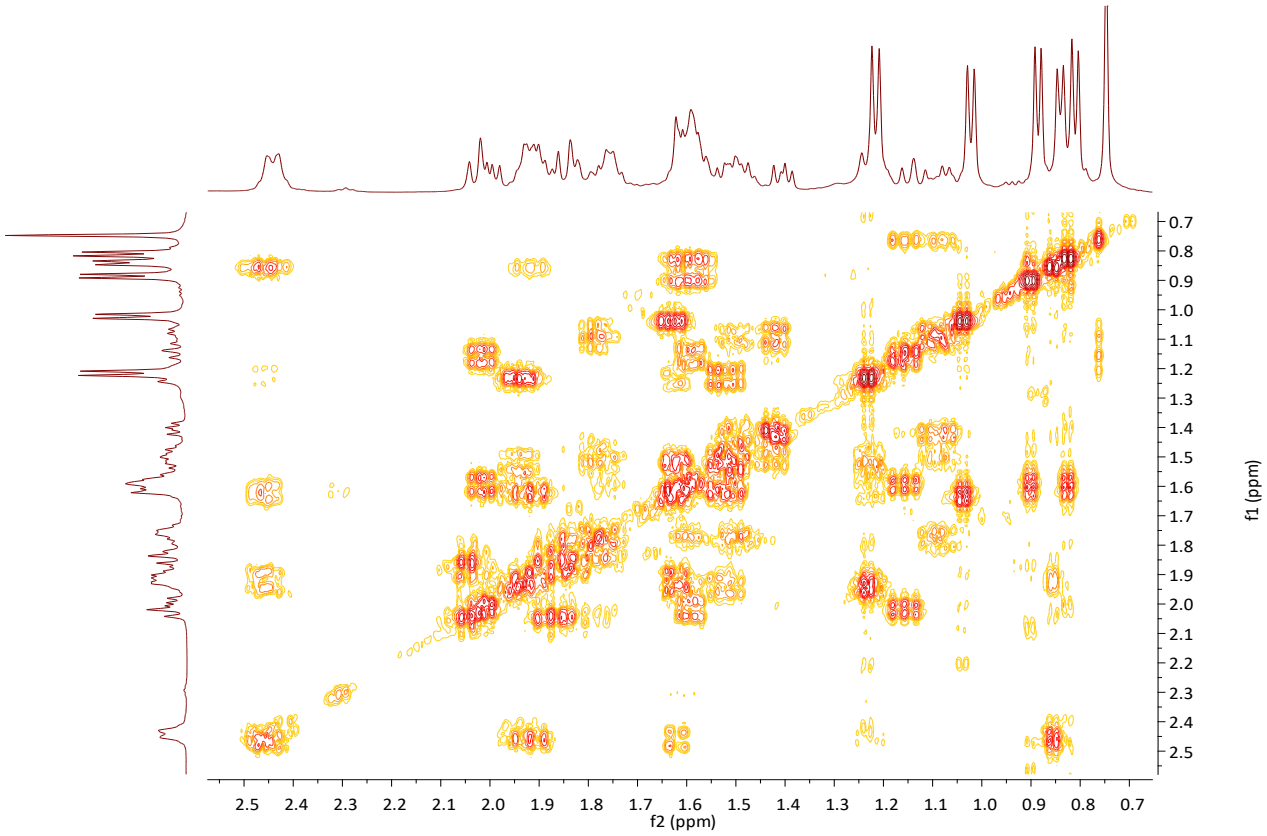

Figure S4. HSQC Spectrum of compound **1** in $CDCl_3$

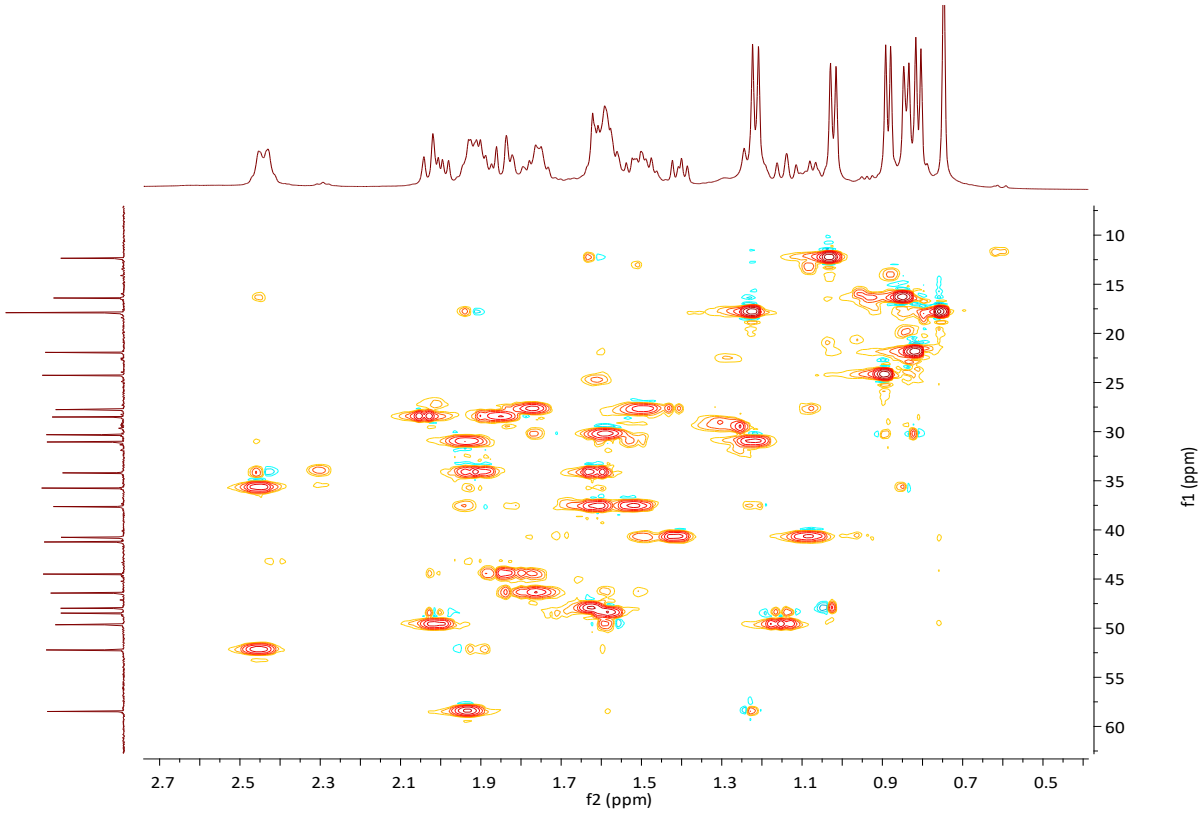

Figure S5. HMBC Spectrum of compound **1** in $CDCl_3$

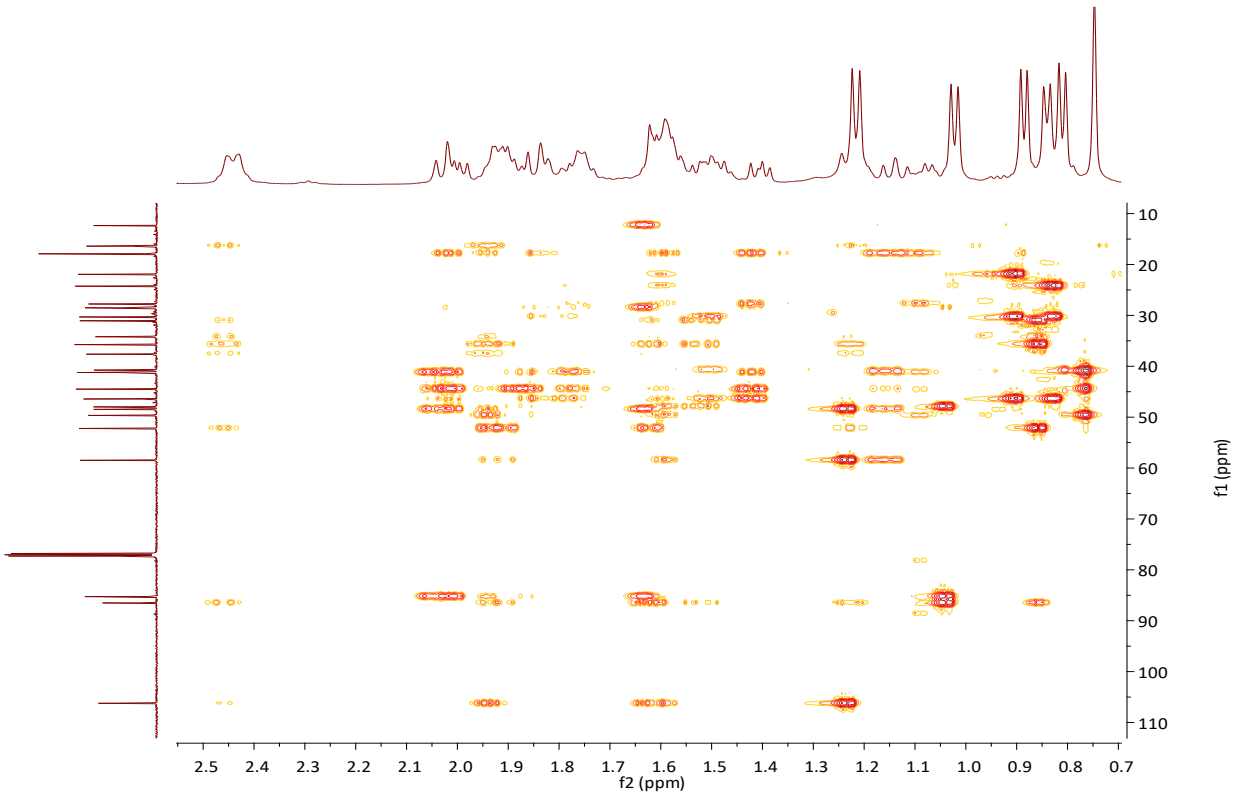

Figure S6. NOESY Spectrum of compound **1** in $CDCl_3$

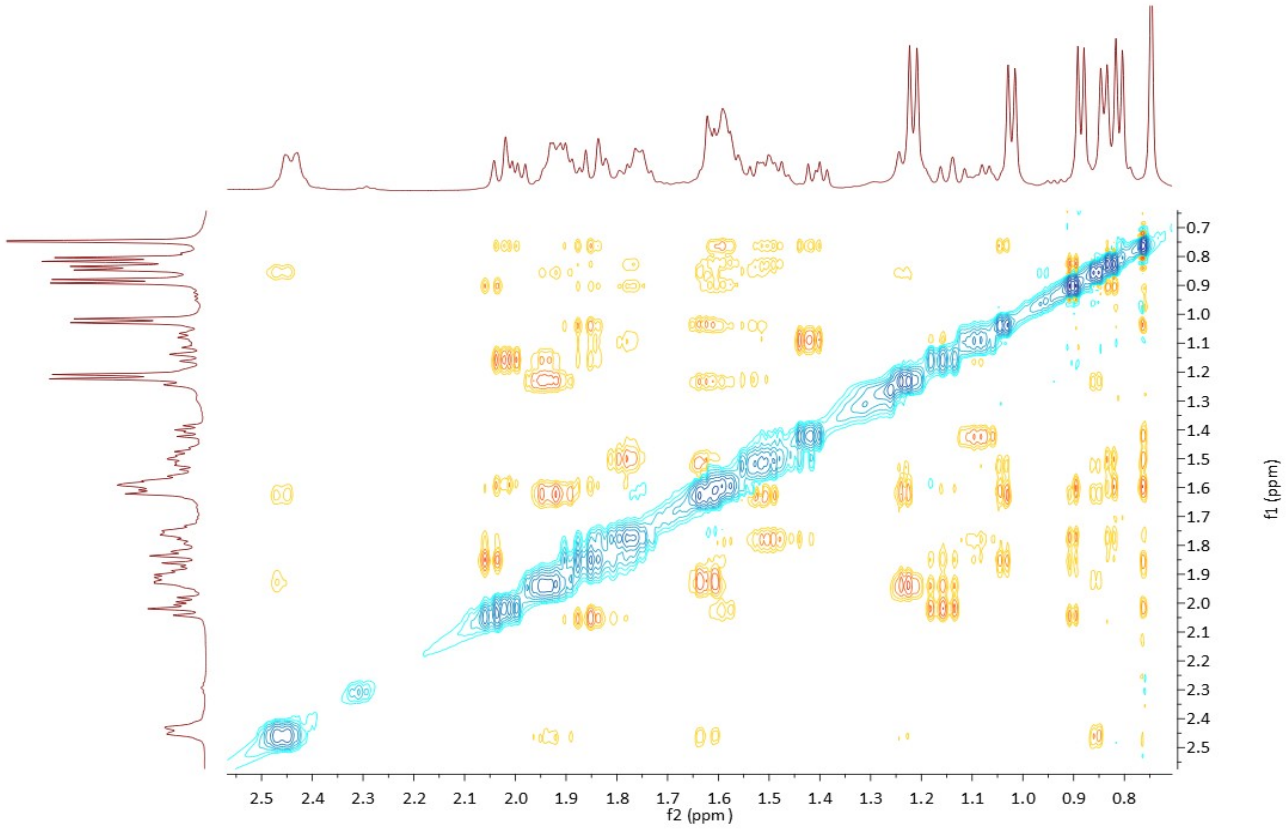

Figure S7. HRESIMS Spectrum of compound **1**

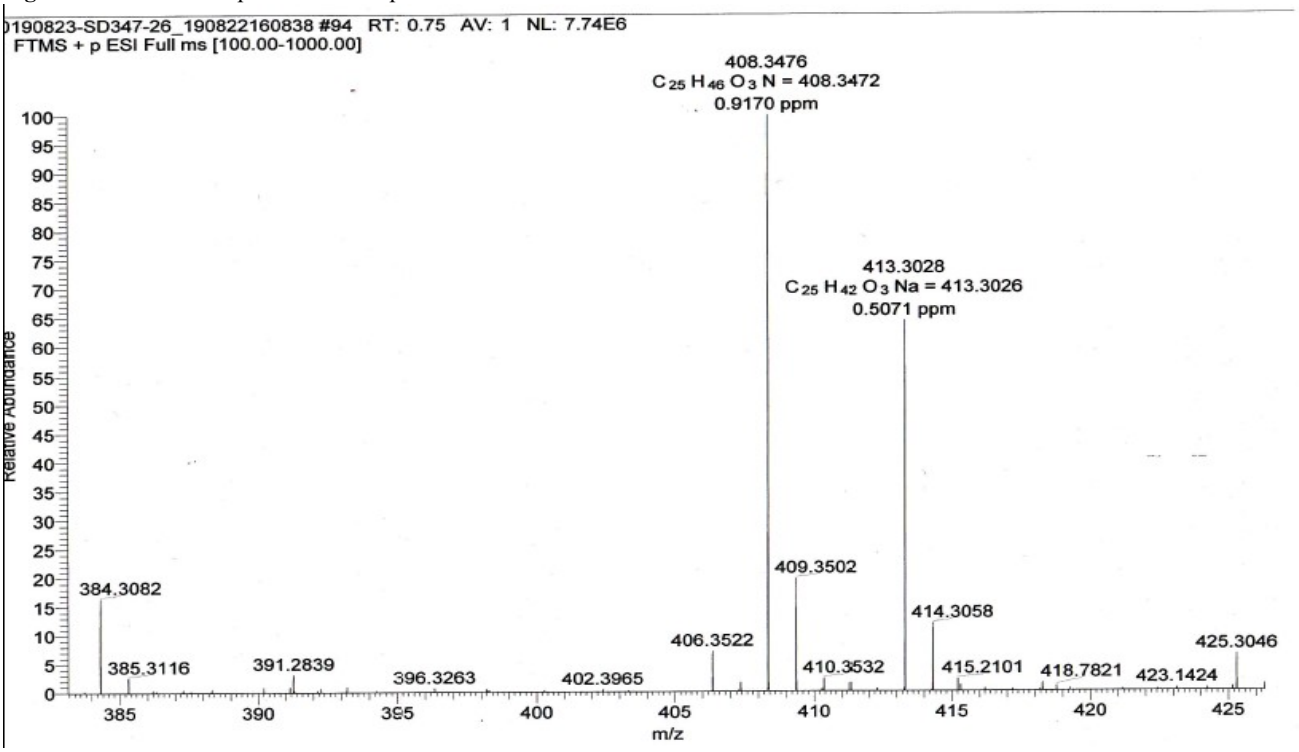

Figure S8. ^{1}H NMR Spectrum (500 MHz) of compound **2** in $CDCl_3$

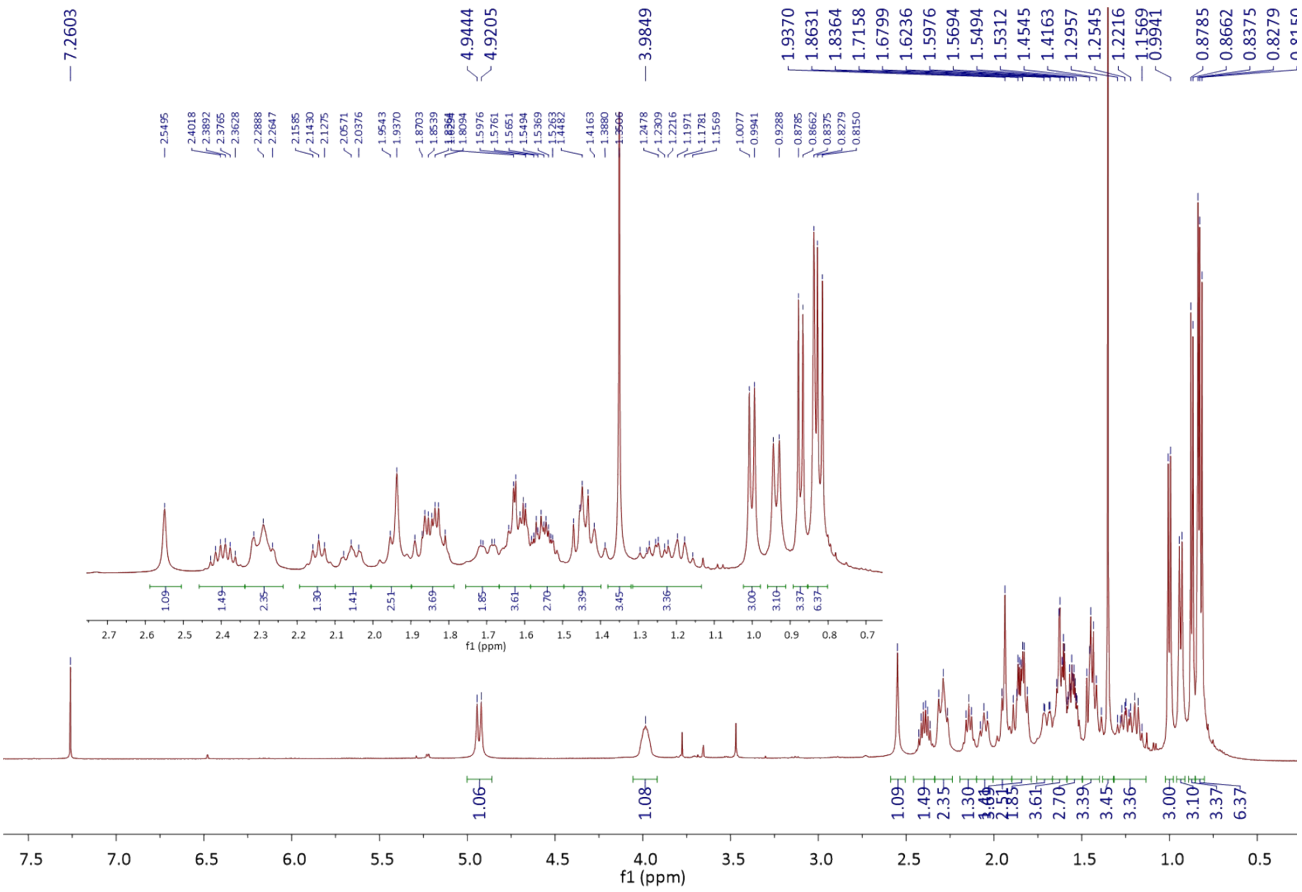

Figure S9. ^{13}C NMR Spectrum (125 MHz) of compound **2** in $CDCl_3$

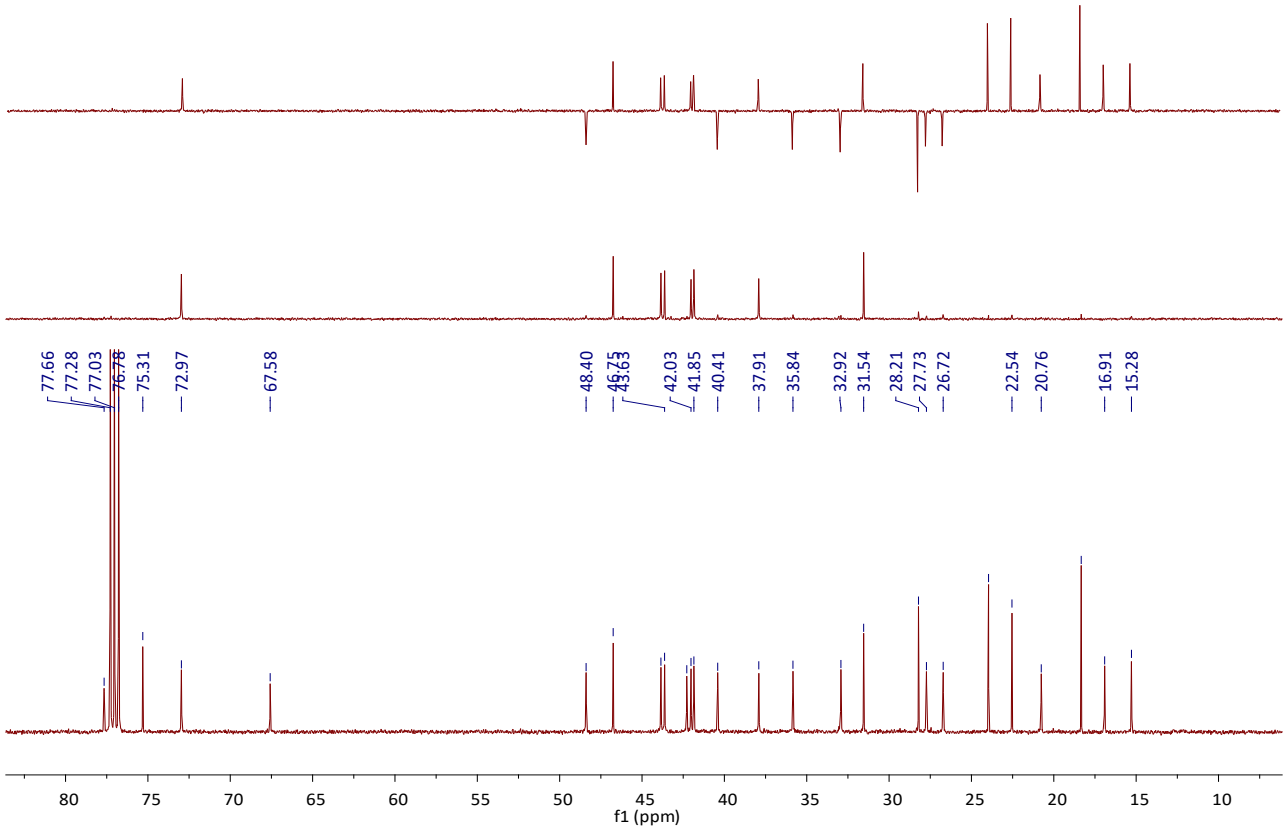

Figure S10. COSY Spectrum of compound **2** in $CDCl_3$

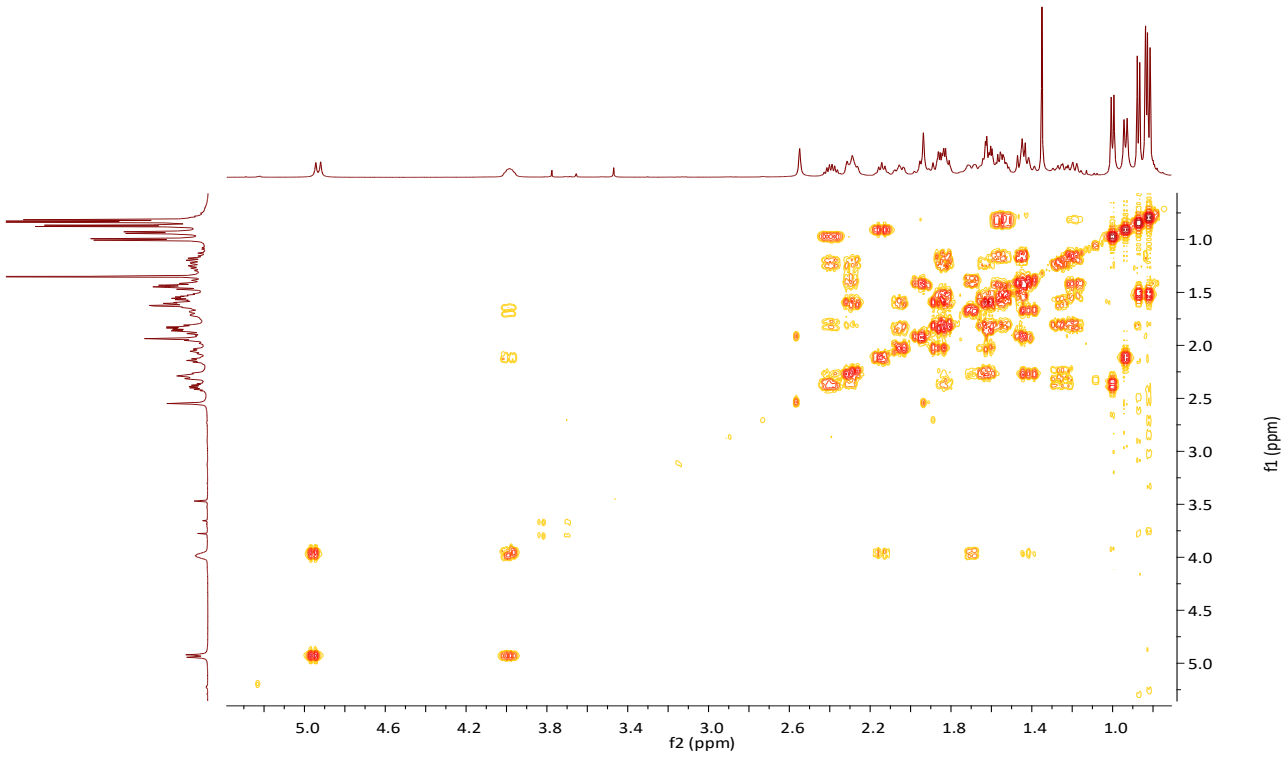

Figure S11. HSQC Spectrum of compound **2** in $CDCl_3$

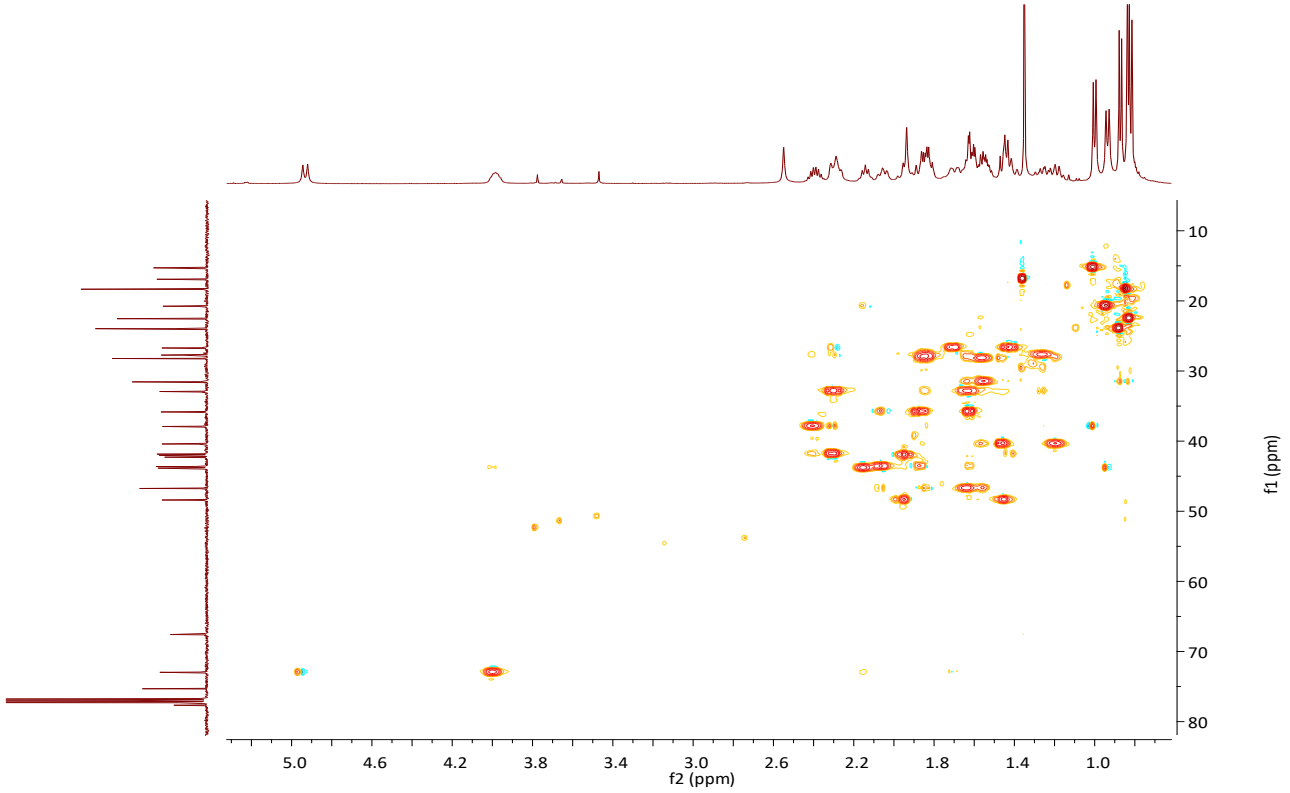

Figure S12. HMBC Spectrum of compound **2** in $CDCl_3$

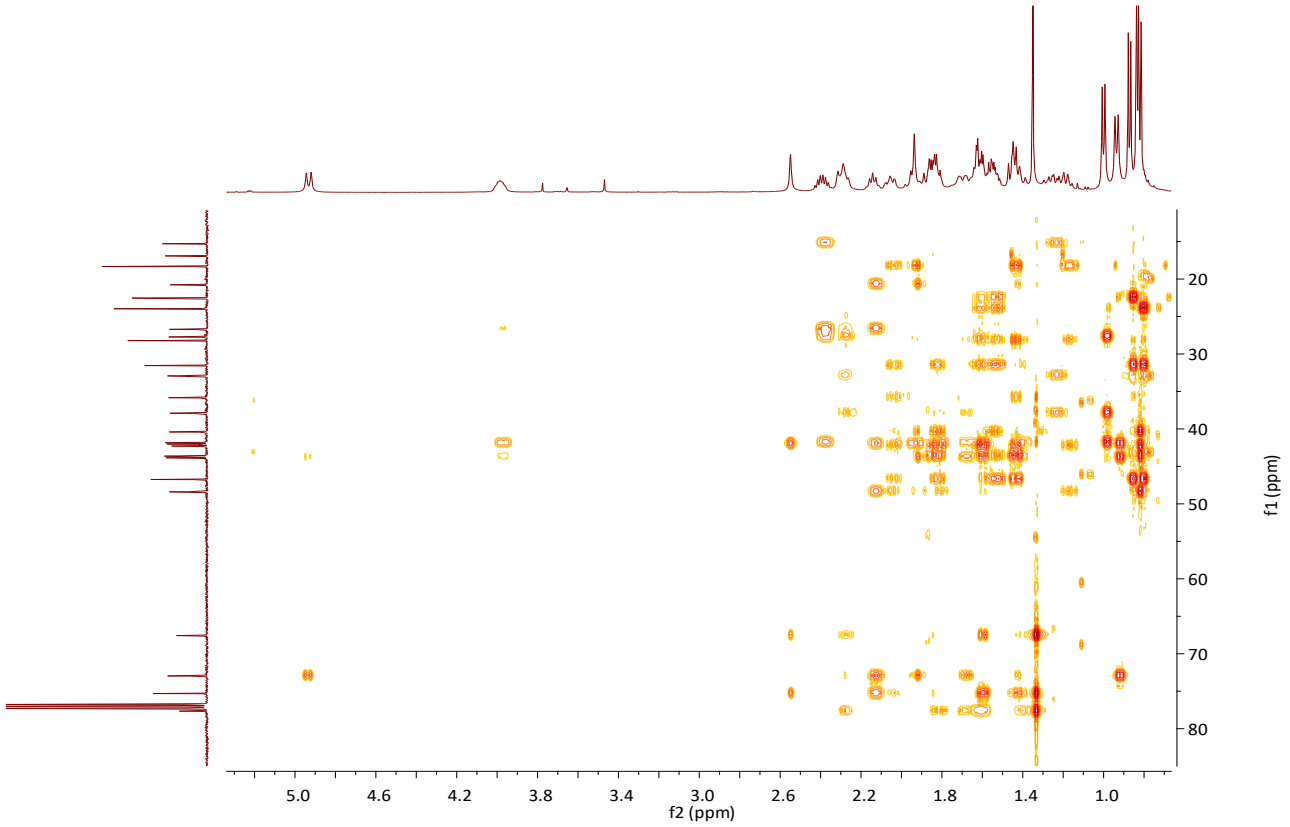

Figure S13. NOESY Spectrum of compound **2** in $CDCl_3$

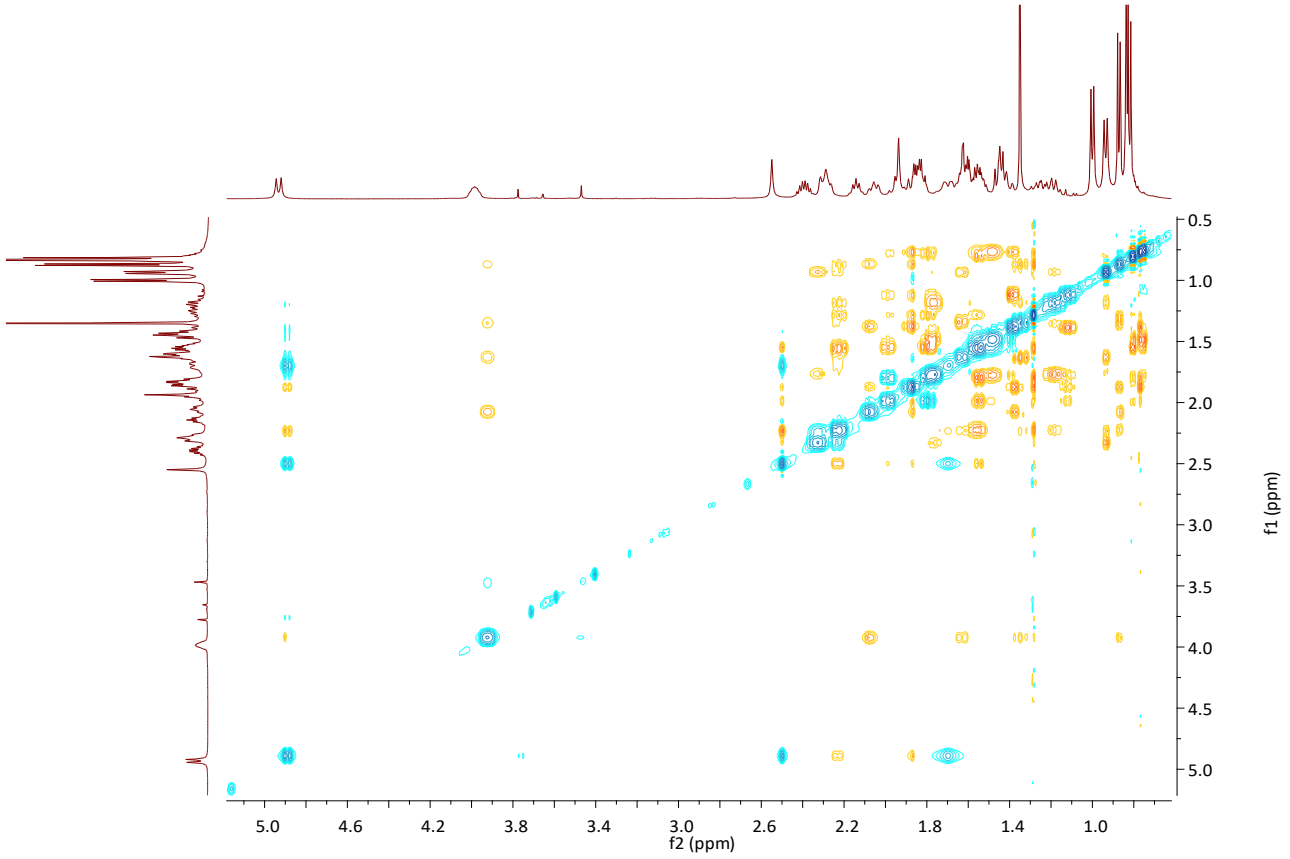

Figure S14. HRESIMS Spectrum of compound **2**

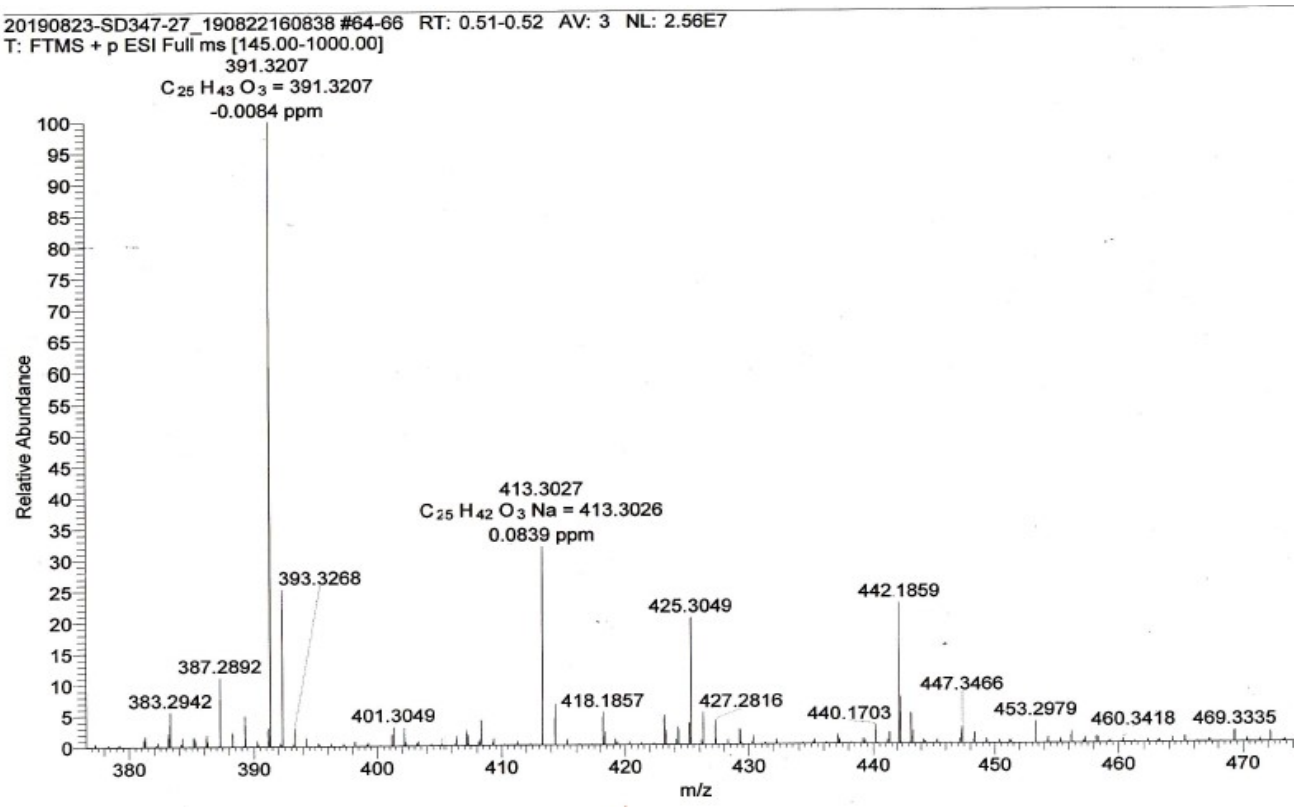

Figure S15. ^{1}H NMR Spectrum (500 MHz) of compounds **3** and **4** in DMSO-d_6

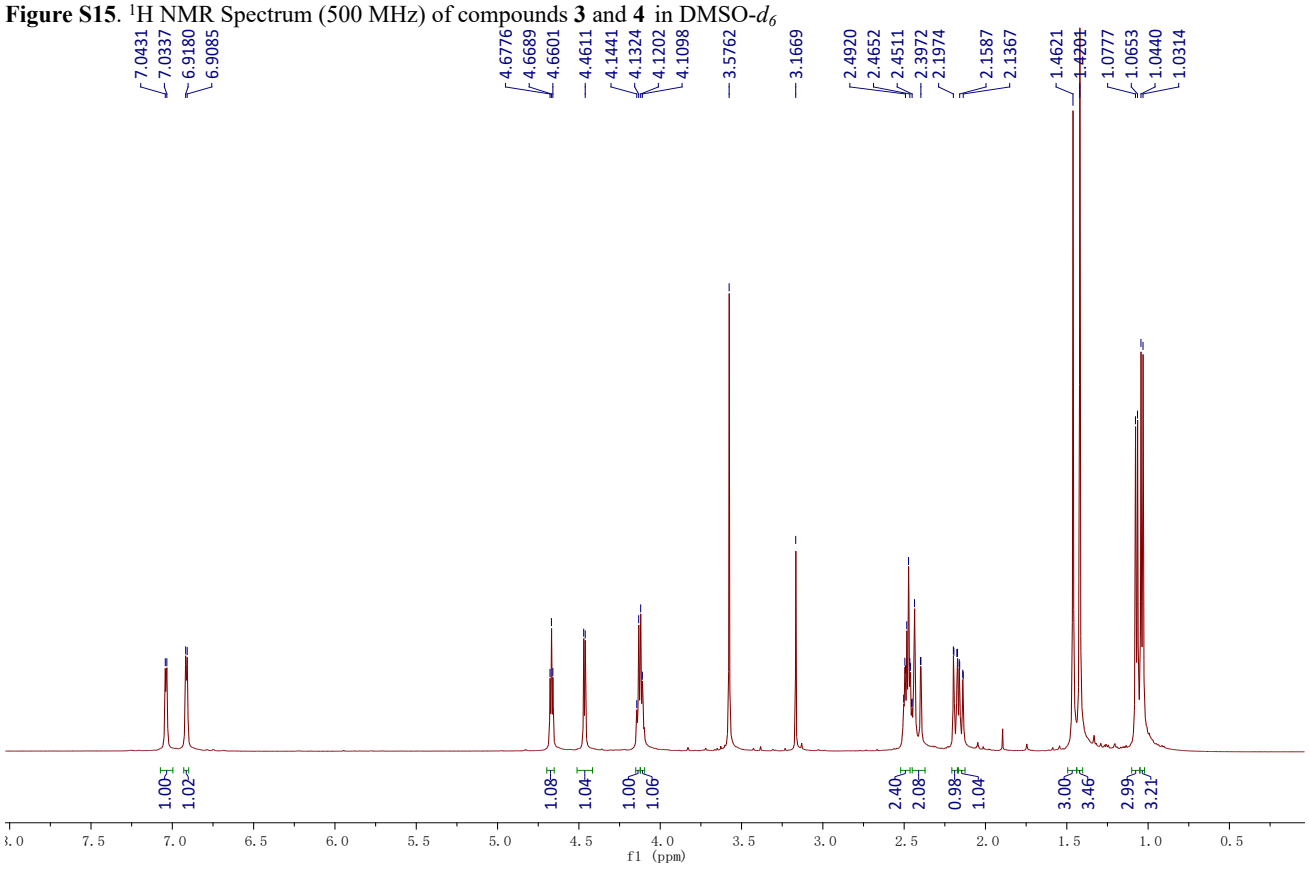

Figure S16. ^{13}C NMR Spectrum (125 MHz) of compounds **3** and **4** in DMSO-d_6

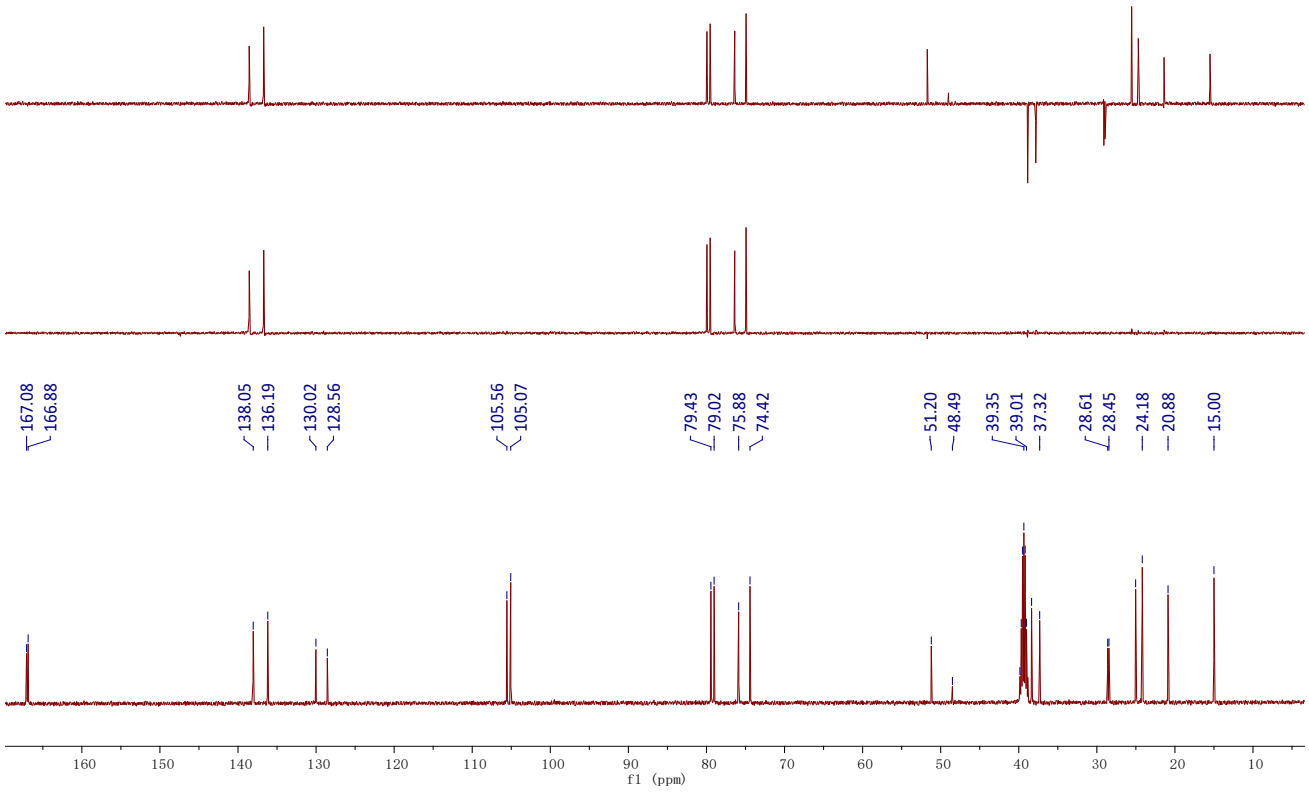

Figure S17. COSY Spectrum of compounds **3** and **4** in DMSO-d_6

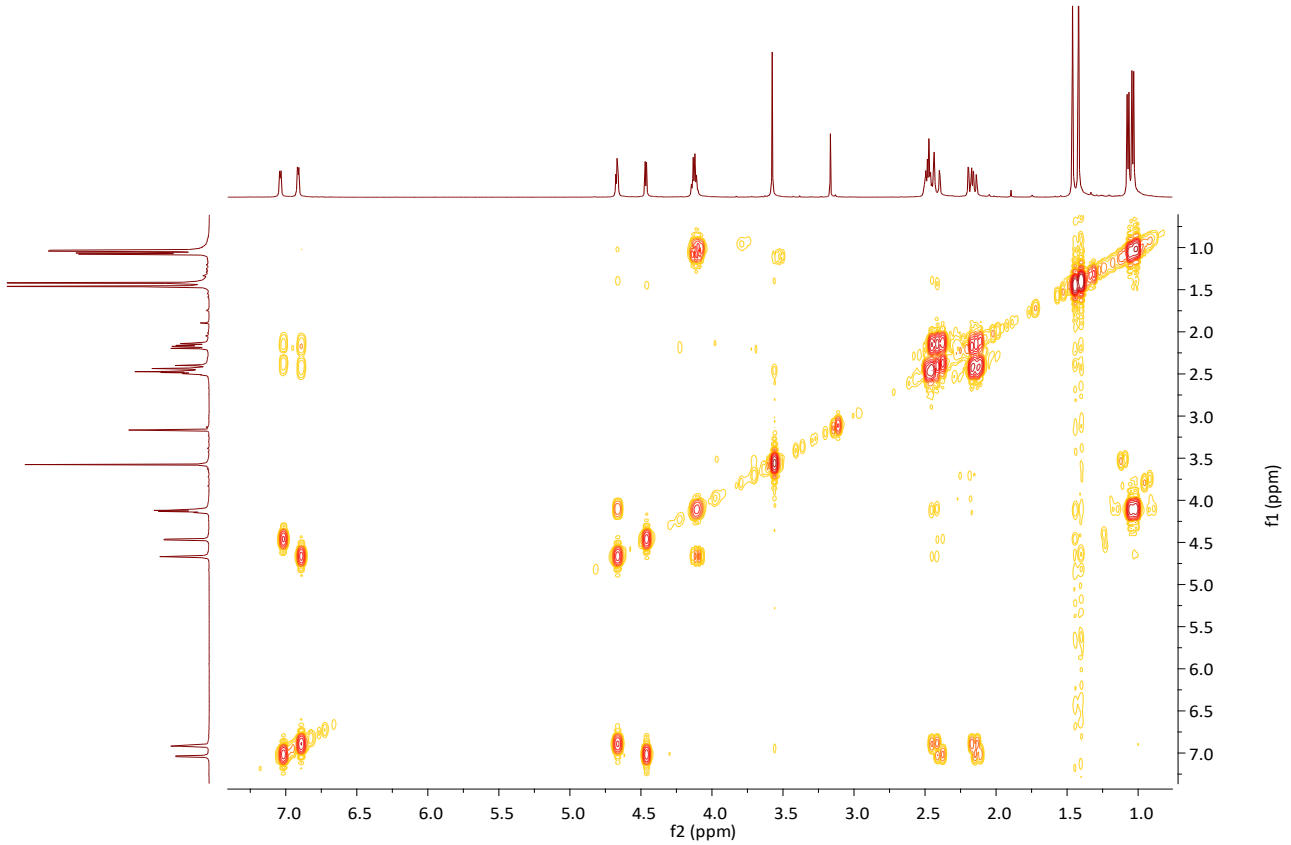

Figure S18. HSQC Spectrum of compounds **3** and **4** in DMSO-d_6

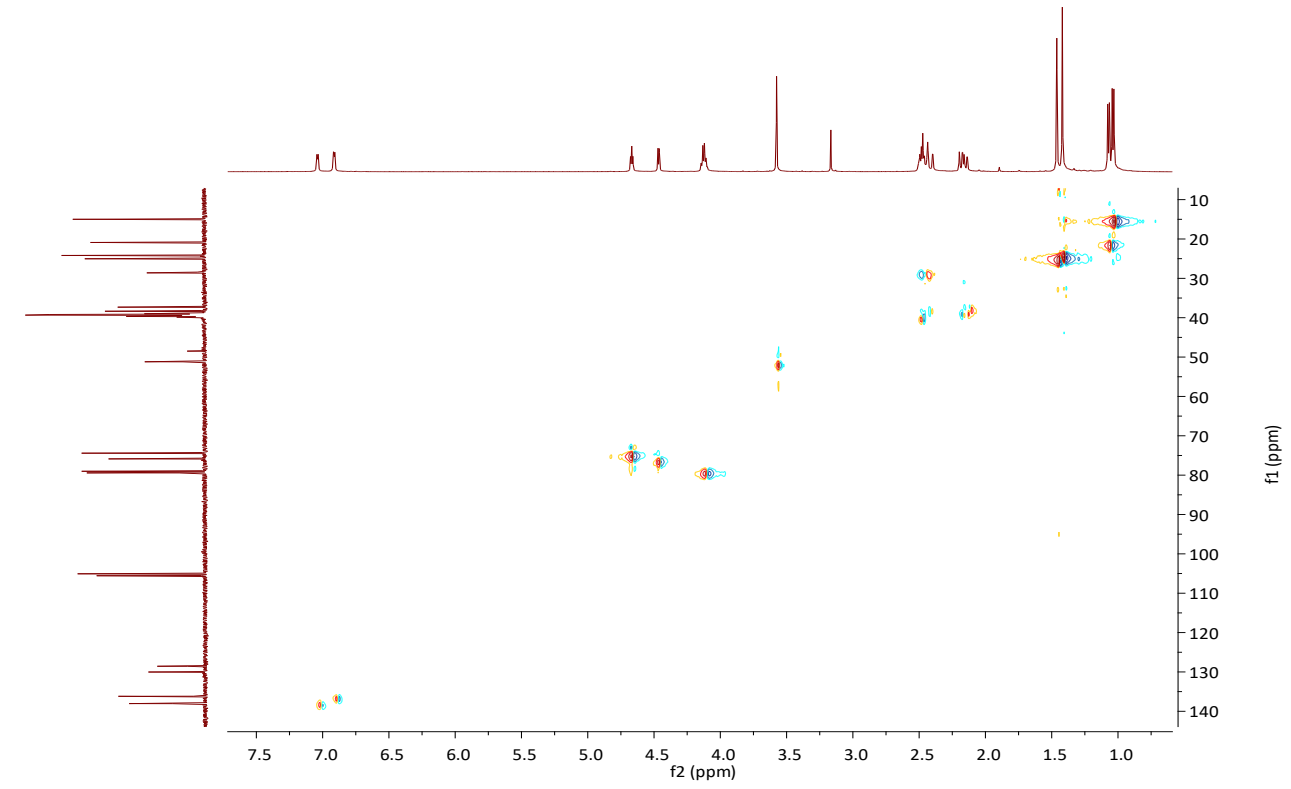

Figure S19. HMBC Spectrum of compounds **3** and **4** in DMSO-d_6

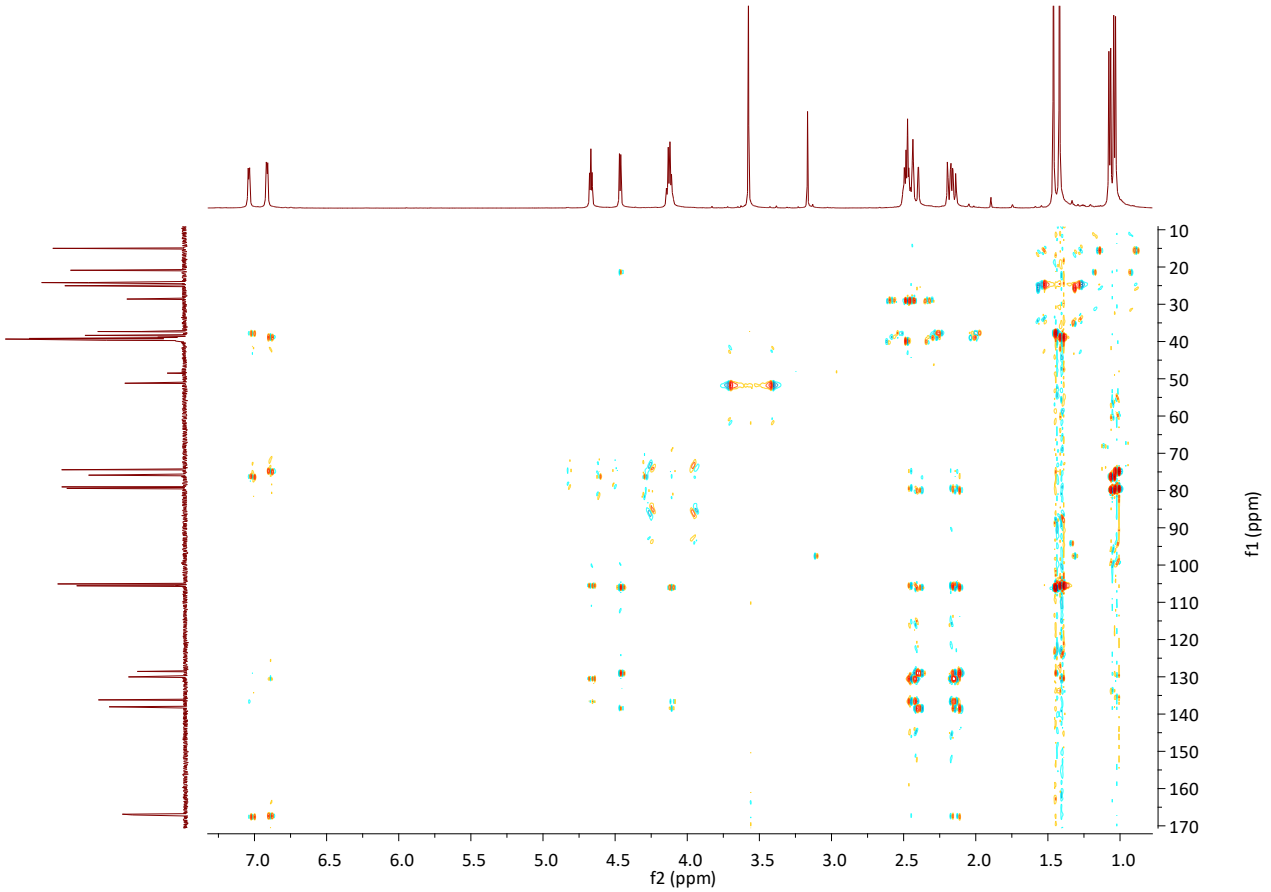

Figure S20. NOESY Spectrum of compounds **3** and **4** in DMSO-d_6

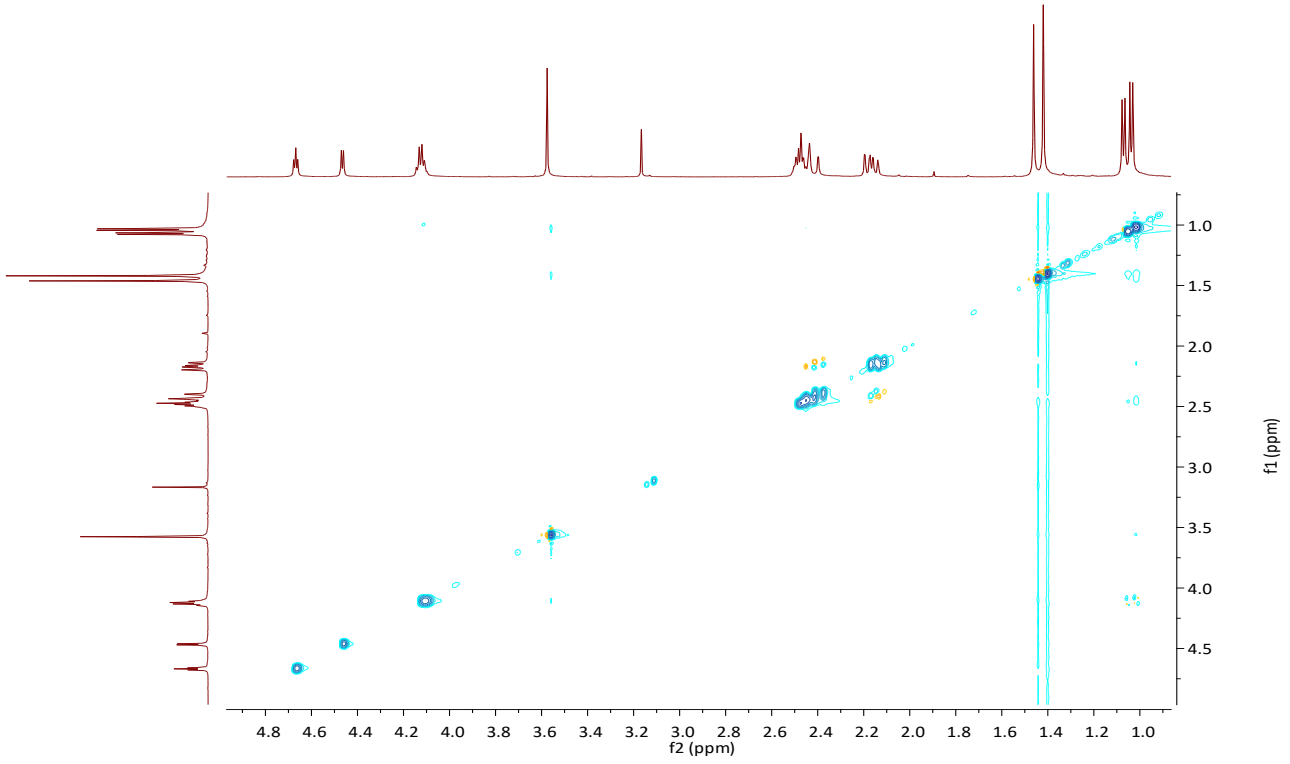

Figure S20. HRESIMS Spectrum of compounds **3** and **4**