Cucurbalsaminones A–C, Rearranged Triterpenoids with a 5/6/3/6/5-Fused Pentacyclic Carbon Skeleton from *Momordica balsamina* as Multidrug Resistance Reversers

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X-ray Crystallography

Table S1. Crystal data and structure refinement details for **1** (CCDC 1878164).

Formula	$C_{27}H_{40}O_3$
Fw	412.59
Crystal form, color	Block, colourless
Crystal size (mm)	0.20×0.10×0.04
cryst. syst.	Orthorhombic
space group	$P2_12_12_1$
a, Å	6.1959(4)
b, Å	14.0177(8)
c, Å	26.2372(16)
Z	4
V, Å^3	2278.8(2)
T, K	150(2)
D_c, g cm^{-3}	1.203
μ(Mo Kα), mm^{-1}	0.076
θ range (°)	2.745–26.436
refl. Collected	26968
independent refl.	4682
R_{int}	0.0813
R_1 [a], wR_2 [b] [$I \geq 2\sigma(I)$]	0.0496, 0.1140
GOF on F^2	1.013

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR_2 = [\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]]^{1/2}$

Table S2. Bond lengths [Å] and angles [°] for compound **1.**

O(2)-C(7)	1.214(4)	C(12)-C(13)-C(18)	110.1(2)	C(3)-C(5)-C(4)	119.9(3)
O(3)-C(23)	1.194(4)	C(12)-C(13)-C(17)	117.5(2)	C(6)-C(5)-C(4)	59.2(2)
C(13)-C(12)	1.524(4)	C(18)-C(13)-C(17)	108.1(2)	C(10)-C(5)-C(4)	123.3(3)
C(13)-C(18)	1.544(4)	C(12)-C(13)-C(14)	107.1(2)	C(19)-C(9)-C(11)	106.8(2)
C(13)-C(17)	1.558(4)	C(18)-C(13)-C(14)	112.2(2)	C(19)-C(9)-C(10)	108.6(2)
C(13)-C(14)	1.571(4)	C(17)-C(13)-C(14)	101.6(2)	C(11)-C(9)-C(10)	109.7(3)
C(8)-C(7)	1.532(4)	C(7)-C(8)-C(14)	111.6(2)	C(19)-C(9)-C(8)	106.9(3)
C(8)-C(14)	1.560(4)	C(7)-C(8)-C(9)	114.5(2)	C(11)-C(9)-C(8)	113.2(2)
C(8)-C(9)	1.584(4)	C(14)-C(8)-C(9)	117.1(2)	C(10)-C(9)-C(8)	111.5(2)
C(17)-C(20)	1.534(4)	C(20)-C(17)-C(13)	119.5(2)	O(3)-C(23)-C(24)	121.5(3)
C(17)-C(16)	1.571(4)	C(20)-C(17)-C(16)	112.0(2)	O(3)-C(23)-C(22)	121.8(3)
C(20)-C(21)	1.521(4)	C(13)-C(17)-C(16)	102.7(2)	C(24)-C(23)-C(22)	116.6(3)
C(20)-C(22)	1.535(4)	C(21)-C(20)-C(17)	114.3(2)	C(15)-C(16)-C(17)	107.5(2)
C(7)-C(6)	1.493(4)	C(21)-C(20)-C(22)	108.5(3)	C(2)-C(1)-C(10)	107.6(3)
C(10)-C(5)	1.522(4)	C(17)-C(20)-C(22)	108.3(2)	C(14)-C(15)-C(16)	103.9(2)
C(10)-C(1)	1.558(4)	O(2)-C(7)-C(6)	118.2(3)	C(12)-C(11)-C(9)	118.9(2)
C(10)-C(9)	1.565(4)	O(2)-C(7)-C(8)	120.8(3)	C(23)-C(22)-C(20)	114.6(3)
C(12)-C(11)	1.528(4)	C(6)-C(7)-C(8)	120.8(3)	C(3)-C(2)-C(1)	106.1(3)
C(6)-C(5)	1.506(4)	C(5)-C(10)-C(1)	102.9(2)	O(1)-C(3)-C(5)	126.1(3)
C(6)-C(4)	1.508(4)	C(5)-C(10)-C(9)	110.9(3)	O(1)-C(3)-C(2)	125.1(3)
C(14)-C(30)	1.536(4)	C(1)-C(10)-C(9)	115.3(2)	C(5)-C(3)-C(2)	108.8(3)
C(14)-C(15)	1.537(4)	C(13)-C(12)-C(11)	110.9(3)	C(29)-C(4)-C(6)	122.8(3)
C(5)-C(3)	1.486(4)	C(7)-C(6)-C(5)	118.4(3)	C(29)-C(4)-C(28)	111.8(3)
C(5)-C(4)	1.548(4)	C(7)-C(6)-C(4)	124.3(3)	C(6)-C(4)-C(28)	115.1(3)
C(9)-C(19)	1.543(4)	C(5)-C(6)-C(4)	61.8(2)	C(29)-C(4)-C(5)	120.2(3)
C(9)-C(11)	1.557(4)	C(30)-C(14)-C(15)	106.7(2)	C(6)-C(4)-C(5)	59.0(2)
C(23)-C(24)	1.494(5)	C(30)-C(14)-C(8)	110.2(2)	C(28)-C(4)-C(5)	118.7(3)
C(23)-C(22)	1.504(5)	C(15)-C(14)-C(8)	116.0(2)		
C(16)-C(15)	1.543(5)	C(30)-C(14)-C(13)	112.8(2)		
C(1)-C(2)	1.537(5)	C(15)-C(14)-C(13)	101.2(2)		
O(1)-C(3)	1.211(4)	C(8)-C(14)-C(13)	109.9(2)		
C(2)-C(3)	1.501(5)	C(3)-C(5)-C(6)	120.2(3)		
C(28)-C(4)	1.519(4)	C(3)-C(5)-C(10)	108.9(3)		
C(29)-C(4)	1.507(5)	C(6)-C(5)-C(10)	117.9(2)		

Table S3. Antiproliferative activity of compounds **1 - 3** on *ABCB1*-transfected mouse T-lymphoma (L5178Y) cells.

compound	**PAR[a] ID_{50} (μM)**	**MDR[a] ID_{50} (μM)**
cucurbalsaminone A (**1**)	72.2 ± 1.3	68.3 ± 2.1
cucurbalsaminone B (**2**)	> 100	> 100
cucurbalsaminone C (**3**)	20.7 ± 2.7	37.6 ± 3.9

[a] Values represent the mean ± SD of three independent experiments

HRMS, IR and NMR spectra of compounds 1-3

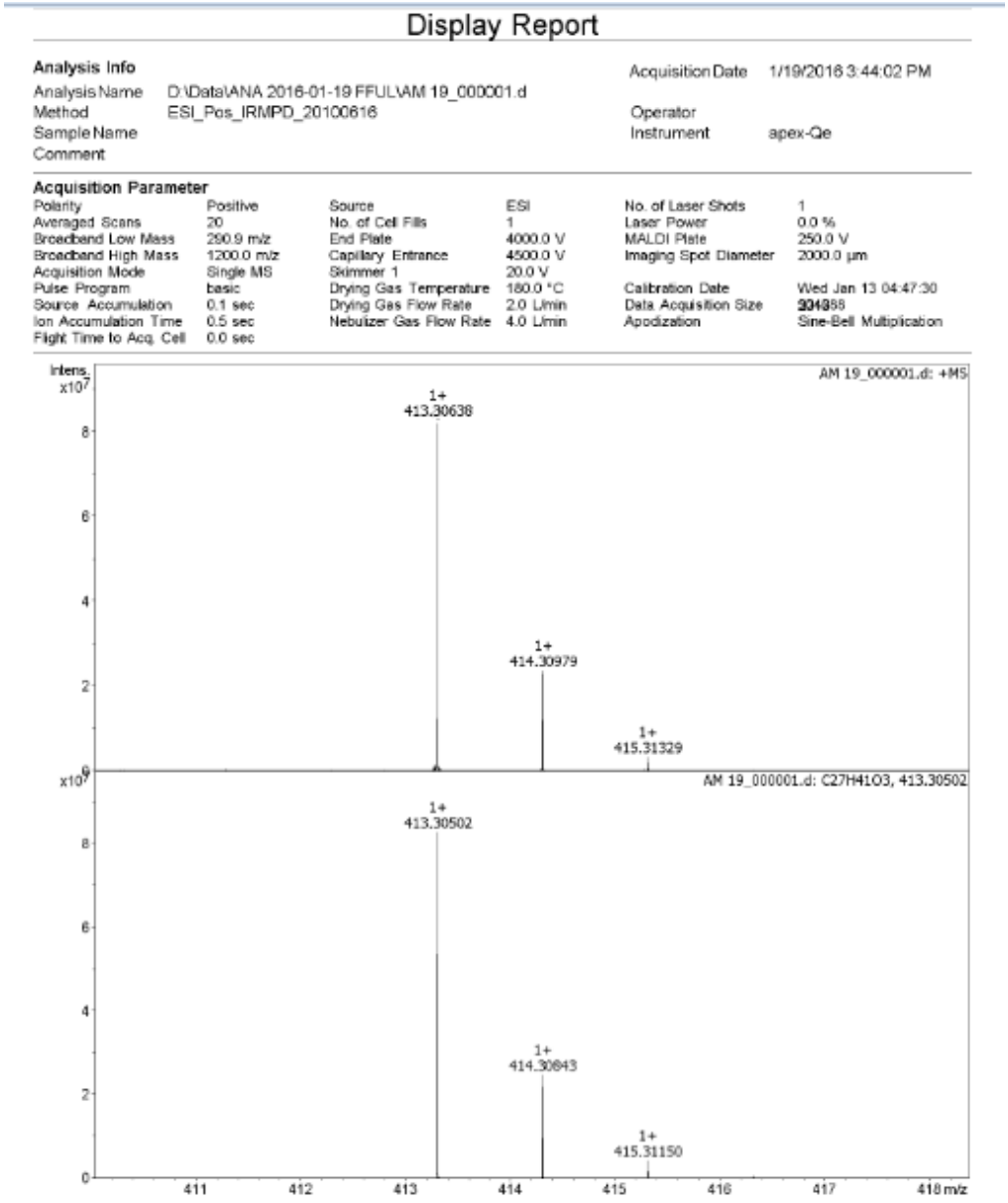

Figure S1. HRMS of compound **1**.

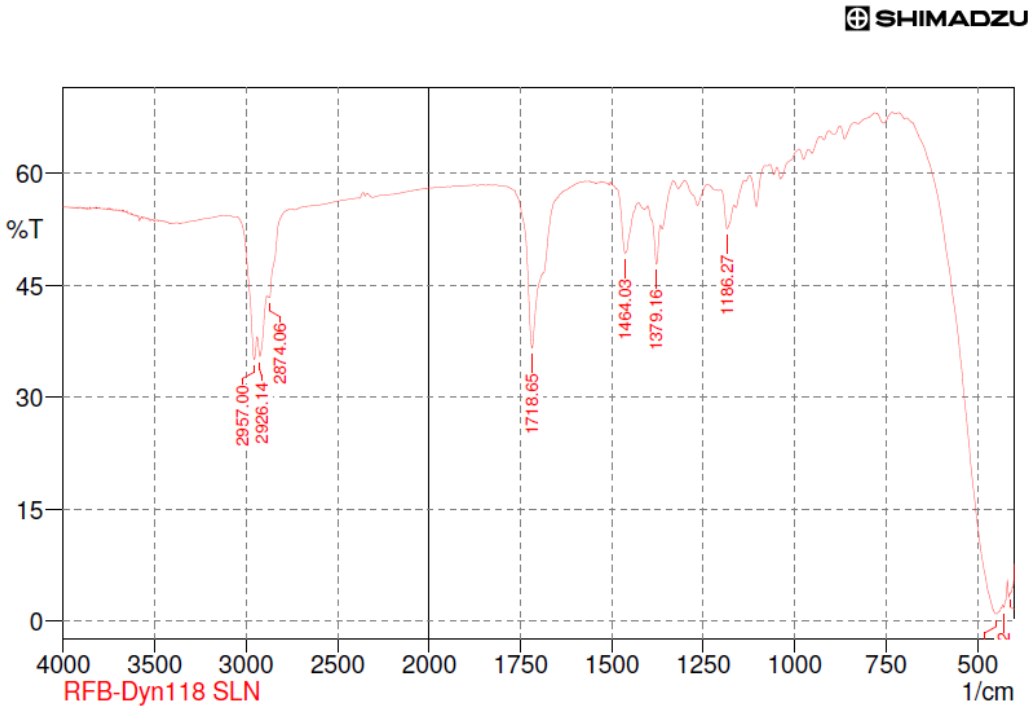

Figure S2. IR of compound **1**.

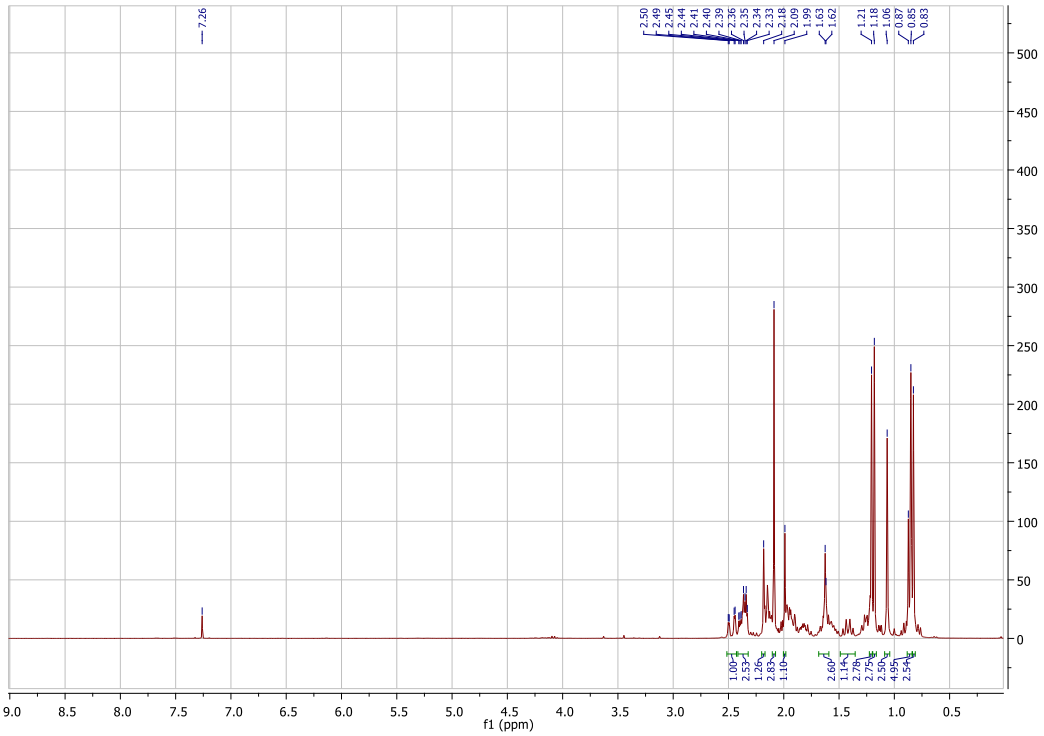

Figure S3. ^{1}H-NMR spectrum of compound **1**, in $CDCl_3$ (300 MHz).

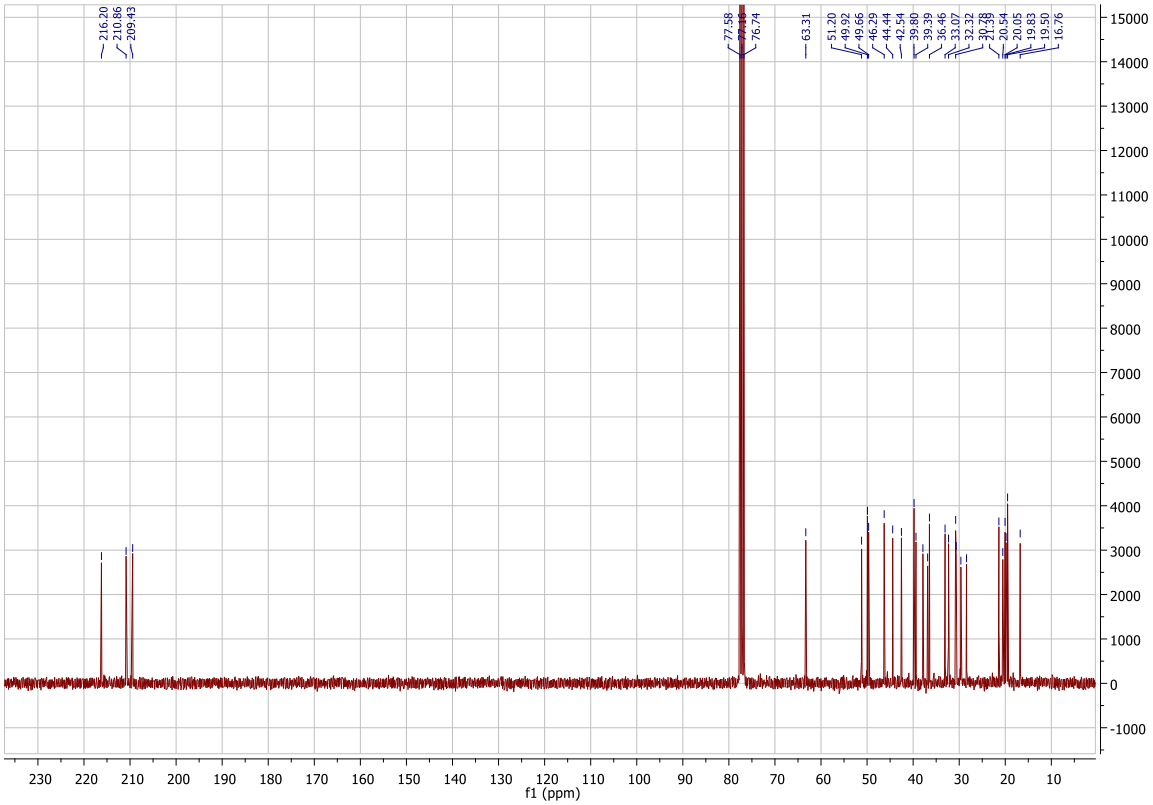

Figure S4. ^{13}C-NMR spectrum of compound **1**, in $CDCl_3$ (75 MHz).

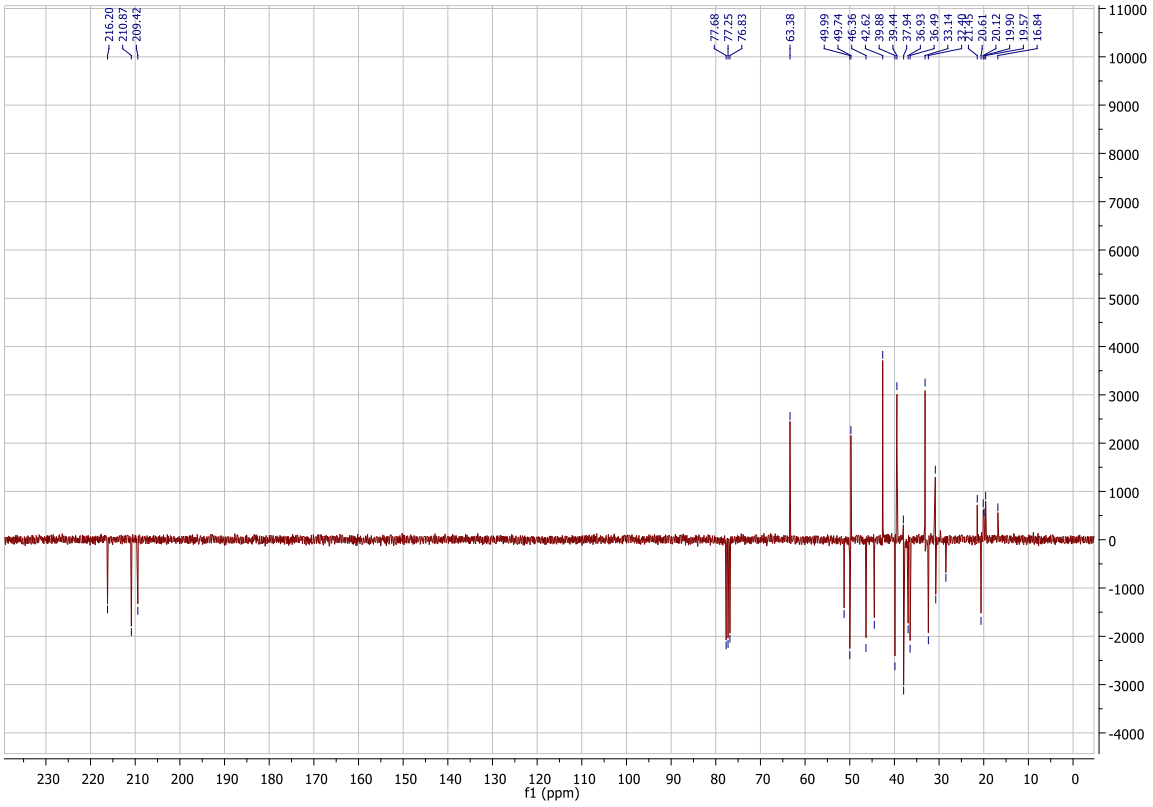

Figure S5. DEPT spectrum of compound **1** in $CDCl_3$ (75 MHz).

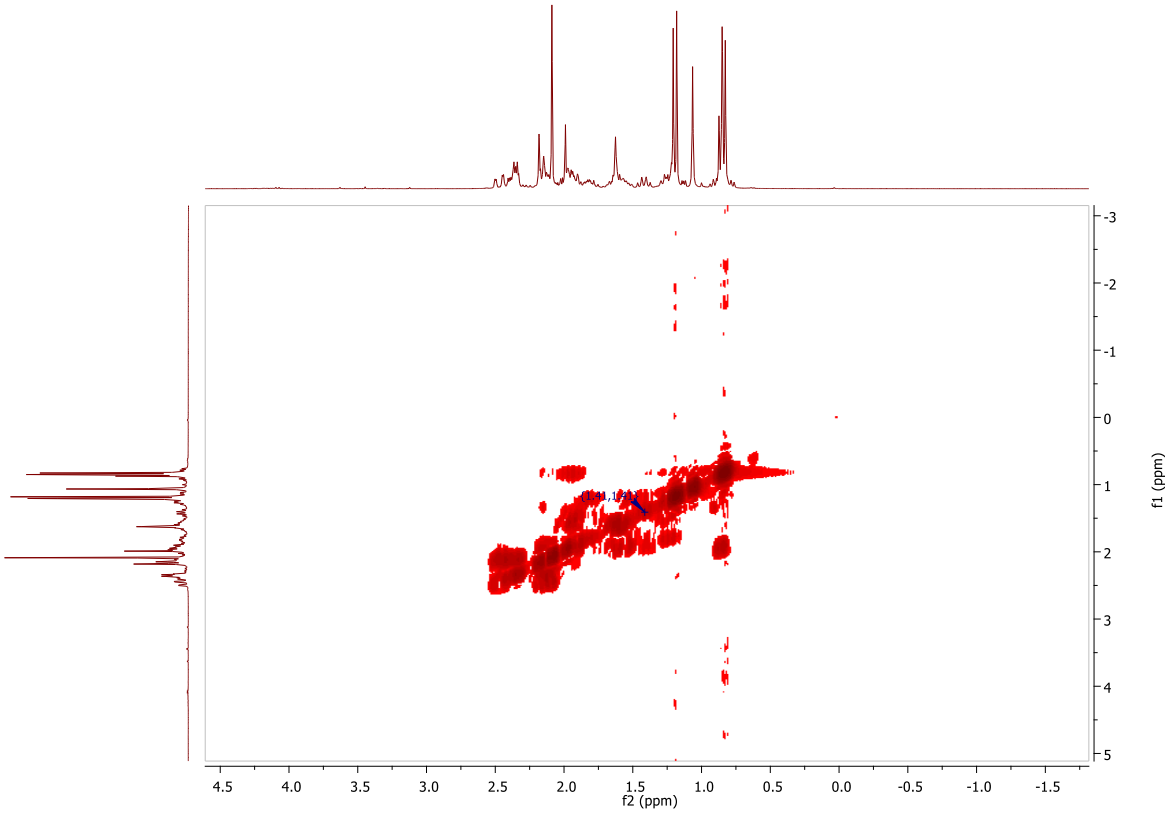

Figure S6. COSY spectrum of compound **1** in $CDCl_3$.

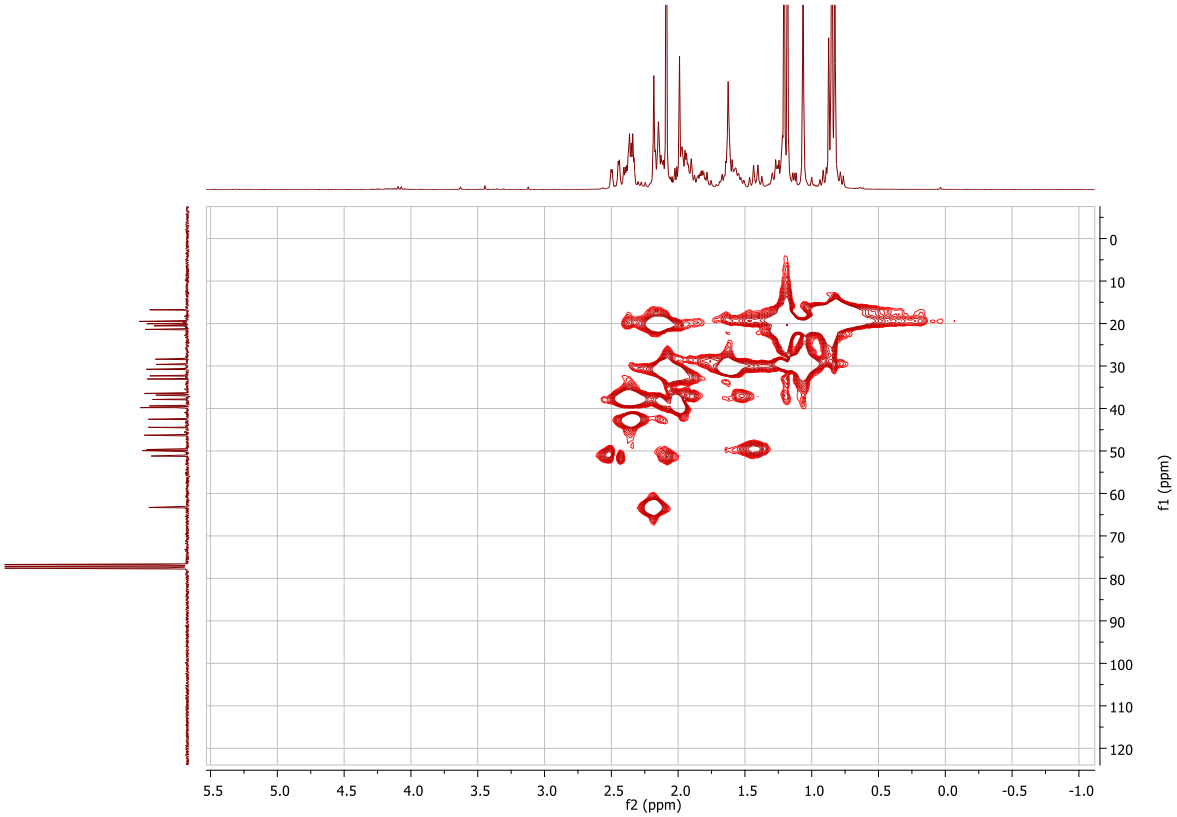

Figure S7. HMQC spectrum of compound **1** in $CDCl_3$.

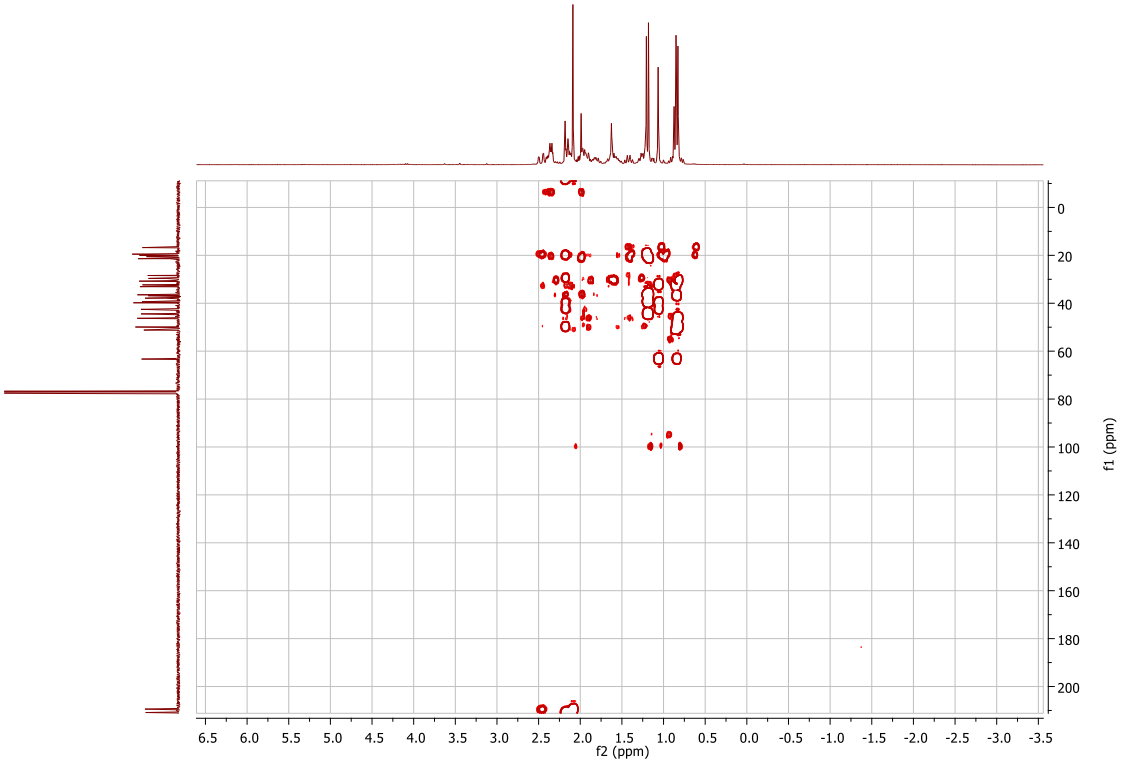

Figure S8. HMBC spectrum of compound **1** in $CDCl_3$

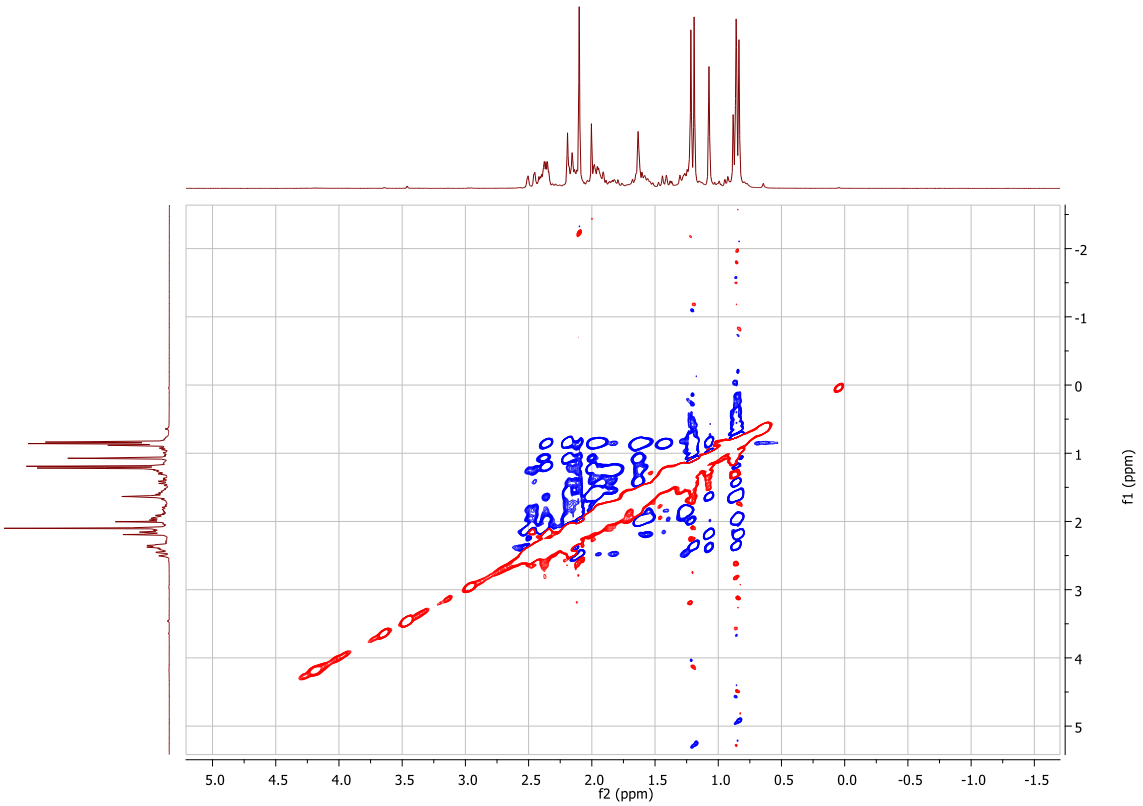

Figure S9. NOESY spectrum of compound **1** in $CDCl_3$.

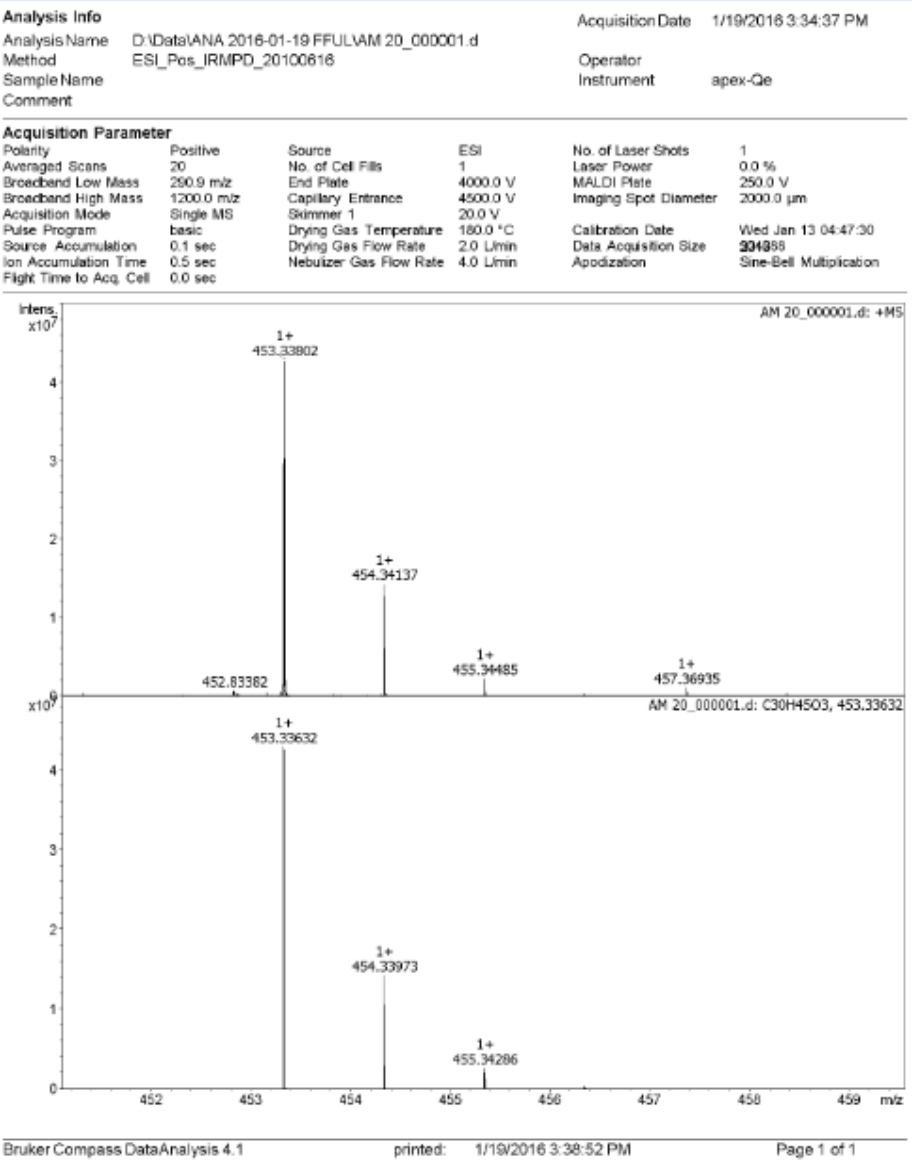

Figure S10. HRMS of compound **2**.

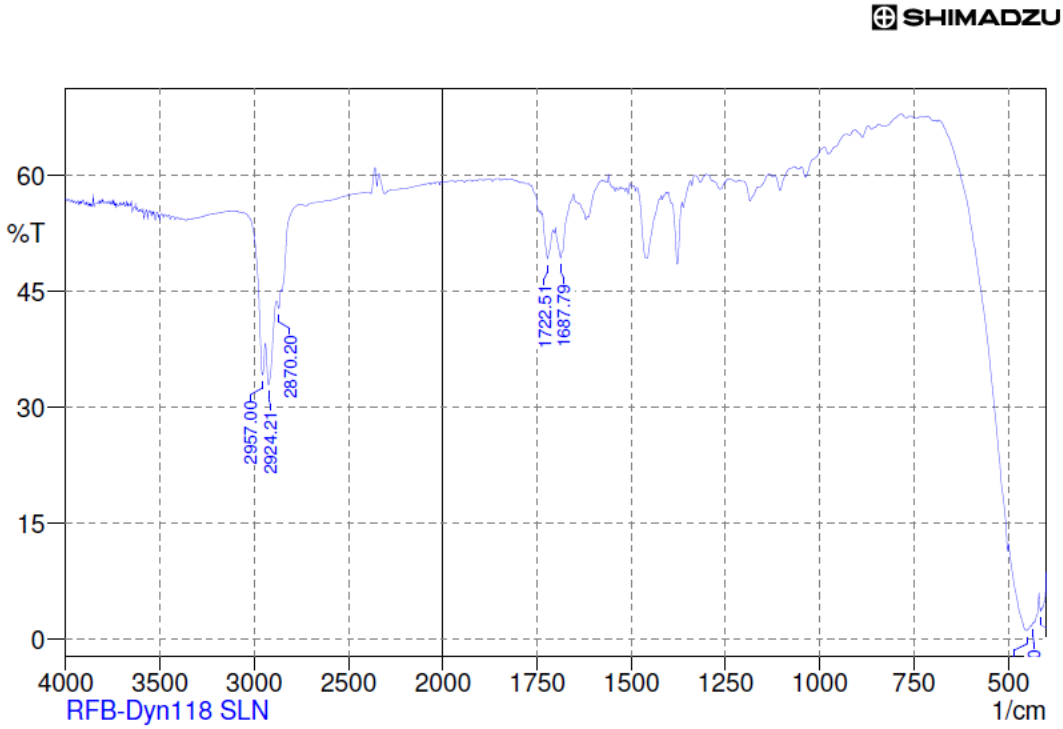

Figure S11. IR of compound **2**.

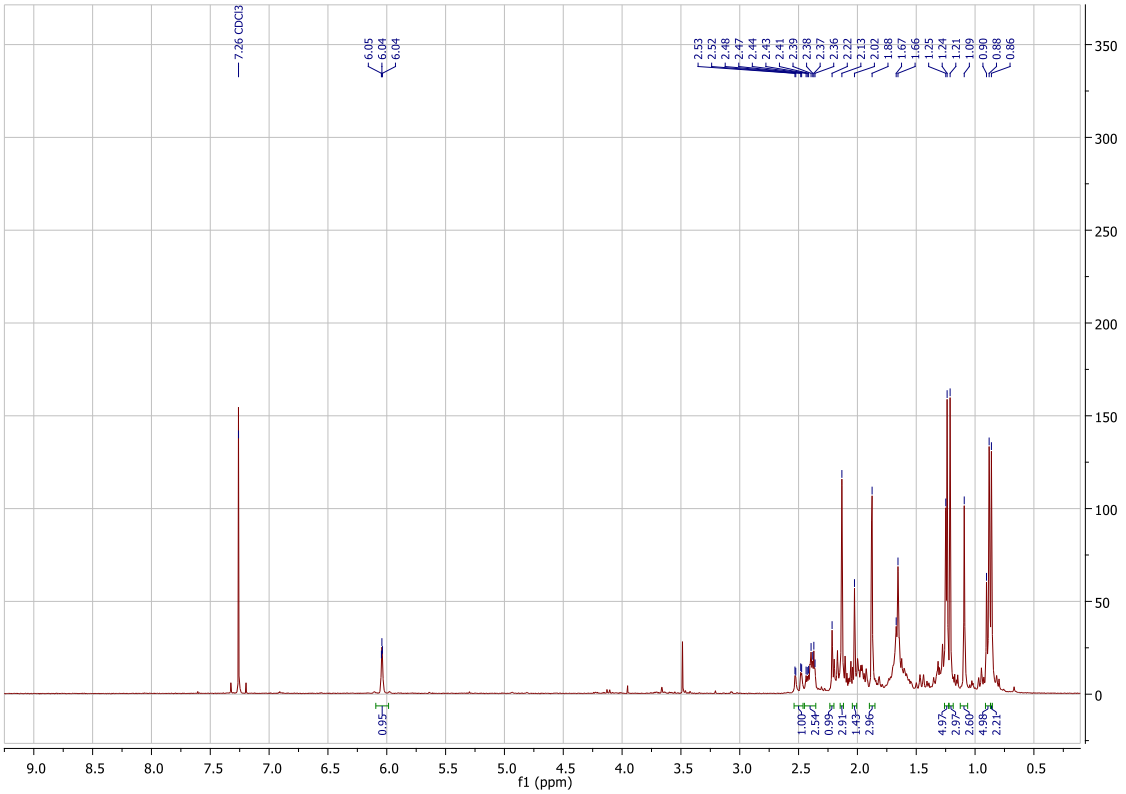

Figure S12. ^{1}H-NMR spectrum of compound **2** in $CDCl_3$ (300 MHz)..

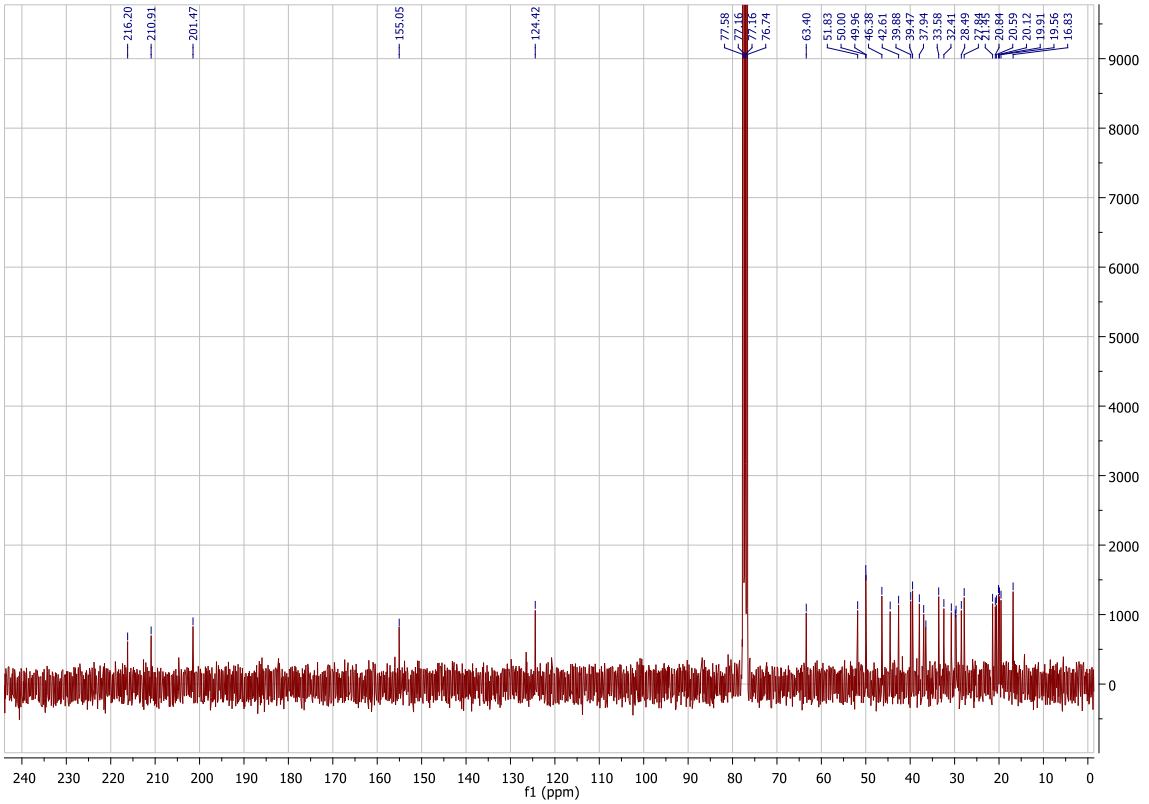

Figure S13. ^{13}C-NMR spectrum of compound **2** in $CDCl_3$ (75 MHz).

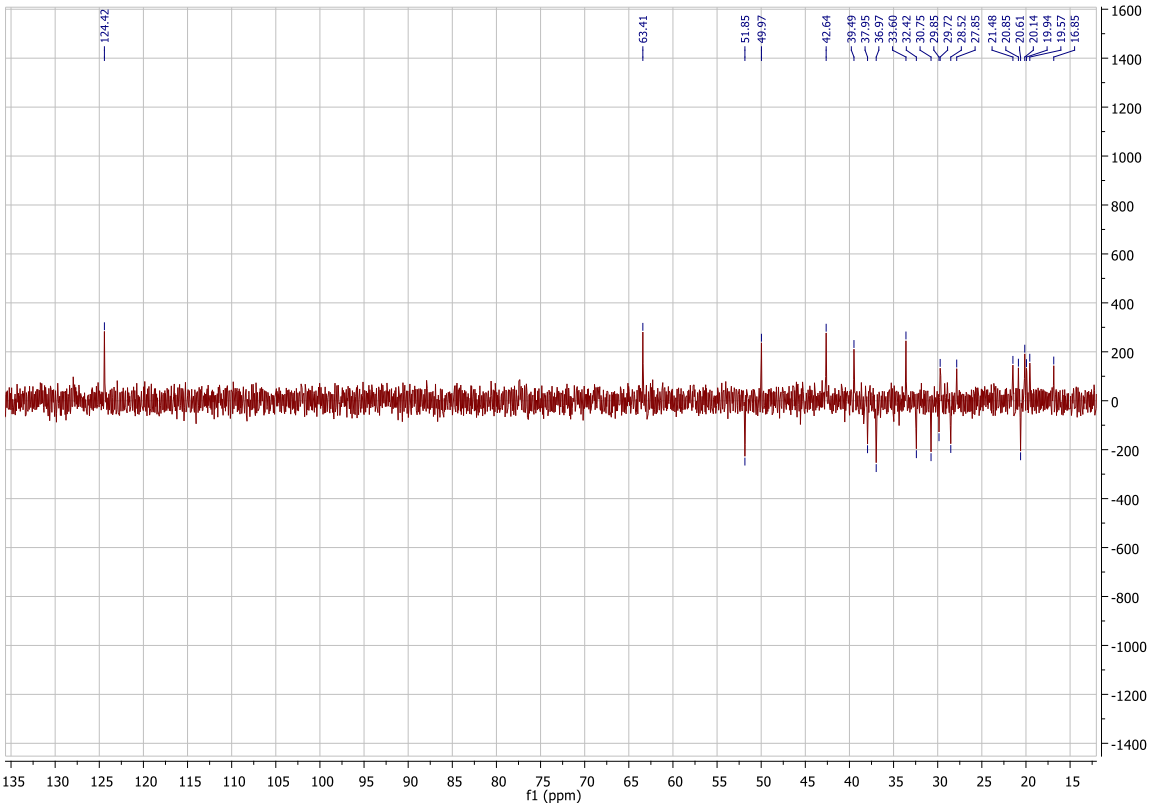

Figure S14. DEPT spectrum of compound **2** in $CDCl_3$ (75 MHz).

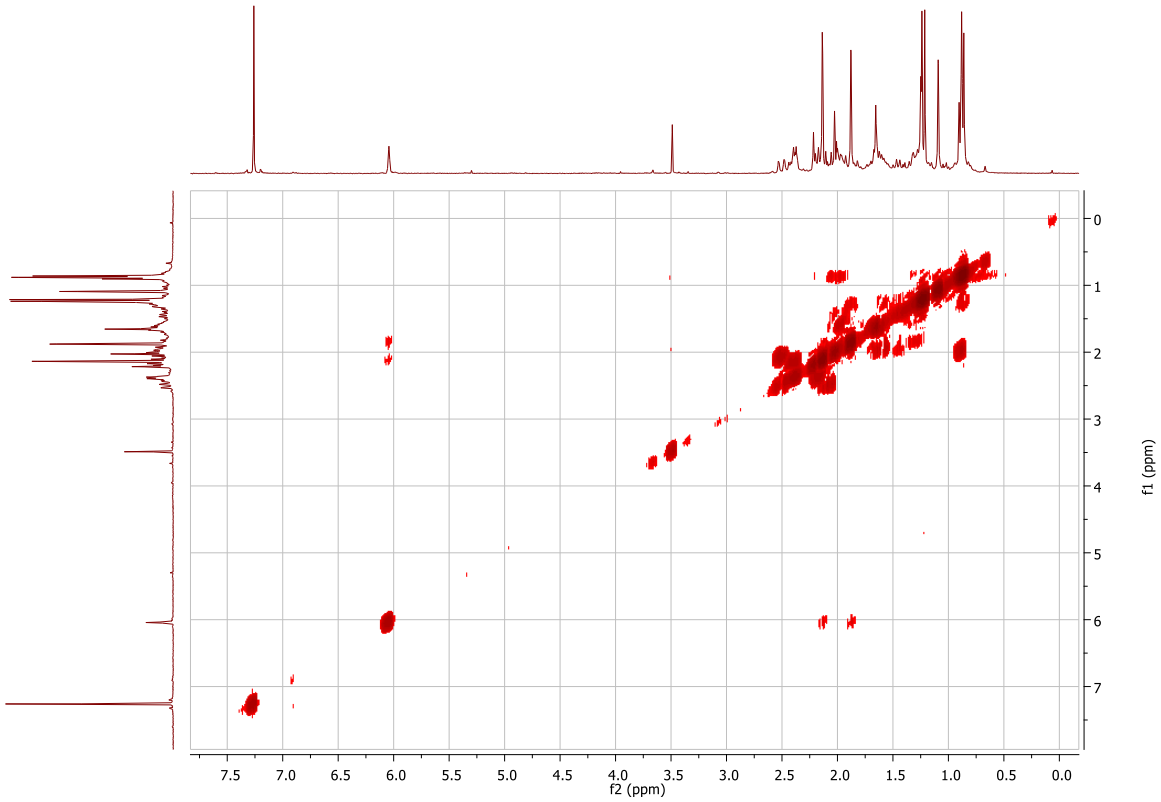

Figure S15. COSY spectrum of compound **2** in $CDCl_3$.

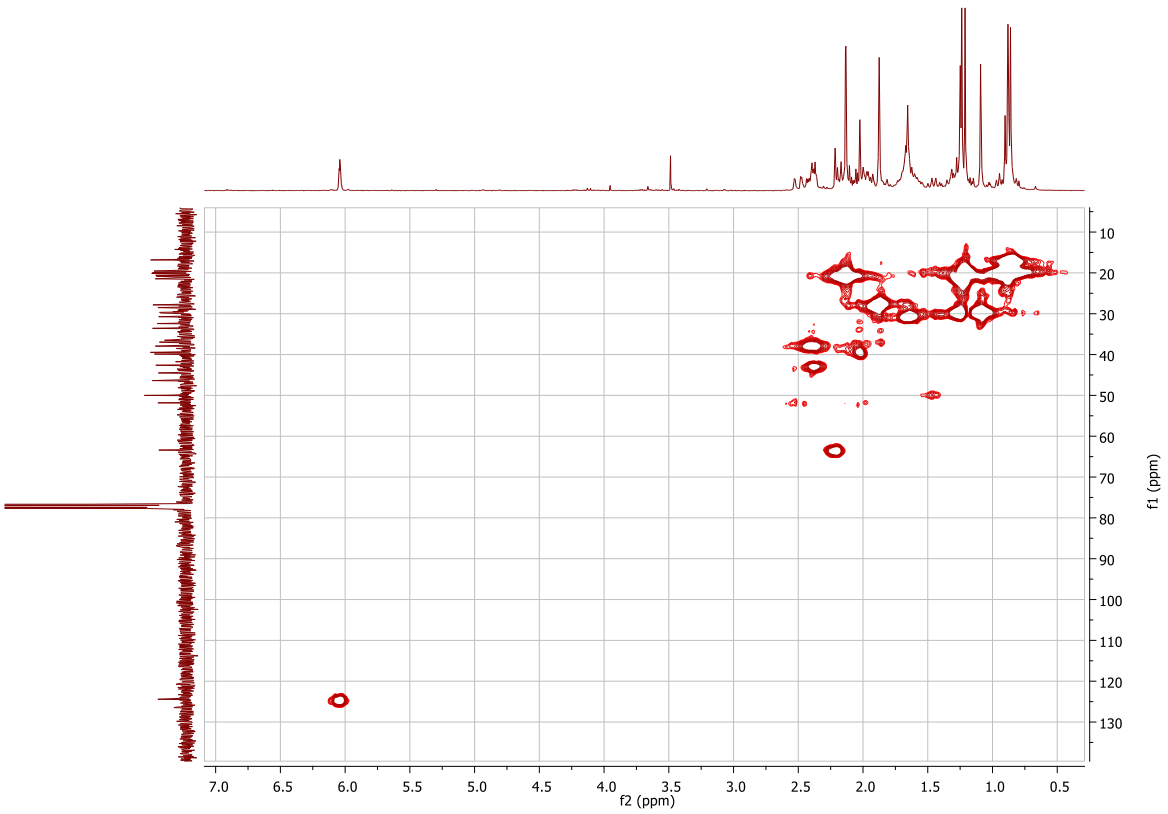

Figure S16. HMQC spectrum of compound **2** in $CDCl_3$.

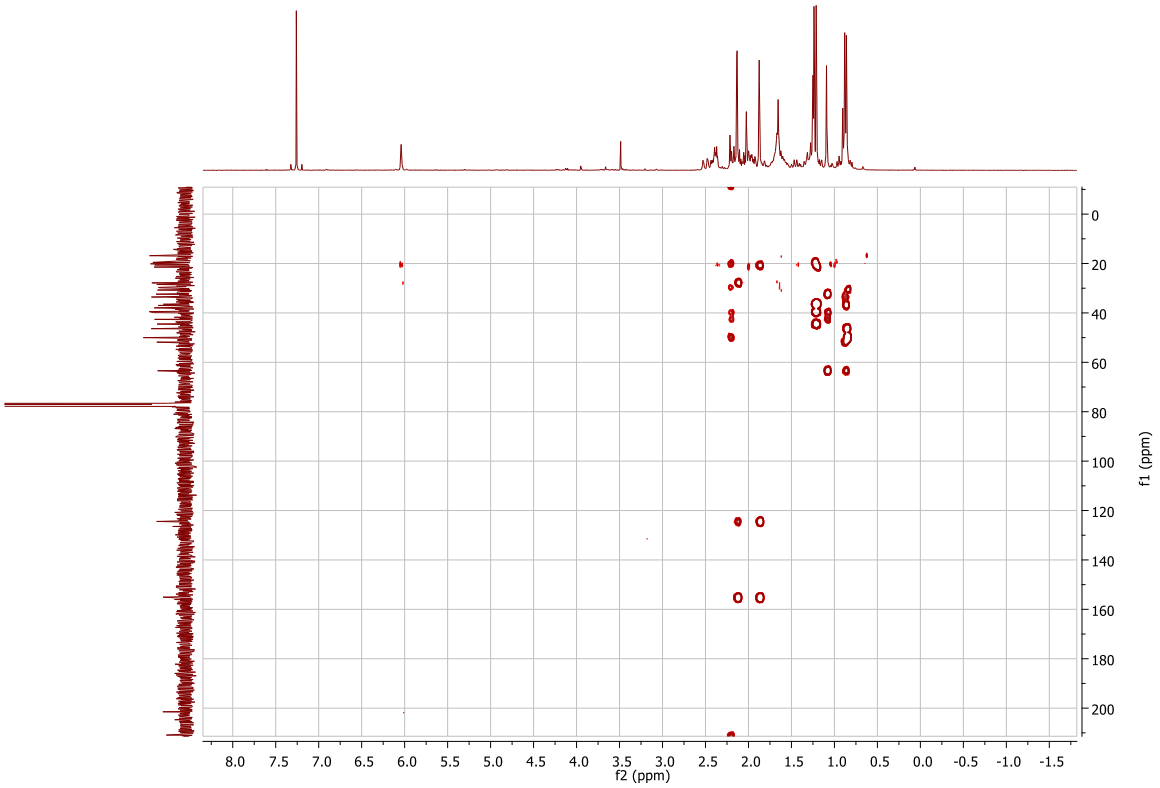

Figure S17. HMBC spectrum of compound **2** in $CDCl_3$.

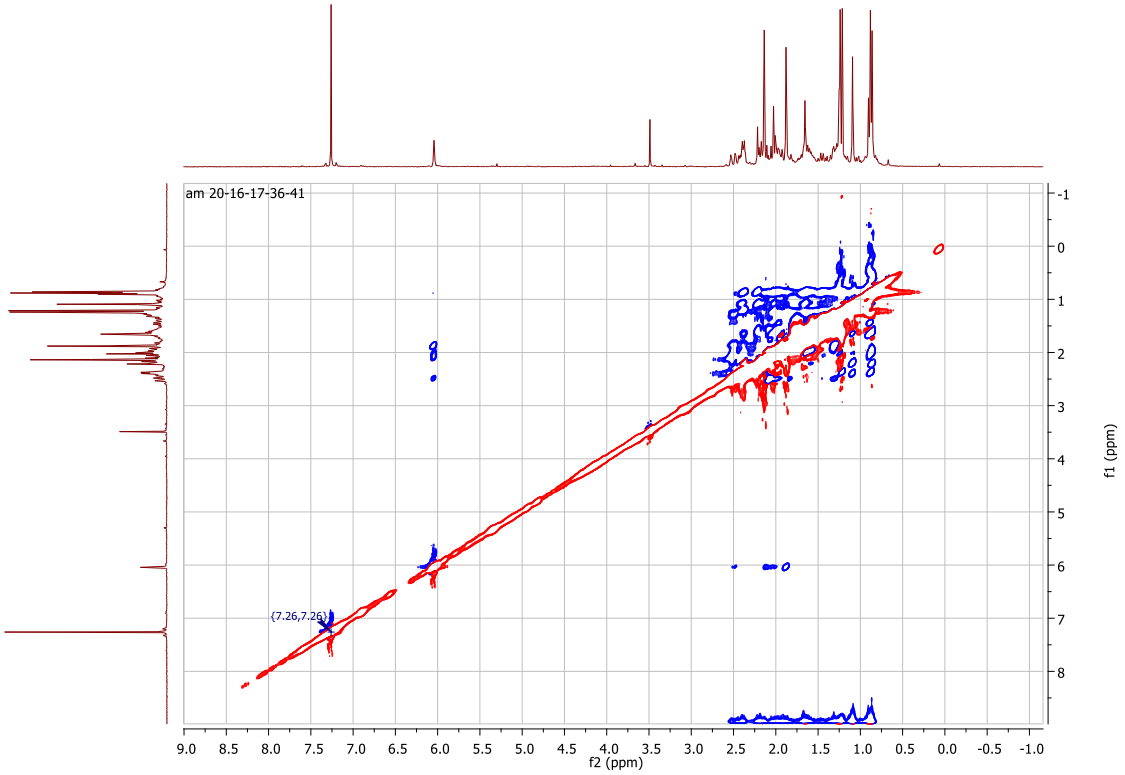

Figure S18. NOESY spectrum of compound **2** in $CDCl_3$.

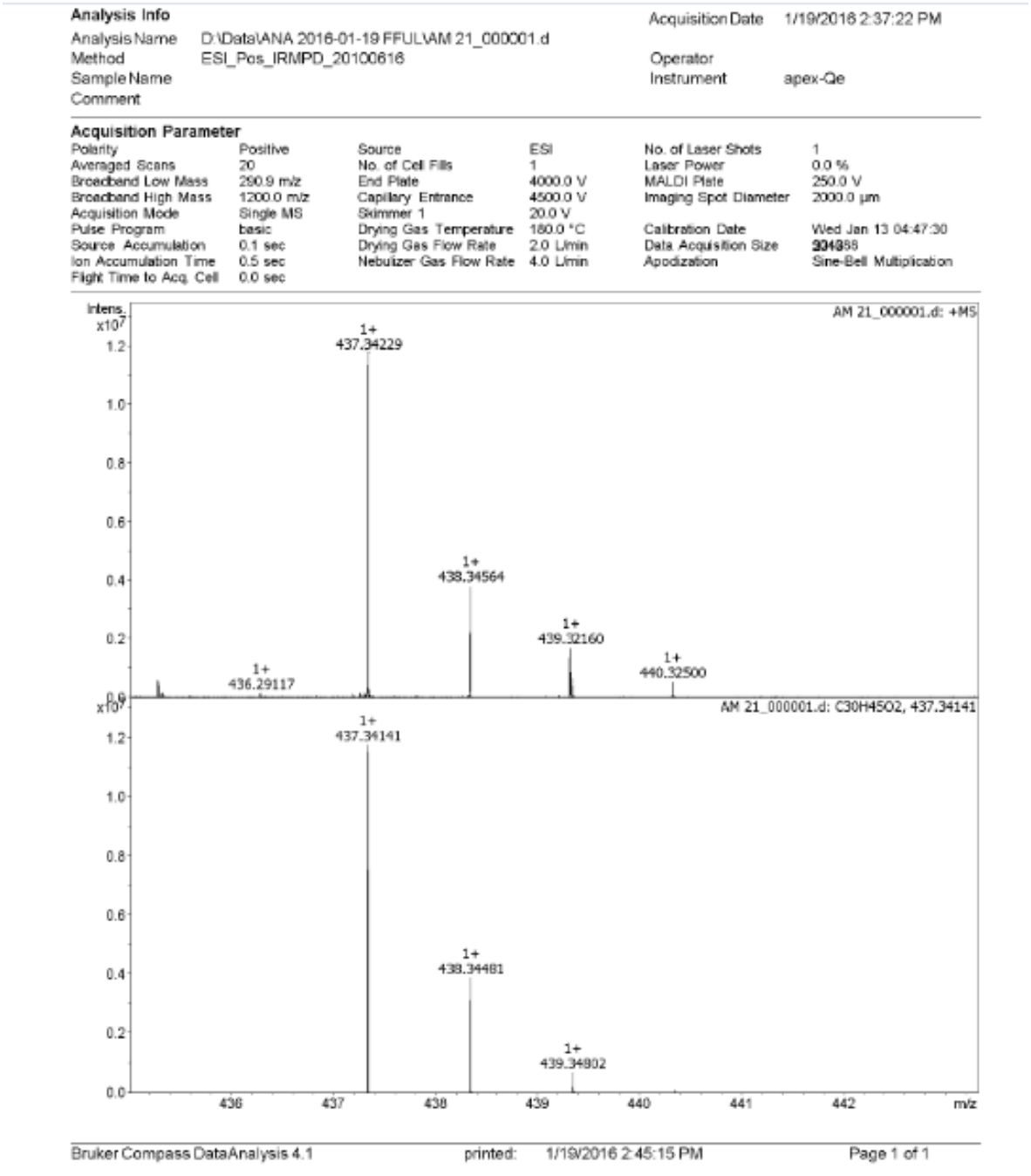

Figure S19. HRMS of compound **3**.

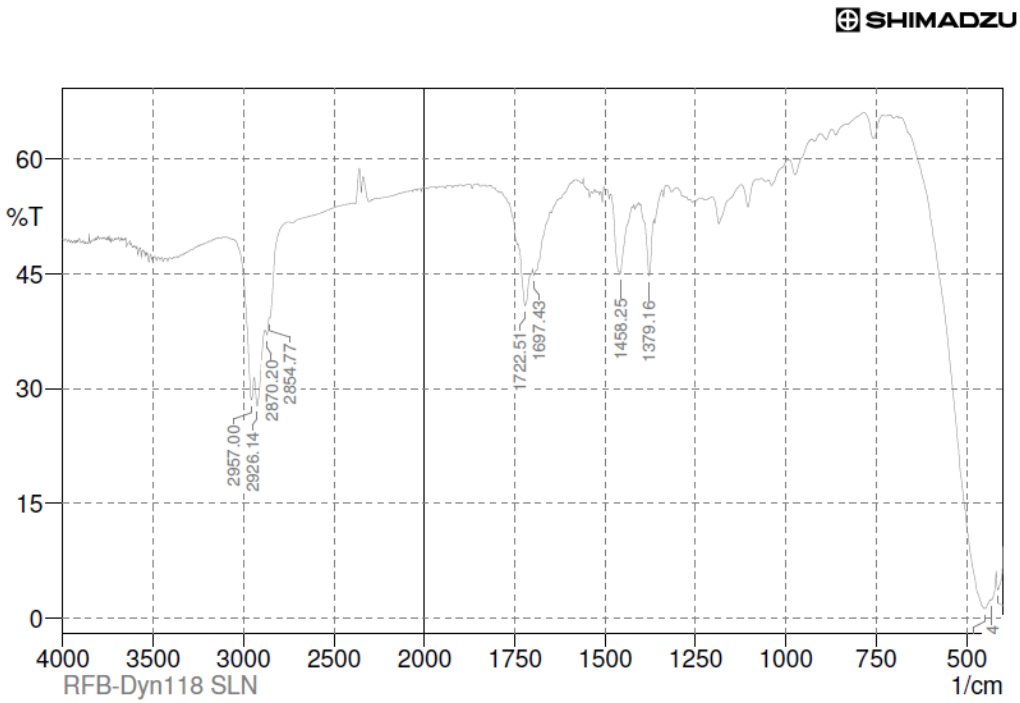

Figure S20. HRMS of compound **3**.

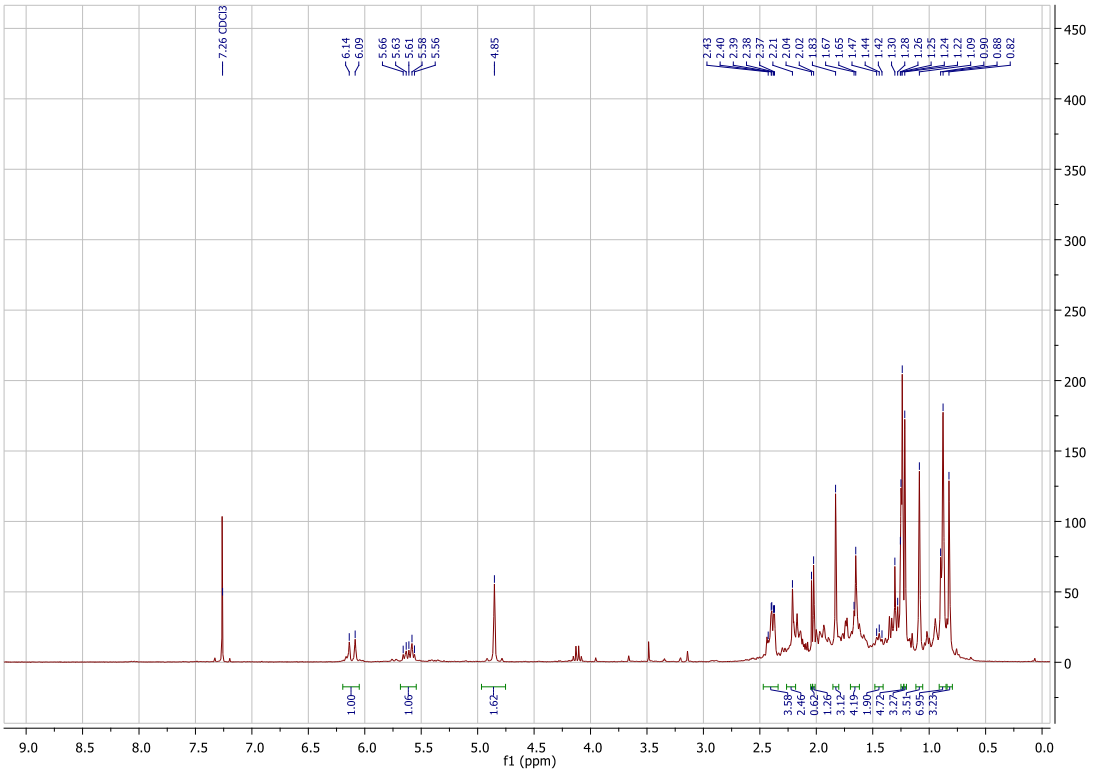

Figure S21 ^{1}H-NMR spectrum of compound **3** in $CDCl_3$ (300 MHz)..

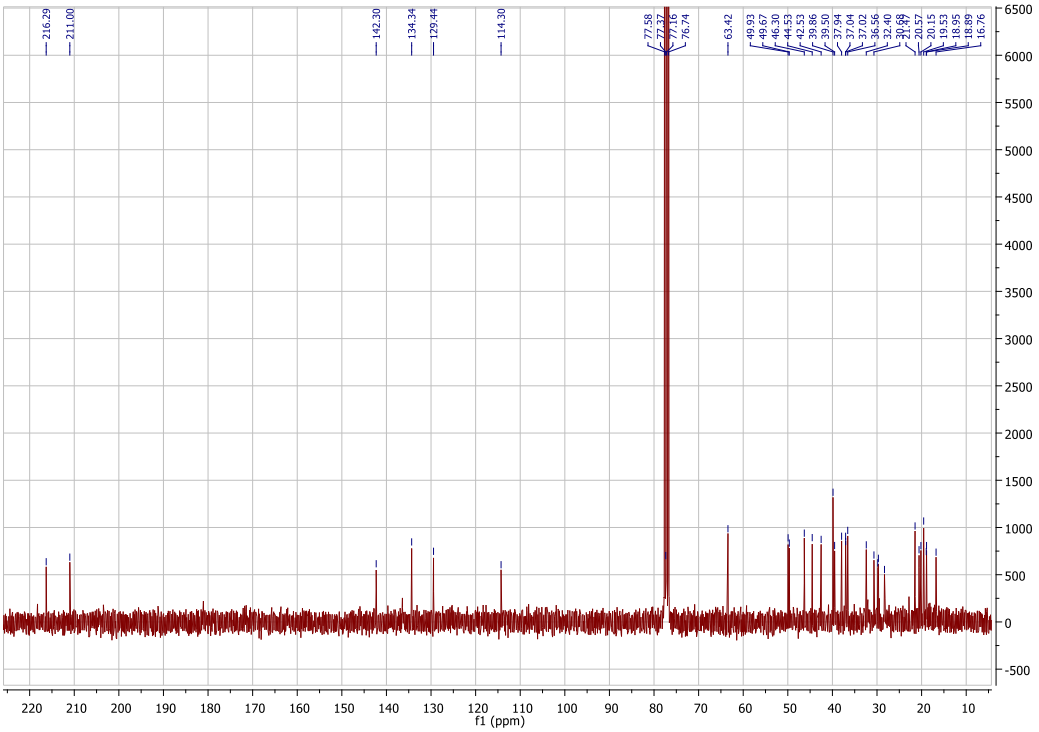

Figure S22. ^{13}C-NMR spectrum of compound **3** in $CDCl_3$ (75 MHz).

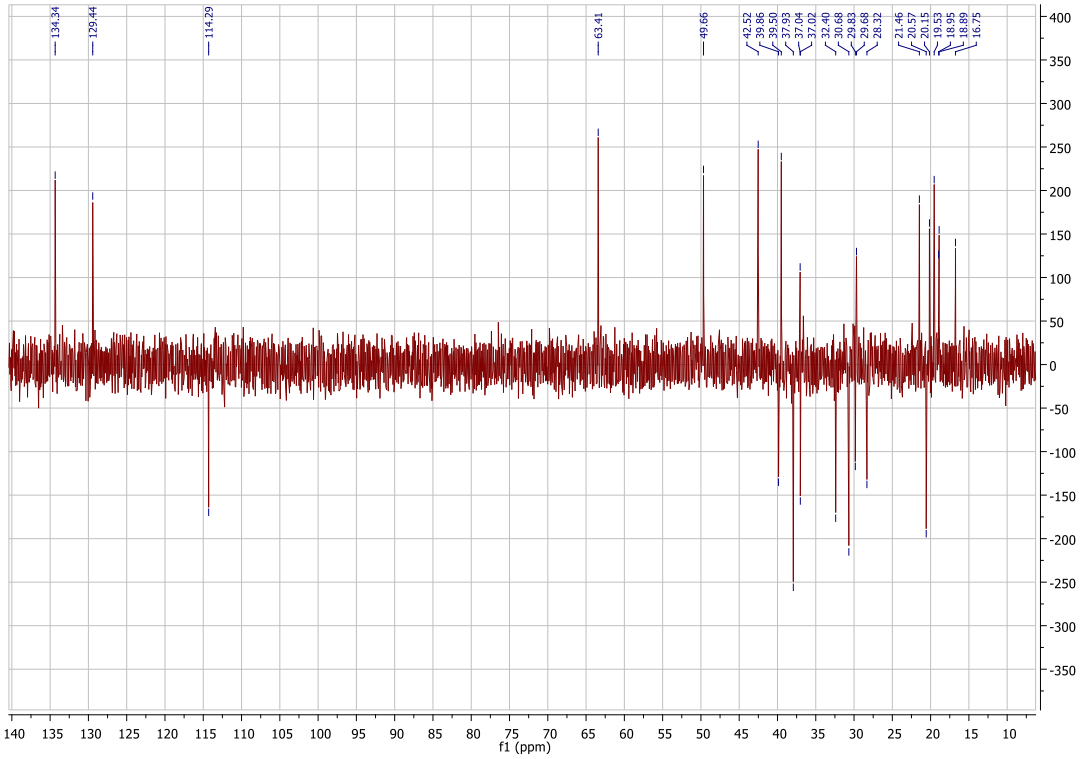

Figure S23. DEPT spectrum of compound **3** in $CDCl_3$ (75 MHz)

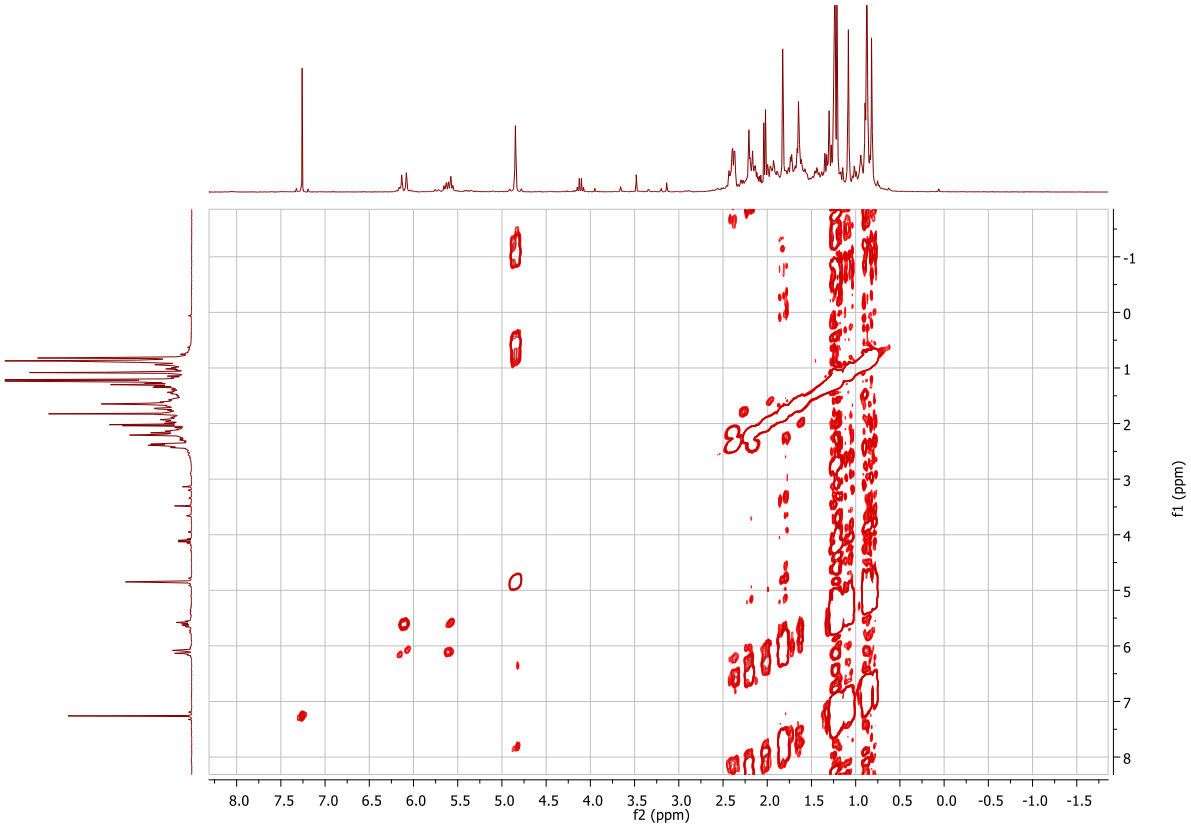

Figure S24. COSY spectrum of compound **3** in $CDCl_3$.

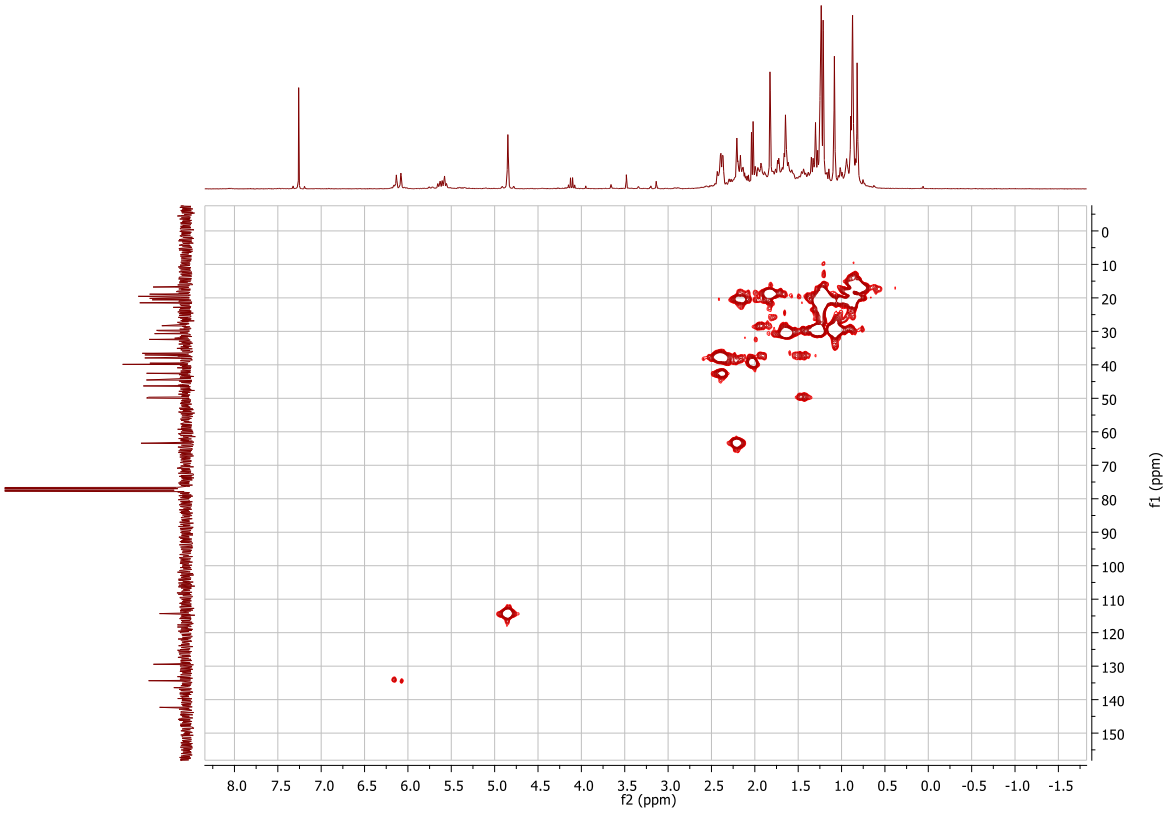

Figure S25. HMQC spectrum of compound **3** in $CDCl_3$.

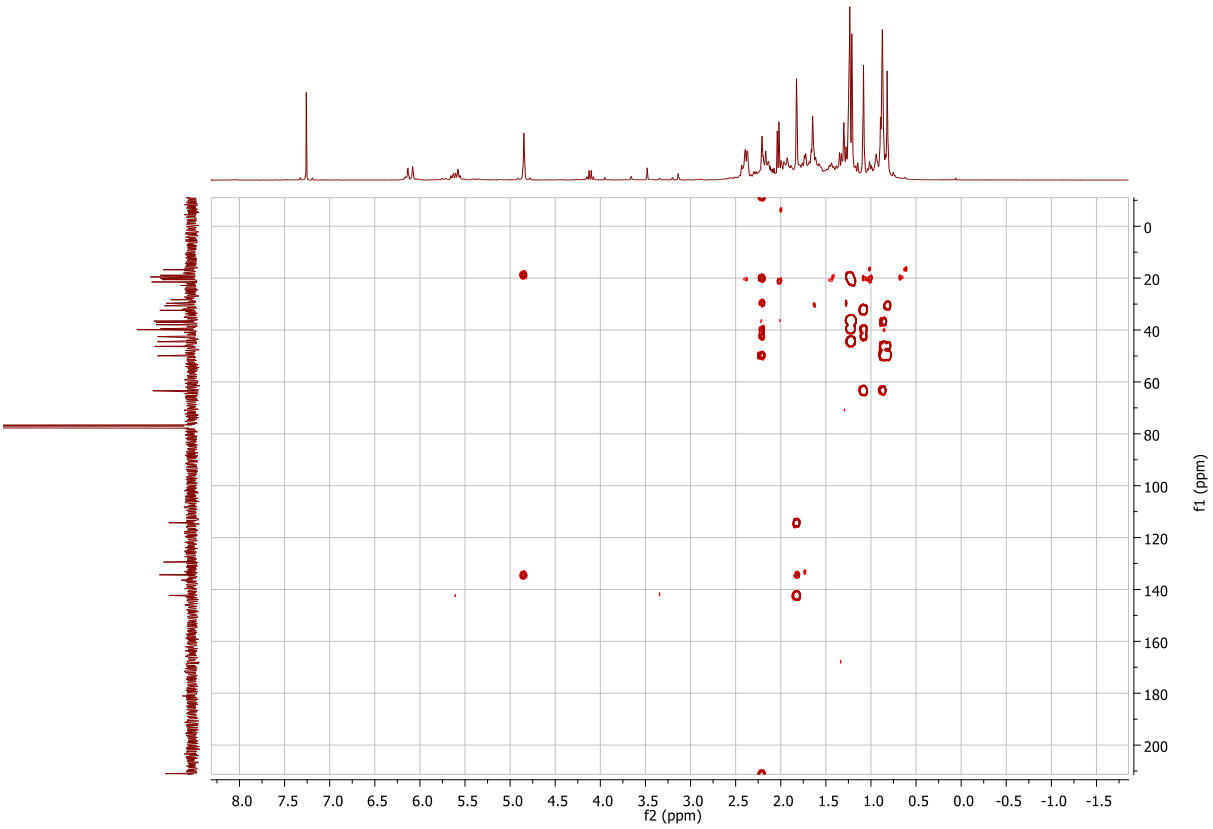

Figure S26. HMBC spectrum of compound **3** in $CDCl_3$