

Eremophilane-type sesquiterpenes from a marine-derived *Penicillium copticola*  
fungus with antitumor and neuroprotective activities

## **Supporting Information**

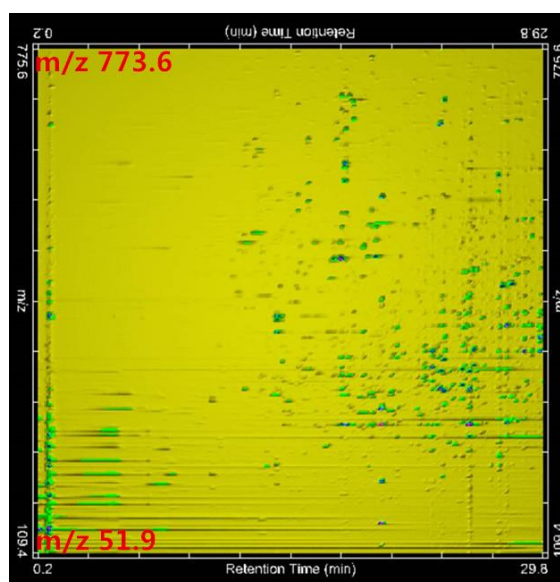
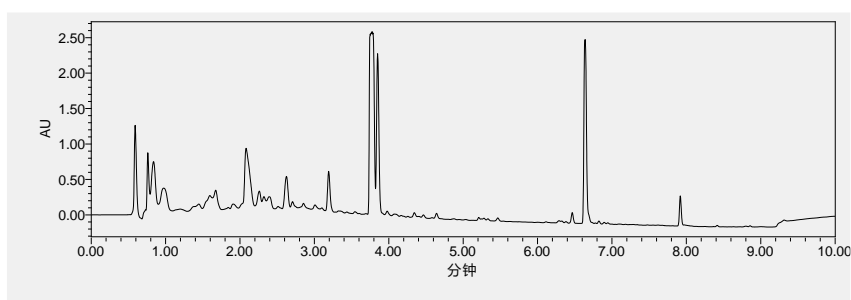
ITS-sequence of fungus

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CTCTGGGTCCACCTCCCACCCGTGTTTTCCGAACCCTGTTGCTTCGGCGGG
CCCGCCTCACGGCCGCCGGGGGGCTTCCGCCCCCGGGCCCGCGCCCGCCG
AAGACACCTGTGAACGCTGTCTGAAGTTGCAGTCTGAGAACTAGCTAGA
TTAGTTAAAACTTTCAACAACGGATCTCTTGGTTCCGGCATCGATGAAGA
ACGCAGCGAAATGCGATAACTAATGTGAATTGCACAATTCAGGAATCATC
GAGTCTTTGAACGCACATGGCGCCCTCTGGTATTCCGGAGGGGCATGCCTG
TCCGAGCGTCATTGCTGCCCTCAAGCACGGCTTGTGTGTTGGGCCCCACCC
CCCCGCCCTGCCCGAAGGCGGGGGCGCGGGGGGGGGGCAGAACCGAGCC
CAATCCTAATGACGAATGGGAGGTGAGACCACACCTGTTTGTATTGACCC
GATCGCCAGCCGCTGACCCACCTAAATTATTTTTTCAGGTTGA
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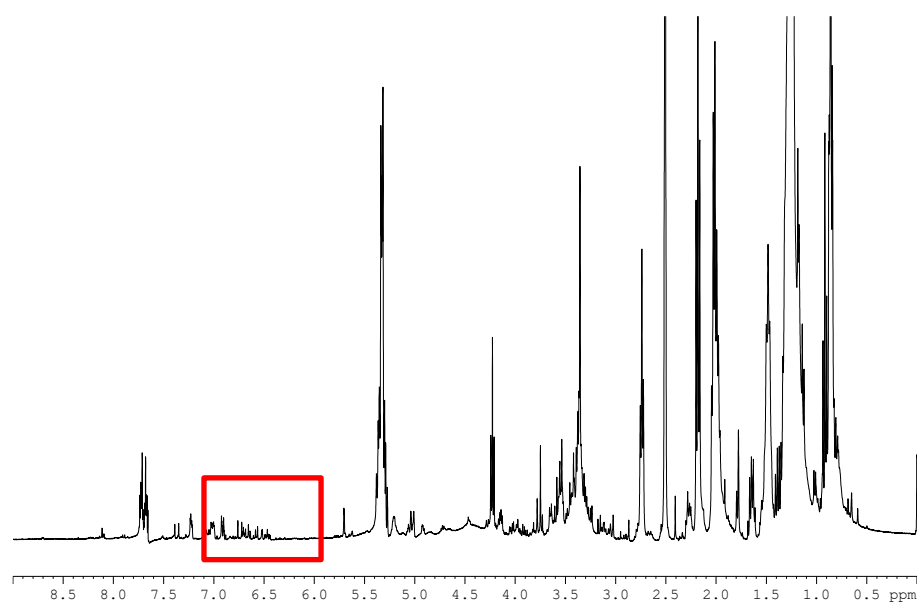
UPLC screening:

t/min	(mL/min)	A (MeCN)	B (H <sub>2</sub> O +0.04%TFA )
0	0.4	10	90
7	0.4	100	0
8	0.4	100	0
8.01	0.4	10	90
10	0.4	10	90

WZXY-SX-10-26-1



LC-MS spectrum of EtOAc extract of WZXY-SX-10-26-1 fungal strain



$^1\text{H}$  NMR spectrum of EtOAc extract of WZXY-SX-10-26-1 fungal strain

Figure S1. IR spectrum of **1**

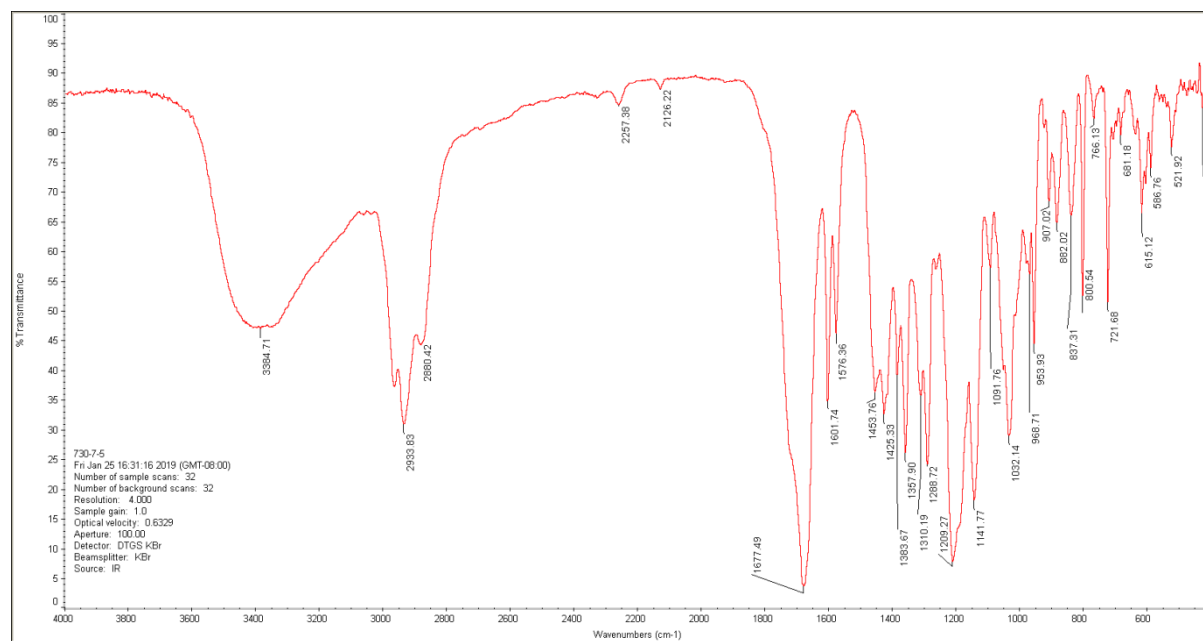


Figure S2.  $^1\text{H}$  NMR (600 MHz) spectrum of **1** in  $\text{DMSO-}d_6$

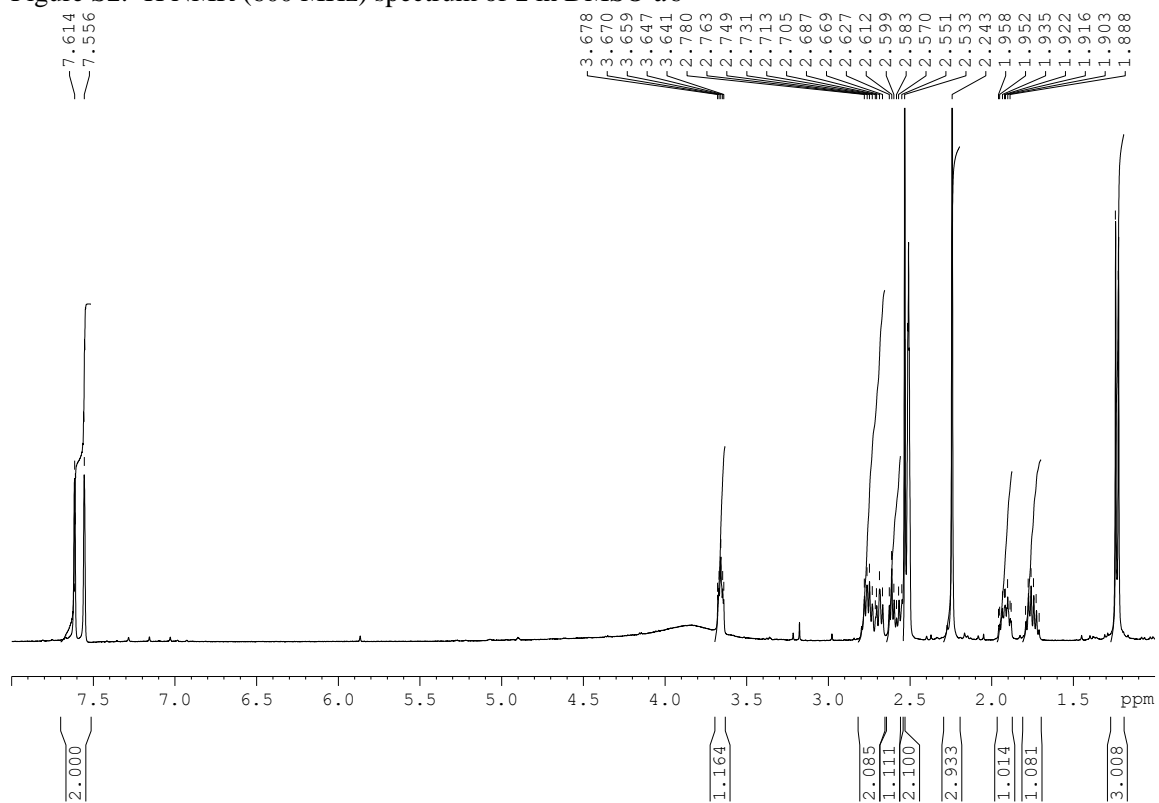




Figure S3.  $^{13}\text{C}$  NMR (150 MHz) spectrum of **1** in  $\text{DMSO-}d_6$

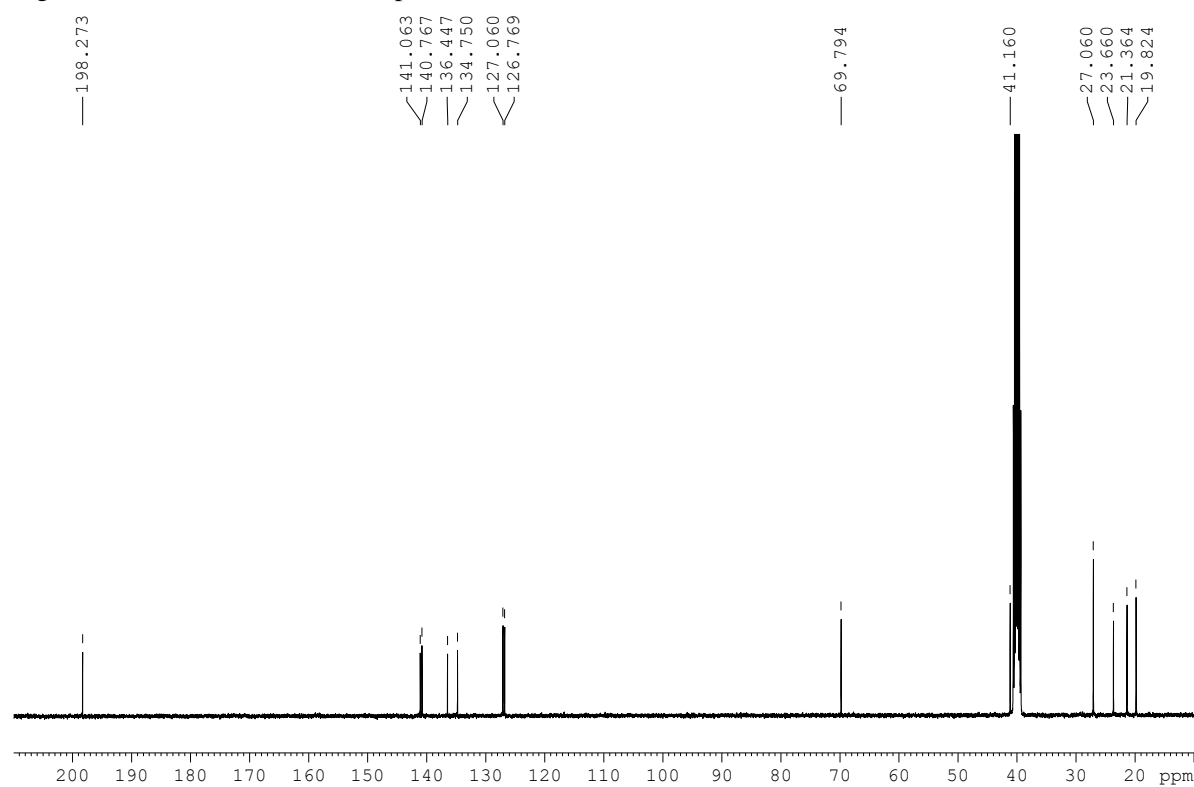


Figure S4.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1** in  $\text{DMSO-}d_6$

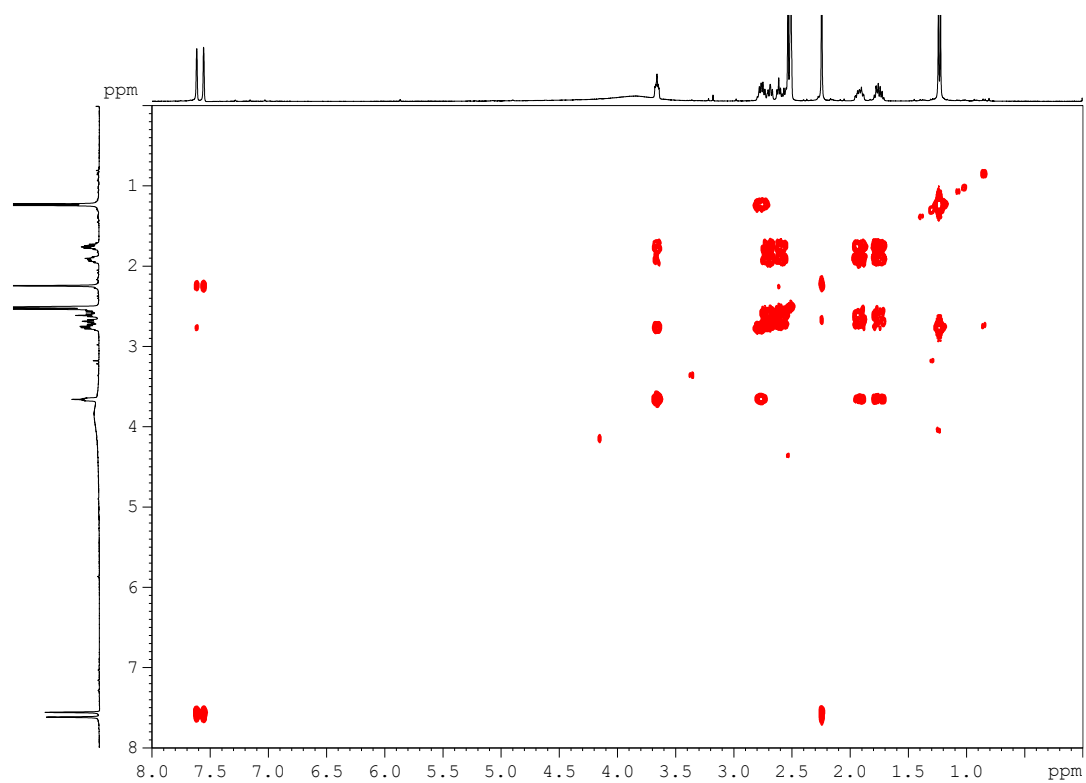


Figure S5. HSQC spectrum of **1** in DMSO-*d*<sub>6</sub>

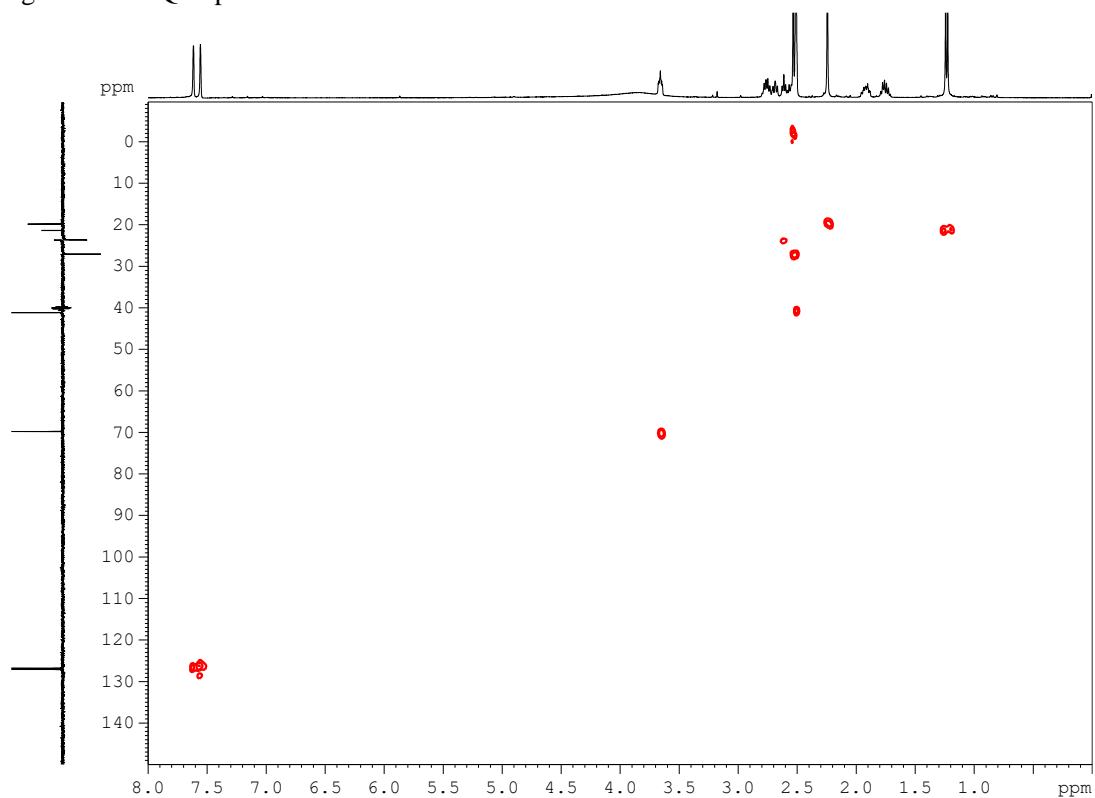


Figure S6. HMBC spectrum of **1** in DMSO-*d*<sub>6</sub>

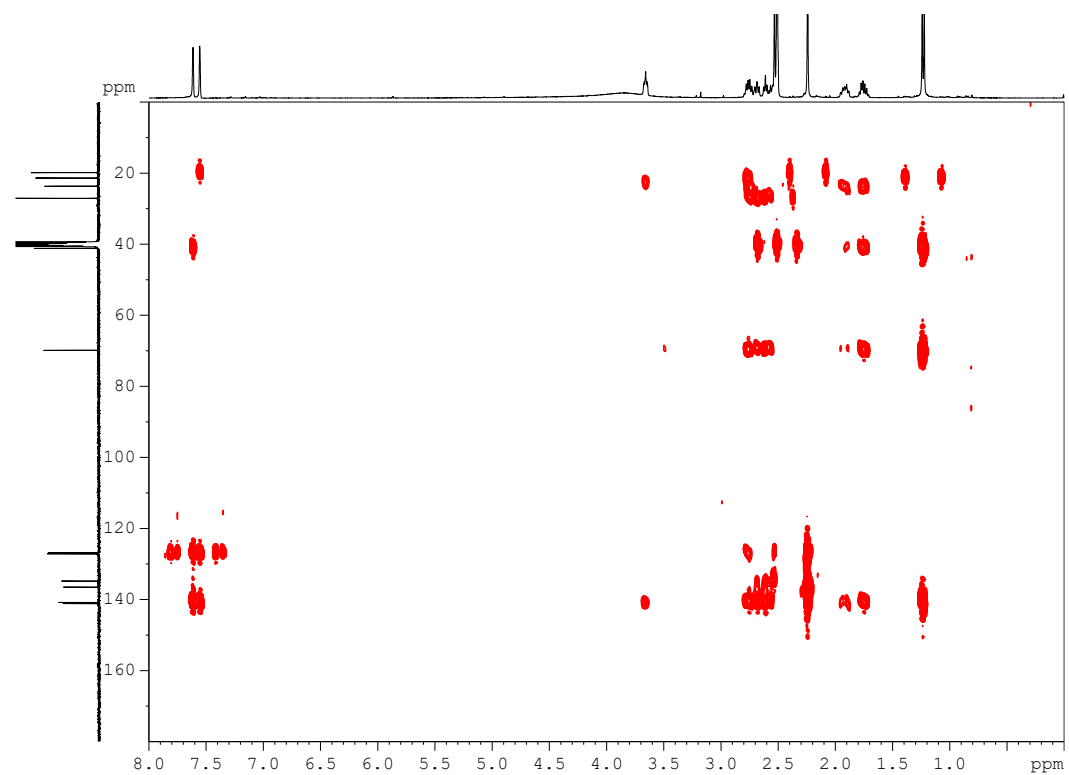


Figure S7. NOESY spectrum of **1** in DMSO-*d*<sub>6</sub>

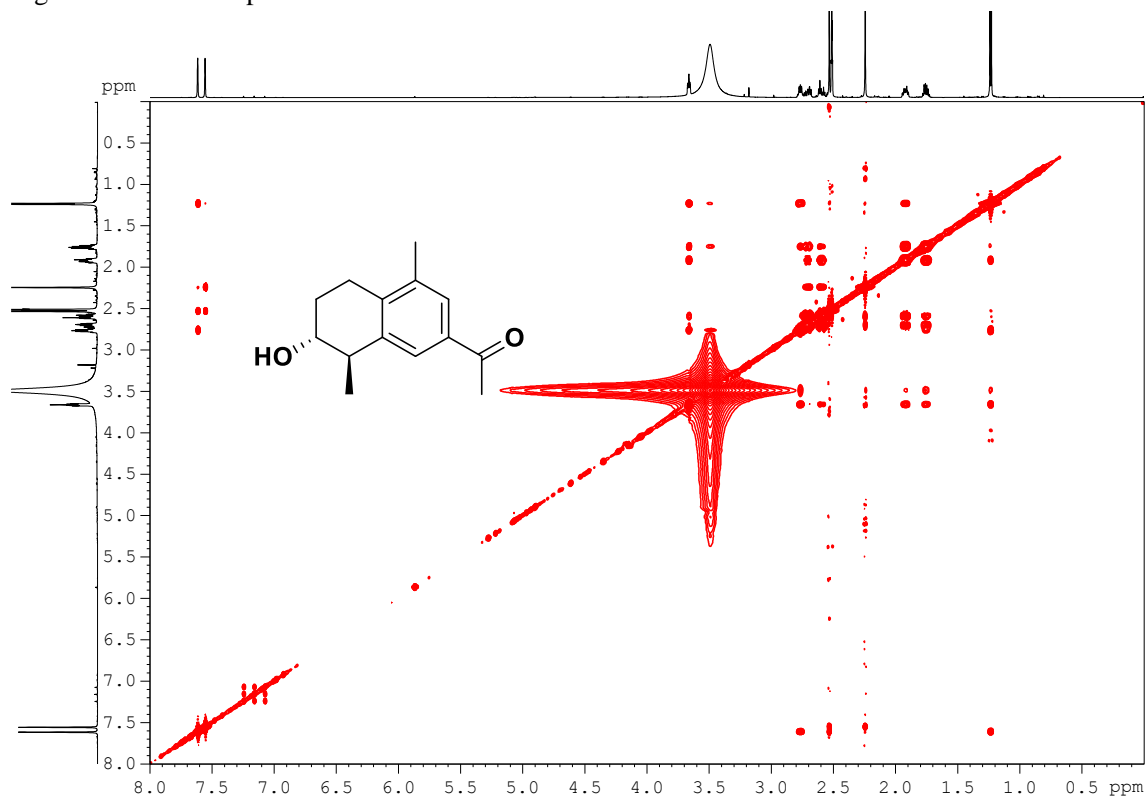
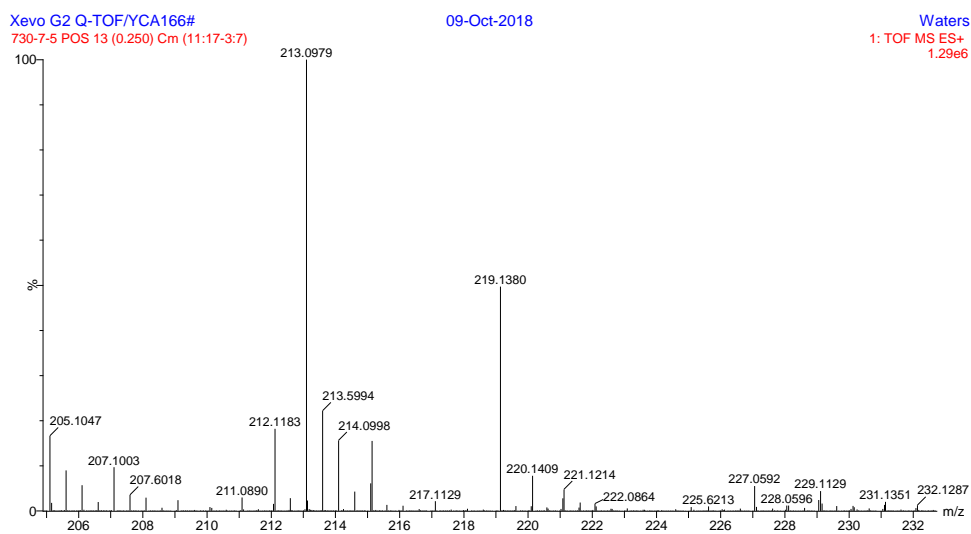


Figure S8. HRESIMS spectrum of **1**



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
219.1380	219.1385	-0.5	-2.3	5.5	767.1	n/a	n/a	C <sub>14</sub> H <sub>19</sub> O <sub>2</sub>

Figure S9. IR spectrum of **2**

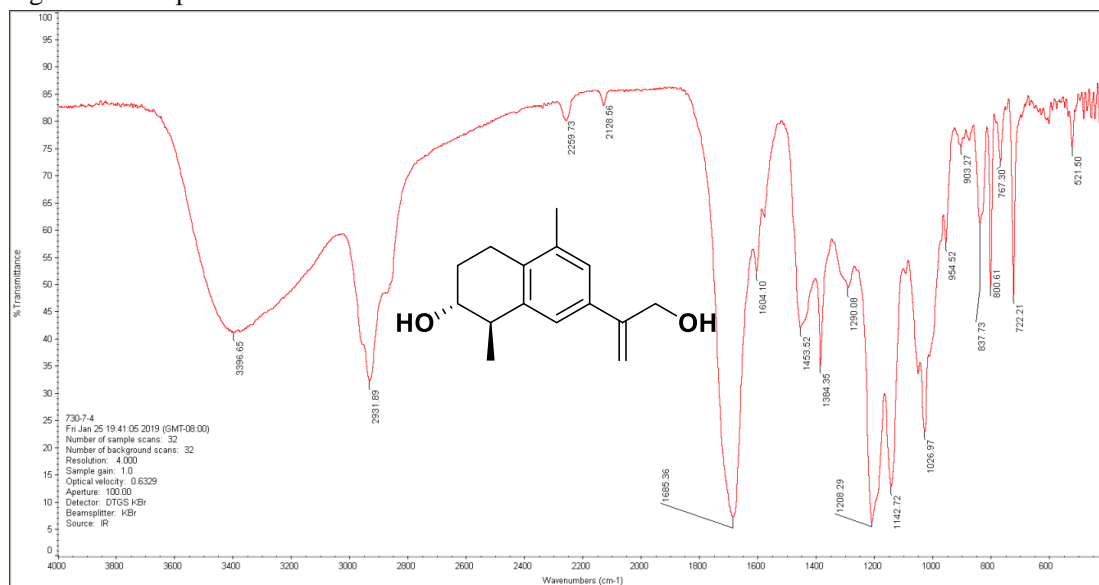


Figure S10. <sup>1</sup>H NMR (600 MHz) spectrum of **2** in DMSO-*d*<sub>6</sub>

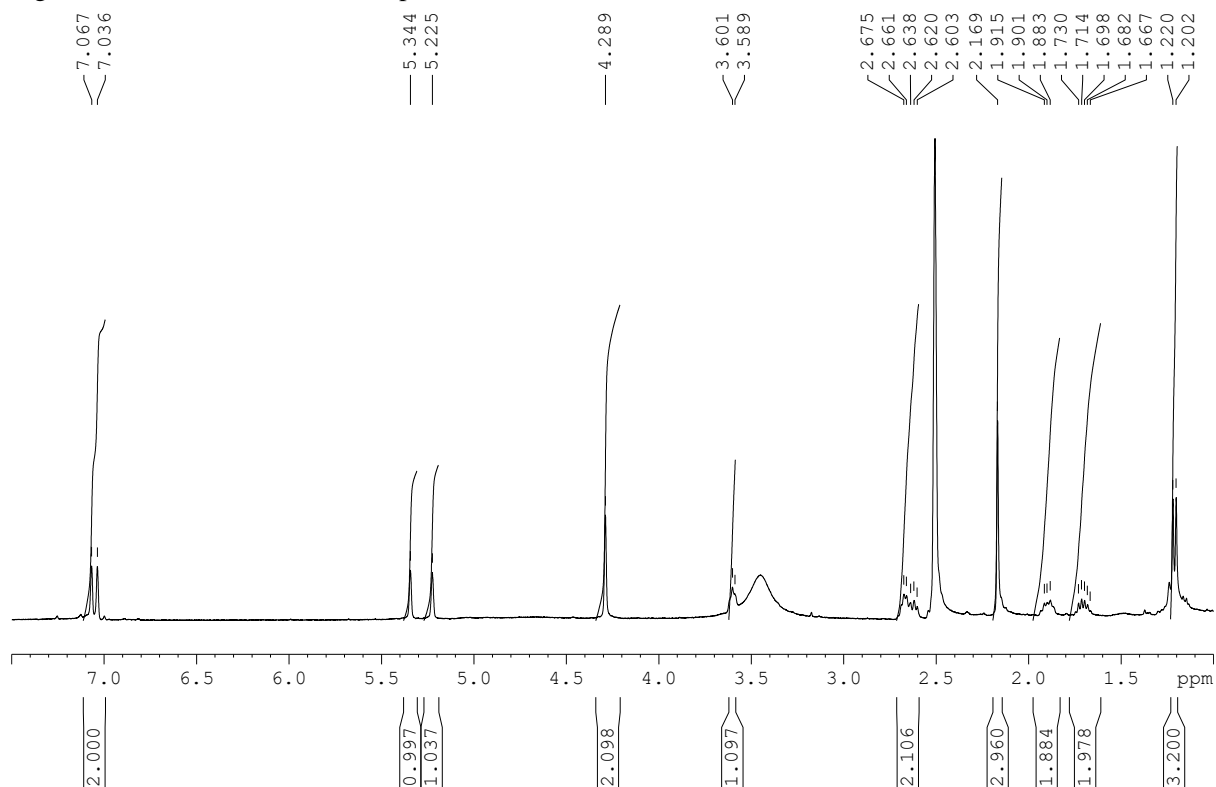


Figure S11.  $^{13}\text{C}$  NMR and DEPT (150 MHz) spectra of **2** in  $\text{DMSO-}d_6$

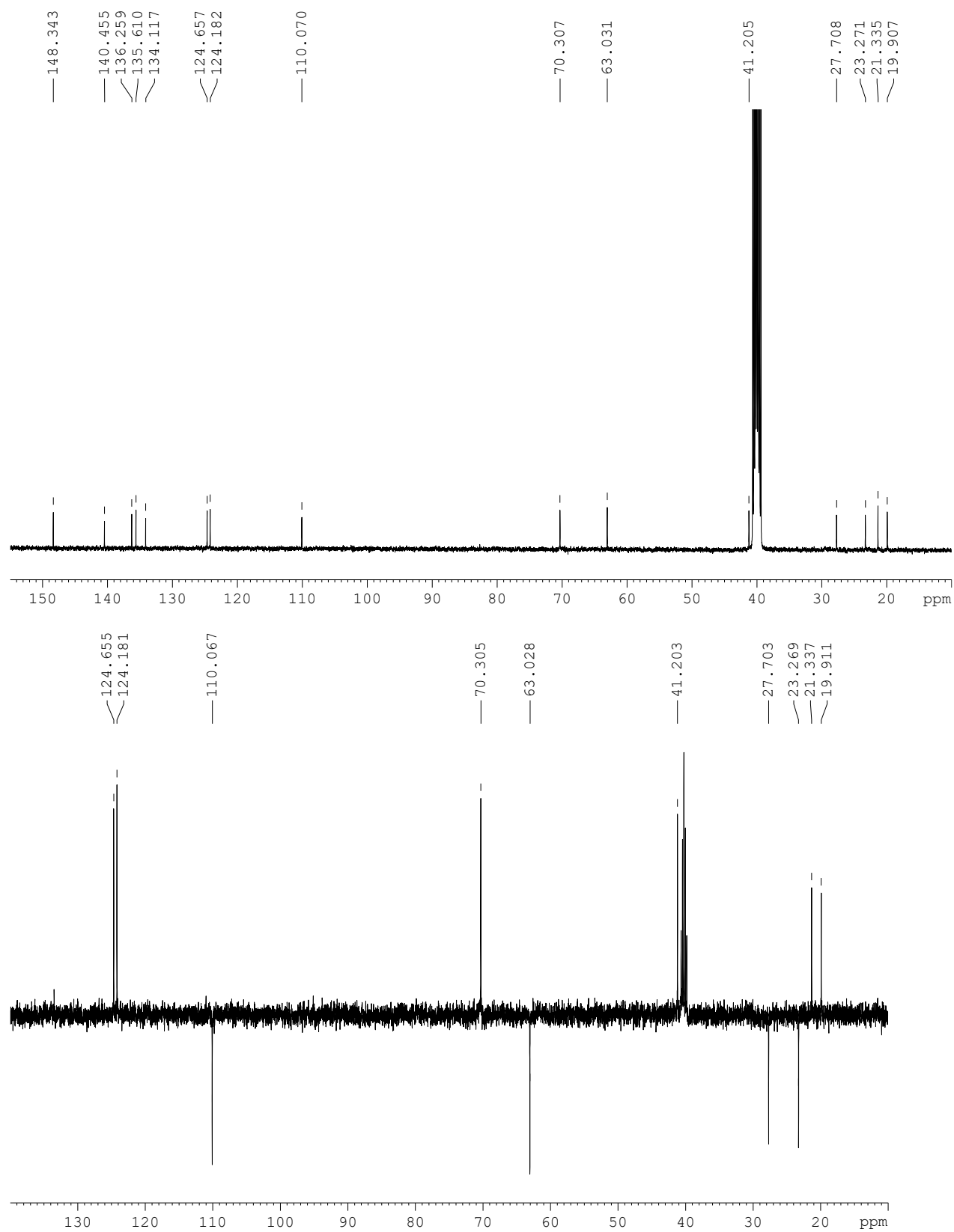


Figure S12.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **2** in DMSO- $d_6$

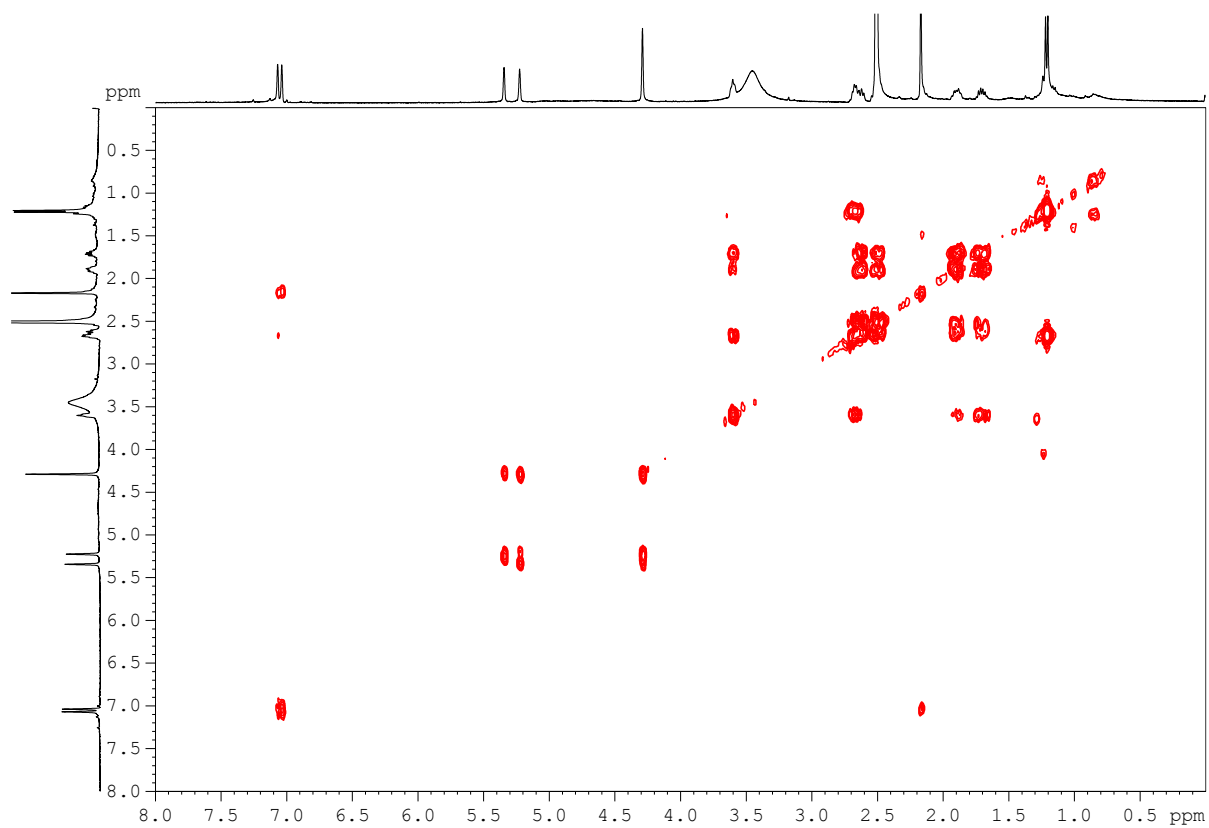


Figure S13. HSQC spectrum of **2** in DMSO- $d_6$

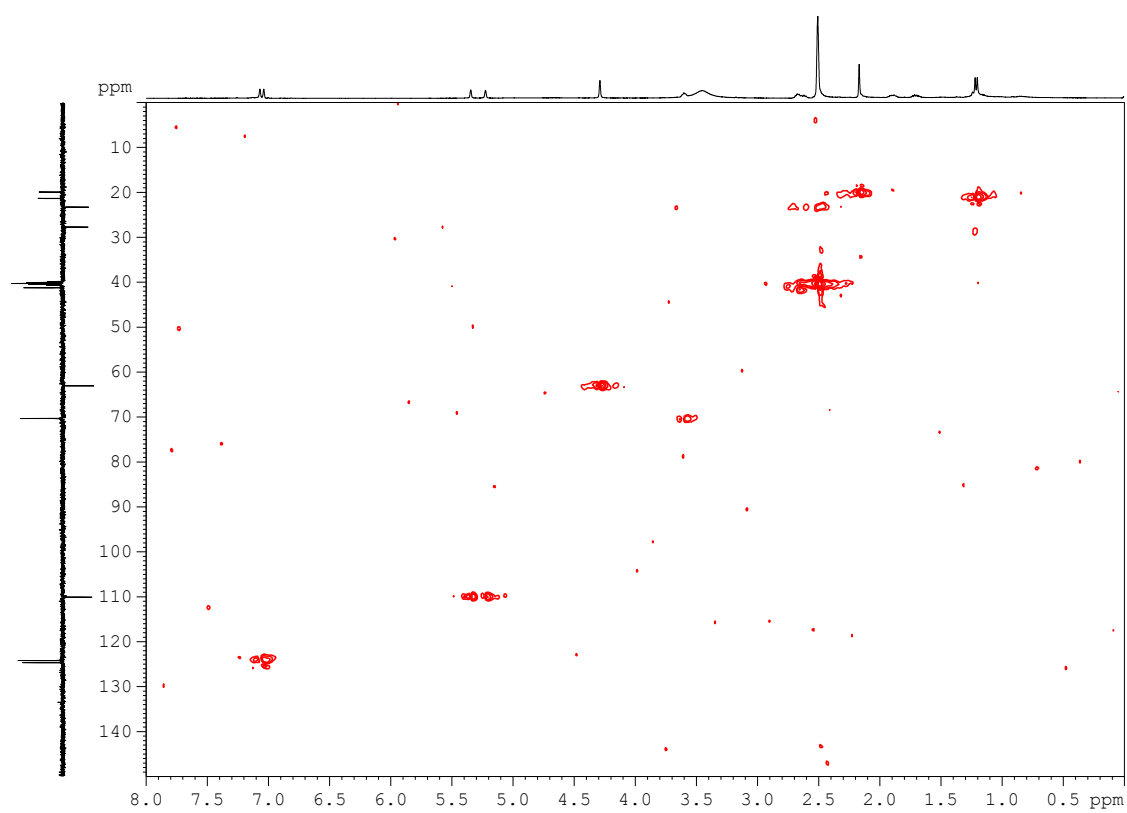


Figure S14. HMBC spectrum of **2** in DMSO-*d*<sub>6</sub>

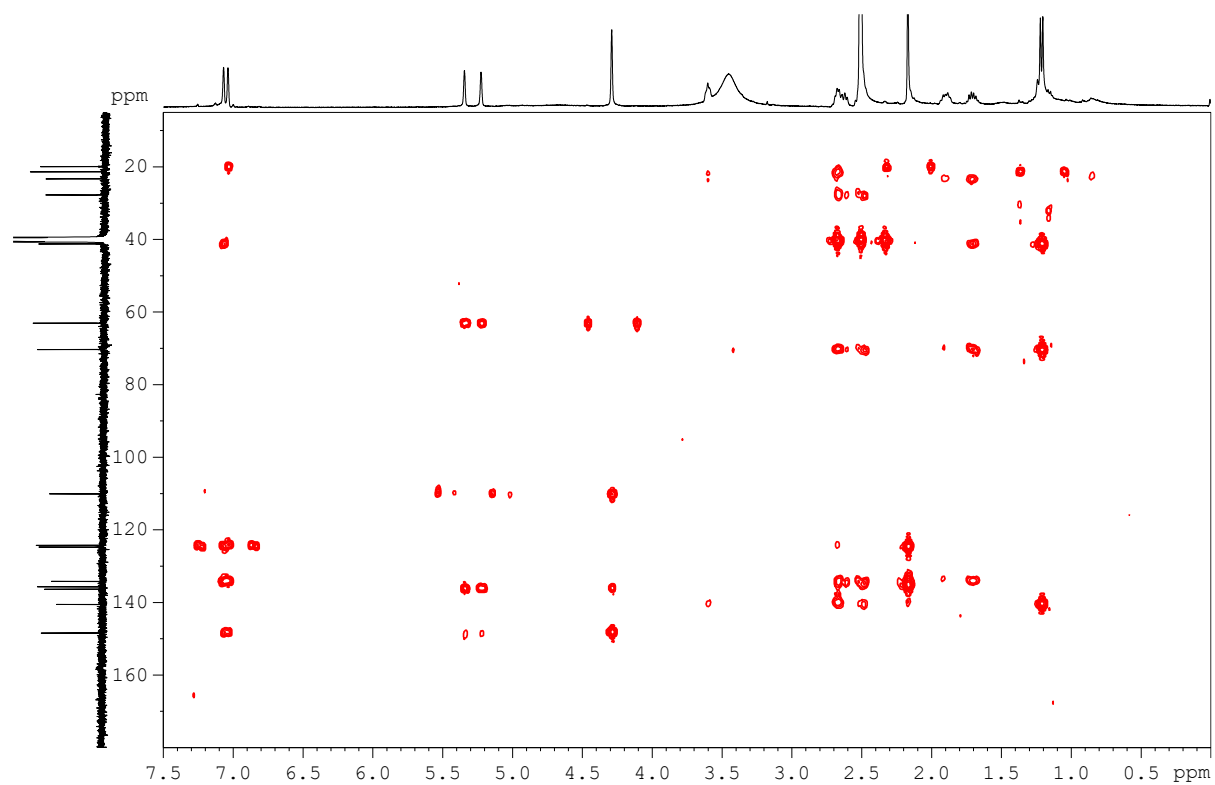


Figure S15. NOESY spectrum of **2** in DMSO-*d*<sub>6</sub>

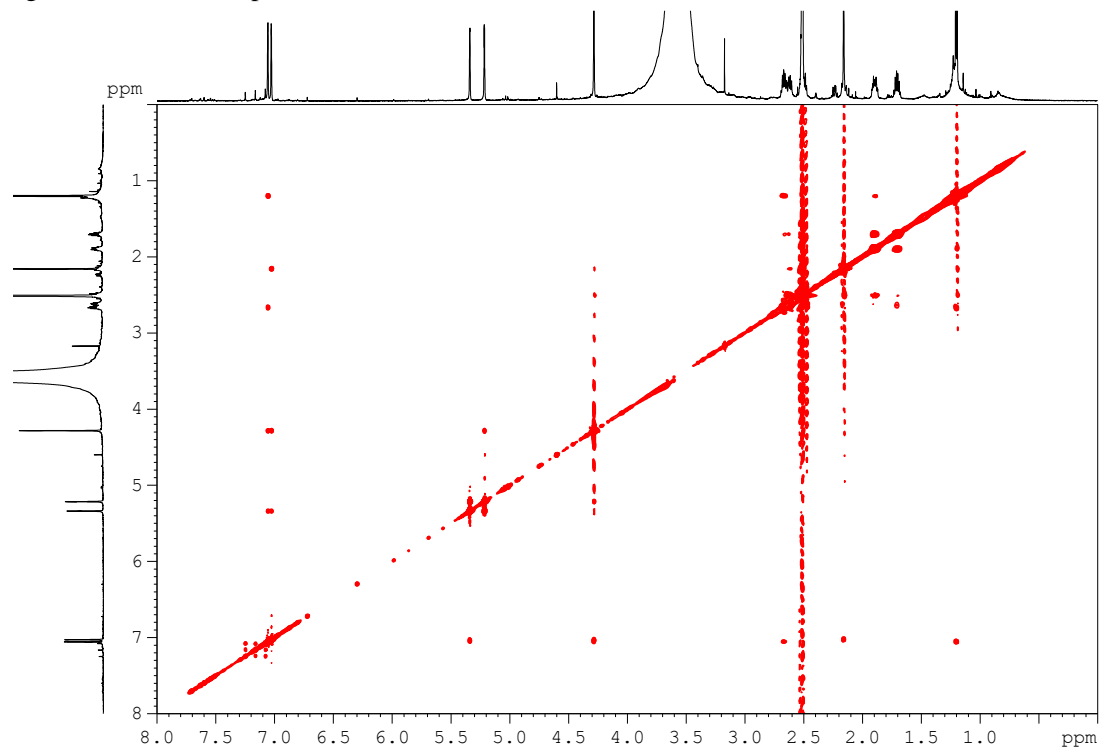
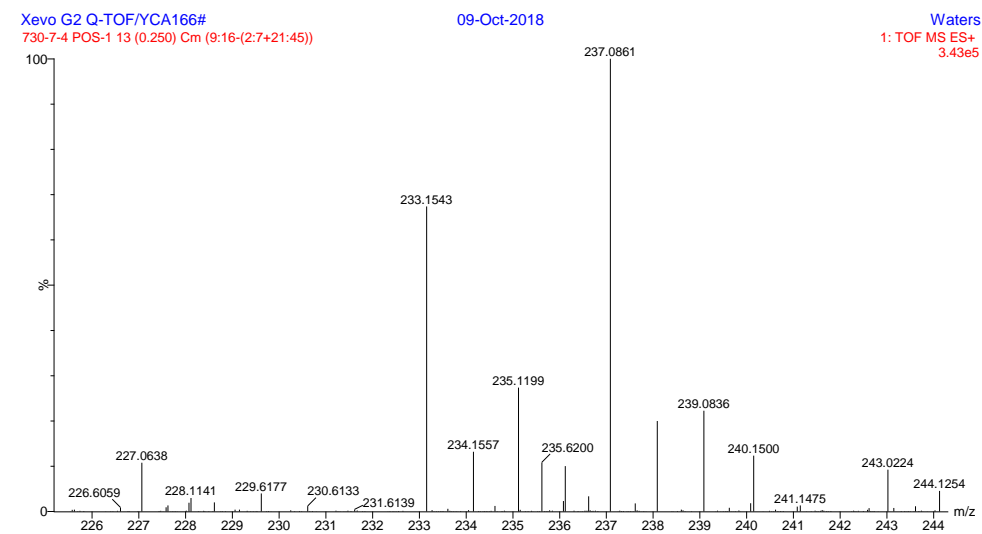


Figure S16. HRESIMS spectrum of **2**



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
233.1543	233.1542	0.1	0.4	5.5	430.1	n/a	n/a	C <sub>15</sub> H <sub>21</sub> O <sub>2</sub>

Figure S17. IR spectrum of **3**

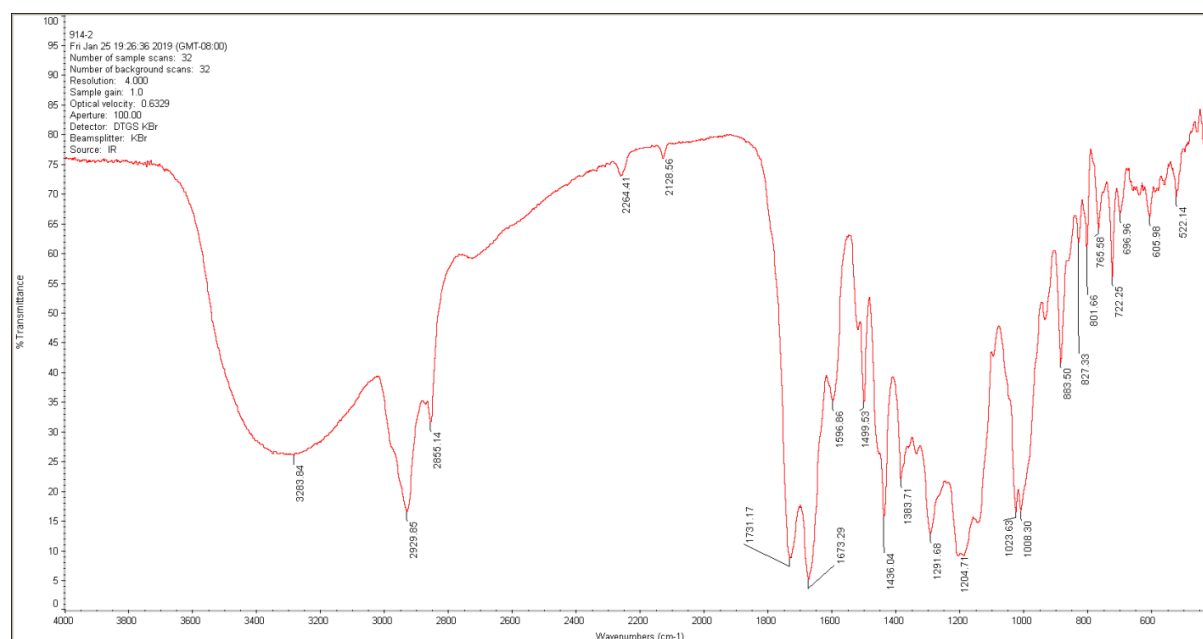




Figure S18.  $^1\text{H}$  NMR (600 MHz) spectrum of **3** in  $\text{DMSO}-d_6$

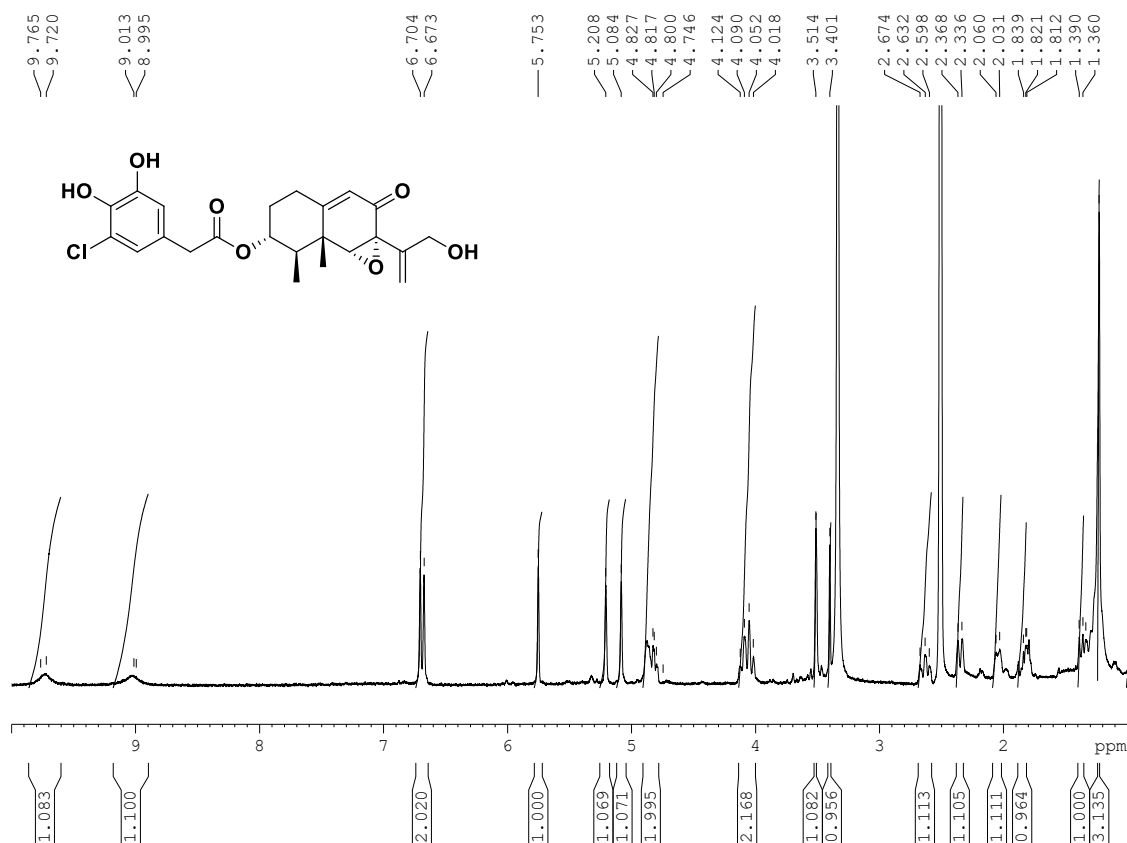


Figure S19.  $^{13}\text{C}$  NMR (150 MHz) spectrum of **3** in  $\text{DMSO}-d_6$

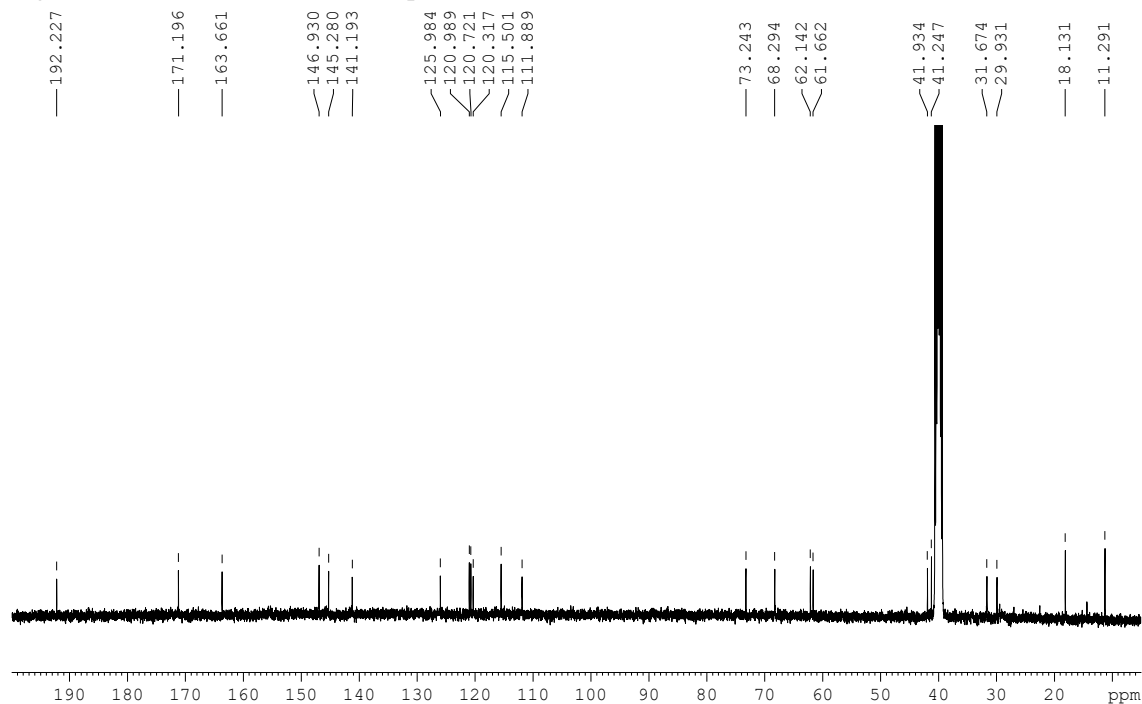


Figure S20. DEPT spectrum of **3** in DMSO-*d*<sub>6</sub>

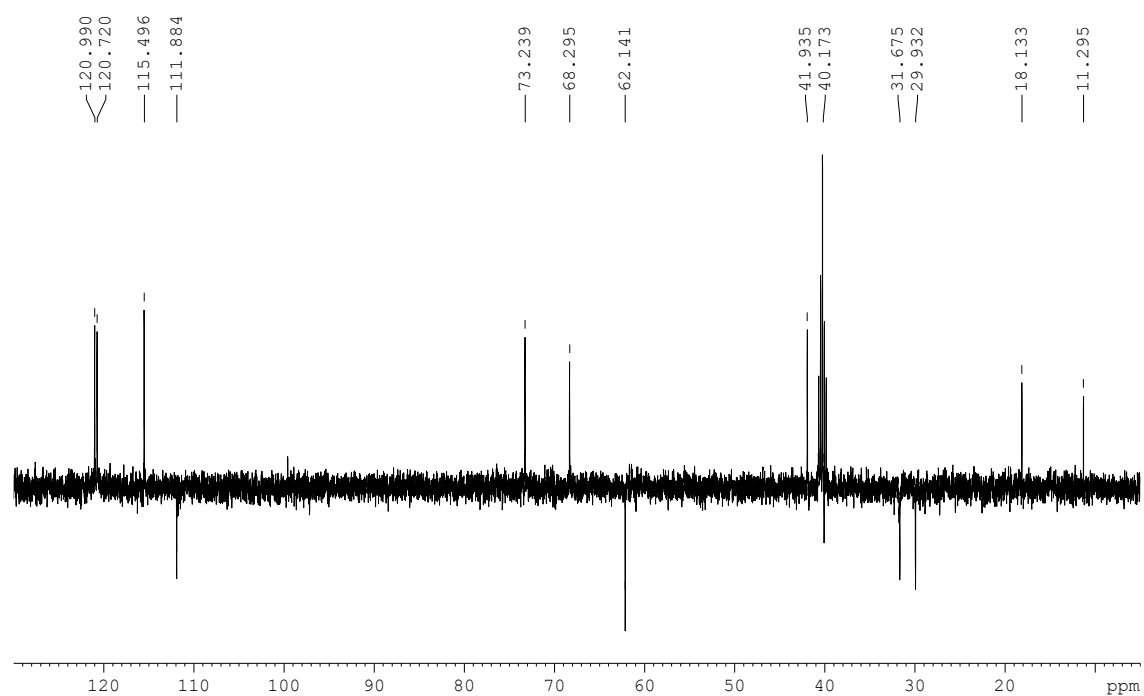


Figure S21. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **3** in DMSO-*d*<sub>6</sub>

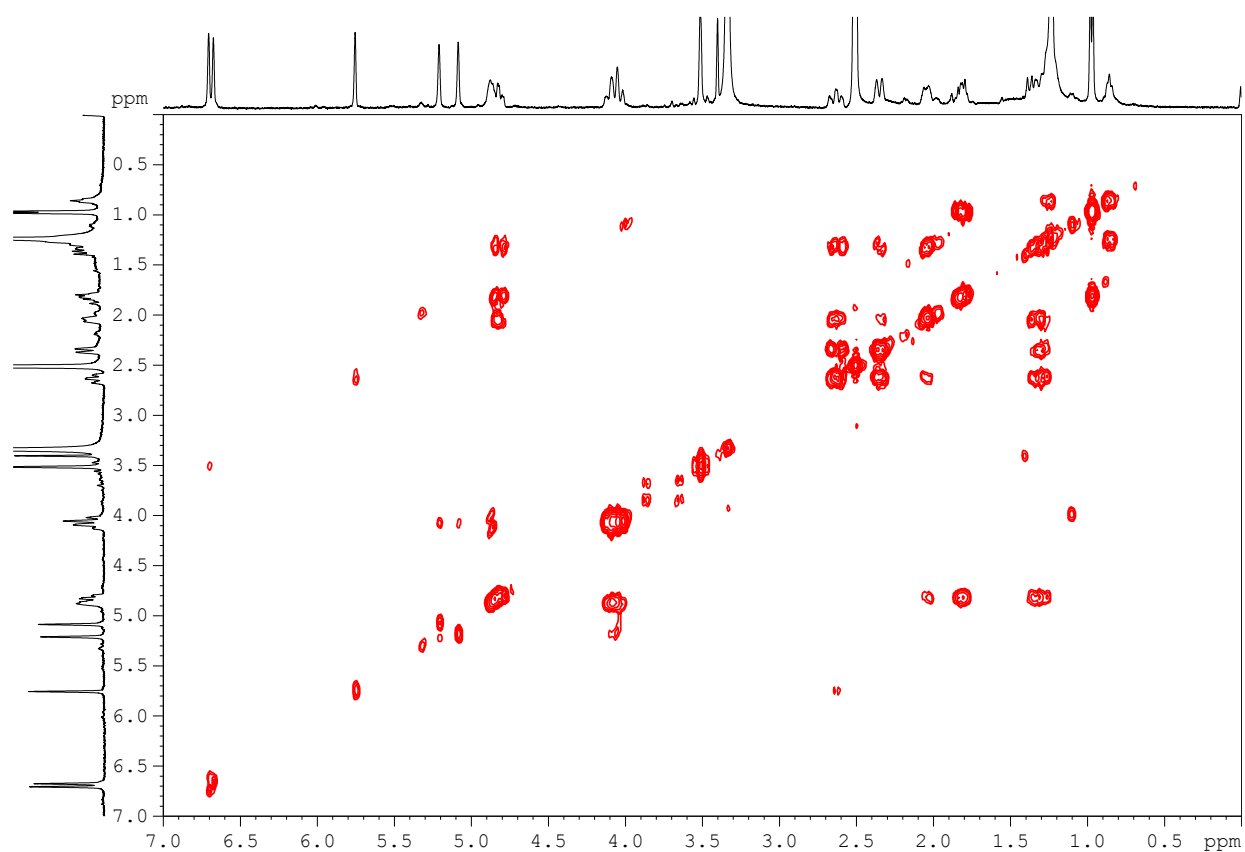


Figure S22. HSQC spectrum of **3** in DMSO-*d*<sub>6</sub>

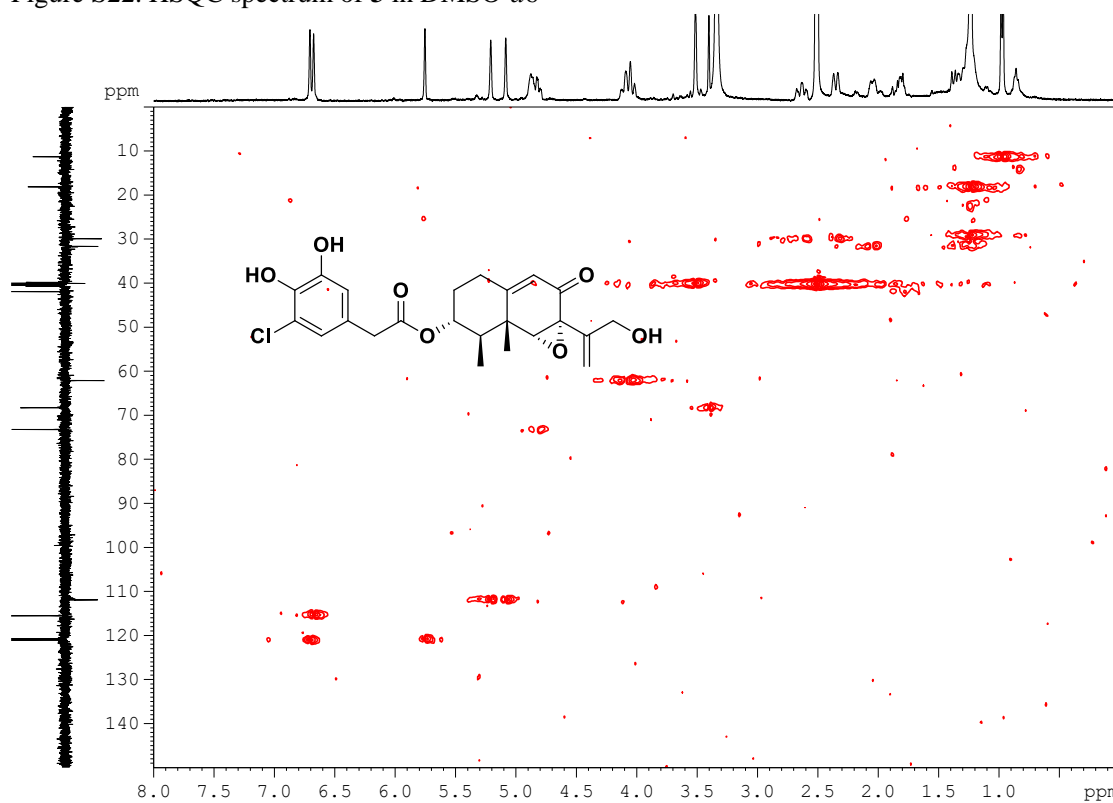


Figure S23. HMBC spectrum of **3** in DMSO-*d*<sub>6</sub>

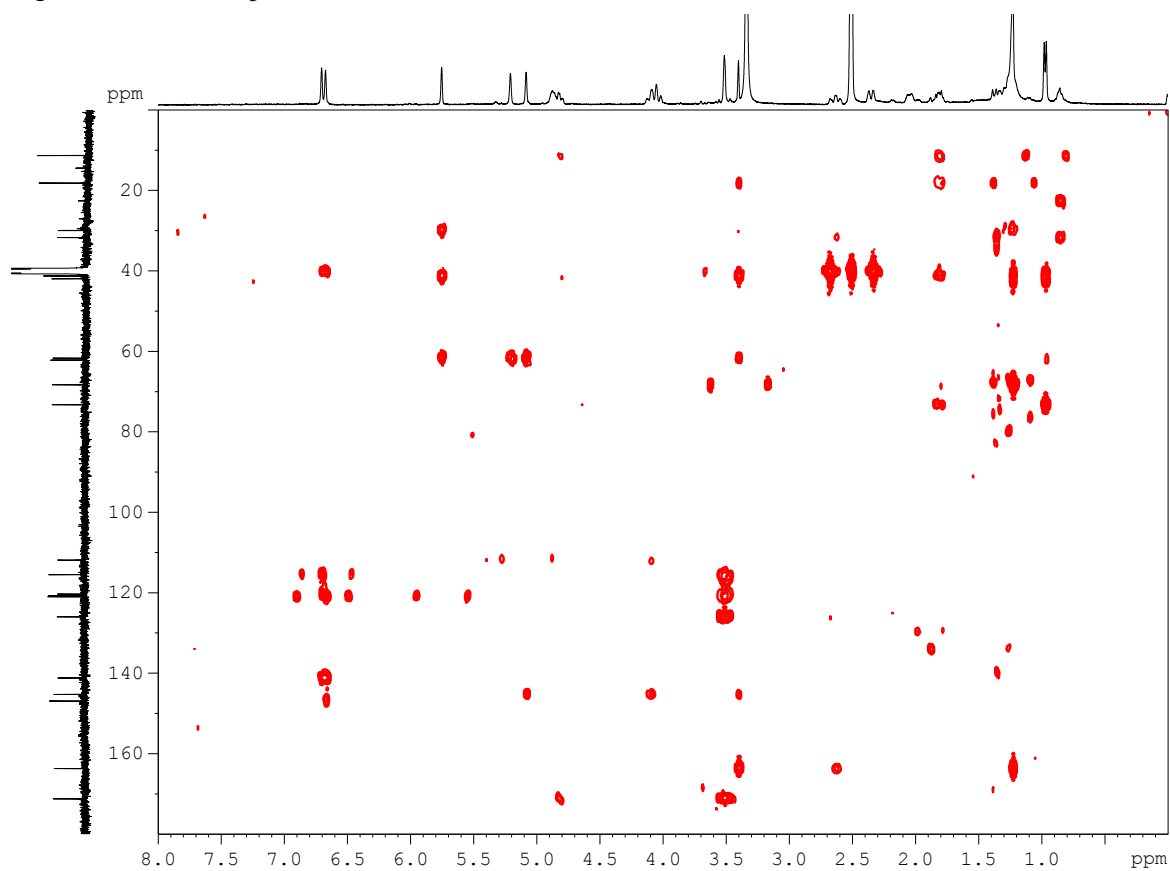


Figure S24. NOESY spectrum of **3** in DMSO-*d*<sub>6</sub>

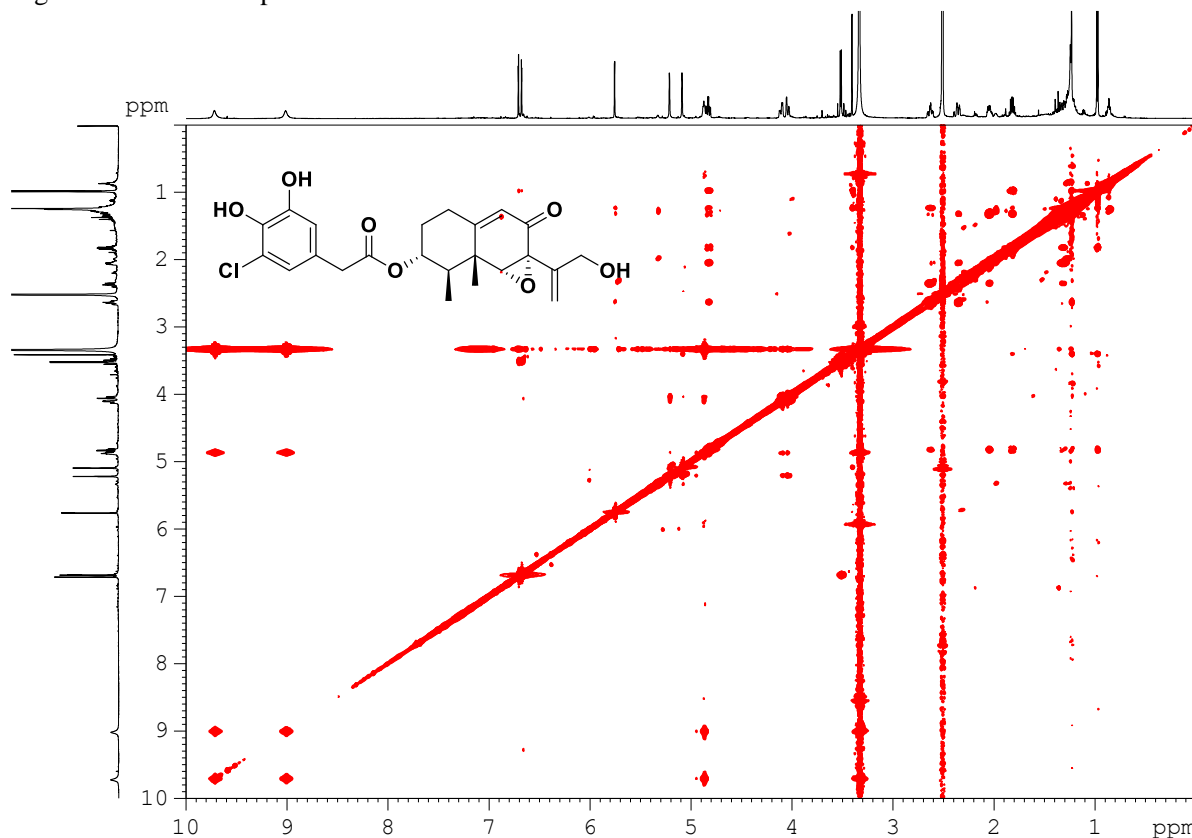
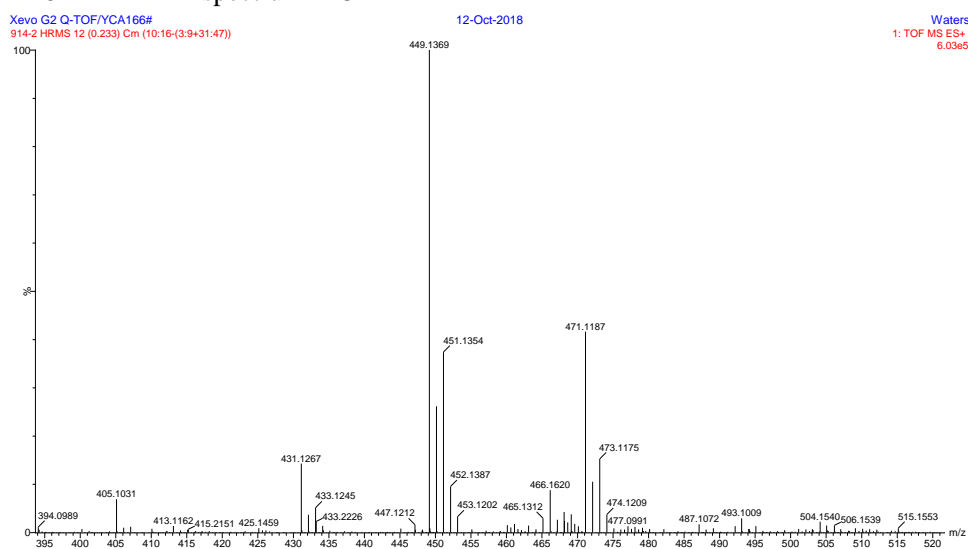


Figure S25. HRESIMS spectrum of **3**



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
449.1369	449.1367	0.2	0.4	2.5	278.2	0.023	97.68	C <sub>23</sub> H <sub>26</sub> O <sub>7</sub> Cl

10-3-7  
 Fri Jan 25 20:47:49 2019 (GMT-08:00)  
 Number of sample scans: 32  
 Number of background scans: 32  
 Resolution: 4.000  
 Sample gain: 1.0  
 Optical velocity: 0.6329  
 Aperture: 100.00  
 Detector: DTGS KBr  
 Beamsplitter: KBr  
 Source: IR

Wavenumber (cm⁻¹)
3260.84
2941.98
2297.38
2128.56
1732.28
1670.29
1596.65
1521.78
1500.08
1435.37
1359.21
1291.67
1205.35
1025.33
1000.54
881.35
827.76
801.16
765.09
721.79
699.42
608.10
524.74

Chemical structure of compound 10 is shown above the spectrum. The structure is a complex polycyclic molecule with a hydroxyl group, a ketone, and a chlorophenyl group.

<sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>) of compound 10. The x-axis represents the chemical shift in ppm, ranging from 0 to 10. The spectrum shows several peaks, with integration values provided below the baseline and chemical shift values labeled above the peaks.

Integration values (from left to right): 1.000, 1.021, 2.088, 0.996, 2.063, 2.098, 2.012, 1.018, 3.068, 3.085, 0.500, 0.504, 1.151, 1.099, 1.091, 2.094, 6.104.

Chemical shift values (from left to right): 9.741, 9.021, 6.631, 6.614, 5.702, 5.366, 5.293, 4.691, 4.661, 3.469, 3.429, 3.416, 3.378, 3.176, 2.545, 2.533, 2.509, 2.476, 2.462, 2.280, 2.244, 1.993, 1.964, 1.567, 1.551, 1.535, 1.527, 1.510, 1.493, 1.252, 1.242.

Figure S28.  $^{13}\text{C}$  NMR (150 MHz) and DEPT spectra of **4** in  $\text{DMSO-}d_6$

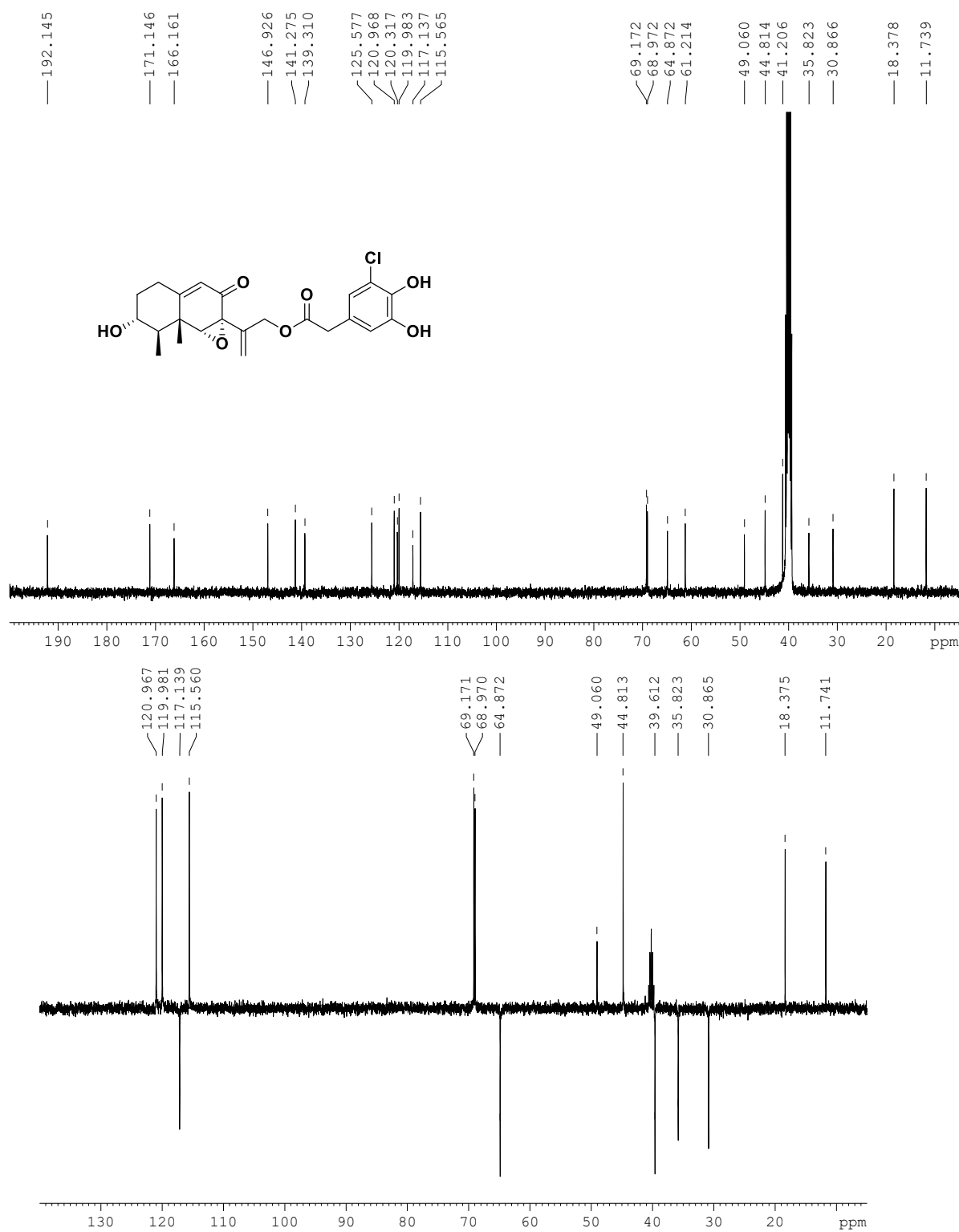


Figure S29.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **4** in  $\text{DMSO-}d_6$

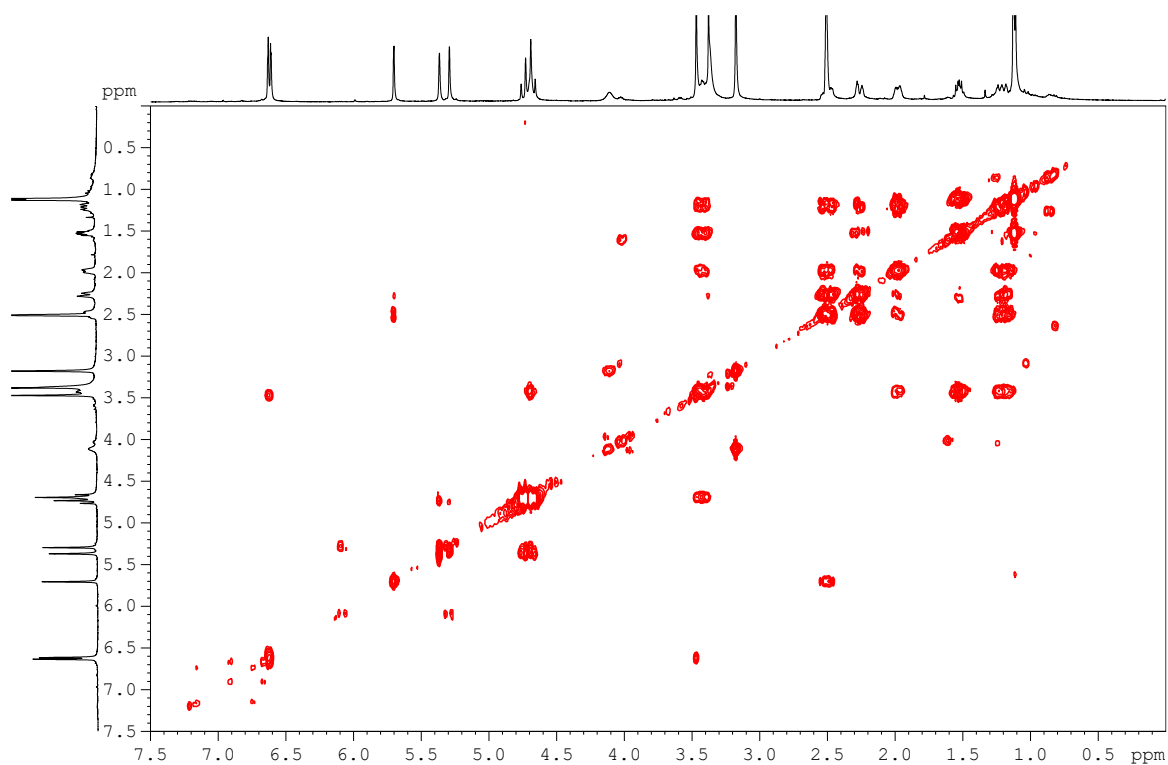


Figure S30. HSQC spectrum of **4** in  $\text{DMSO-}d_6$

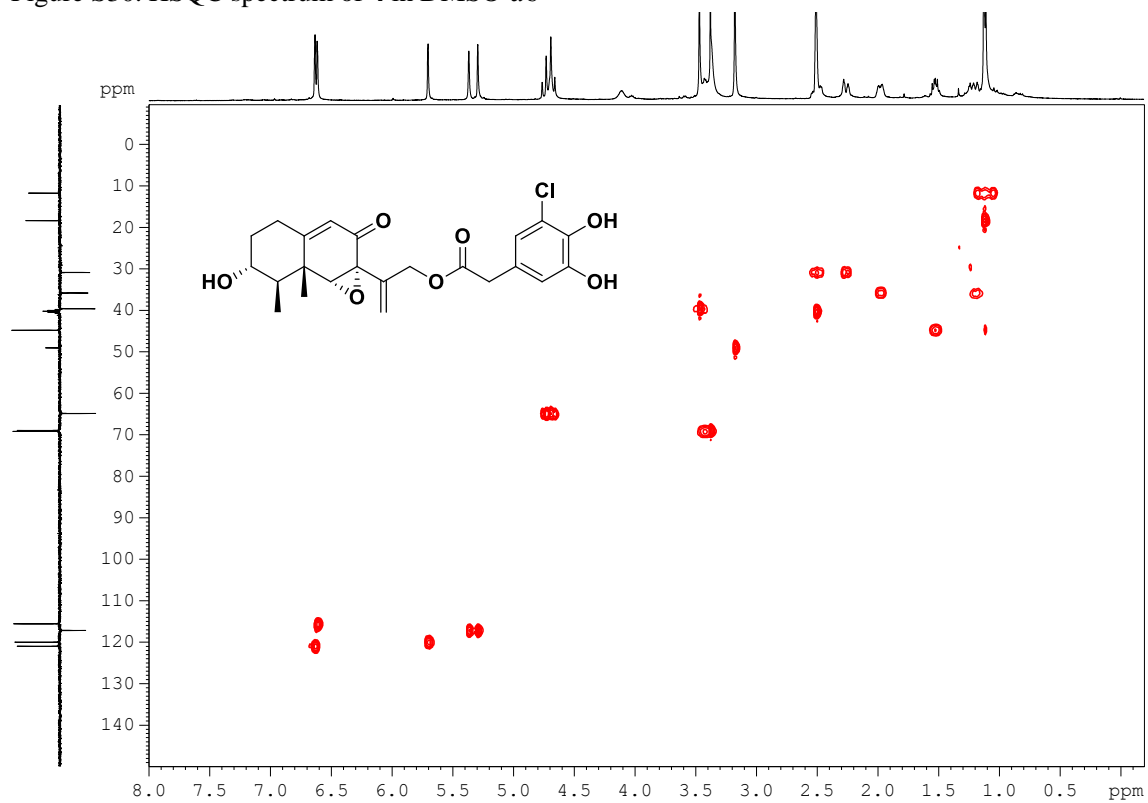


Figure S31. HMBC spectrum of **4** in DMSO-*d*<sub>6</sub>

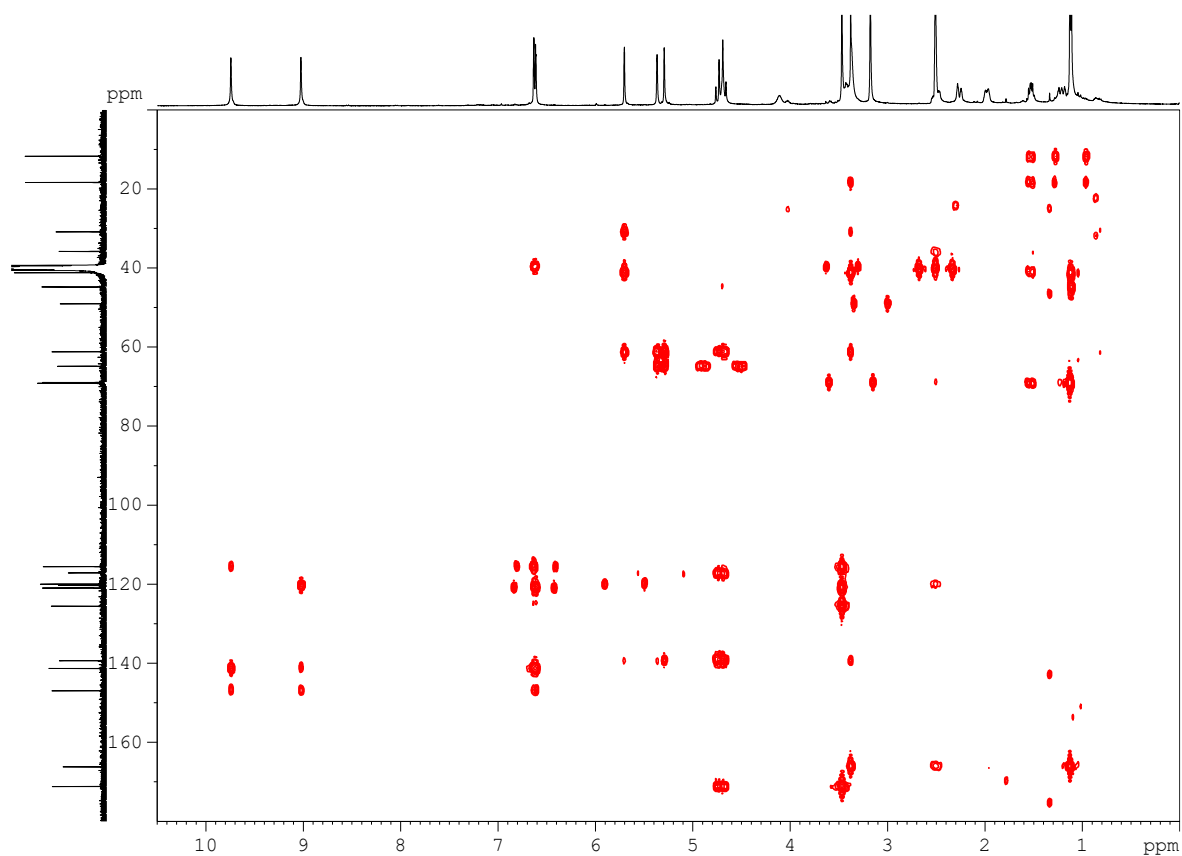


Figure S32. NOESY spectrum of **4** in DMSO-*d*<sub>6</sub>

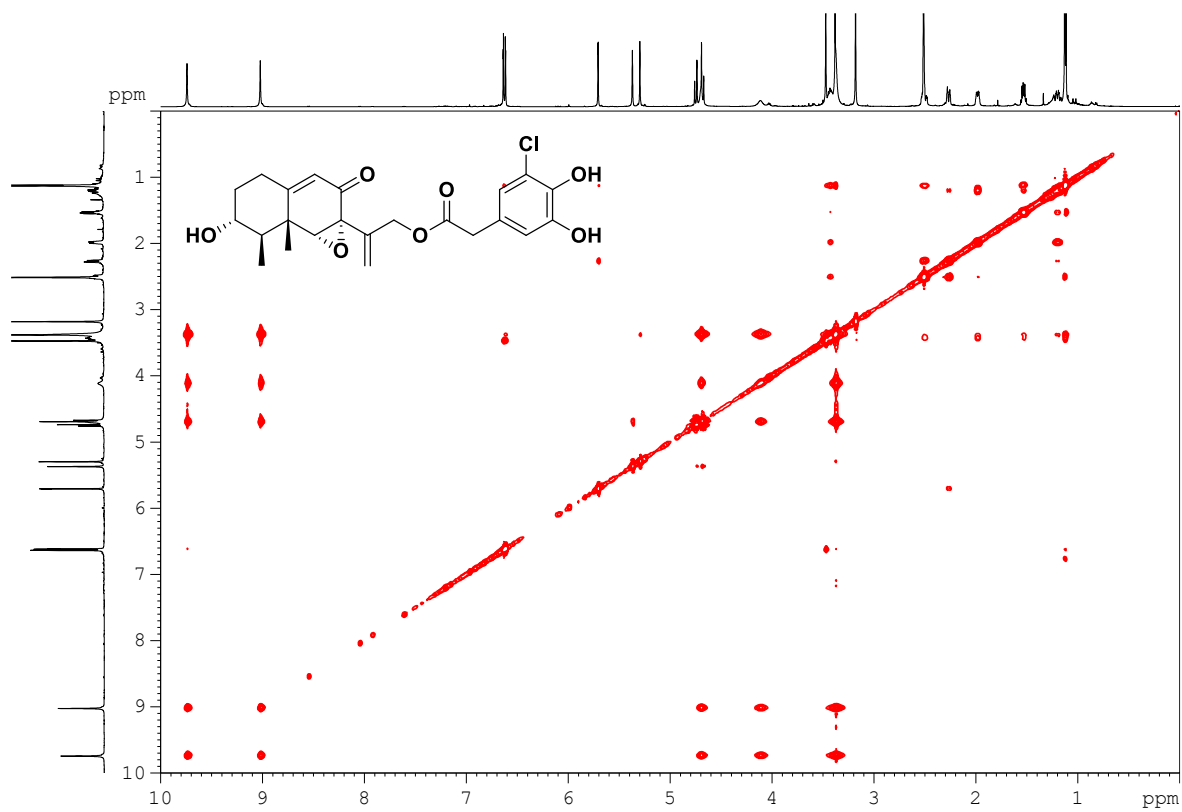
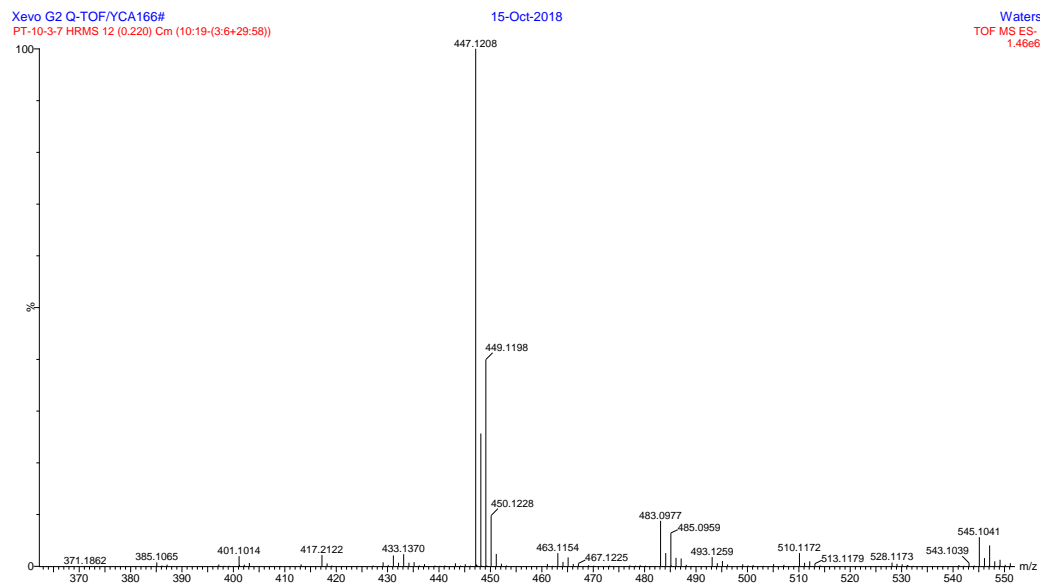




Figure S33. HRESIMS spectrum of **4**



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
447.1208	447.1211	-0.3	-0.7	11.5	419.8	0.000	100.00	C <sub>23</sub> H <sub>24</sub> O <sub>7</sub> Cl

Figure S34. IR spectrum of **5**

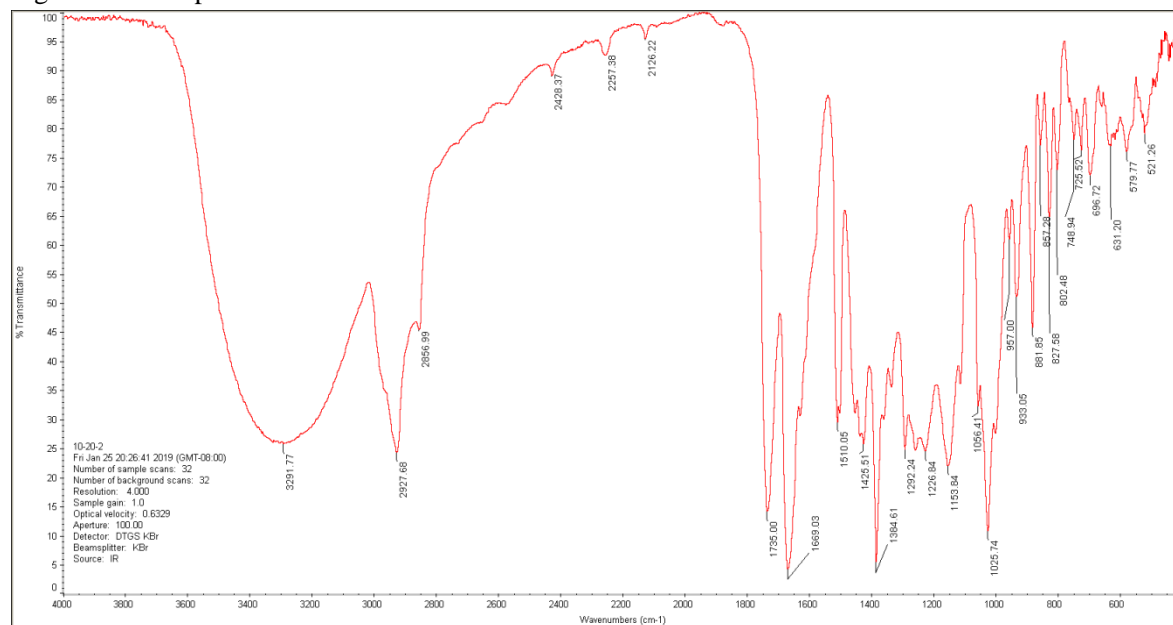


Figure S35.  $^1\text{H}$  NMR (600 MHz) spectrum of **5** in  $\text{DMSO}-d_6$

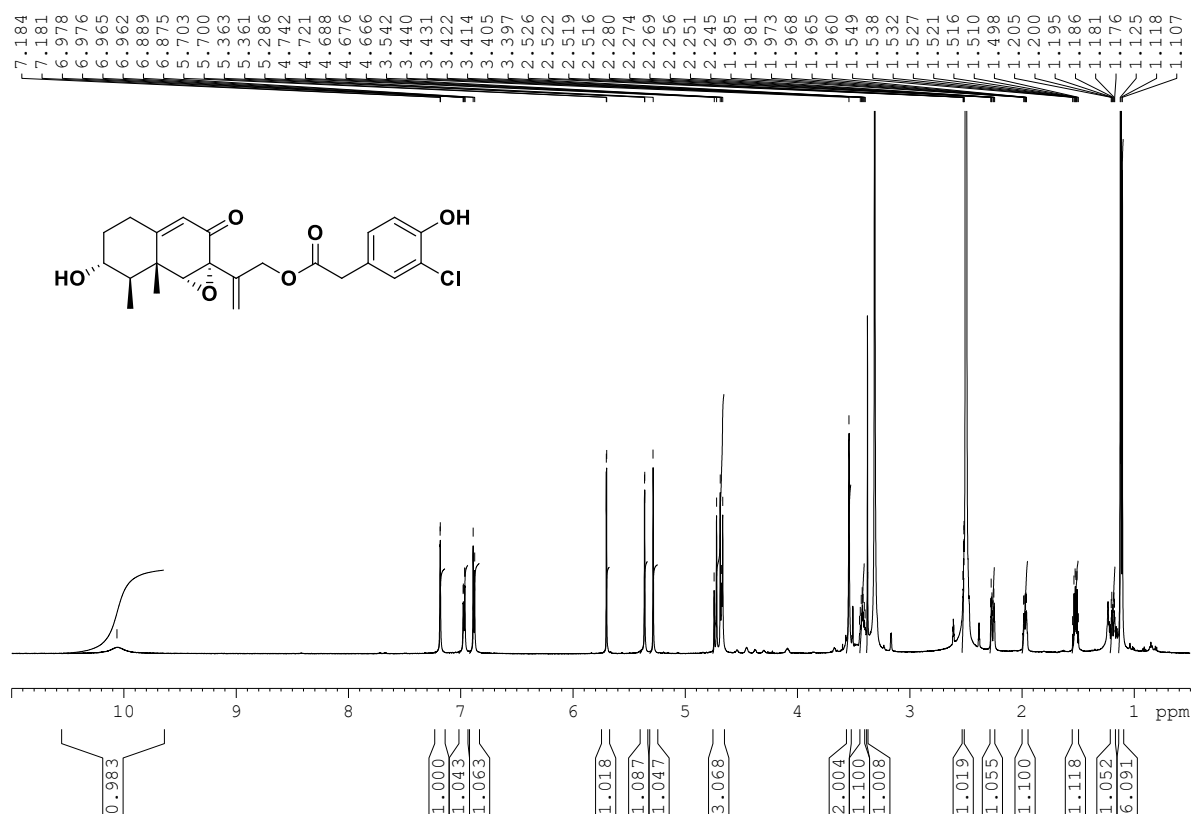


Figure S36.  $^{13}\text{C}$  NMR (150 MHz) spectrum of **5** in  $\text{DMSO}-d_6$

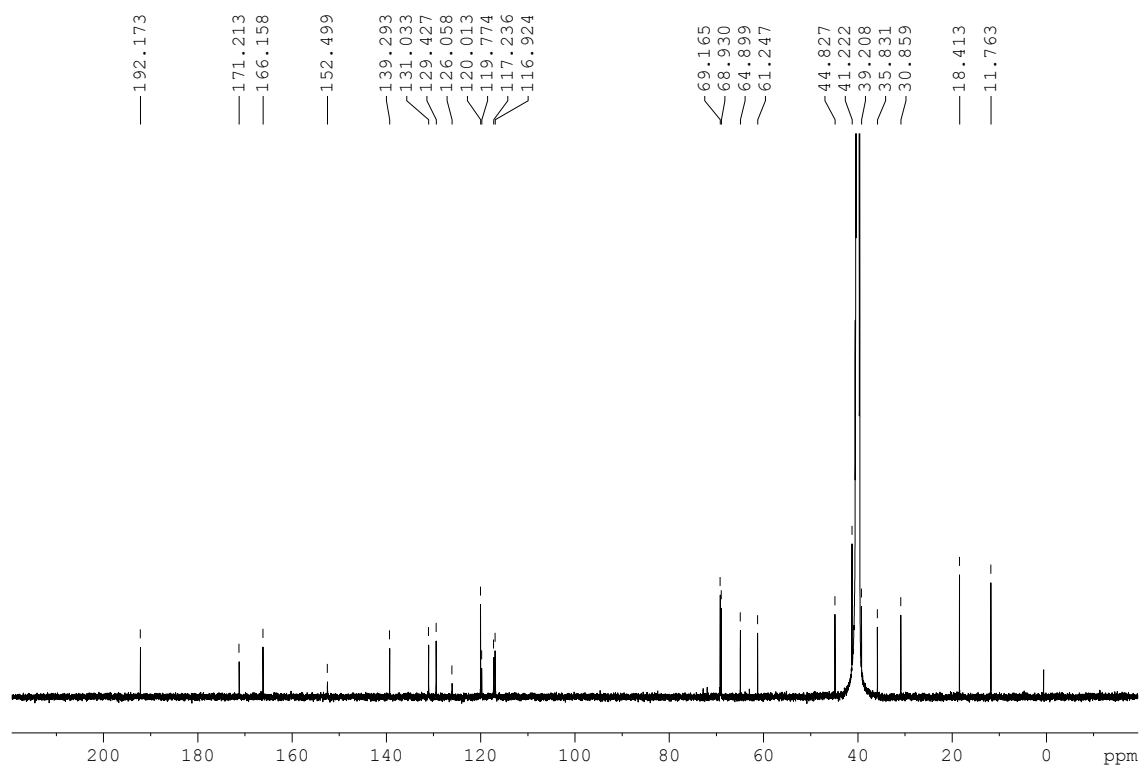


Figure S37. DEPT spectrum of **5** in DMSO-*d*<sub>6</sub>

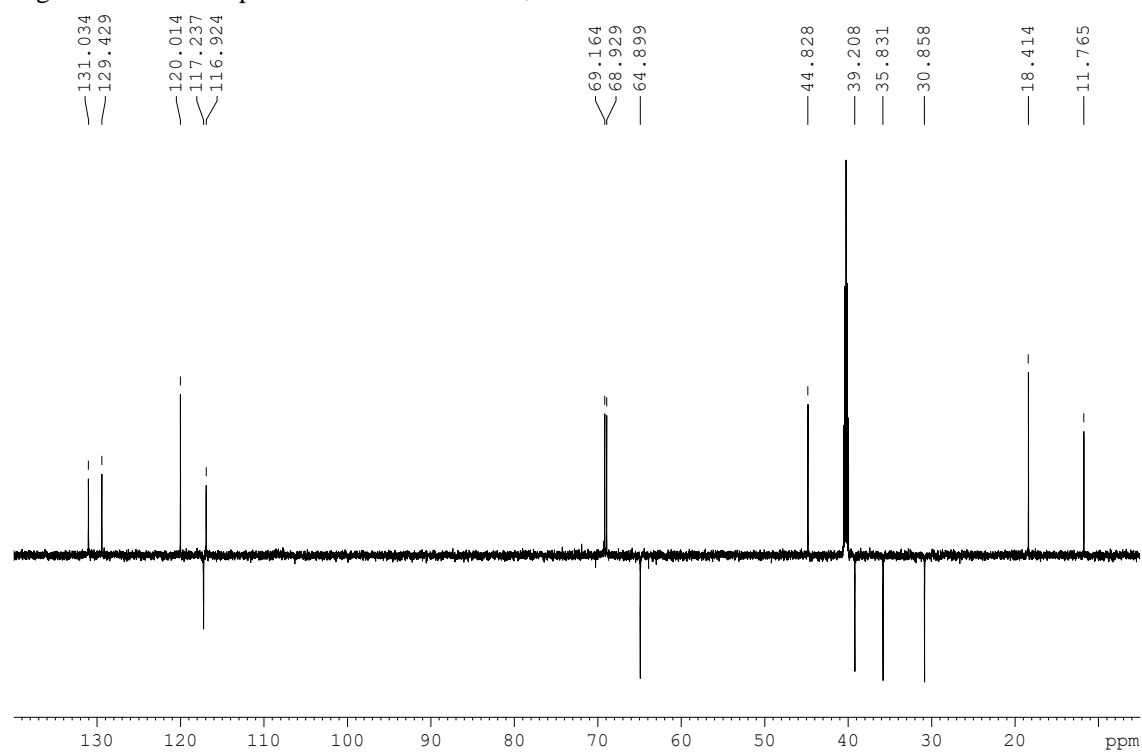


Figure S38. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **5** in DMSO-*d*<sub>6</sub>

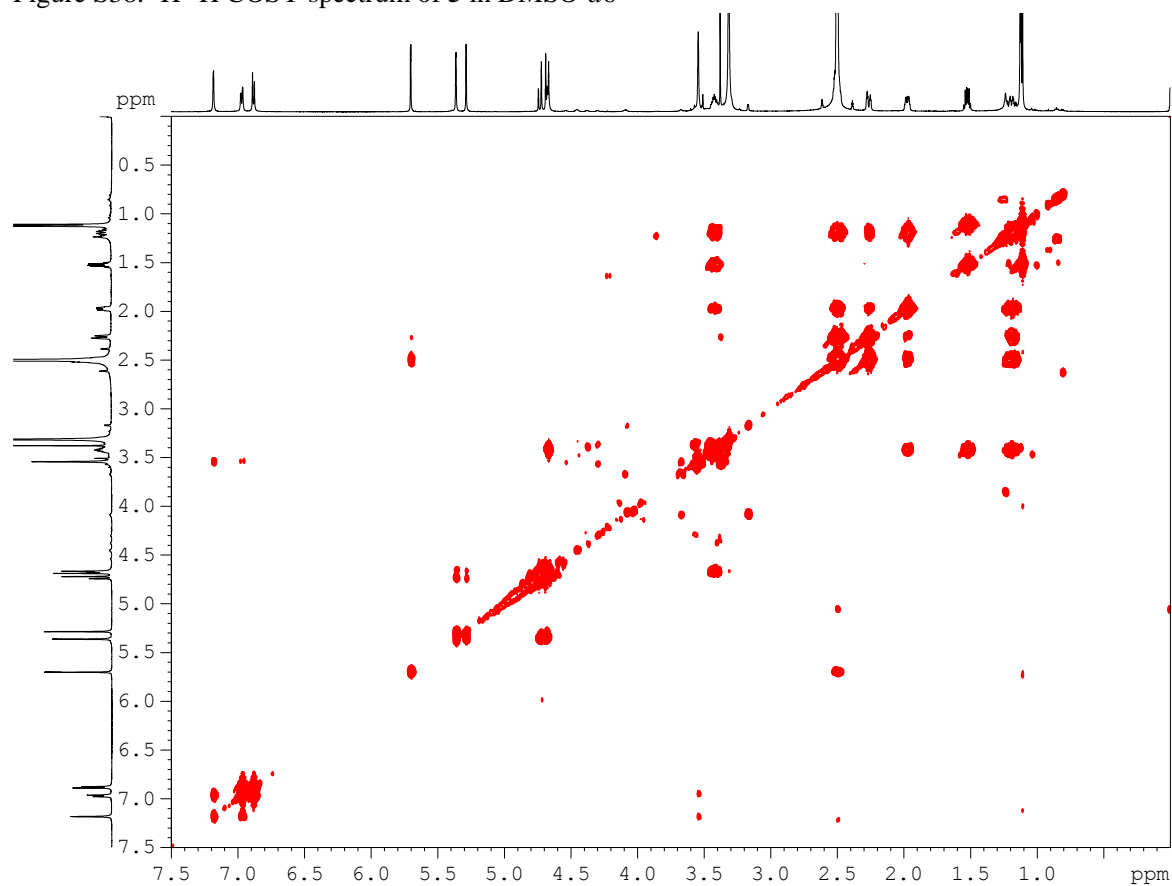


Figure S39. HSQC spectrum of **5** in DMSO-*d*<sub>6</sub>

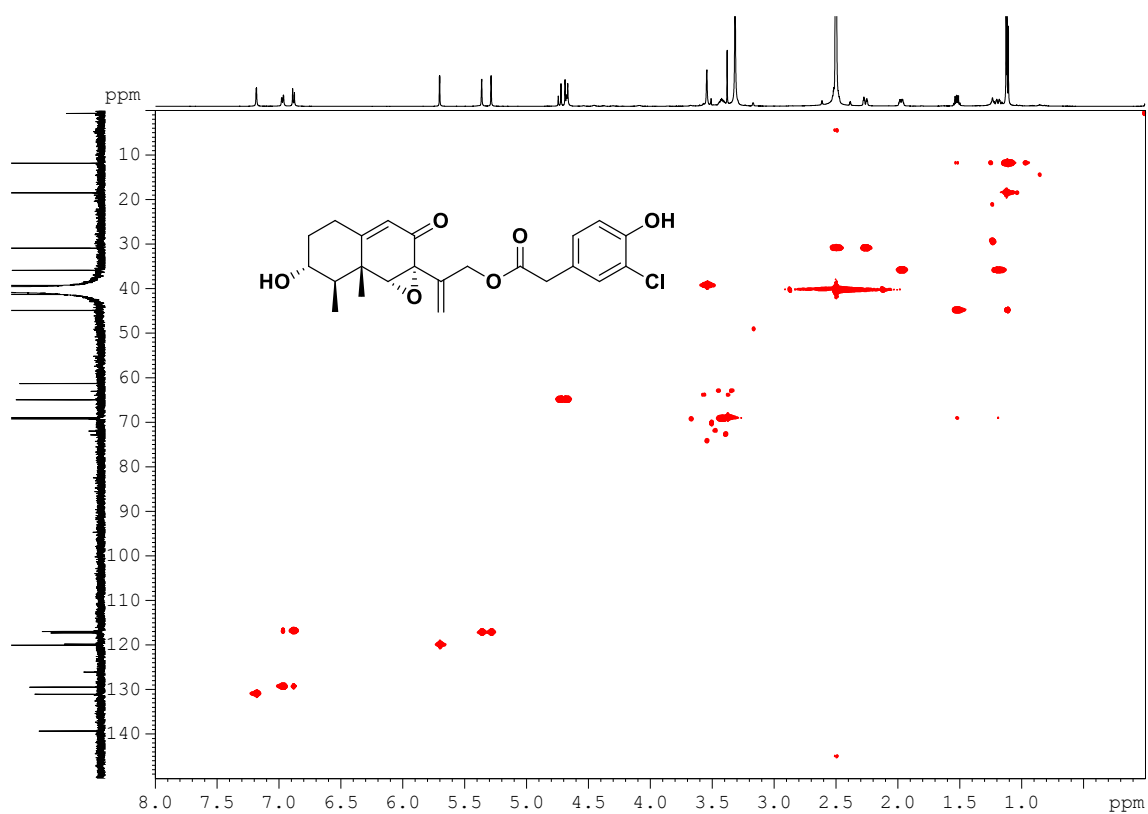


Figure S40. HMBC spectrum of **5** in DMSO-*d*<sub>6</sub>

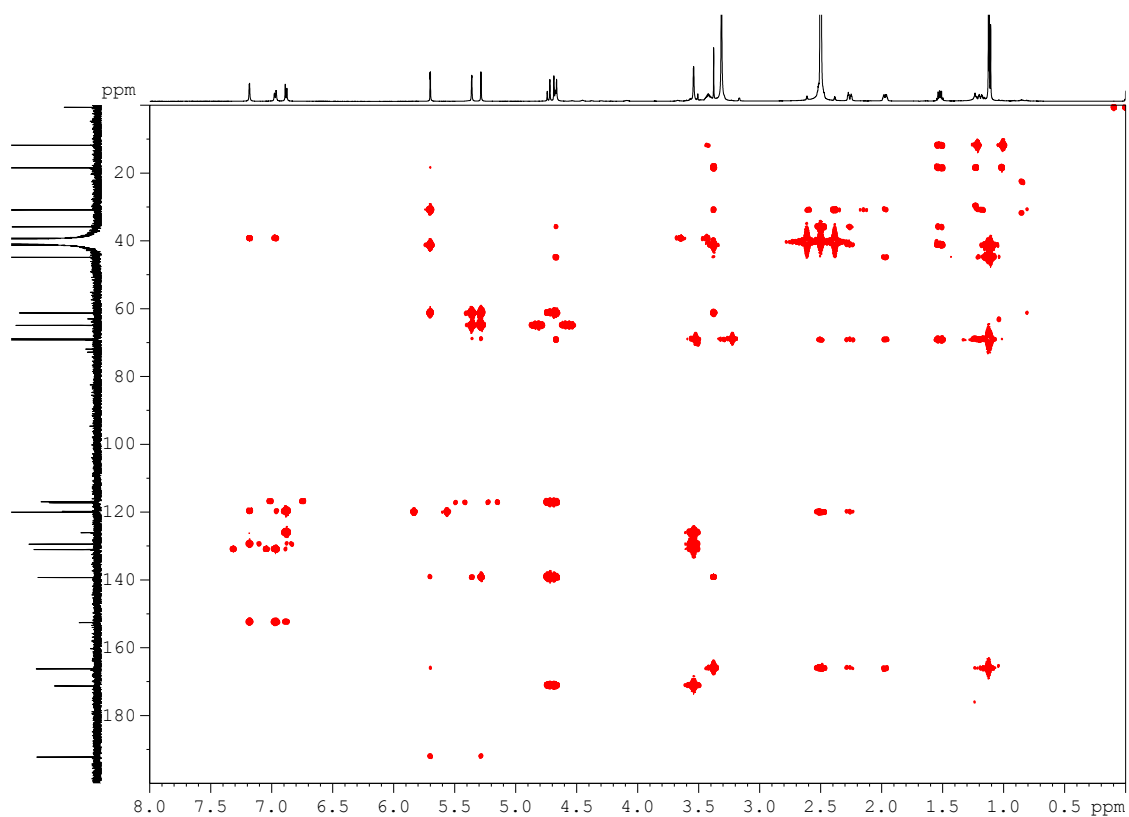


Figure S41. NOESY spectrum of **5** in DMSO-*d*<sub>6</sub>

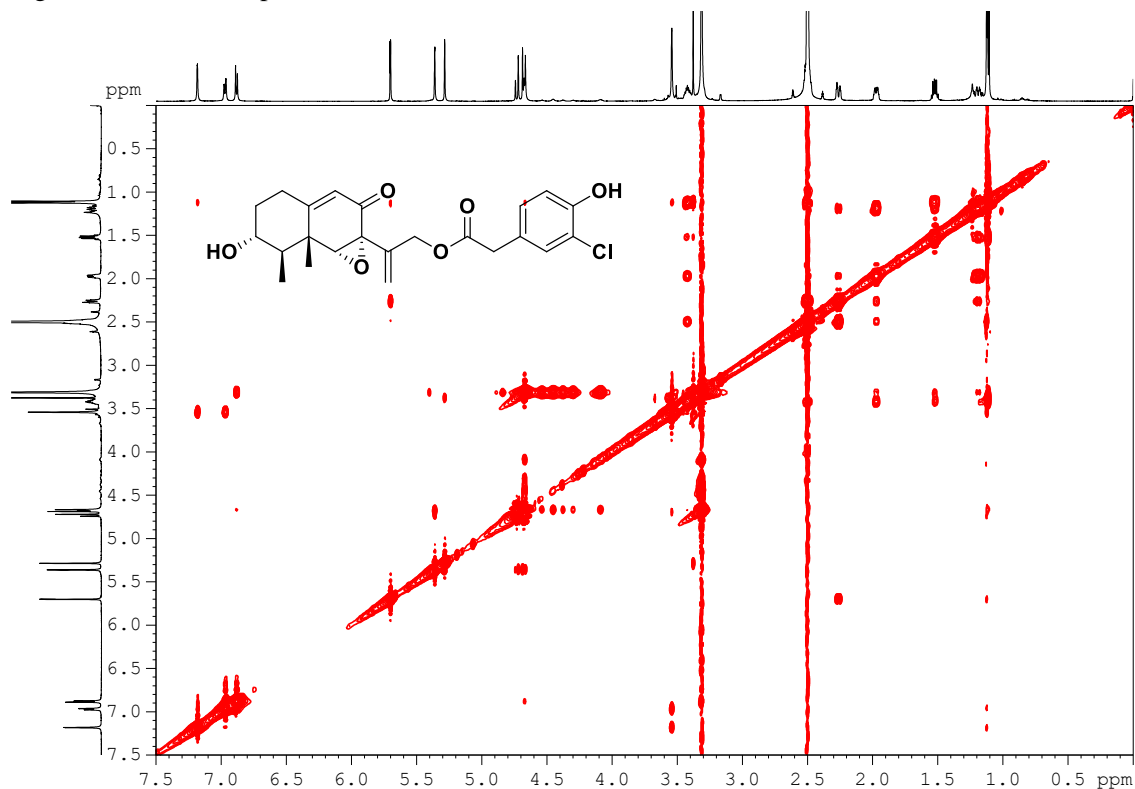
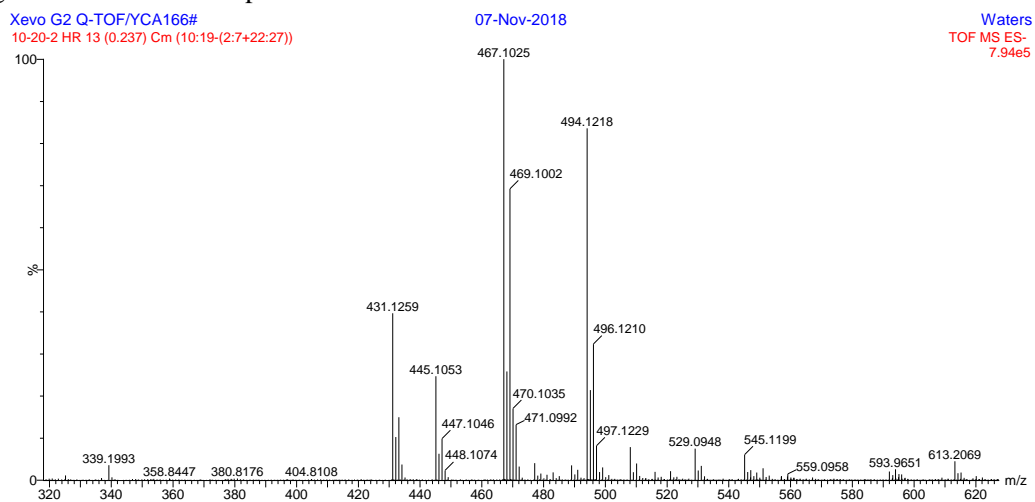


Figure S42. HRESIMS spectrum of **5**



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
431.1259	431.1261	-0.2	-0.5	11.5	369.5	0.000	100.00	C <sub>23</sub> H <sub>24</sub> O <sub>6</sub> Cl

Figure S43. IR spectrum of **6**

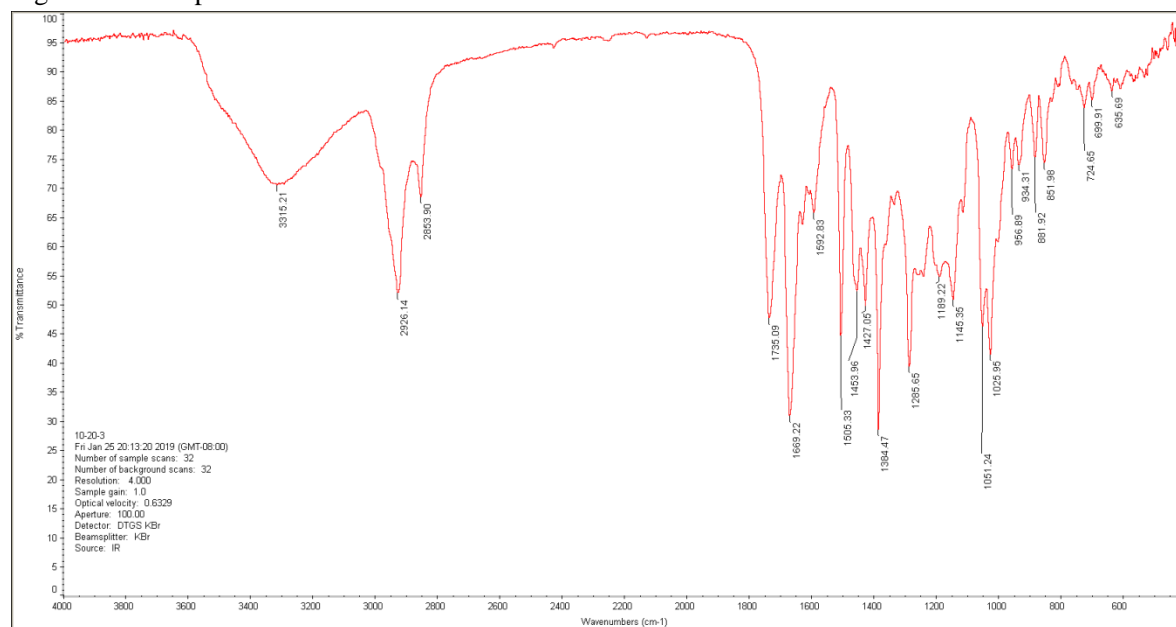


Figure S44. <sup>1</sup>H NMR (600 MHz) spectrum of **6** in DMSO-*d*<sub>6</sub>

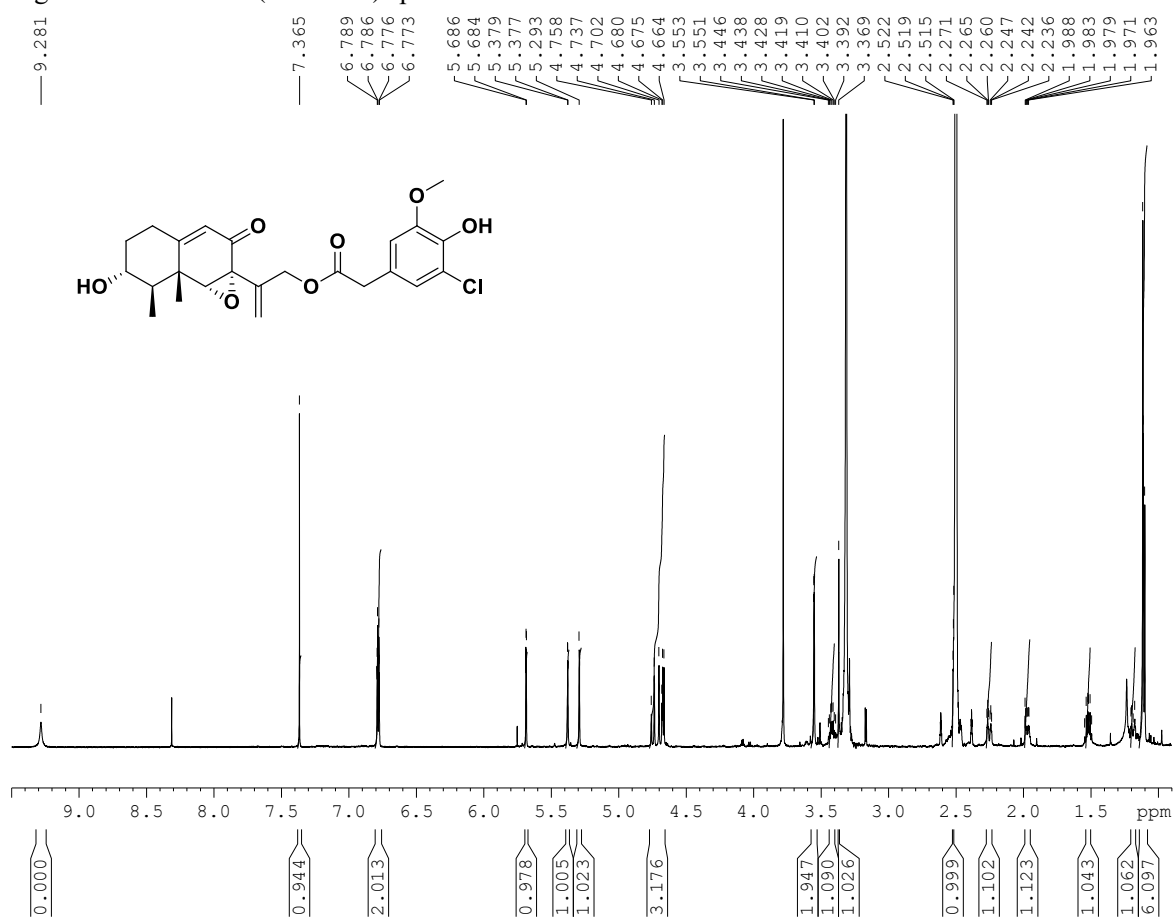


Figure S45.  $^{13}\text{C}$  NMR (150 MHz) and DEPT spectra of **6** in  $\text{DMSO}-d_6$

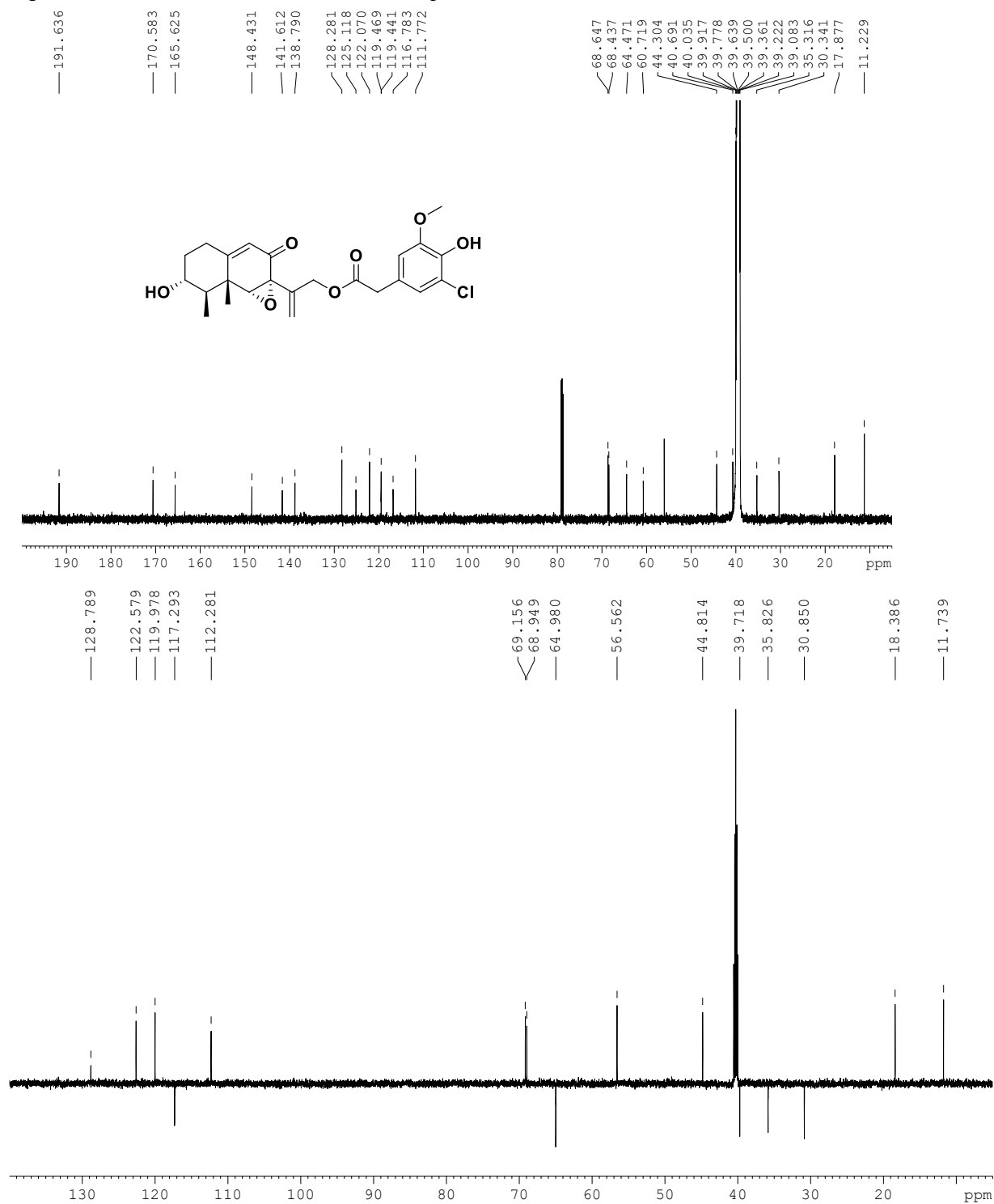


Figure S46.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **6** in  $\text{DMSO-}d_6$

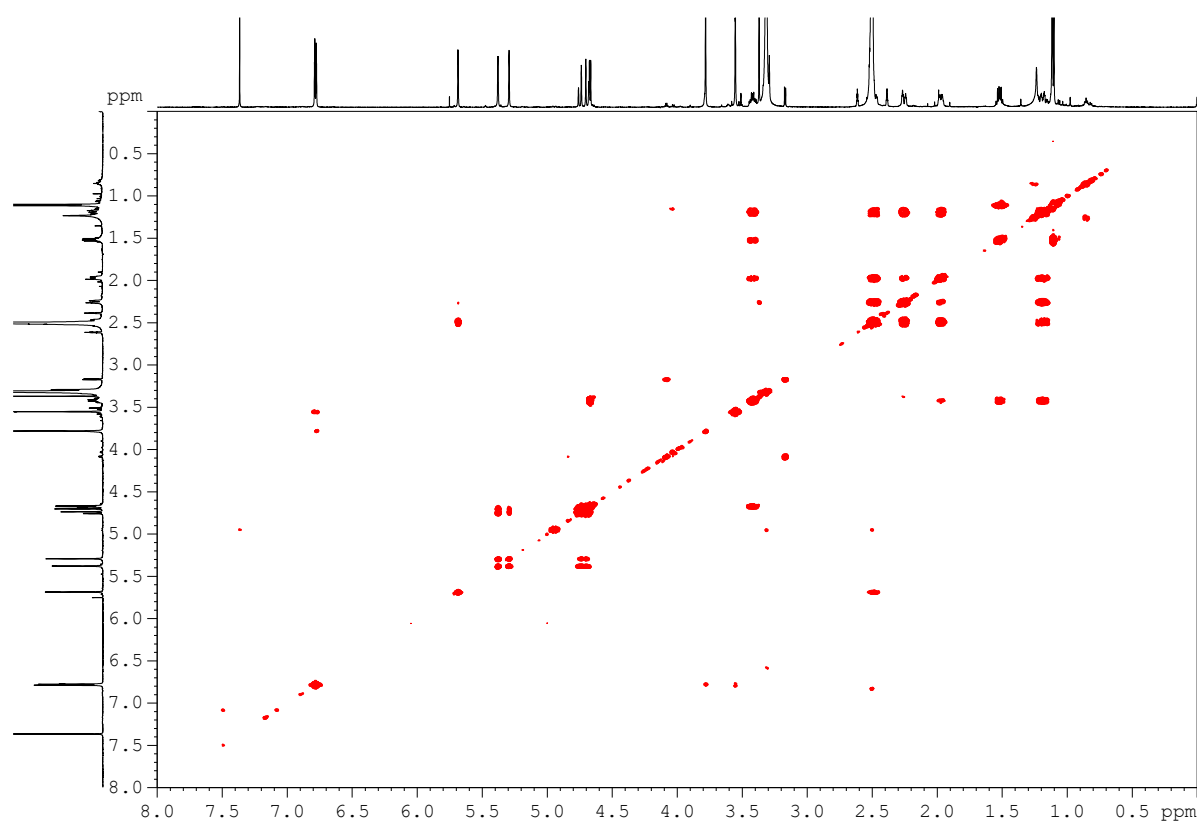


Figure S47. HSQC spectrum of **6** in  $\text{DMSO-}d_6$

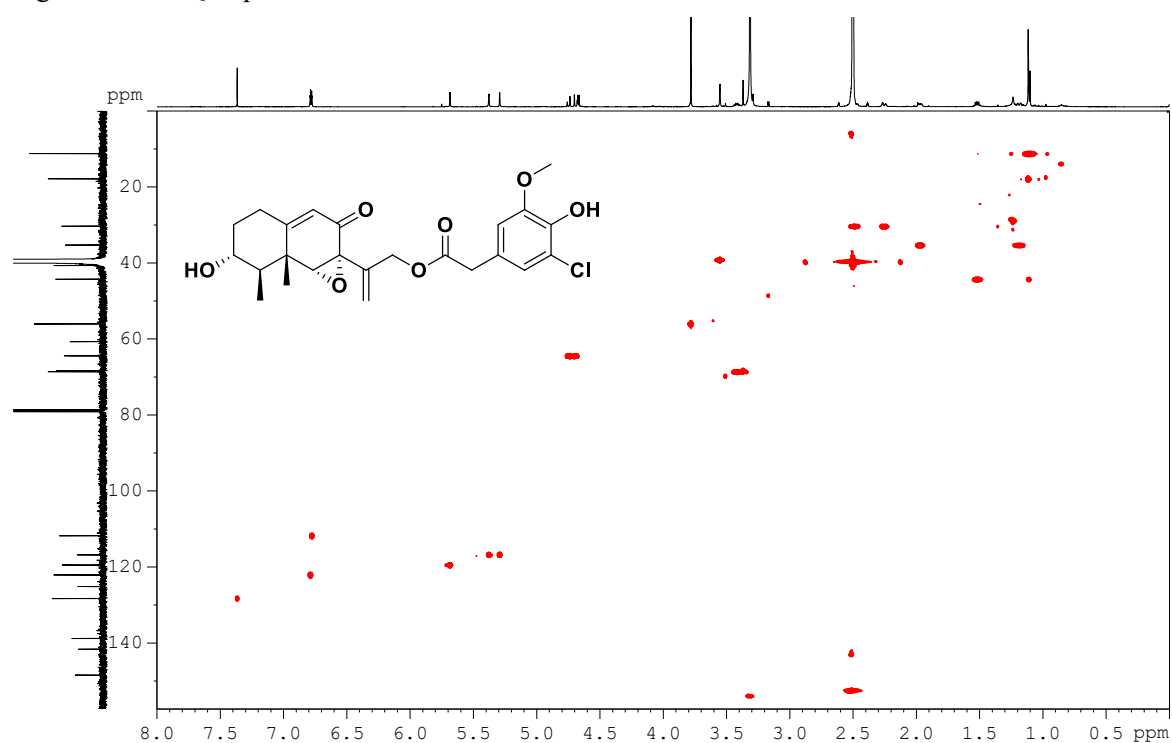




Figure S48. HMBC spectrum of **6** in DMSO-*d*<sub>6</sub>

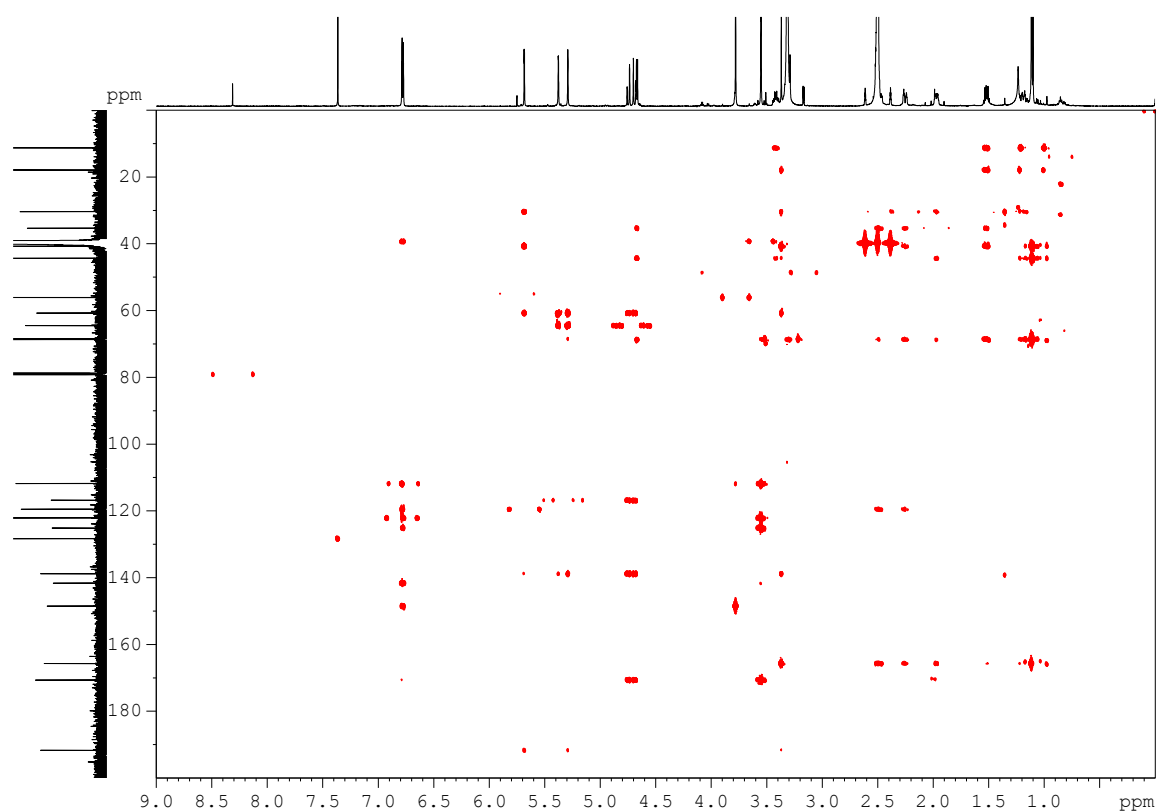


Figure S49. NOESY spectrum of **6** in DMSO-*d*<sub>6</sub>

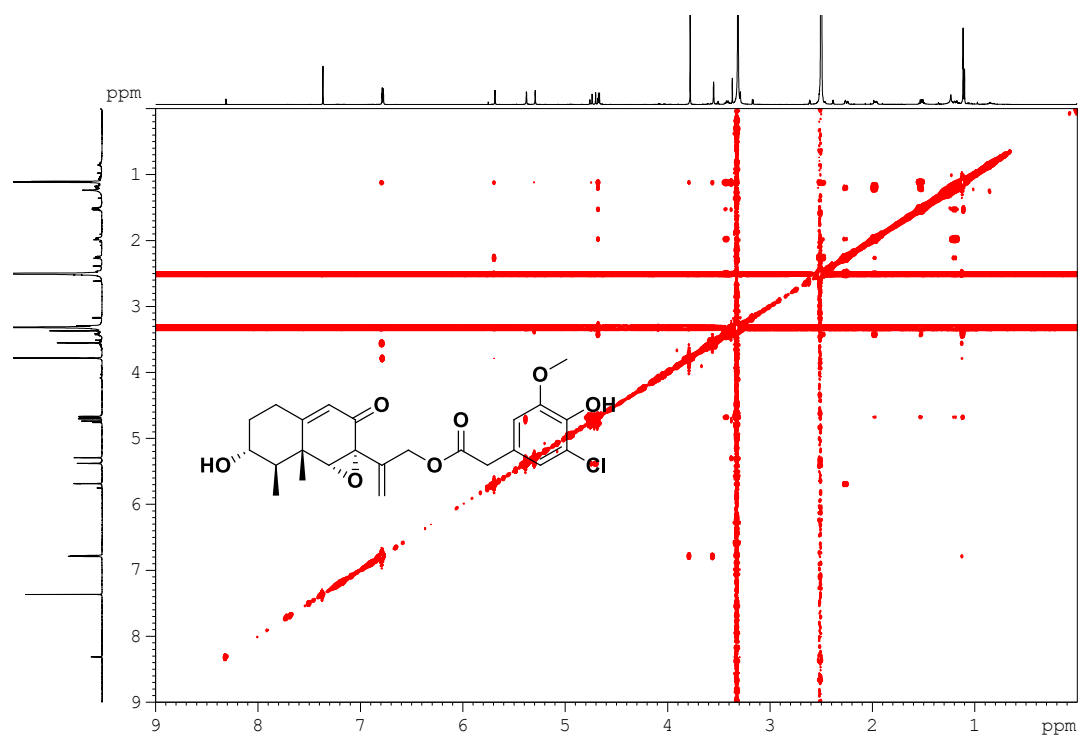
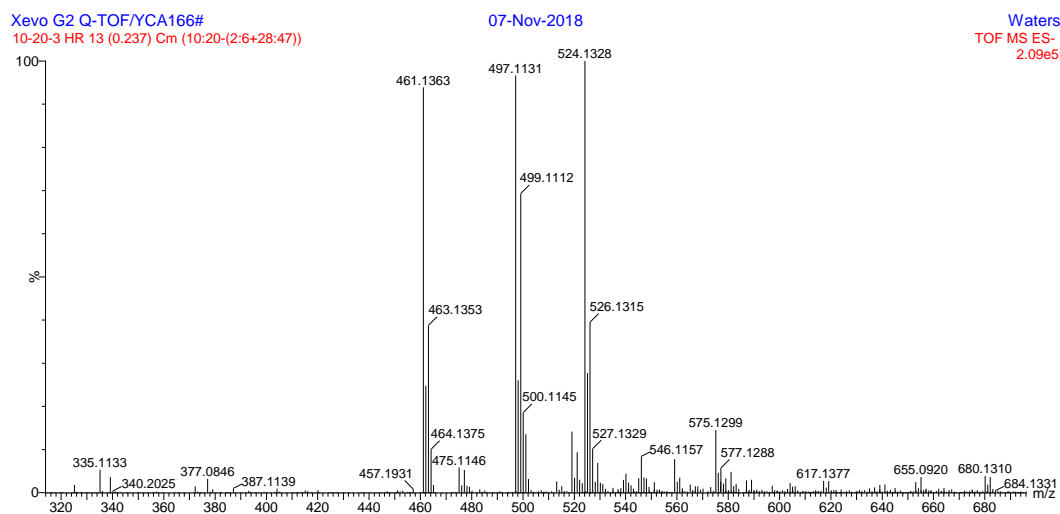


Figure S50. HRESIMS spectrum of **6**



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
461.1363	461.1367	-0.4	-0.9	11.5	185.3	0.000	100.00	C <sub>24</sub> H <sub>26</sub> O <sub>7</sub> Cl

Figure S51. IR spectrum of **7**

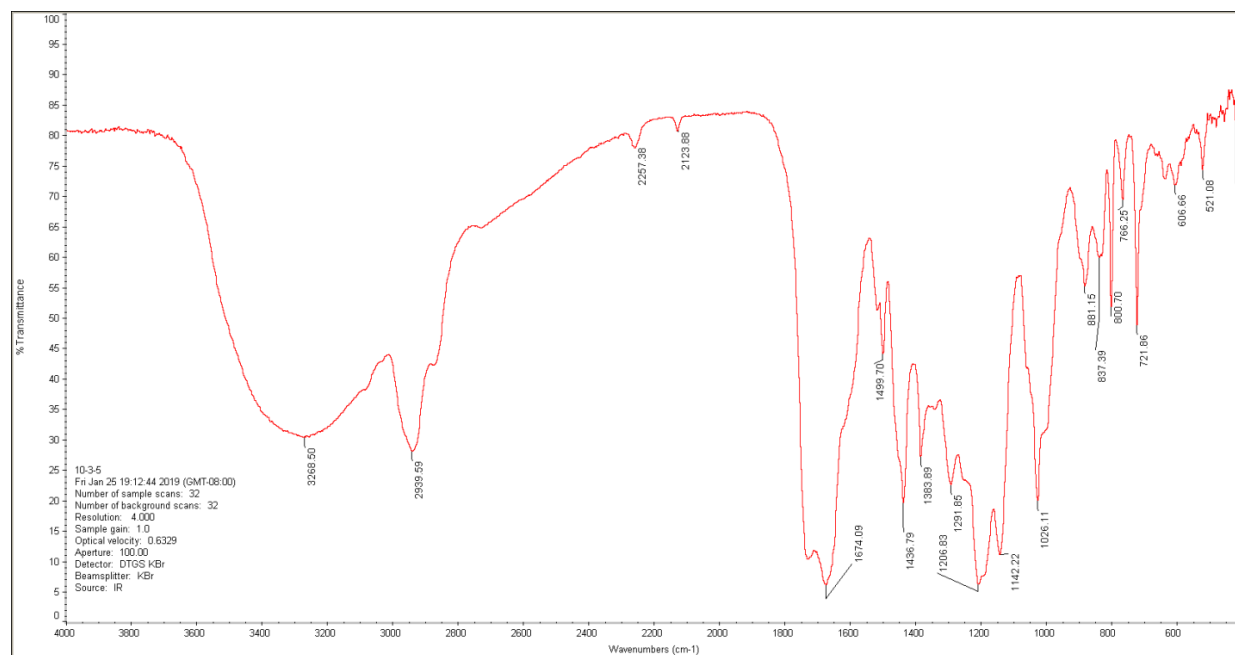


Figure S52.  $^1\text{H}$  NMR (600 MHz) spectrum of **7** in  $\text{DMSO}-d_6$

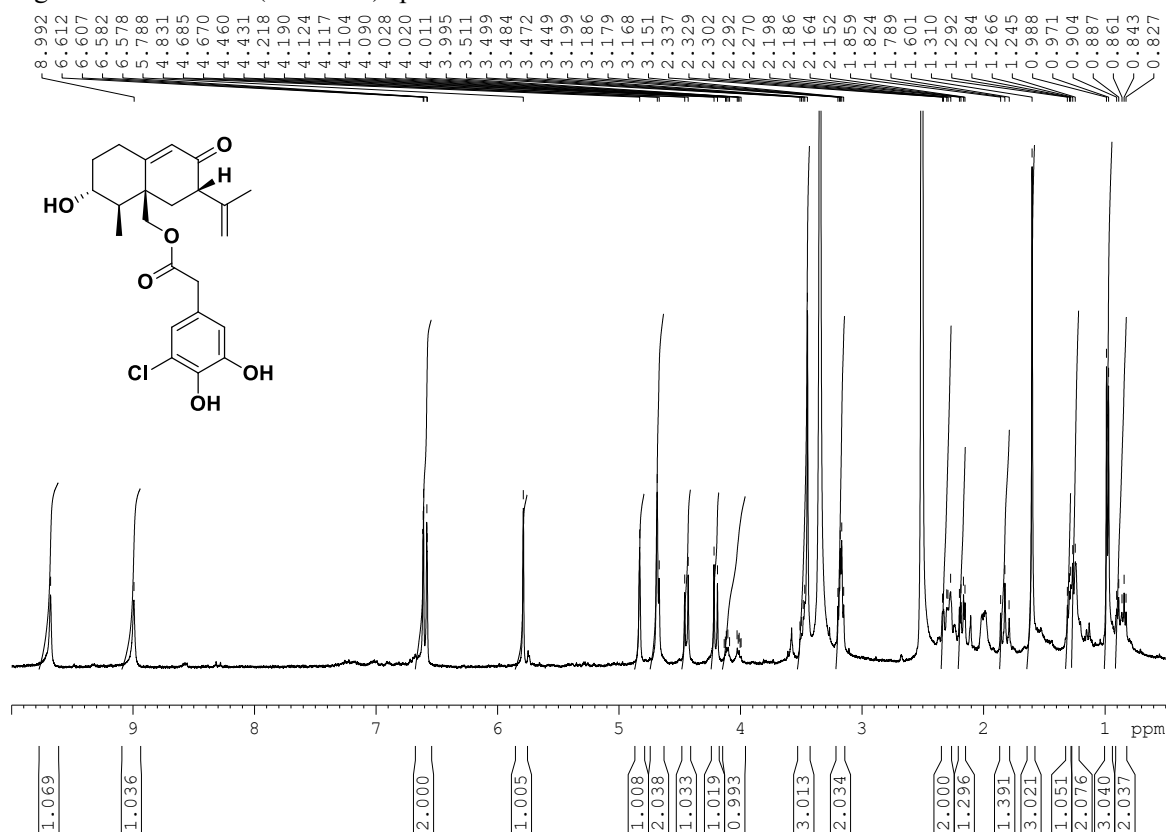


Figure S53.  $^{13}\text{C}$  NMR (150 MHz) spectrum of **7** in  $\text{DMSO}-d_6$

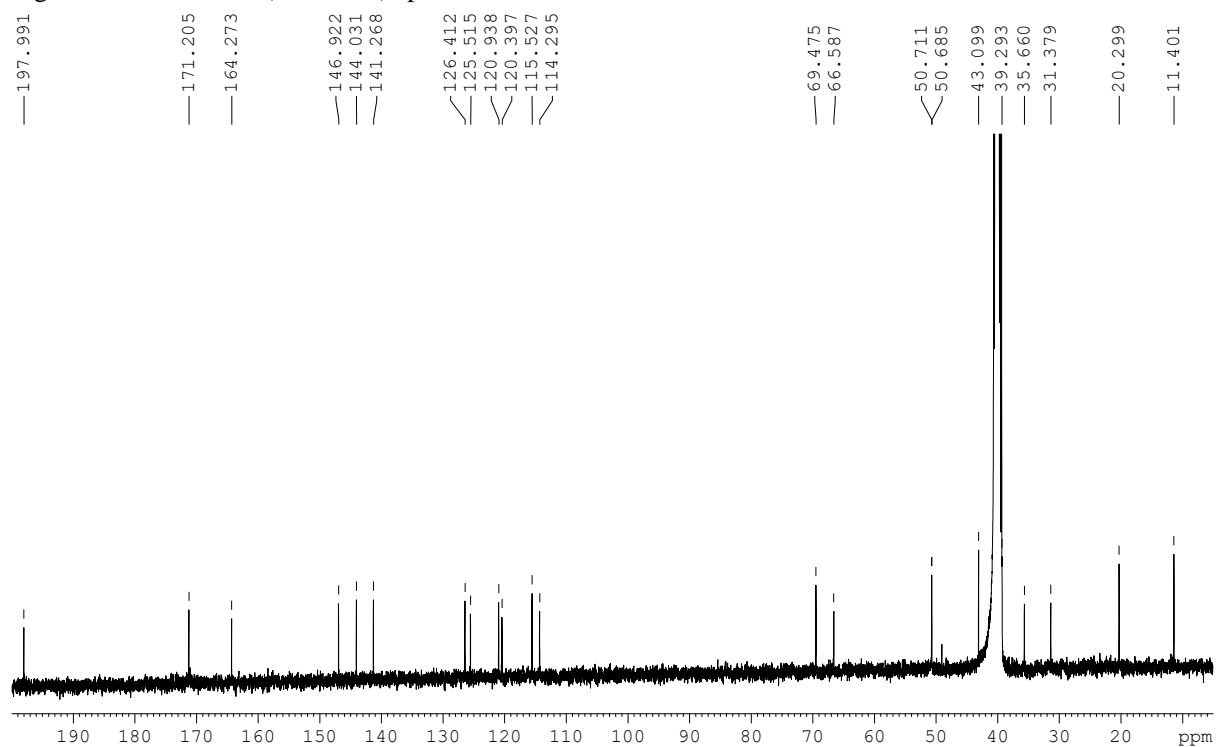


Figure S54. DEPT spectrum of **7** in DMSO-*d*<sub>6</sub>

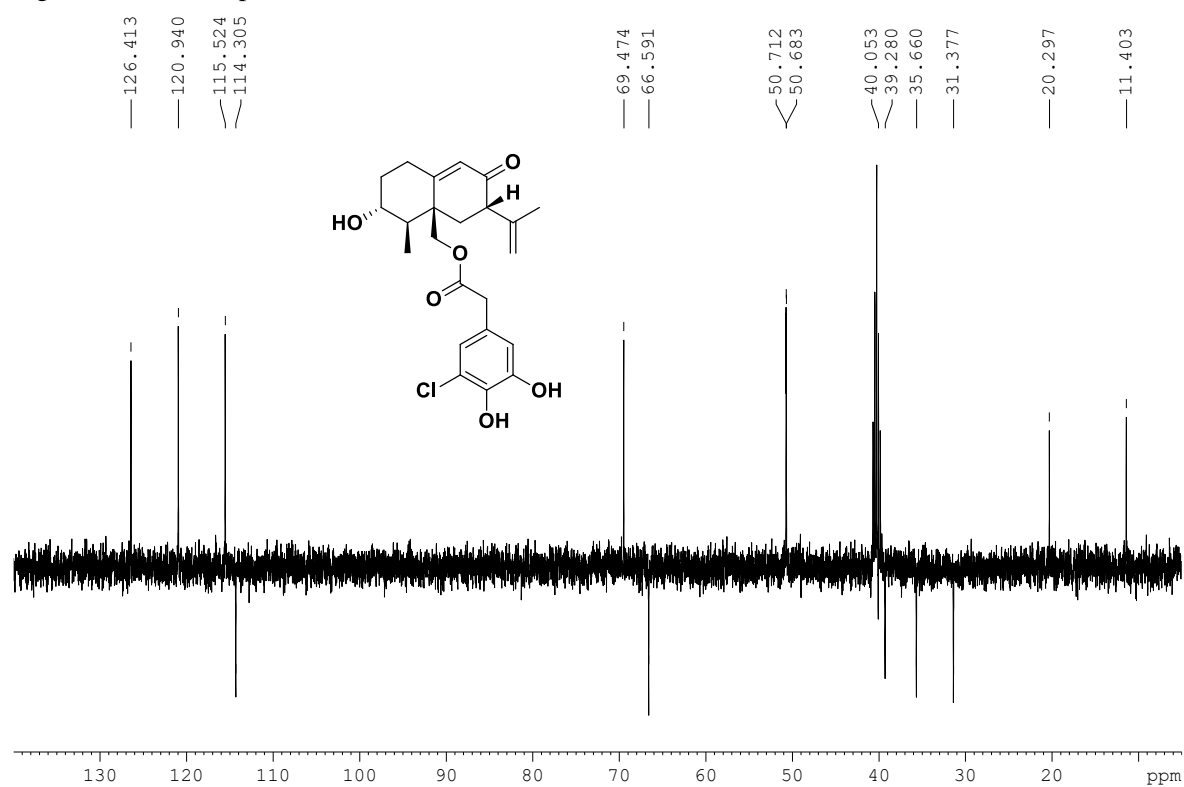


Figure S55. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **7** in DMSO-*d*<sub>6</sub>

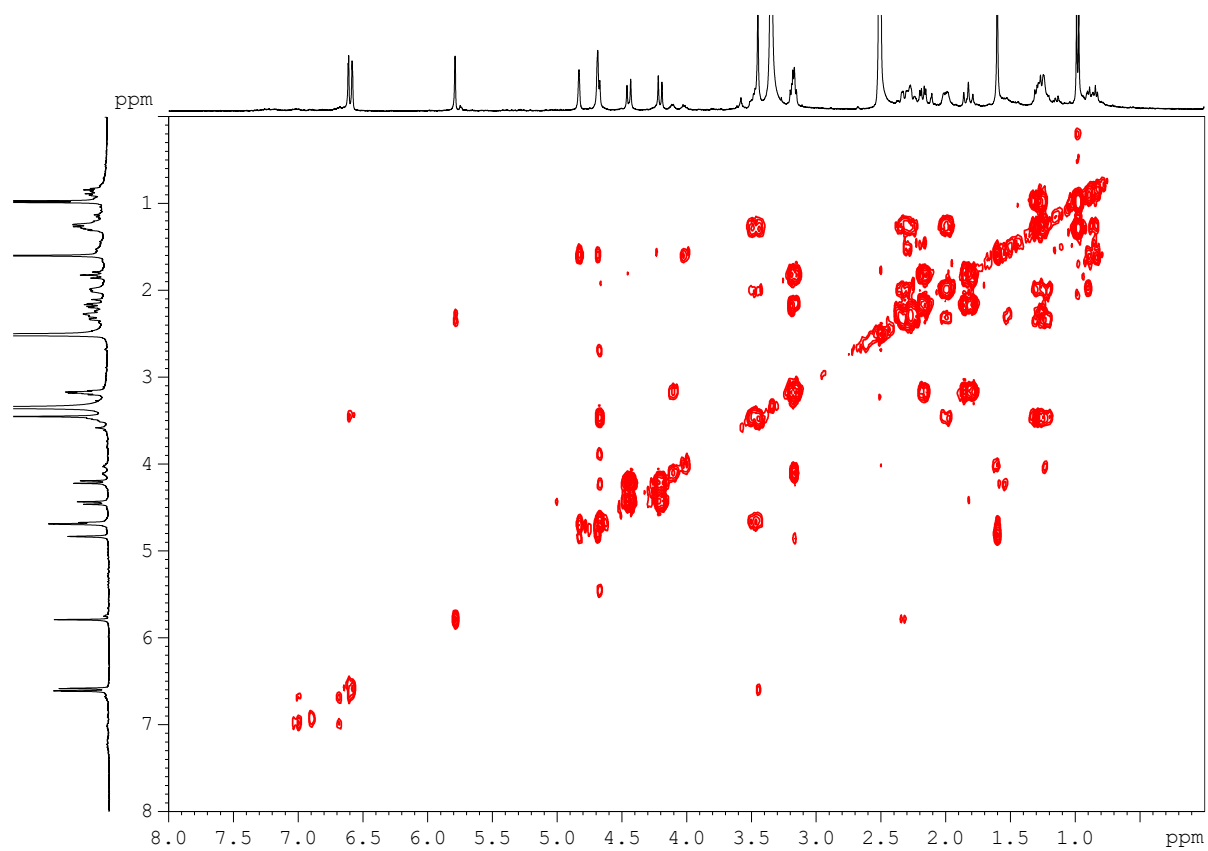


Figure S56. HSQC spectrum of **7** in DMSO-*d*<sub>6</sub>

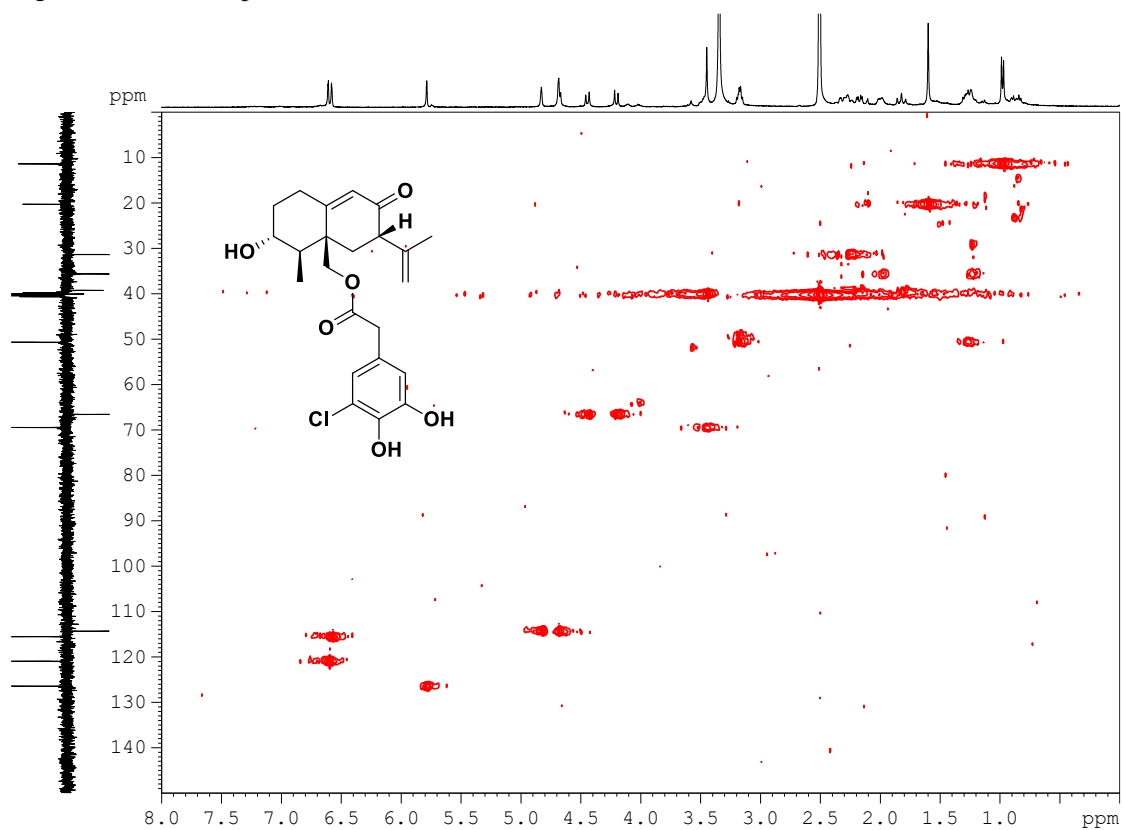


Figure S57. HMBC spectrum of **7** in DMSO-*d*<sub>6</sub>

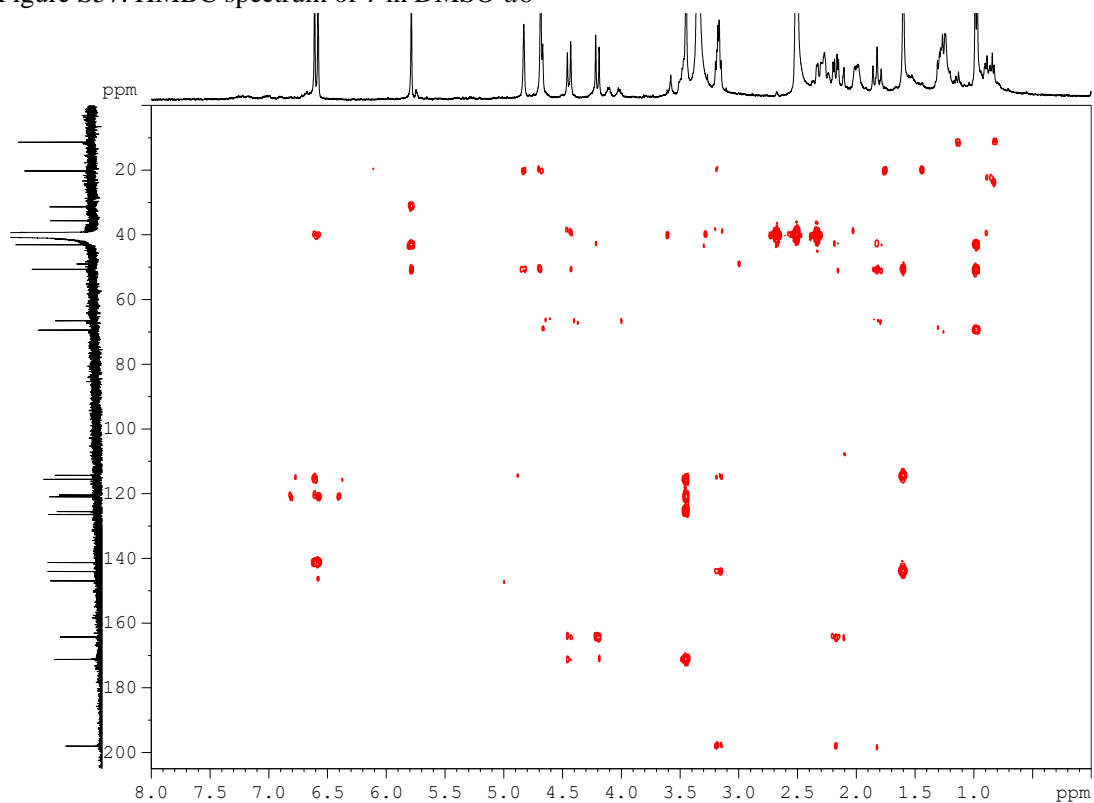


Figure S58. NOESY spectrum of **7** in DMSO-*d*<sub>6</sub>

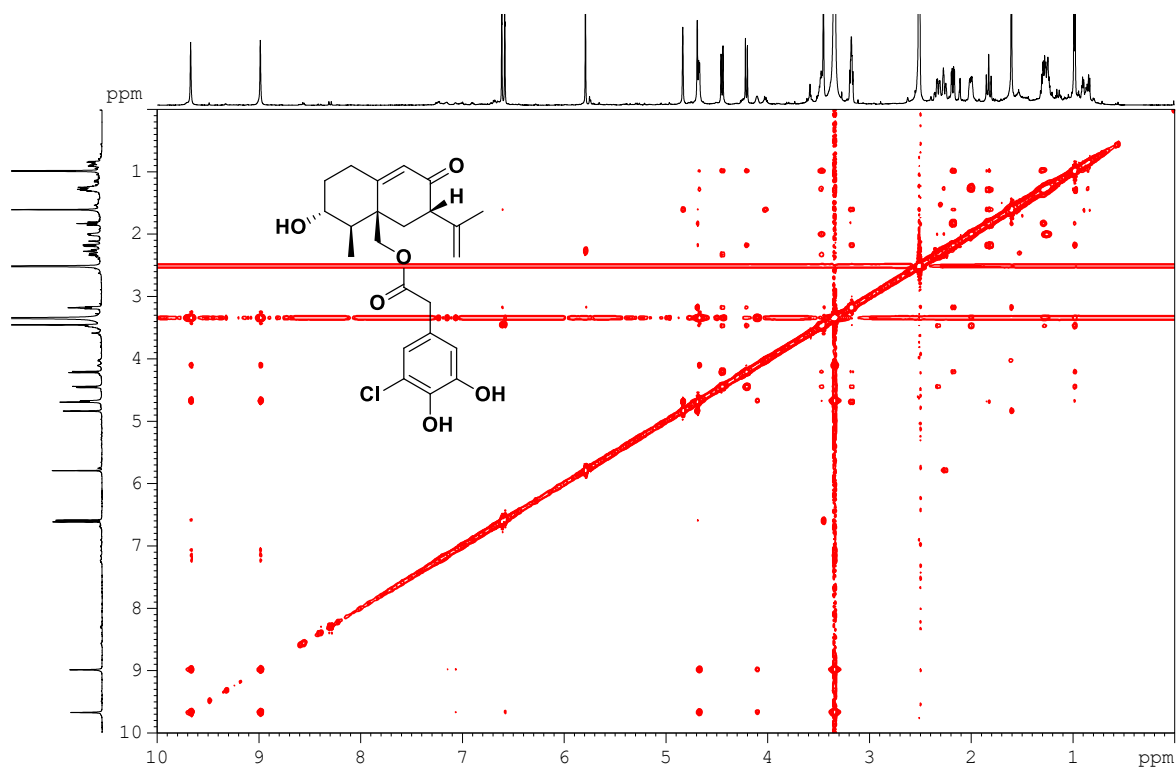
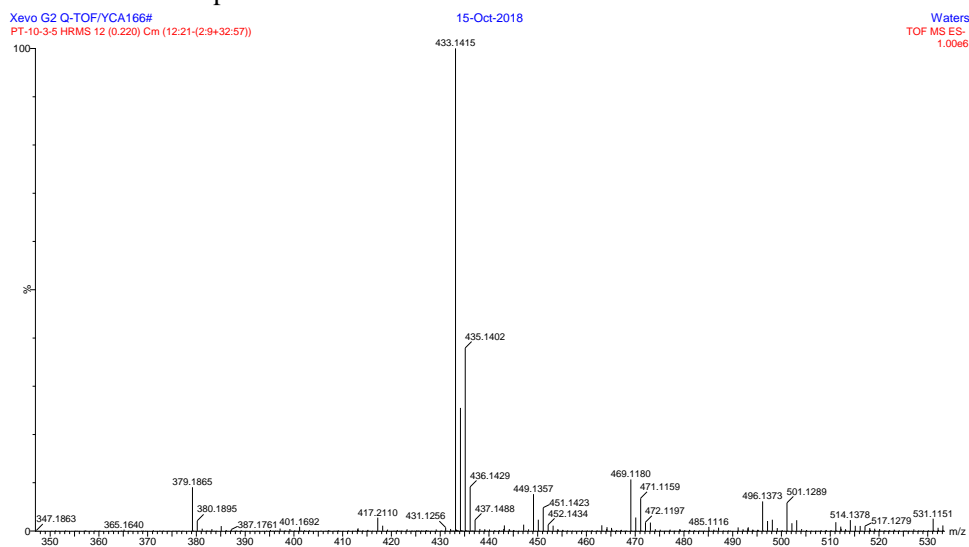


Figure S59. HRESIMS spectrum of **7**



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
443.1415	443.1418	-0.3	-0.7	10.5	646.7	n/a	n/a	C <sub>23</sub> H <sub>26</sub> O <sub>6</sub> Cl

Figure S60. IR spectrum of **8**

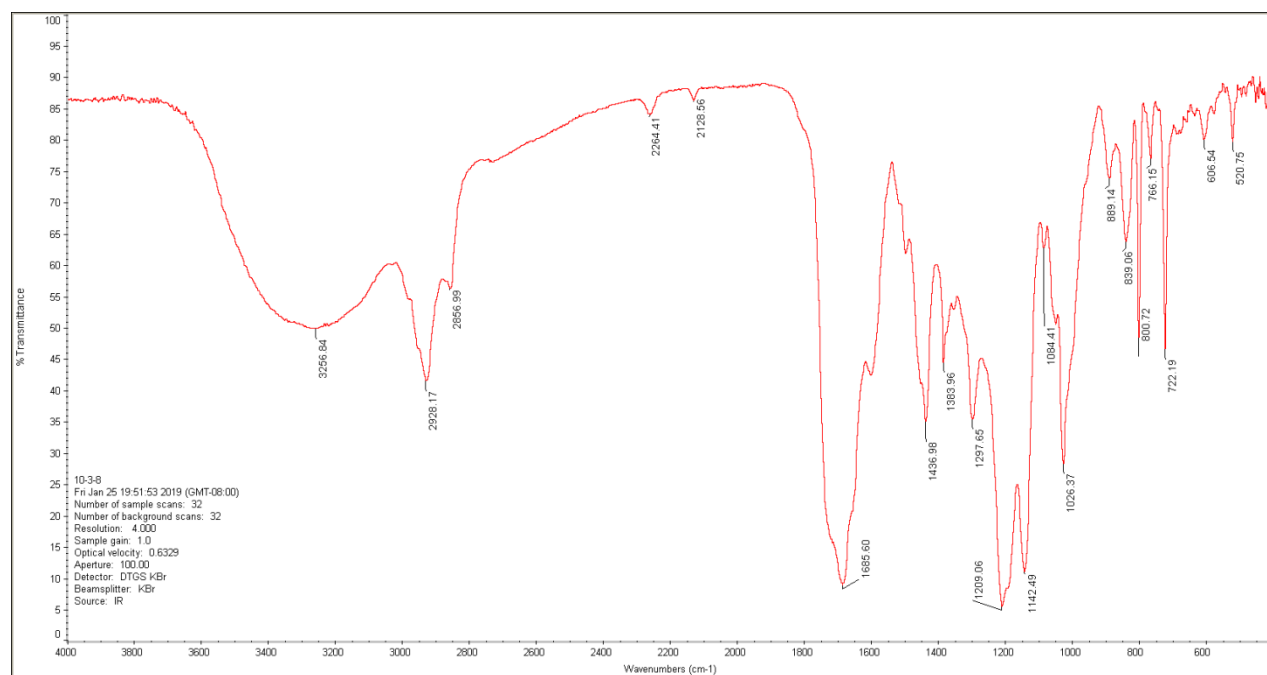


Figure S61. <sup>1</sup>H NMR (600 MHz) spectrum of **8** in DMSO-*d*<sub>6</sub>

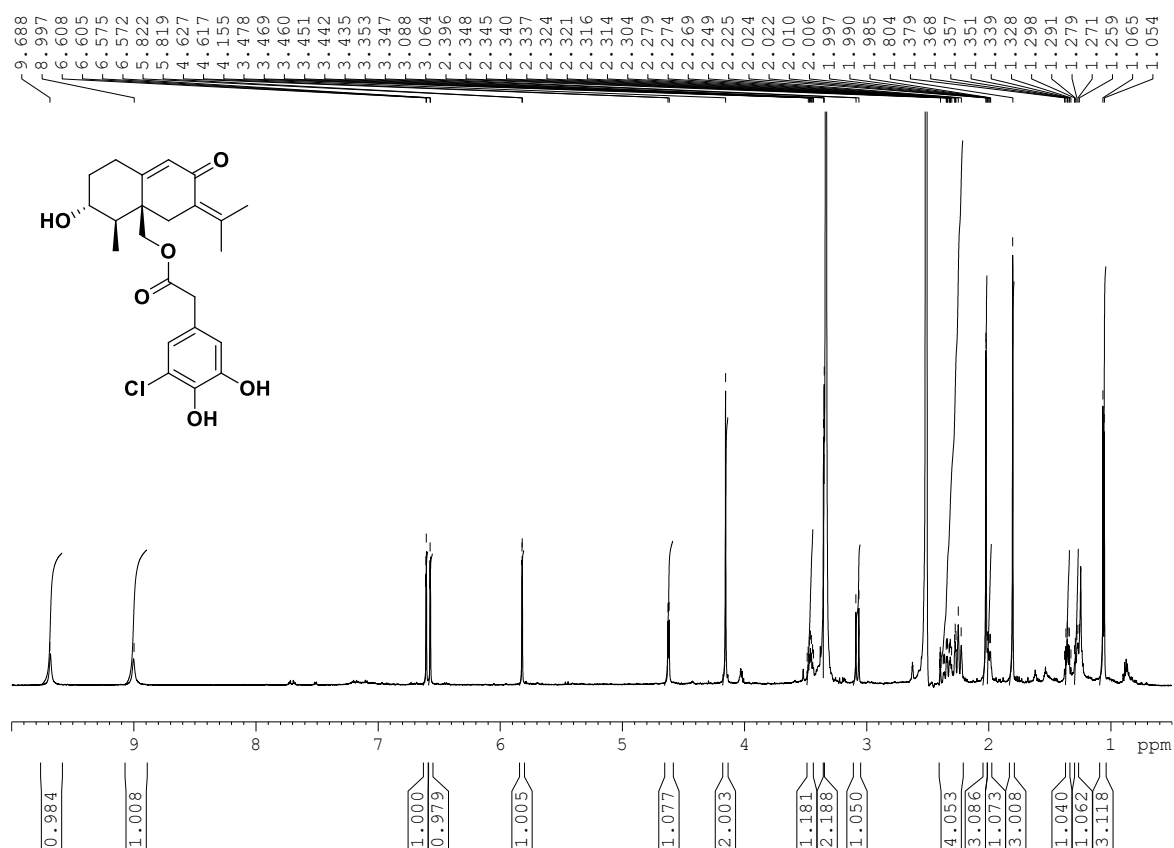


Figure S62.  $^{13}\text{C}$  NMR (150 MHz) and DEPT spectra of **8** in  $\text{DMSO-}d_6$

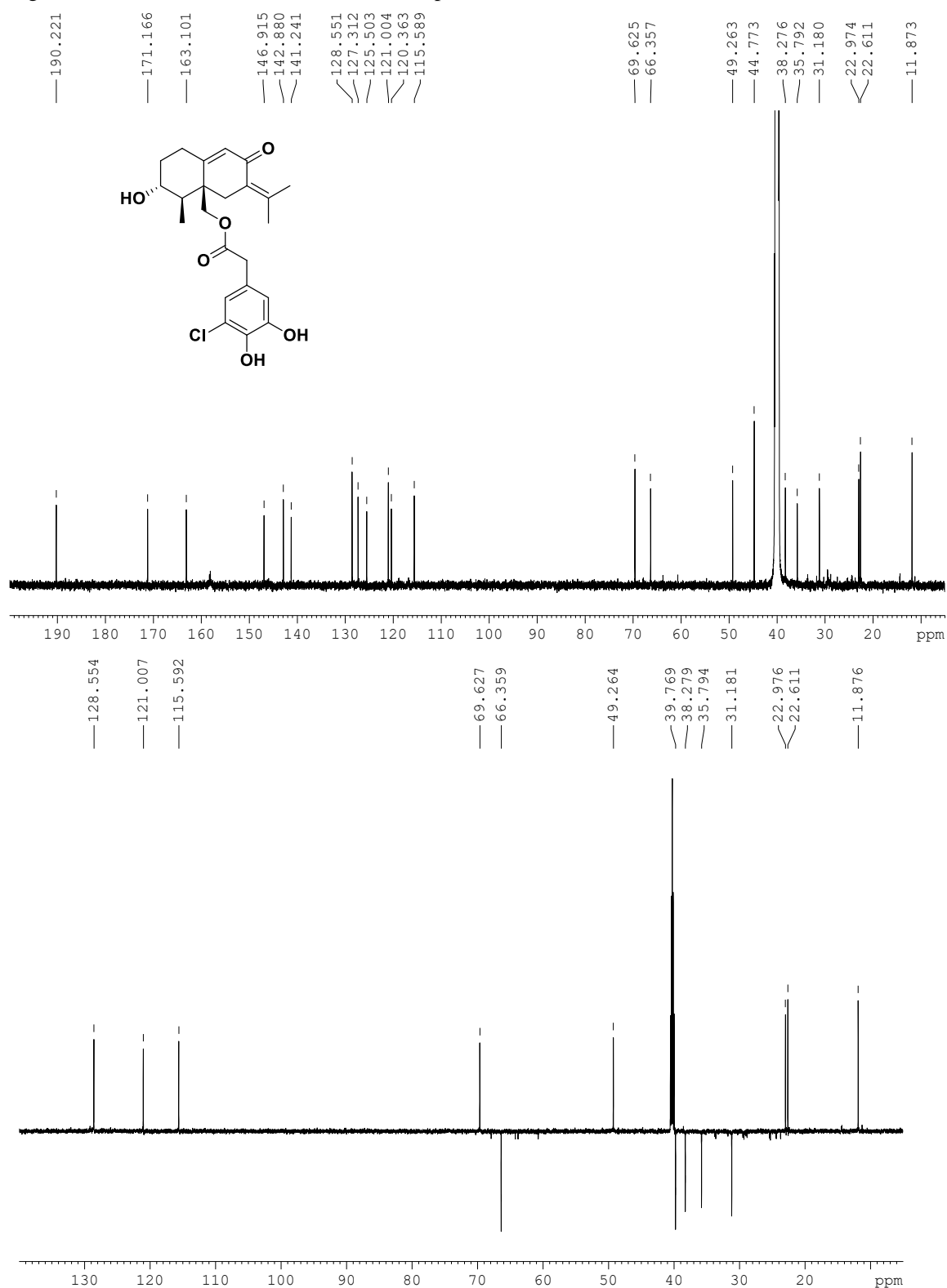




Figure S63.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **8** in DMSO- $d_6$

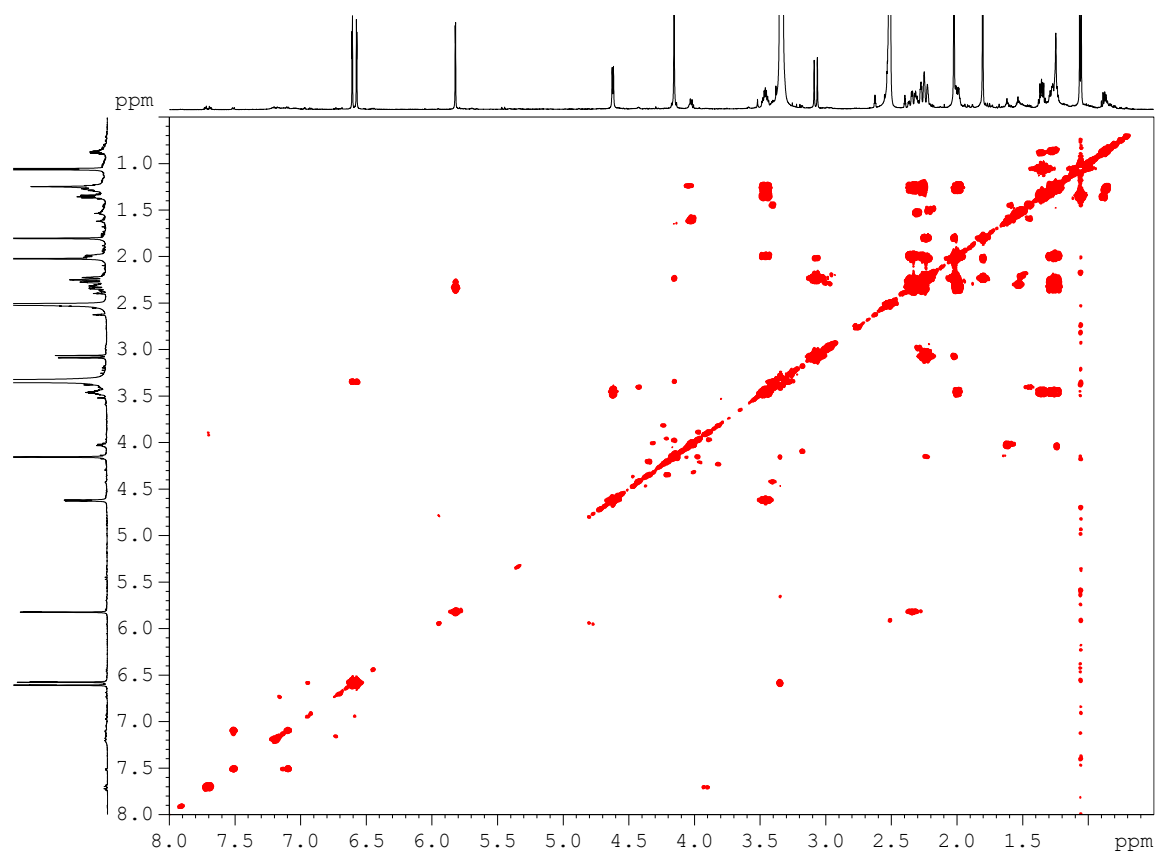


Figure S64. HSQC spectrum of **8** in DMSO- $d_6$

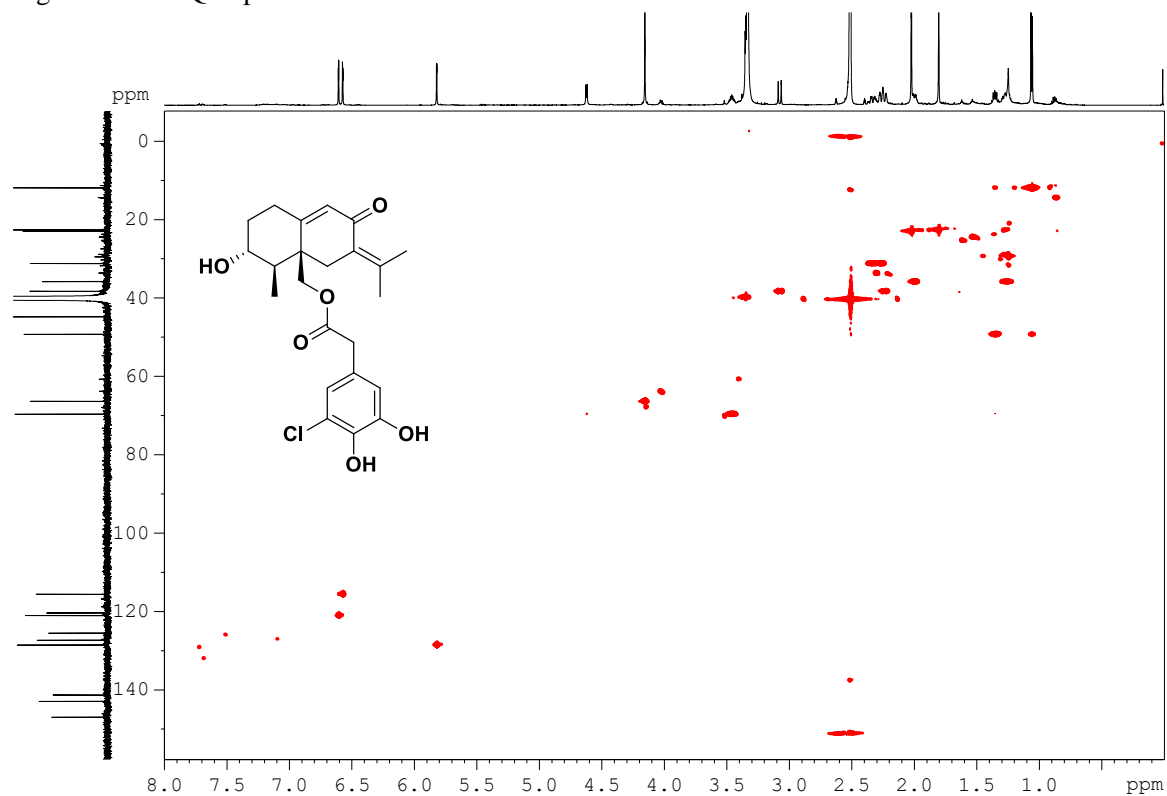


Figure S65. HMBC spectrum of **8** in DMSO-*d*<sub>6</sub>

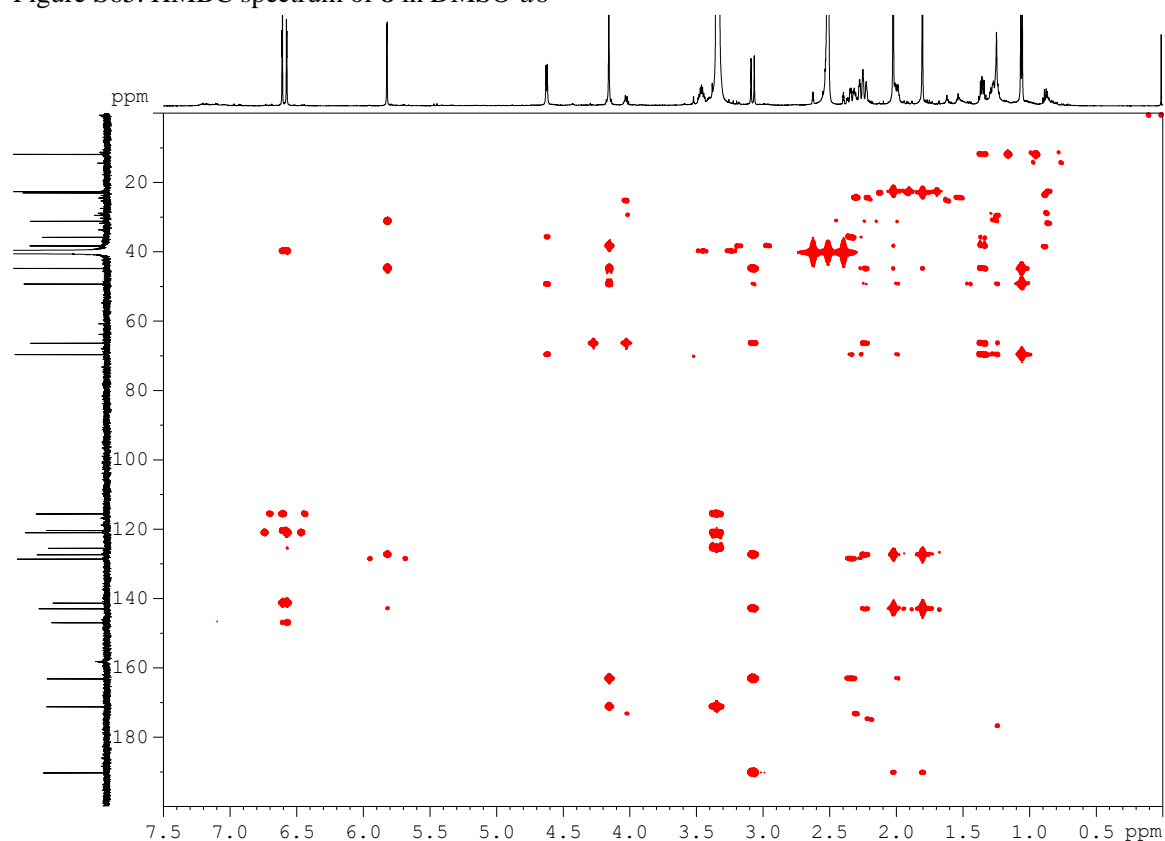


Figure S66. NOESY spectrum of **8** in DMSO-*d*<sub>6</sub>

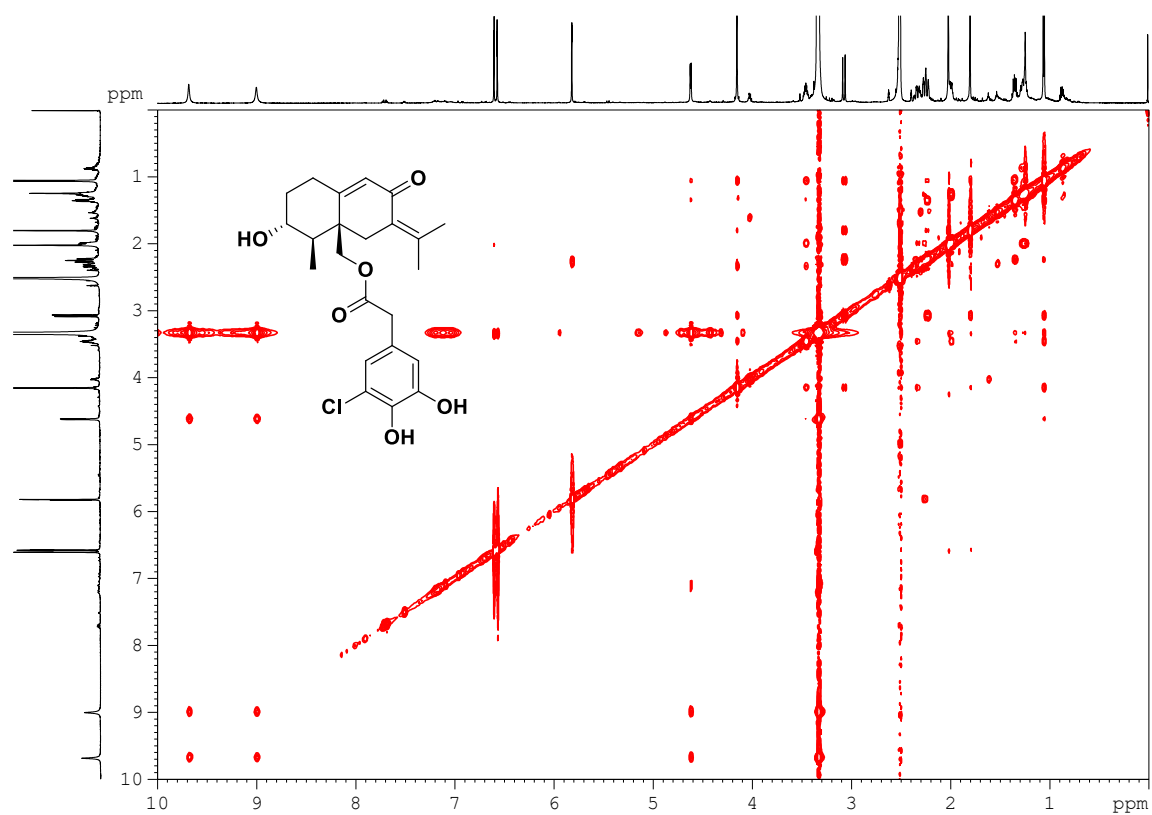
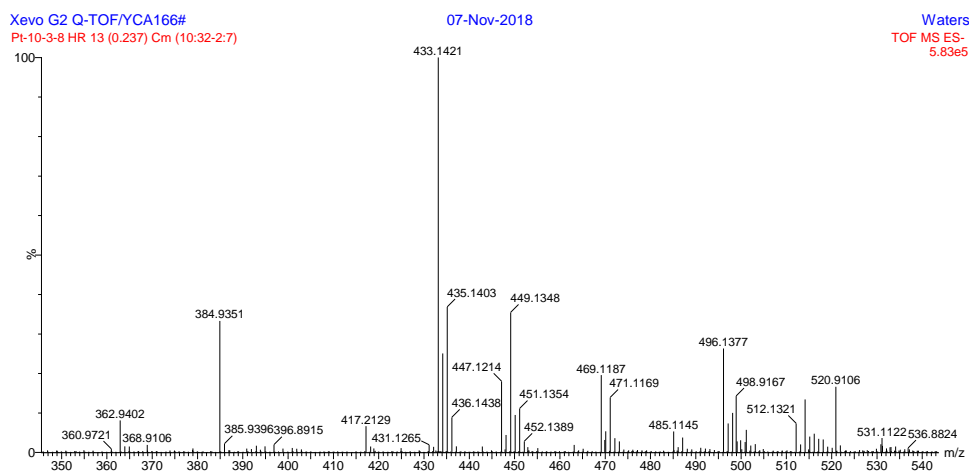


Figure S67. HRESIMS spectrum of **8**



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
443.1421	443.1418	0.3	0.7	10.5	610.1	0.000	100.00	C <sub>23</sub> H <sub>26</sub> O <sub>6</sub> Cl

Figure S68. IR spectrum of **9**

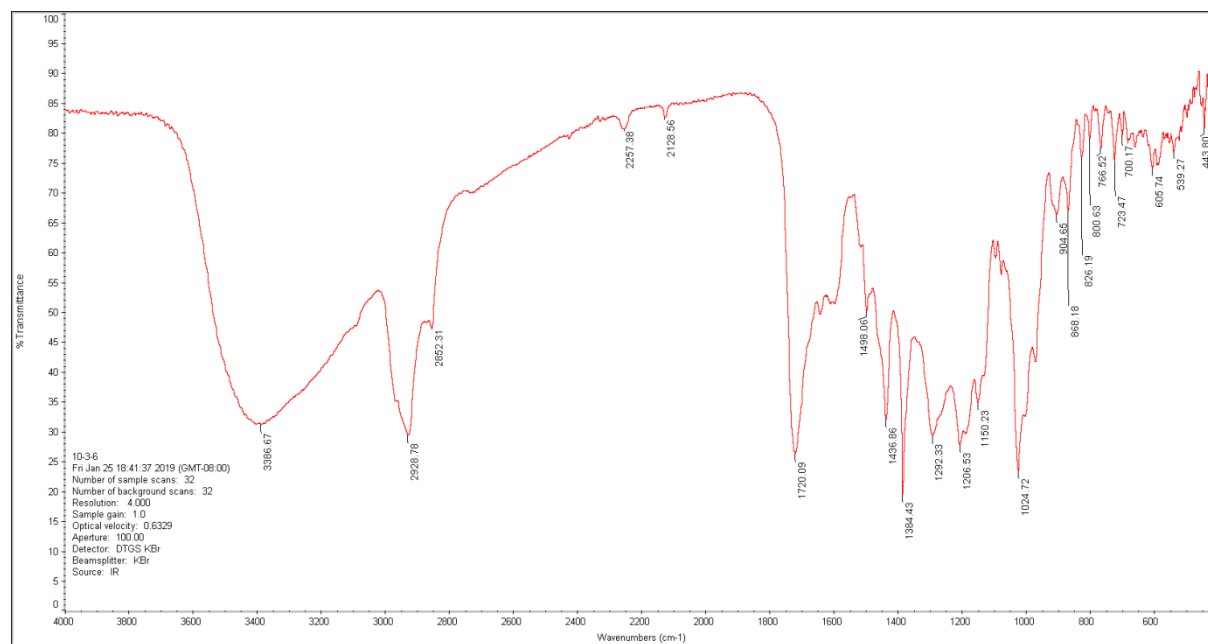


Figure S69.  $^1\text{H}$  NMR (600 MHz) spectrum of **9** in  $\text{DMSO}-d_6$

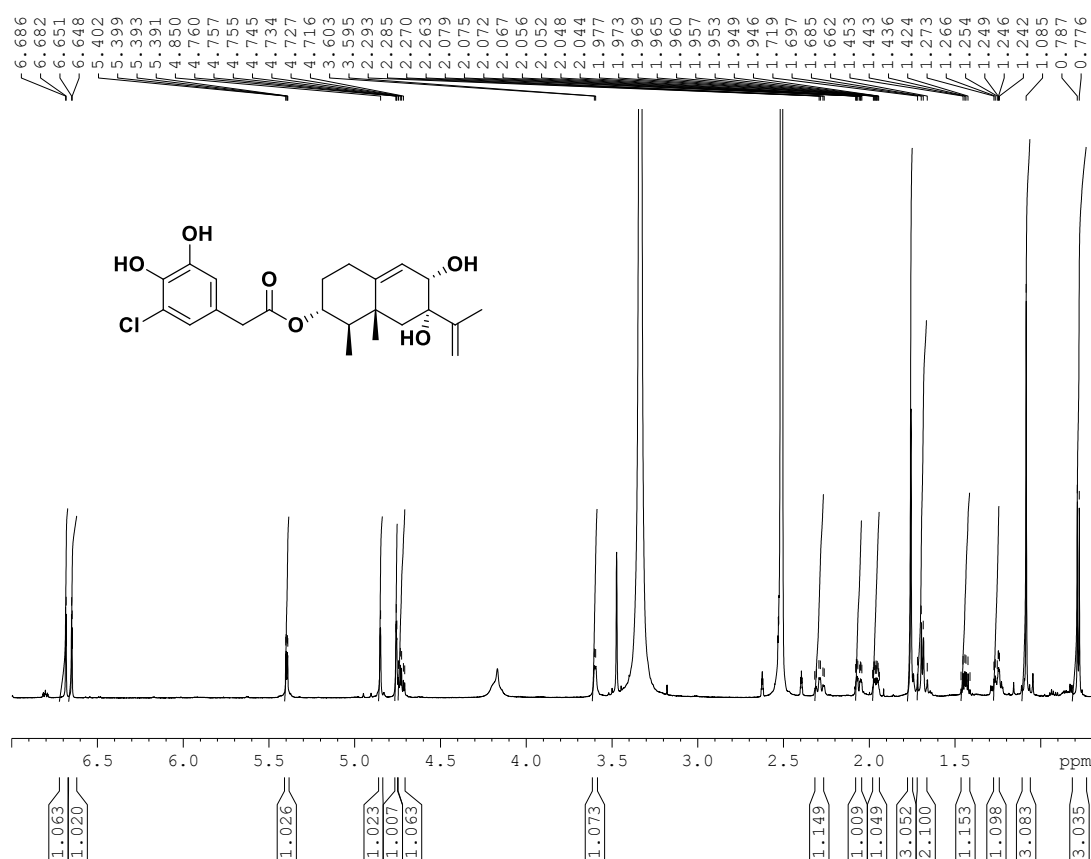


Figure S70.  $^{13}\text{C}$  NMR (150 MHz) spectrum of **9** in  $\text{DMSO}-d_6$

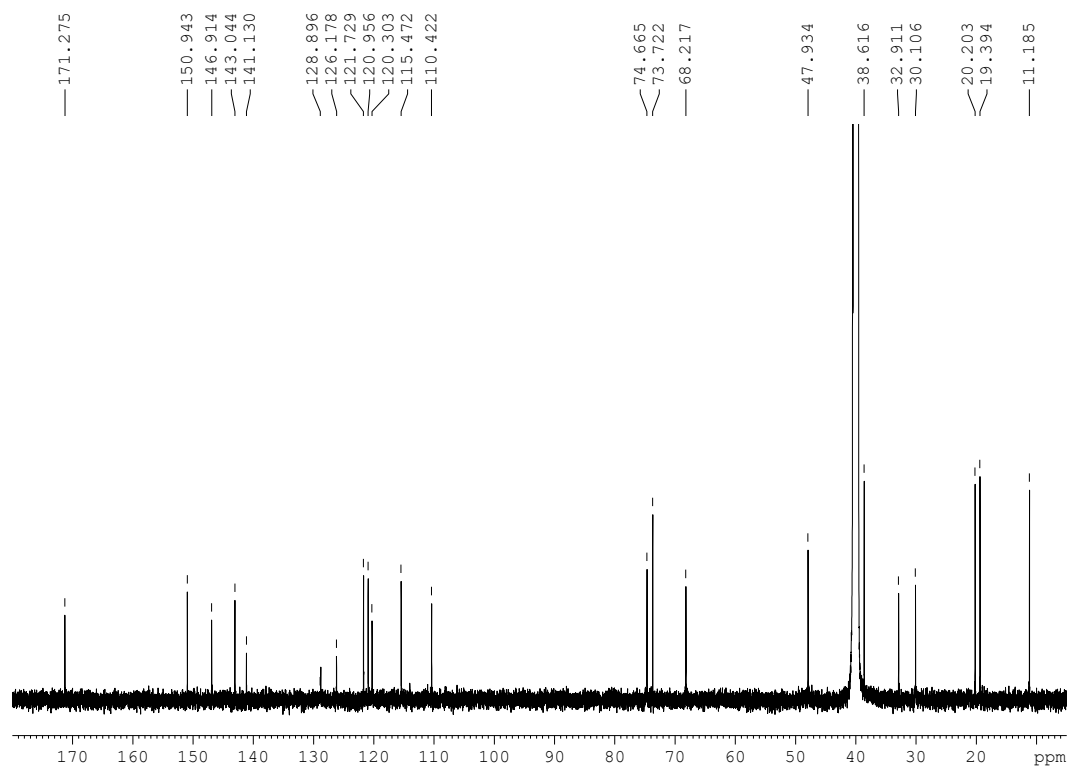


Figure S71. DEPT spectrum of **9** in DMSO-*d*<sub>6</sub>

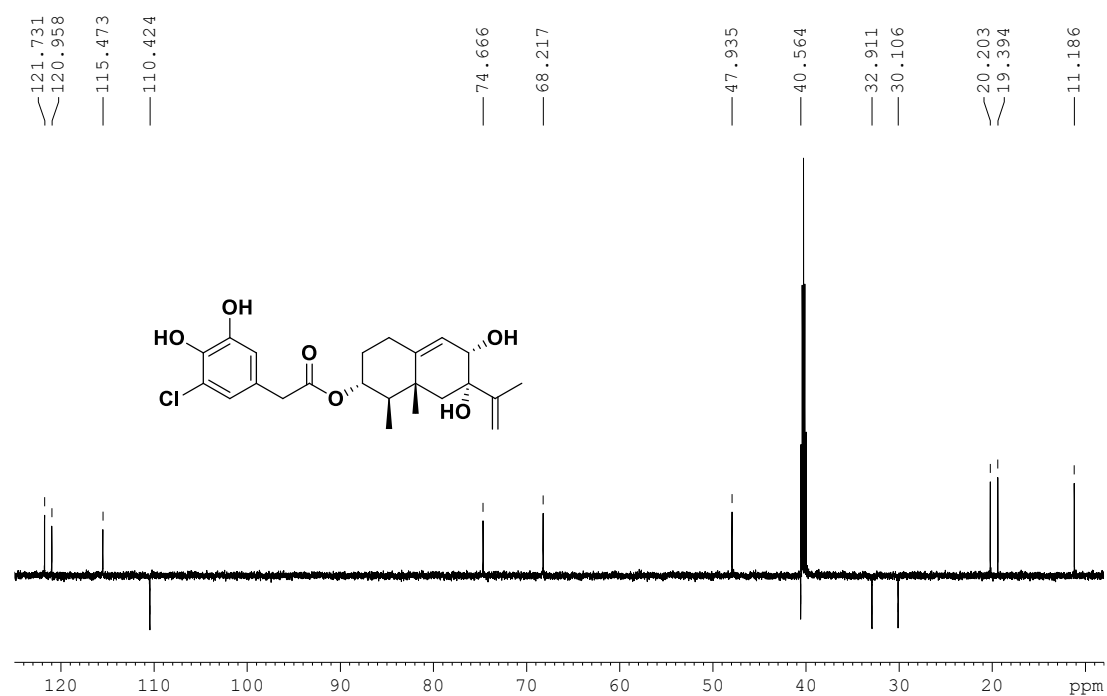


Figure S72. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **9** in DMSO-*d*<sub>6</sub>

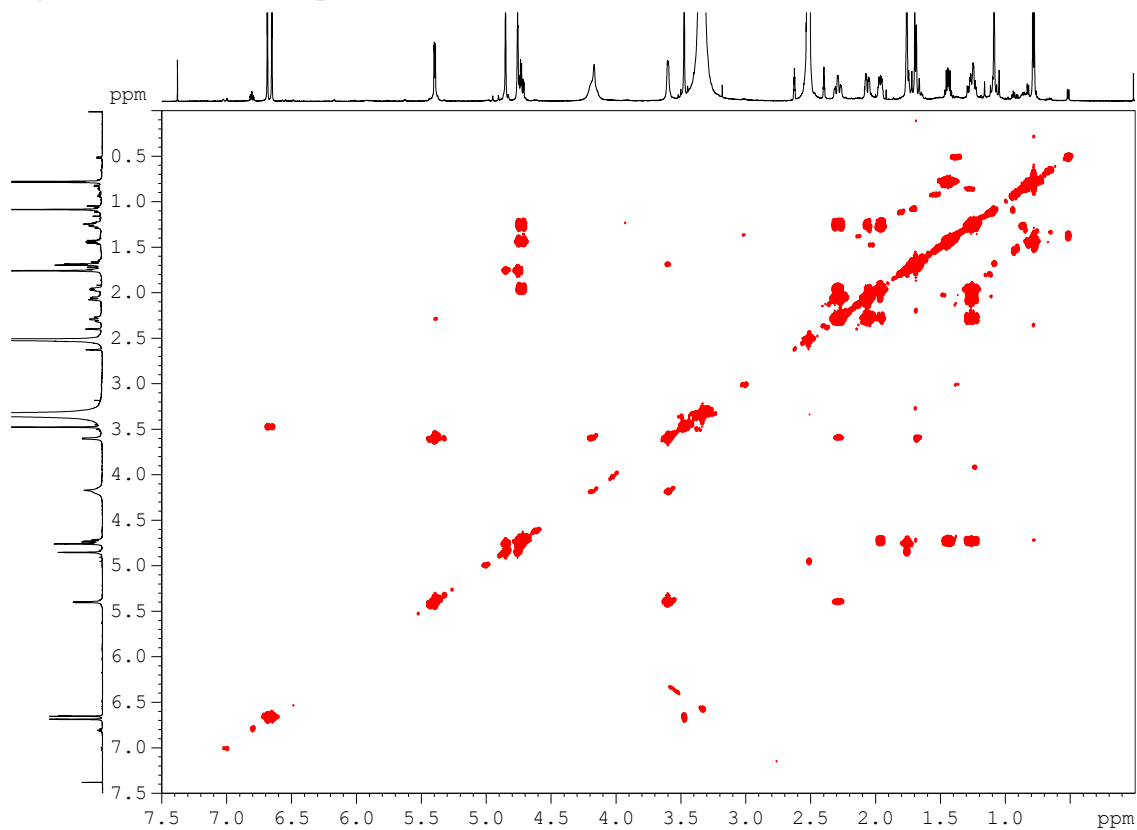


Figure S73. HSQC spectrum of **9** in DMSO-*d*<sub>6</sub>

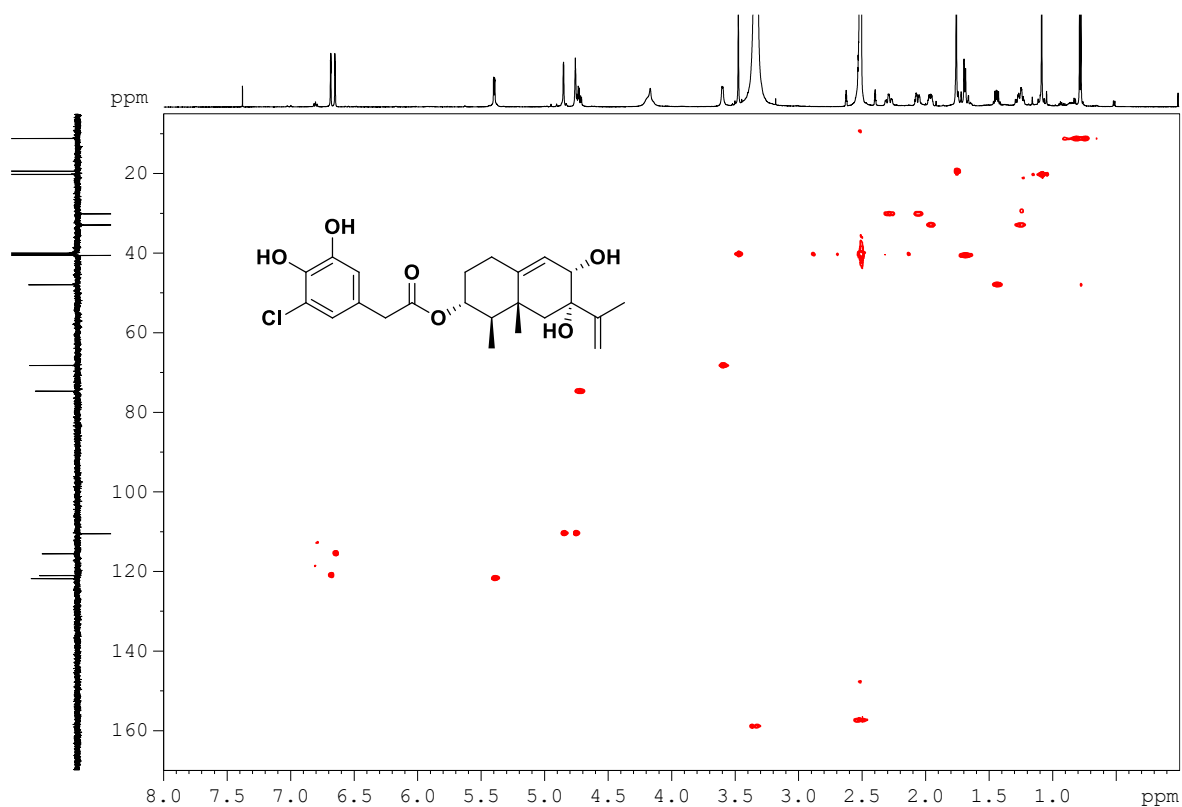


Figure S74. HMBC spectrum of **9** in DMSO-*d*<sub>6</sub>

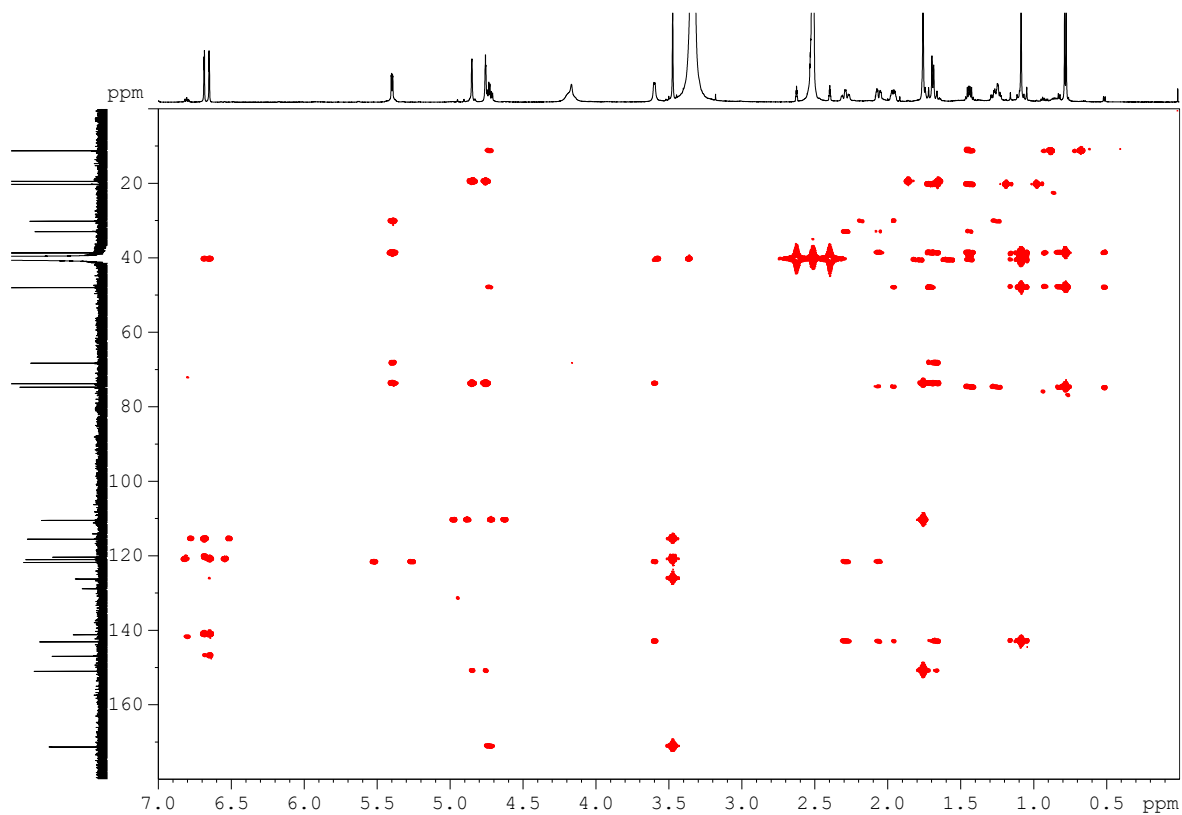


Figure S75. NOESY spectrum of **9** in DMSO-*d*<sub>6</sub>

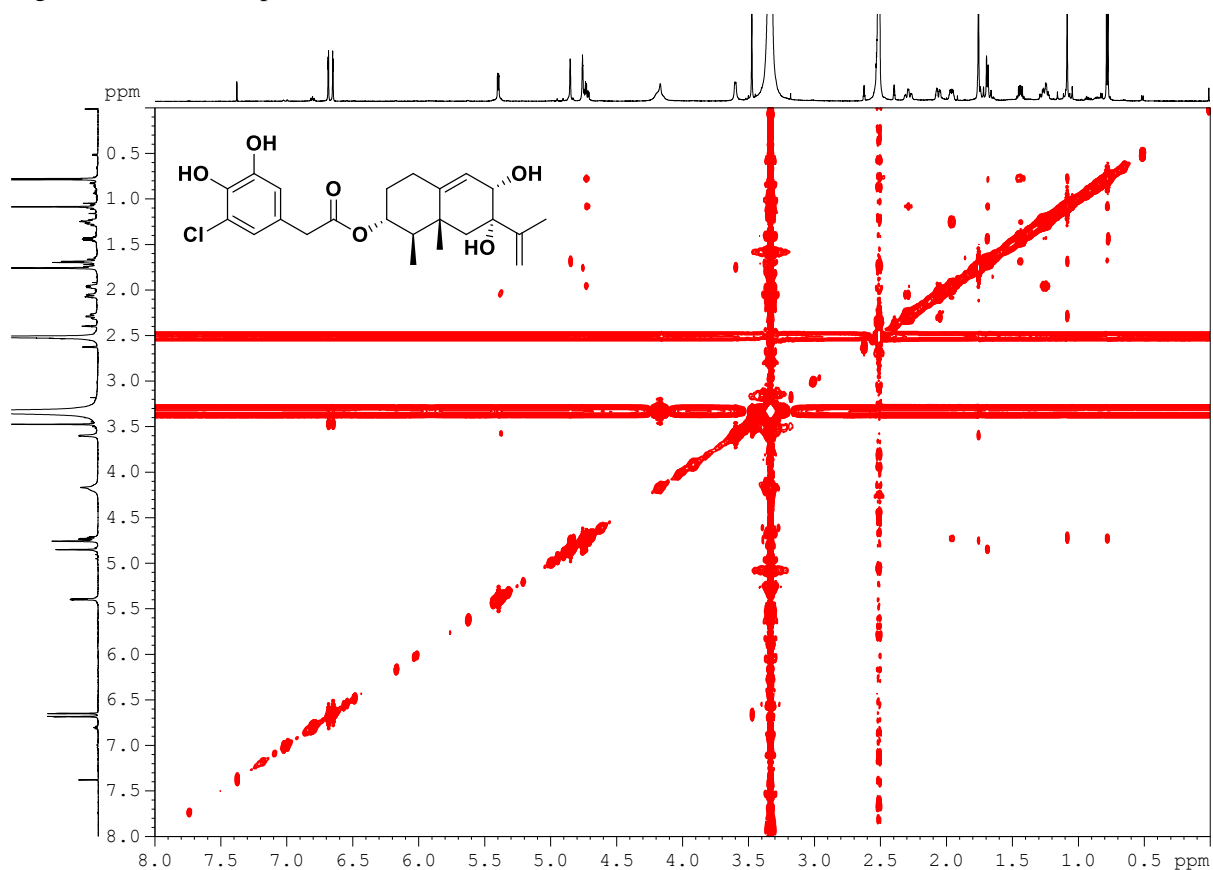
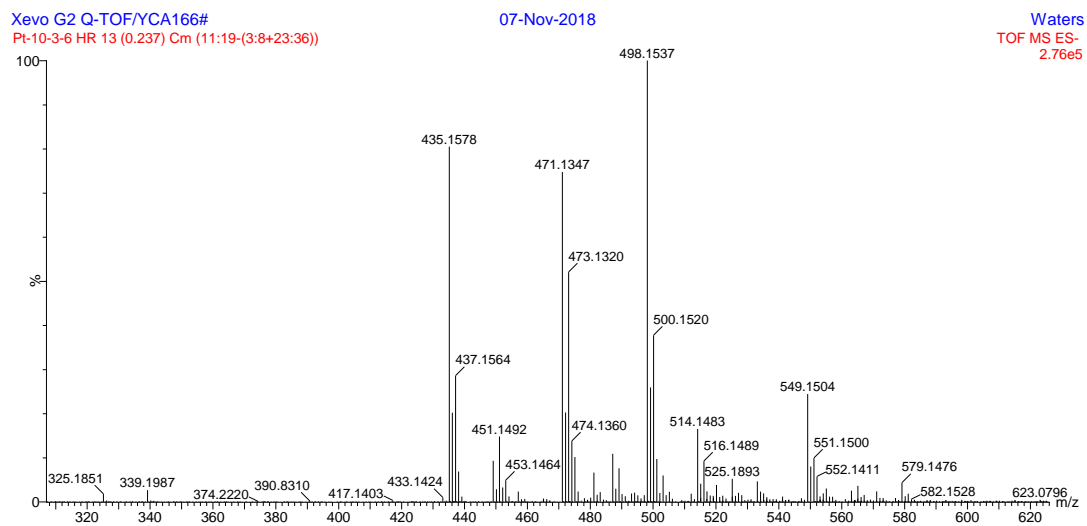


Figure S76. HRESIMS spectrum of **9**



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
435.1578	435.1574	0.4	0.9	9.5	257.3	0.000	100.00	C <sub>23</sub> H <sub>28</sub> O <sub>6</sub> Cl

Figure S77. IR spectrum of **10**

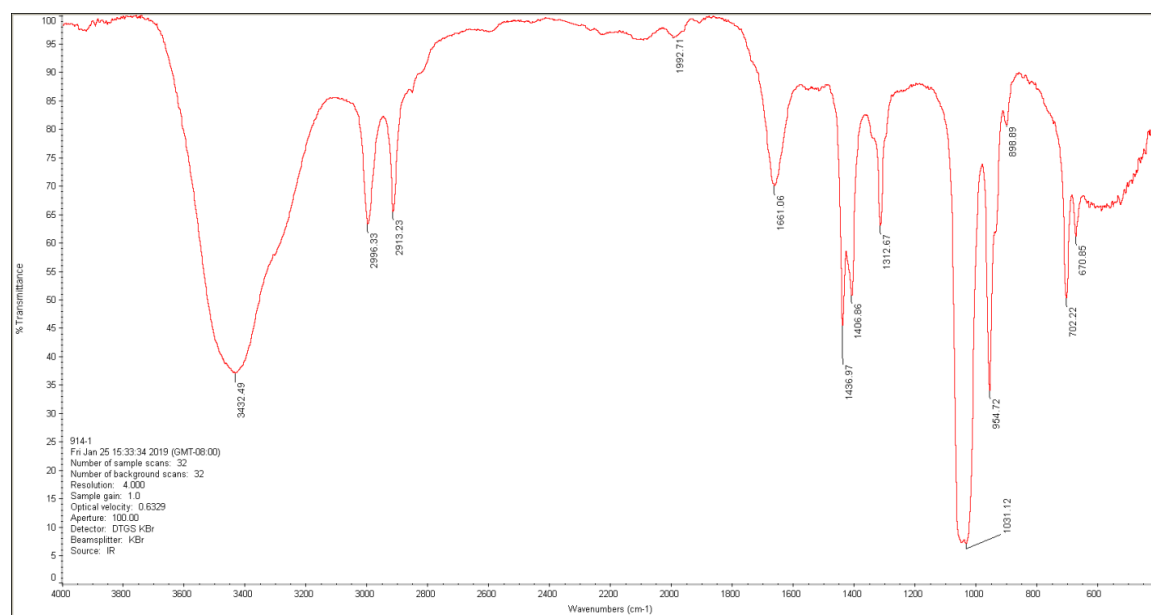


Figure S78. <sup>1</sup>H NMR (600 MHz) spectrum of **10** in DMSO-*d*<sub>6</sub>

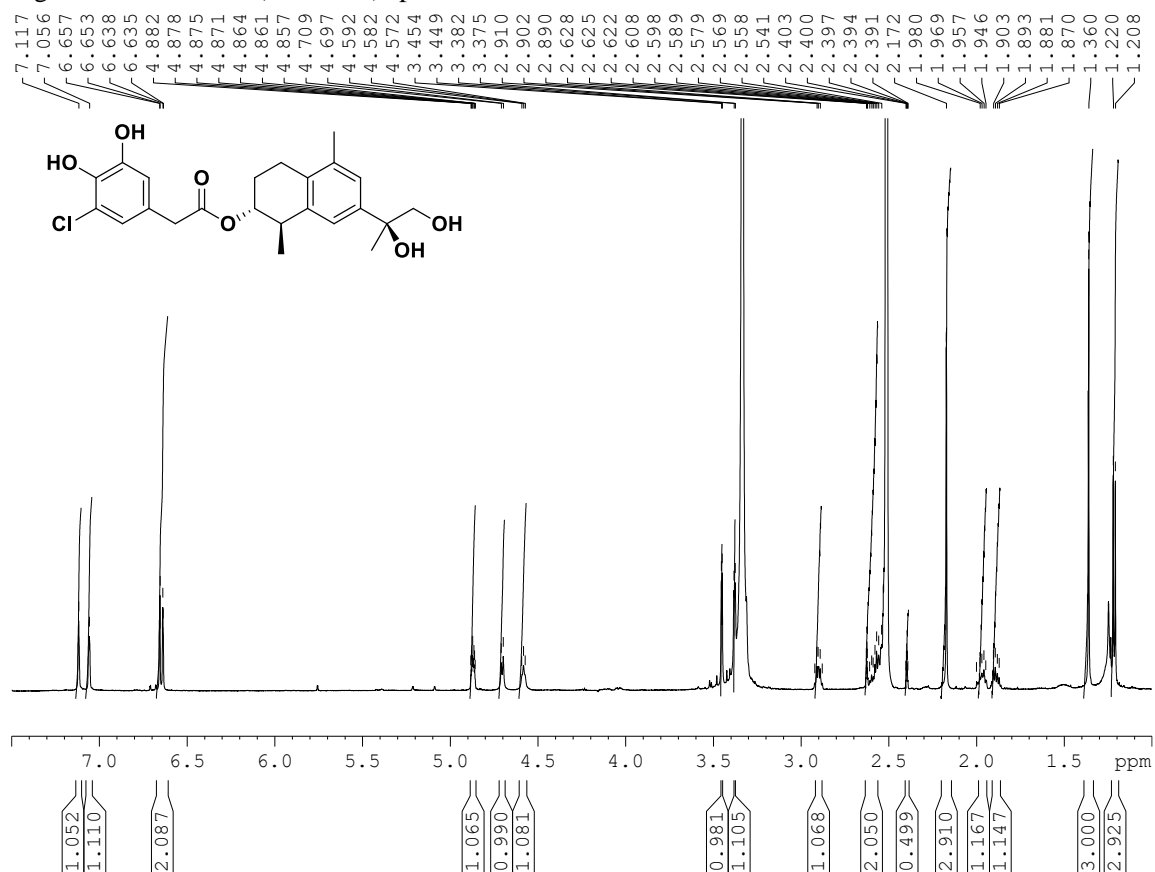




Figure S79.  $^{13}\text{C}$  NMR (150 MHz) and DEPT spectra of **10** in  $\text{DMSO}-d_6$

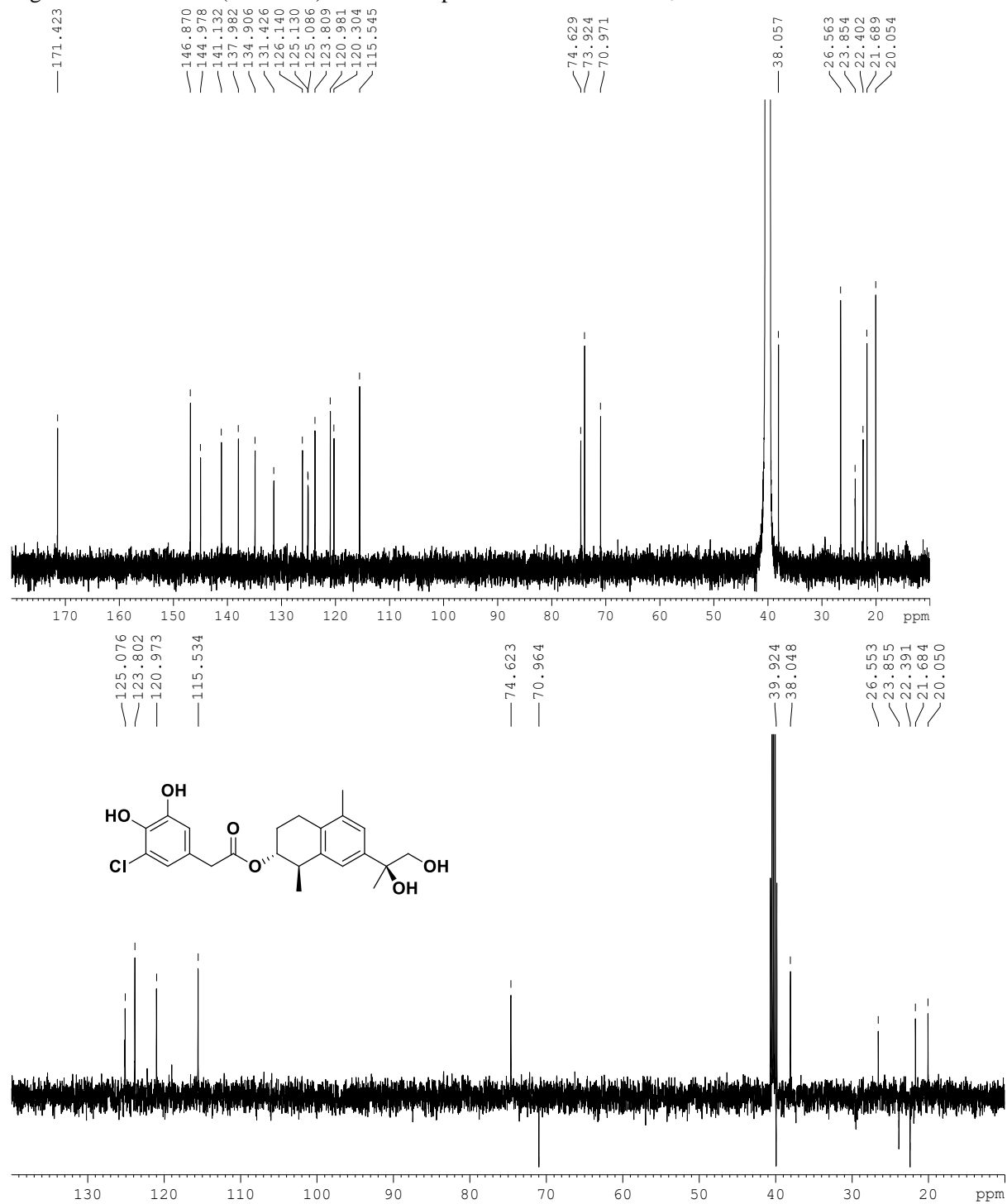




Figure S82. HMBC spectrum of **10** in DMSO-*d*<sub>6</sub>

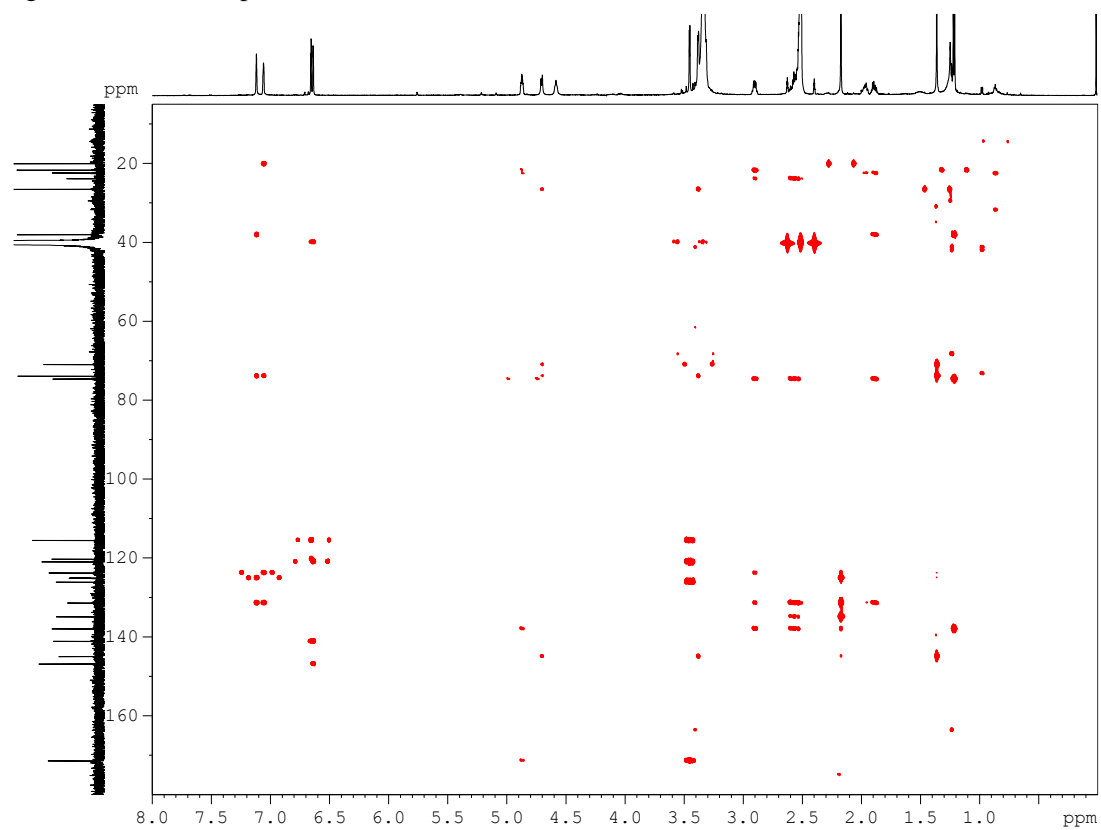


Figure S83. NOESY spectrum of **10** in DMSO-*d*<sub>6</sub>

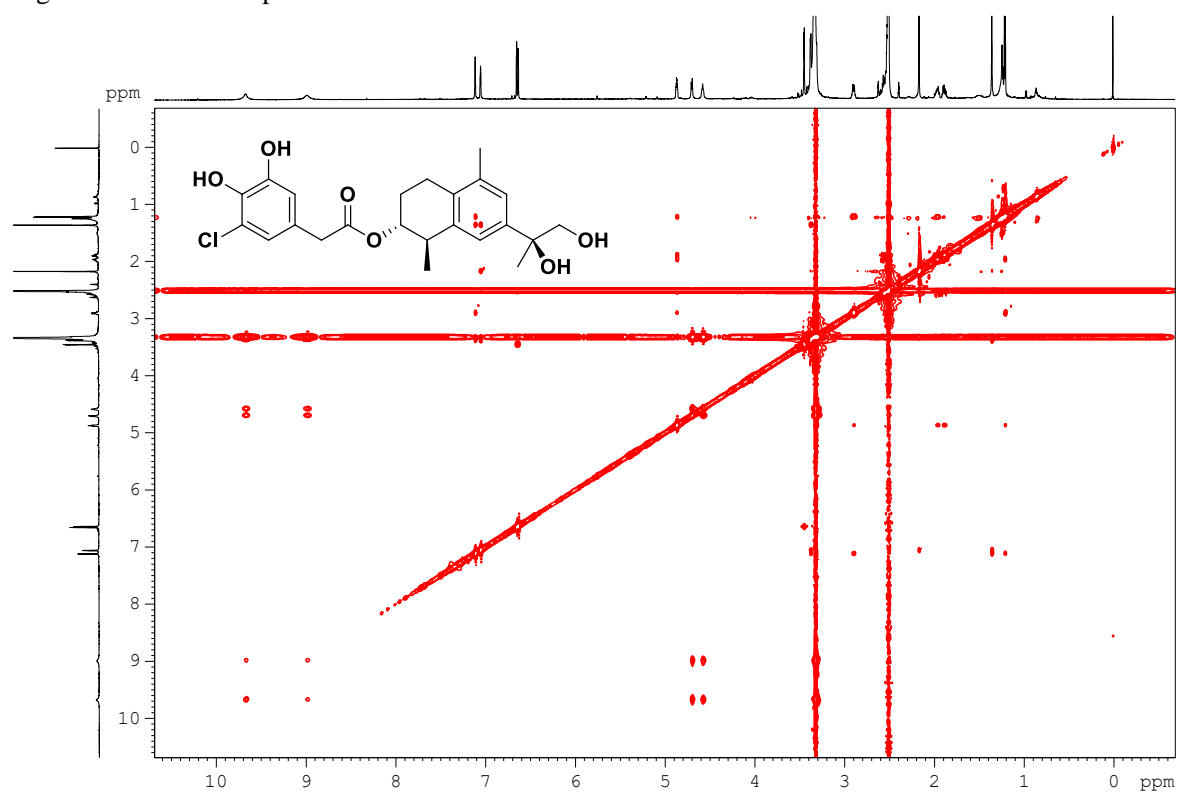


Figure S84. HRESIMS spectrum of **10** in DMSO-*d*<sub>6</sub>

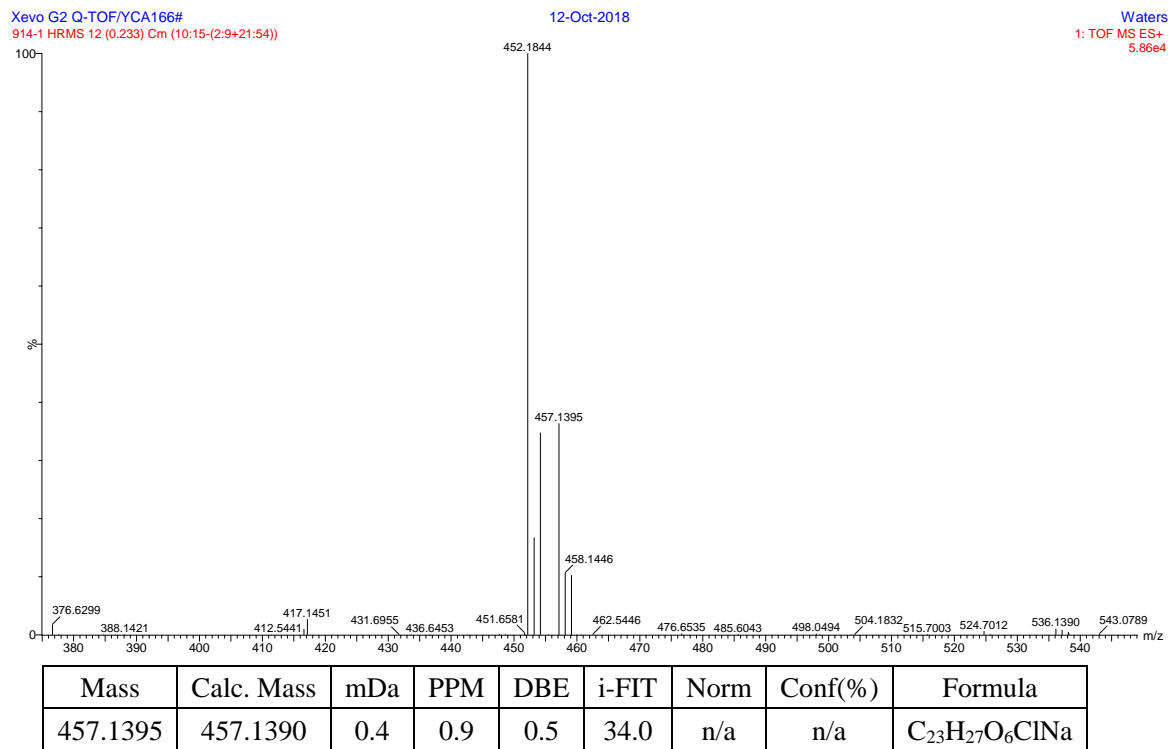


Figure S85. IR spectrum of **11**

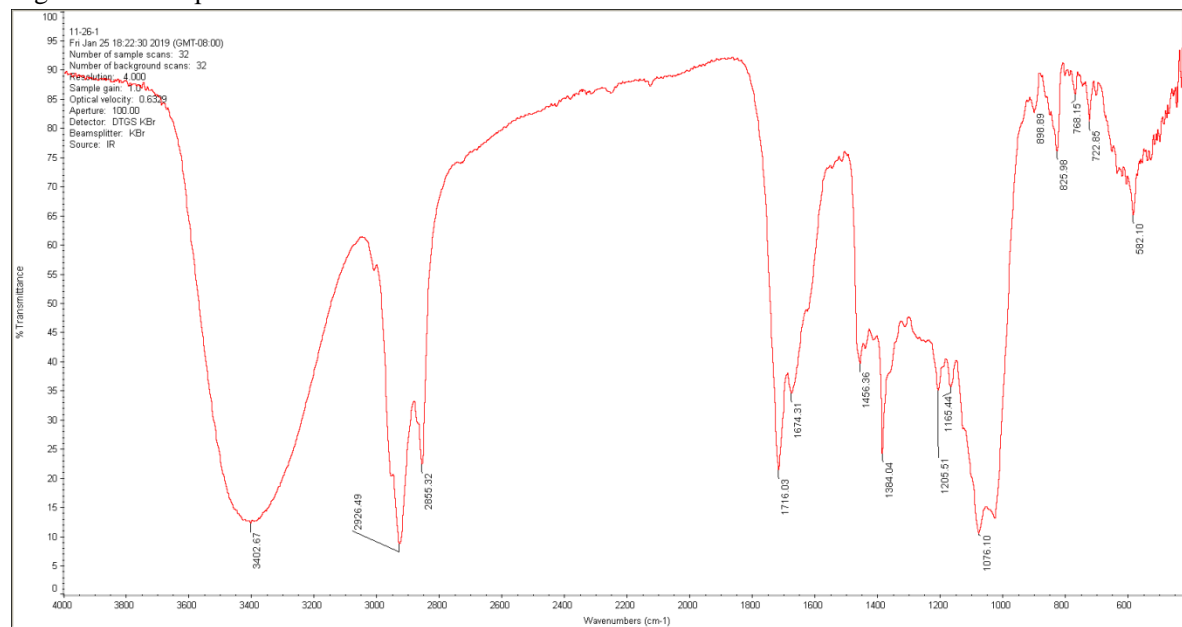


Figure S86.  $^1\text{H}$  NMR (600 MHz) spectrum of **11** in  $\text{DMSO}-d_6$

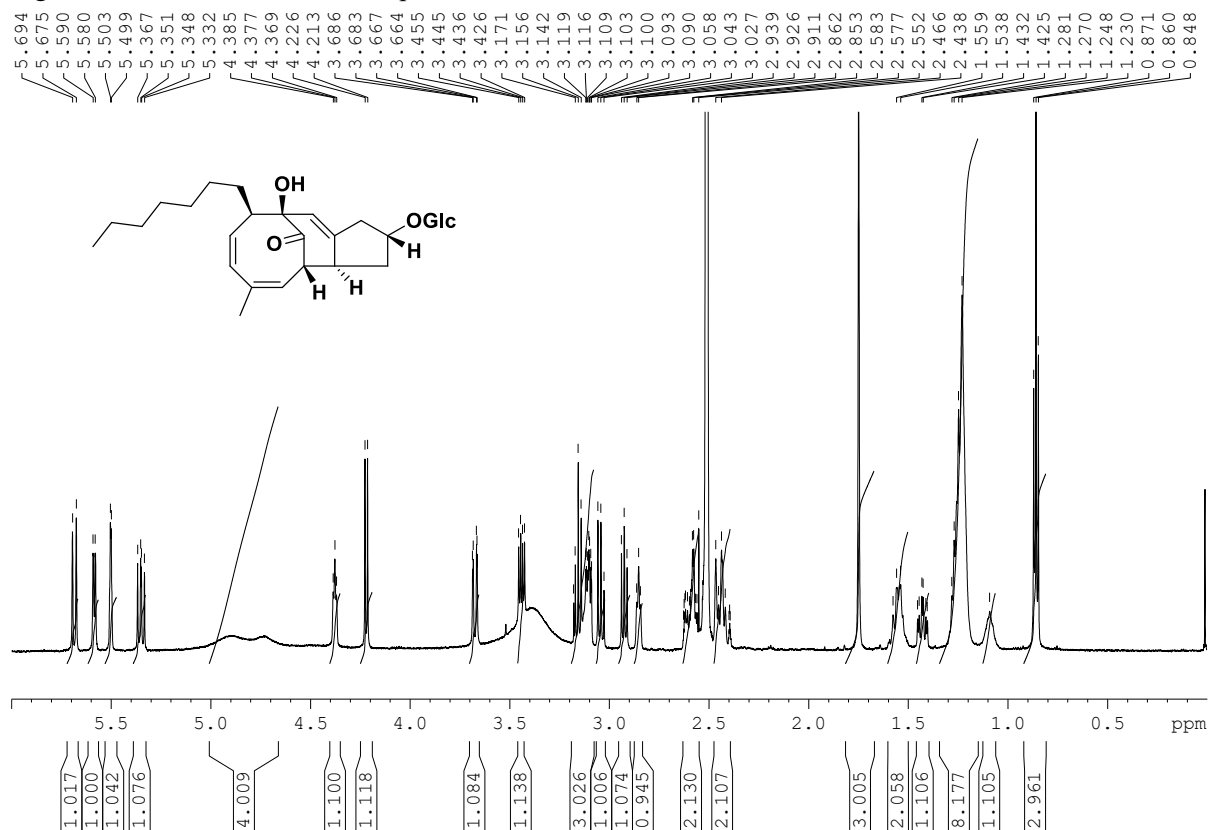
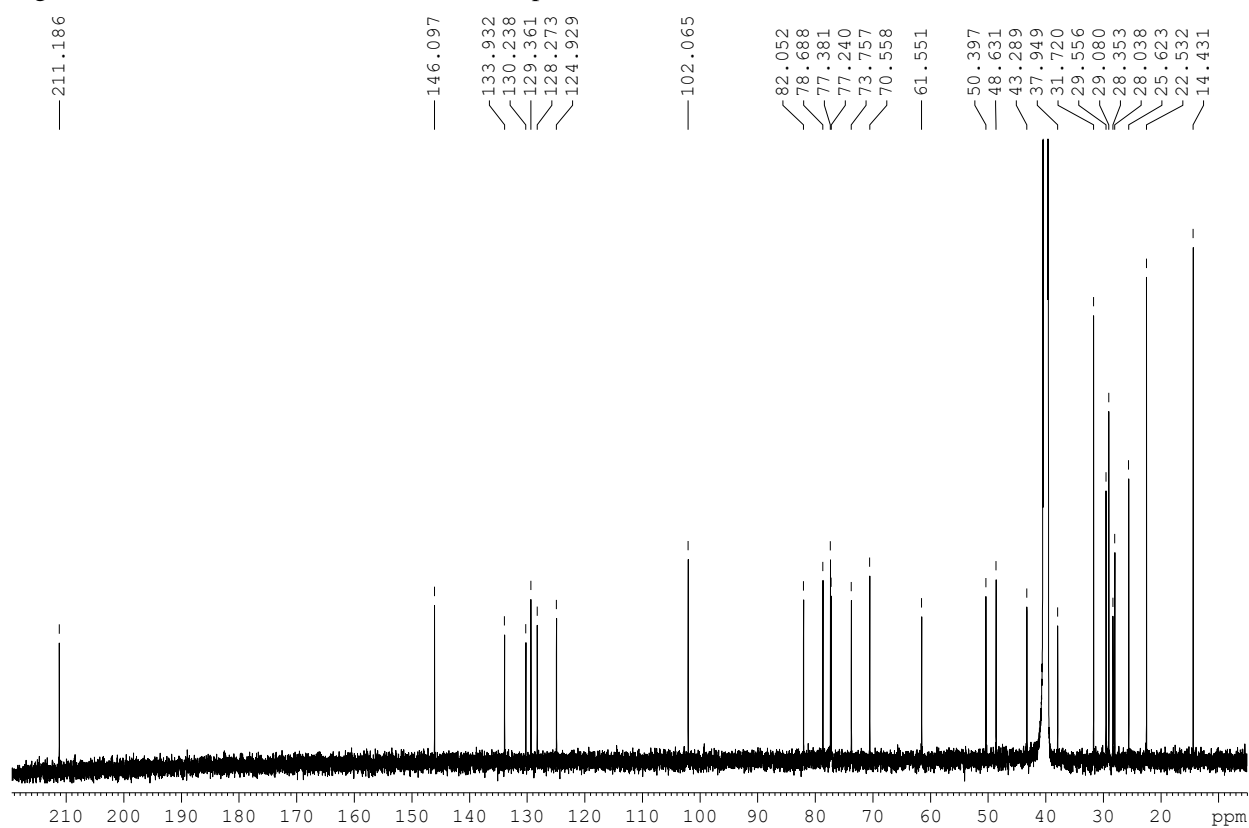


Figure S87.  $^{13}\text{C}$  NMR and DEPT (150 MHz) spectra of **11** in  $\text{DMSO}-d_6$



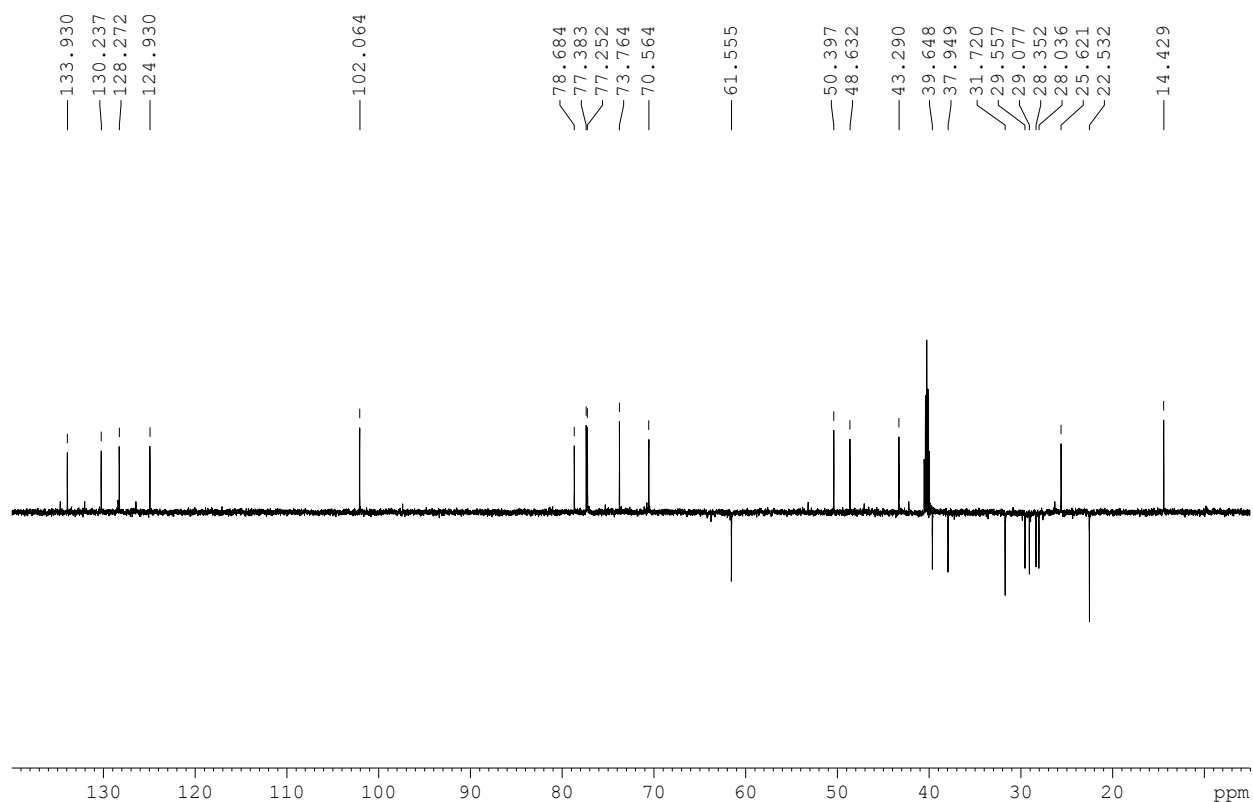


Figure S88.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **11** in DMSO- $d_6$

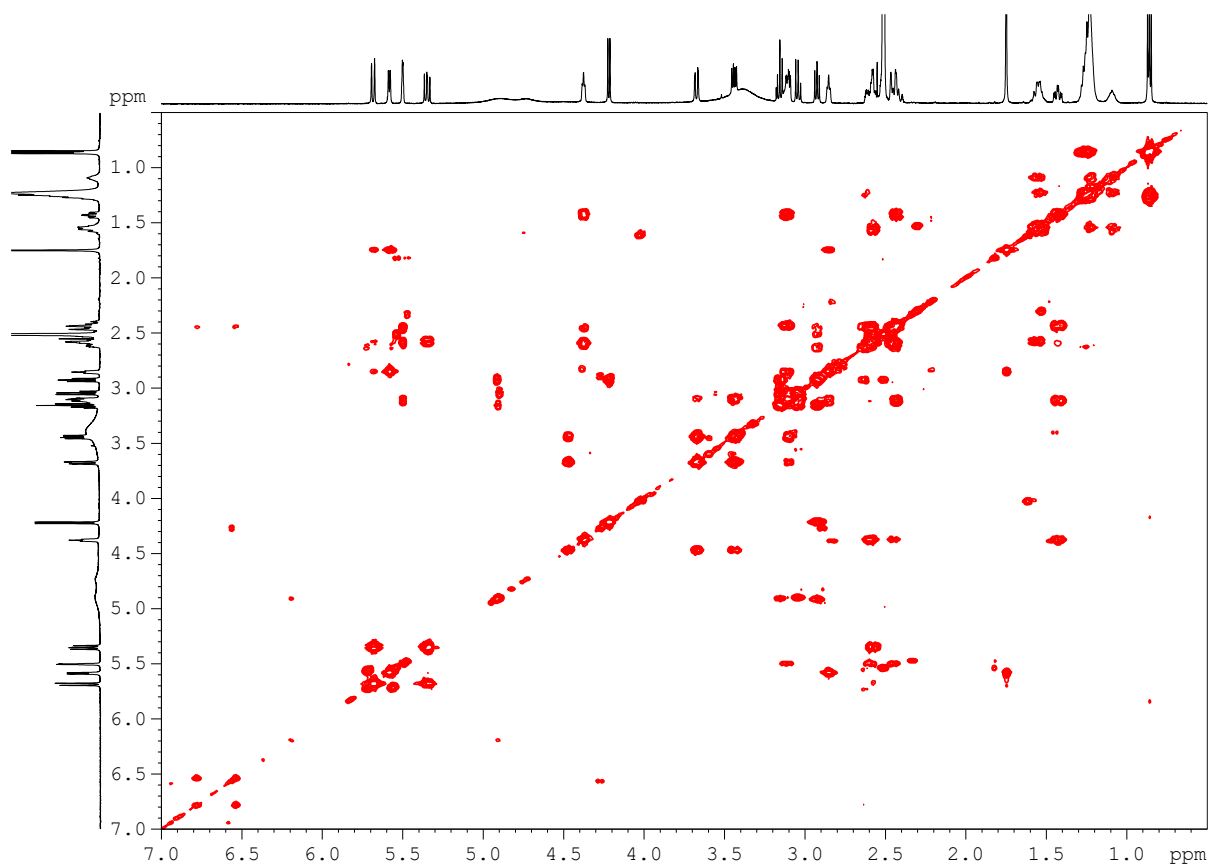


Figure S89. HSQC spectrum of **11** in DMSO-*d*<sub>6</sub>

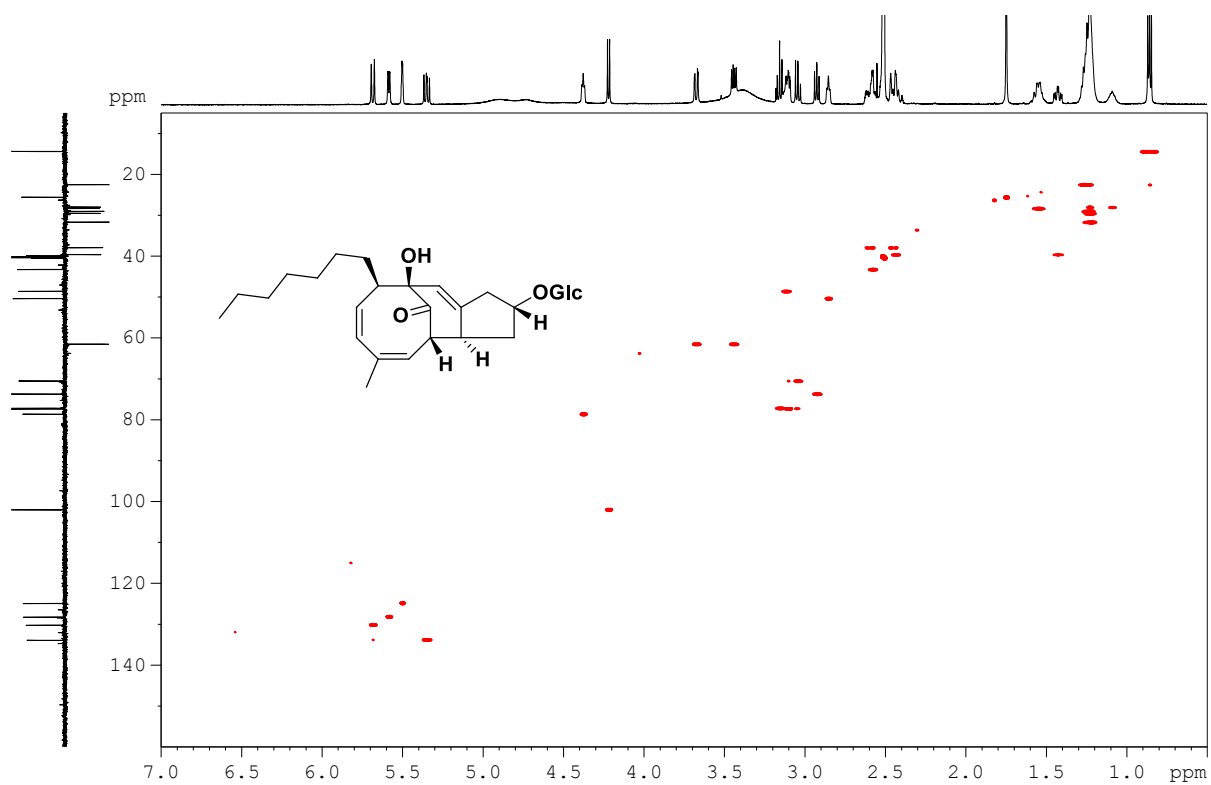


Figure S90. HMBC spectrum of **11** in DMSO-*d*<sub>6</sub>

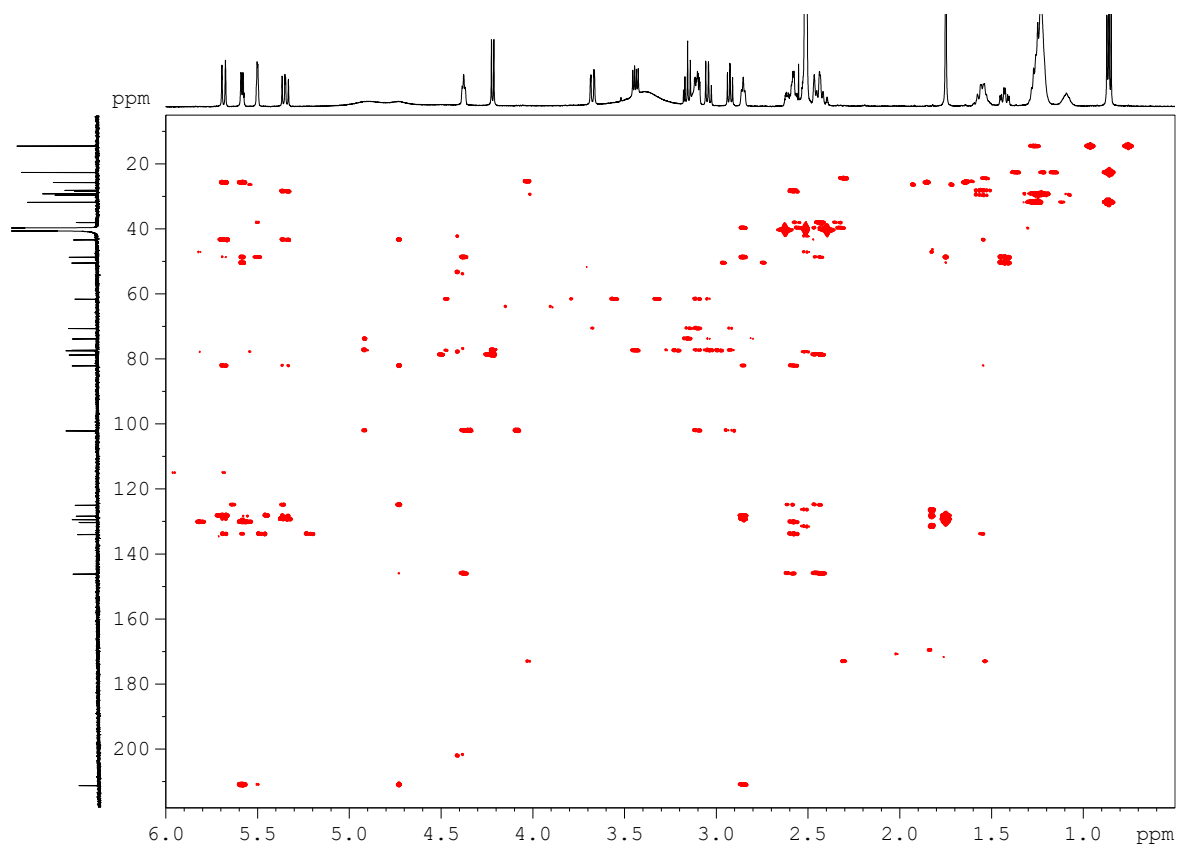


Figure S91. NOESY spectrum of **11** in DMSO-*d*<sub>6</sub>

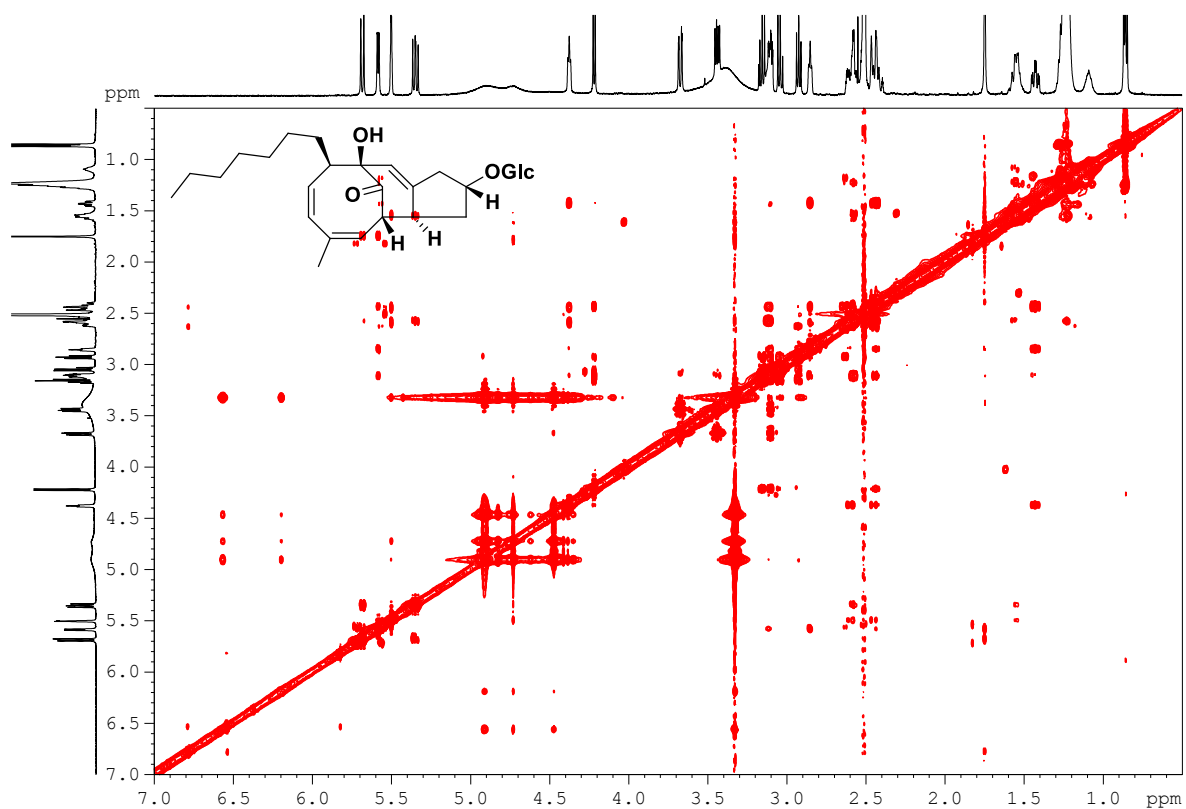


Figure S92. ROESY spectrum of **11** in DMSO-*d*<sub>6</sub>

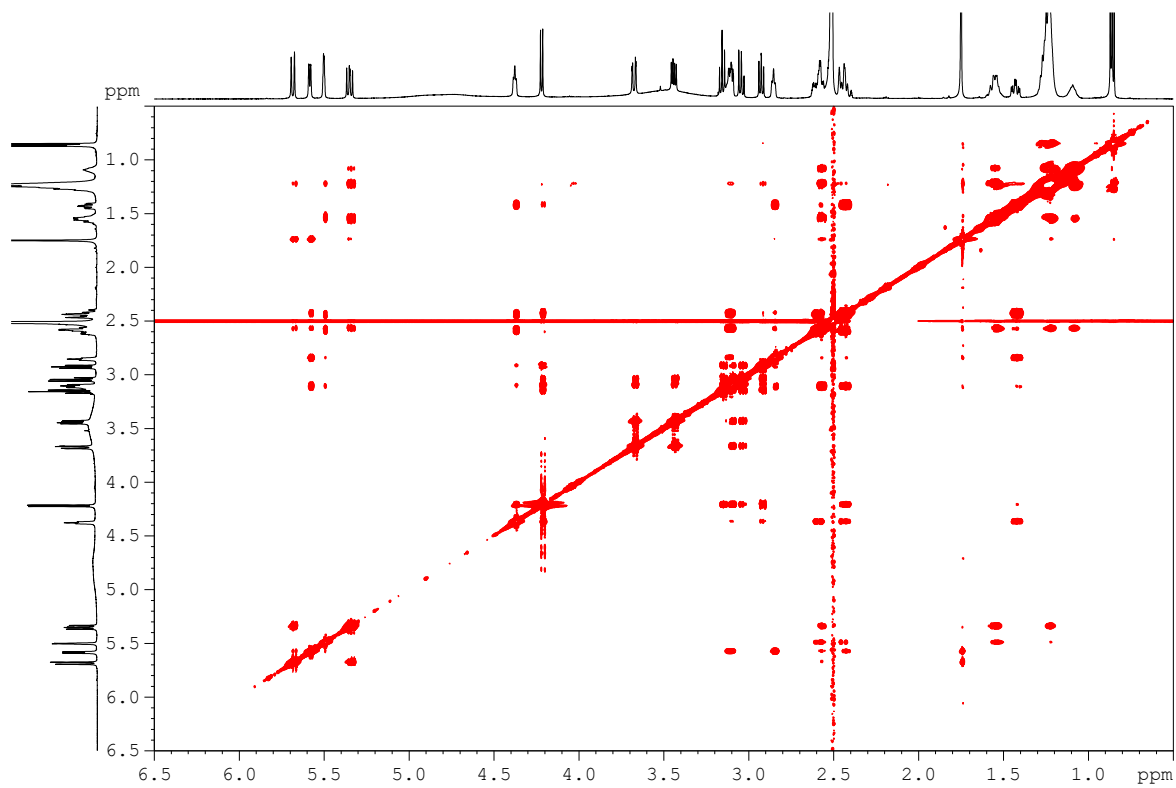
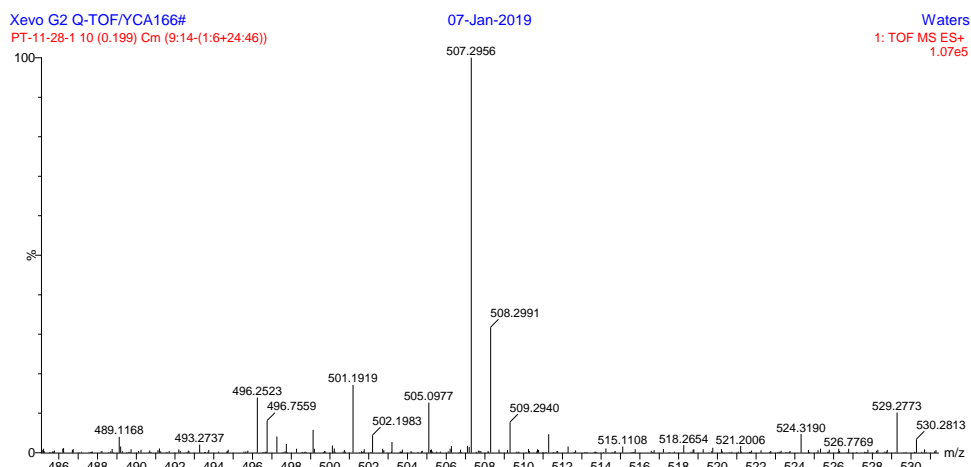




Figure S93. HRESIMS spectrum of **11**



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
507.2956	507.2958	-0.2	-0.4	7.5	166.9	1.373	25.33	C <sub>28</sub> H <sub>43</sub> O <sub>8</sub>

Figure S94. IR spectrum of **12**

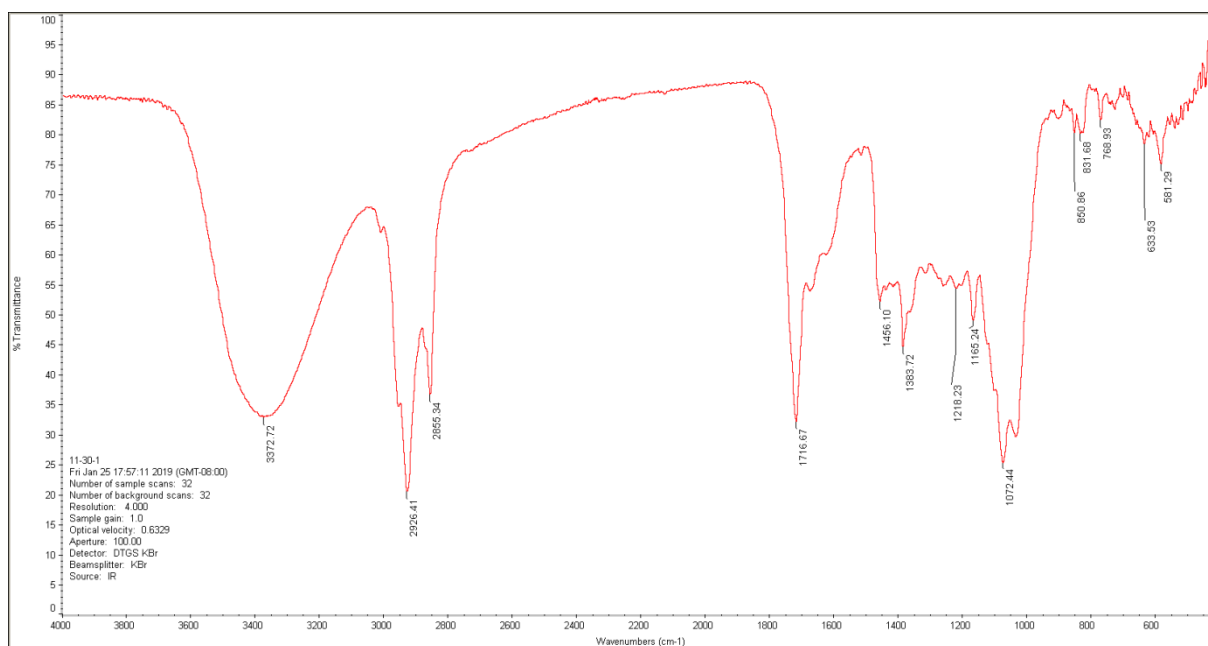


Figure S95.  $^1\text{H}$  NMR (600 MHz) spectrum of **12** in  $\text{DMSO}-d_6$

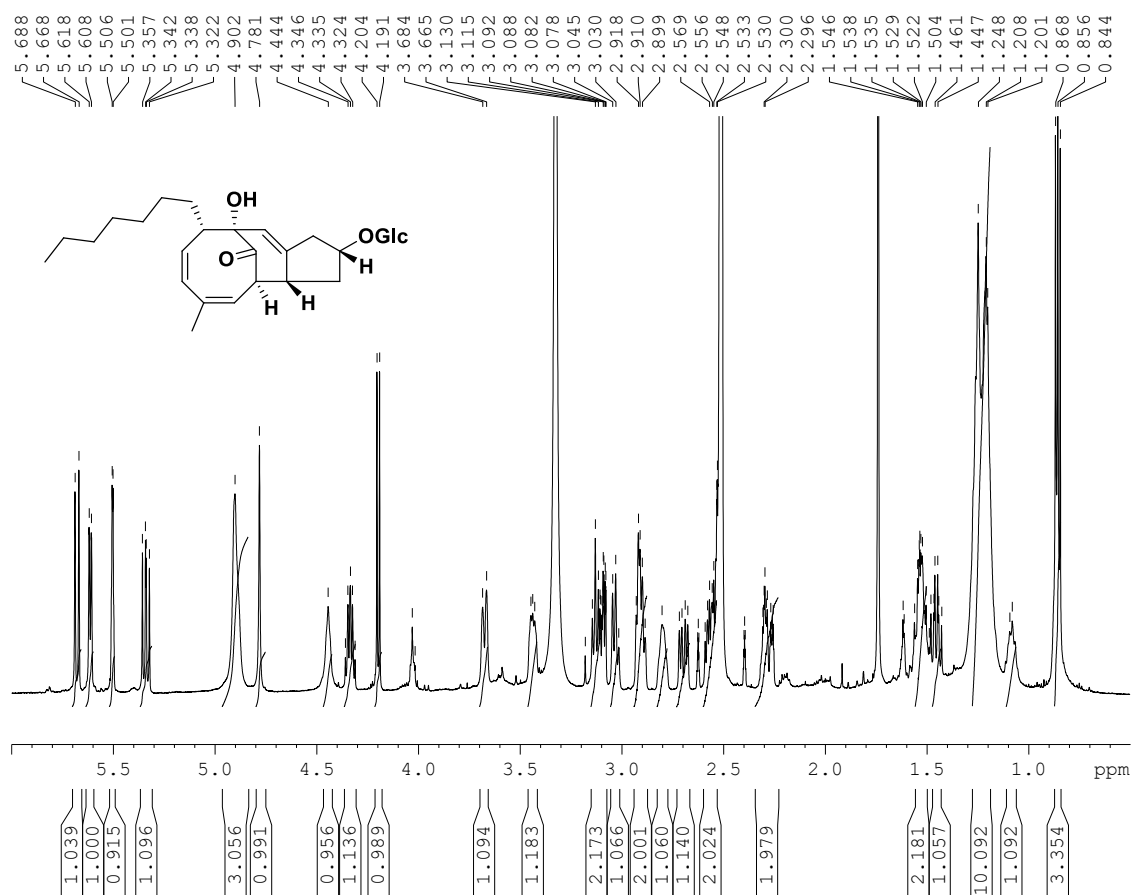


Figure S96.  $^{13}\text{C}$  NMR (150 MHz) spectrum of **12** in  $\text{DMSO}-d_6$

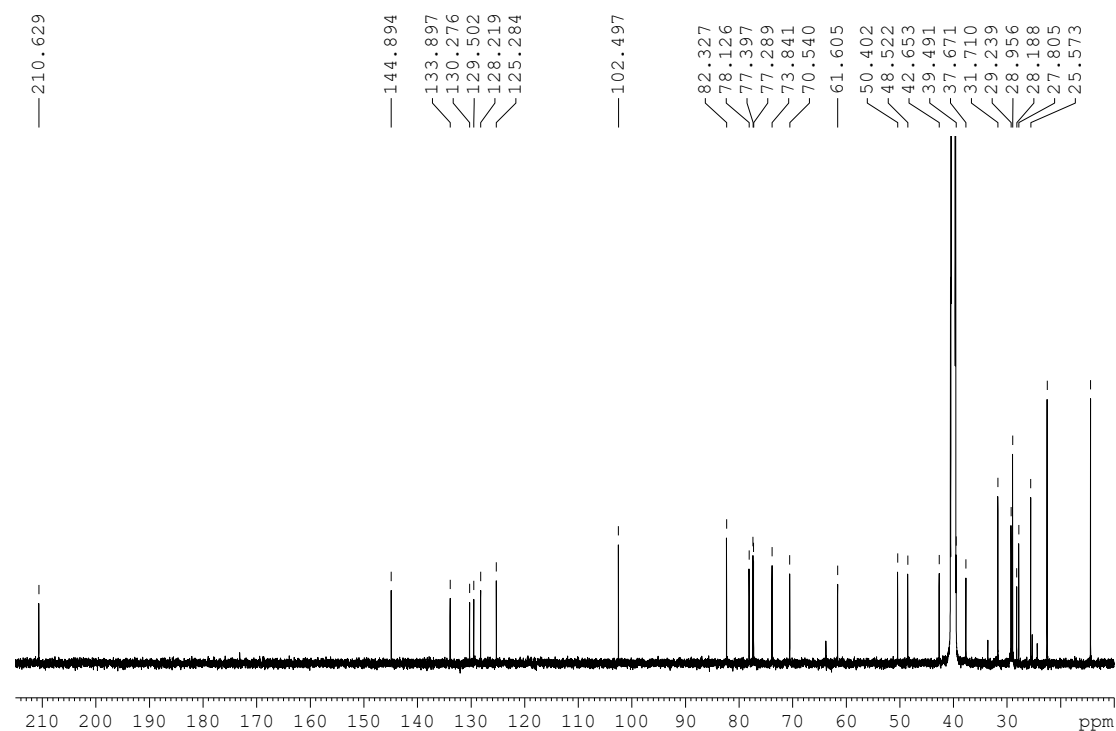


Figure S97. DEPT spectrum of **12** in DMSO-*d*<sub>6</sub>

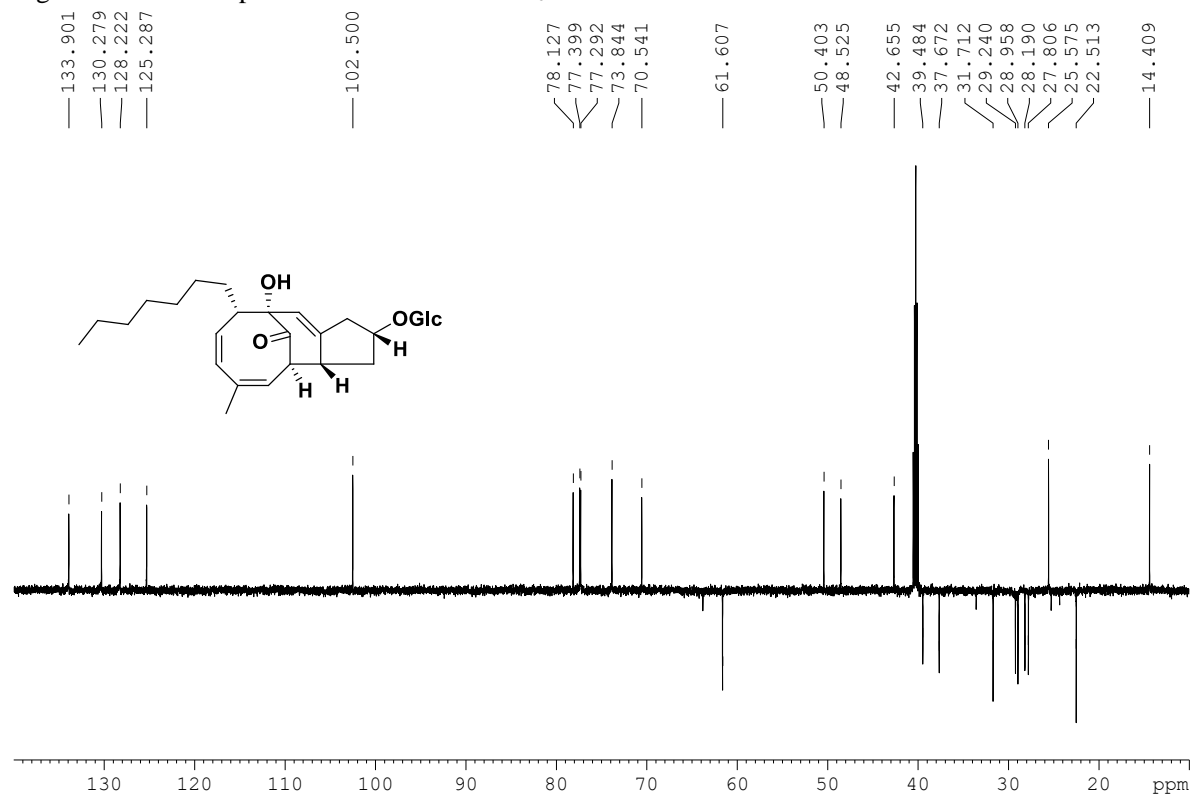


Figure S98. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **12** in DMSO-*d*<sub>6</sub>

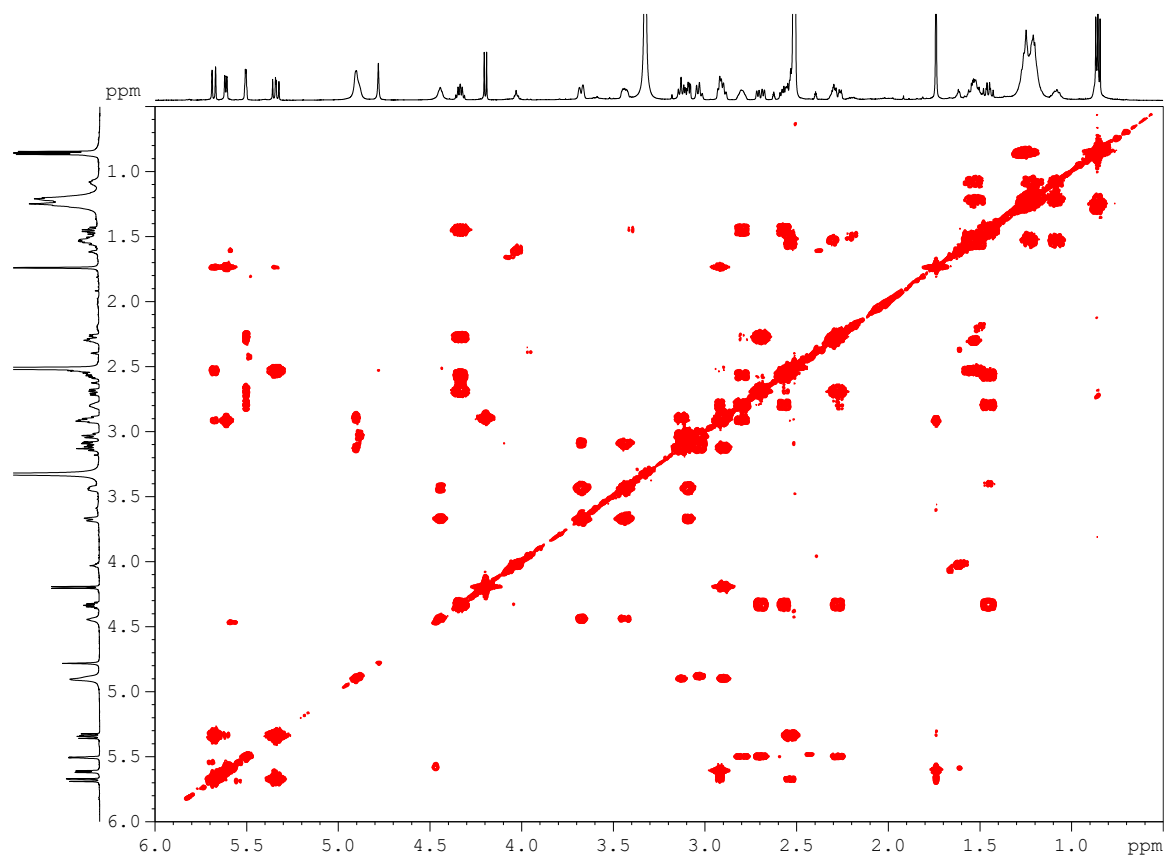


Figure S99. HSQC spectrum of **12** in DMSO-*d*<sub>6</sub>

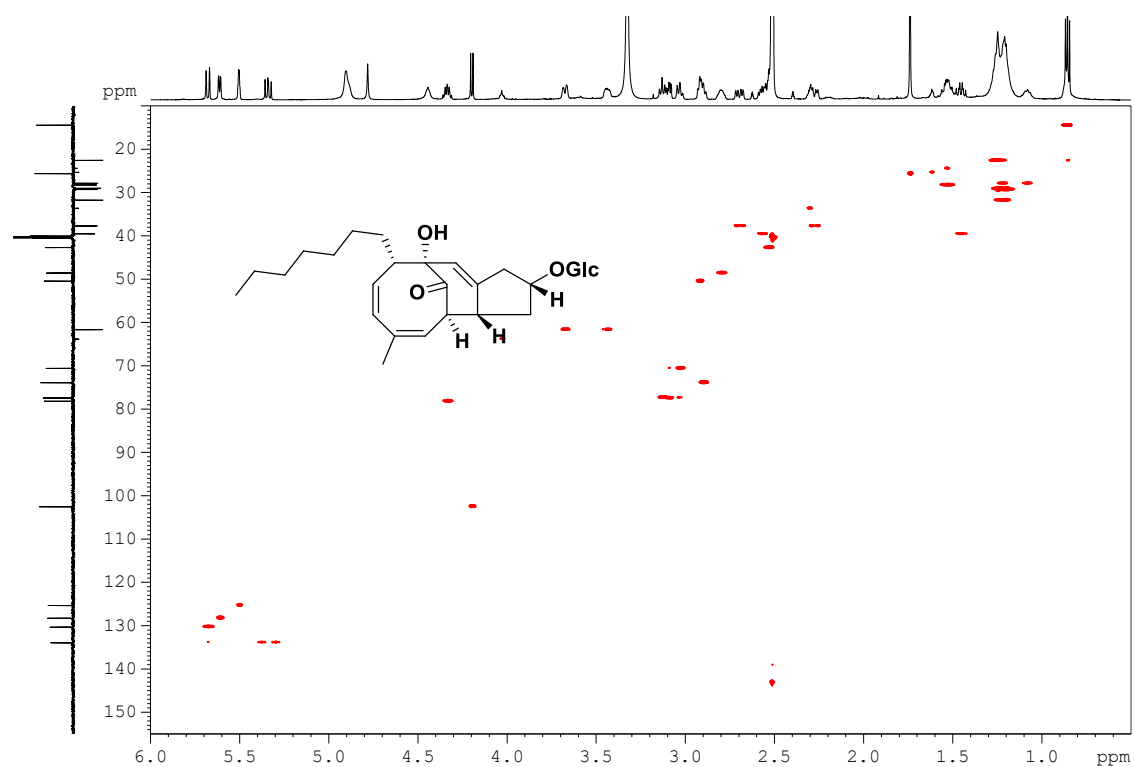


Figure S100. HMBC spectrum of **12** in DMSO-*d*<sub>6</sub>

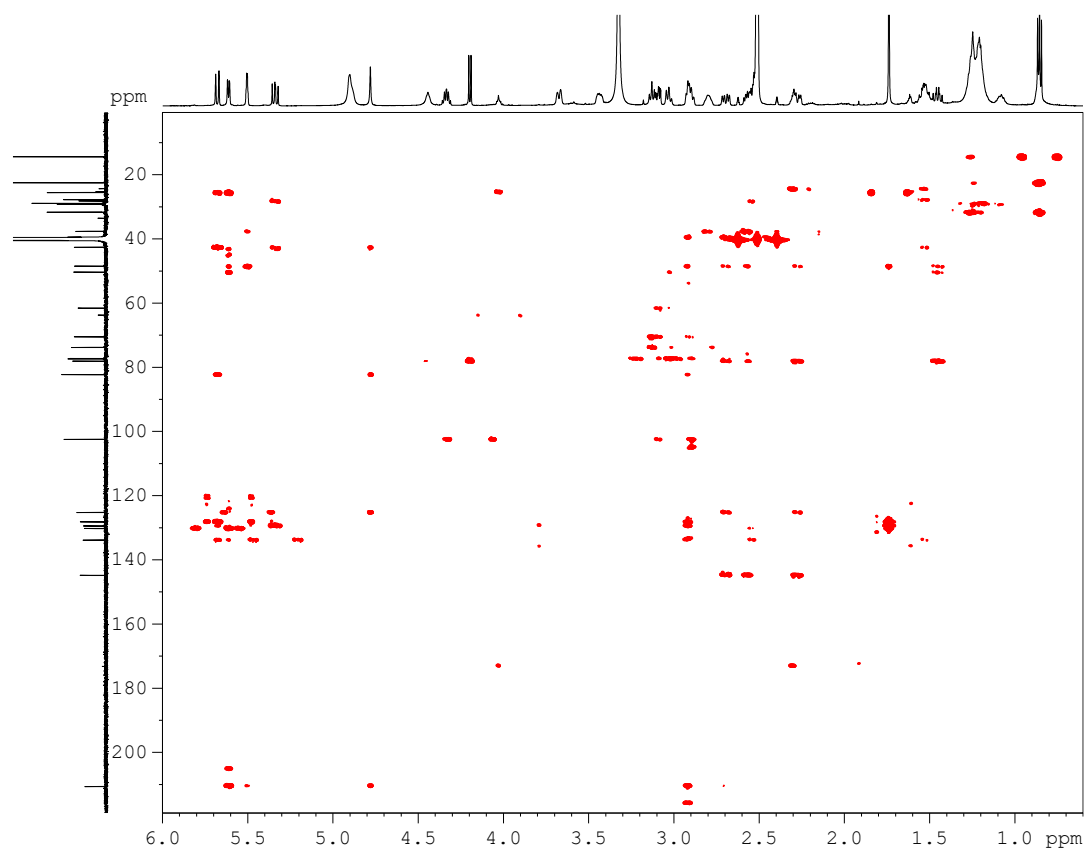


Figure S101. NOESY spectrum of **12** in DMSO-*d*<sub>6</sub>

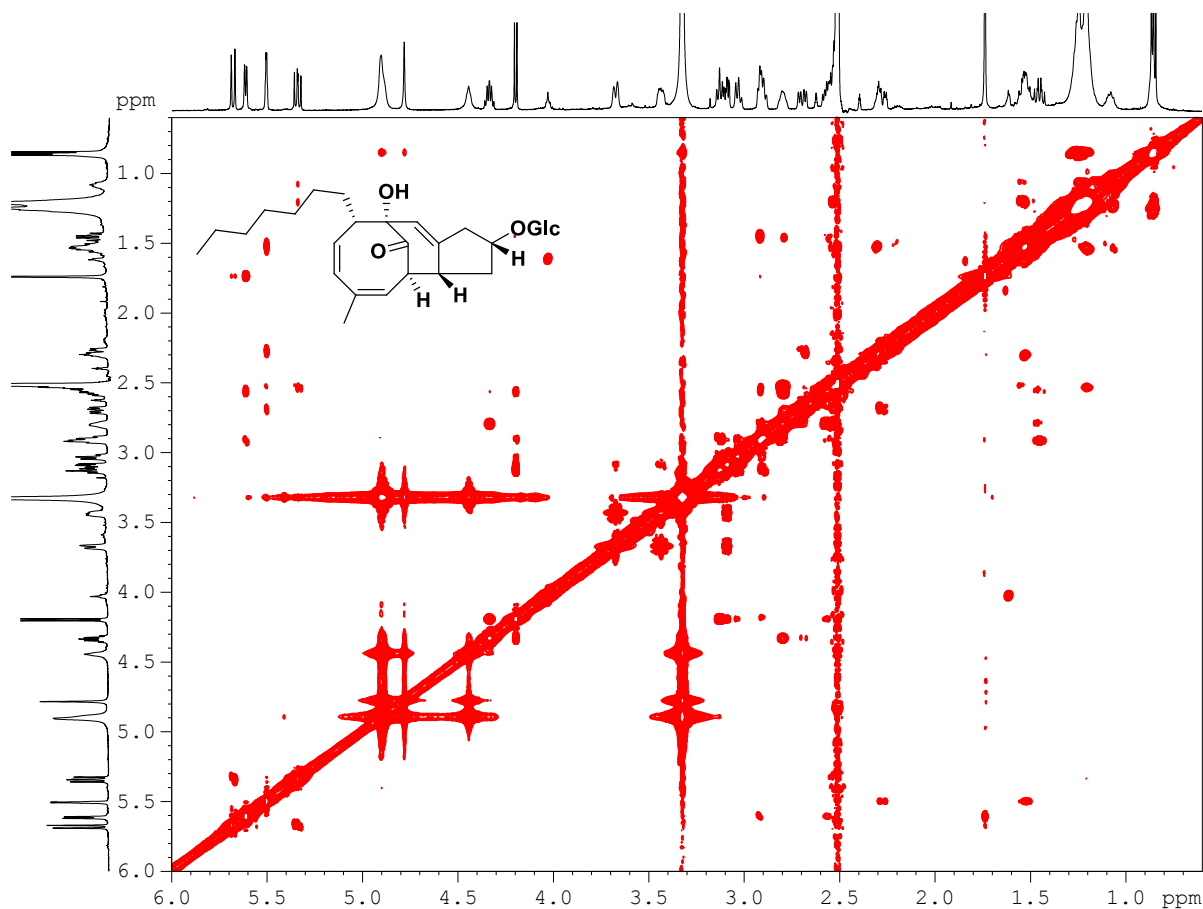
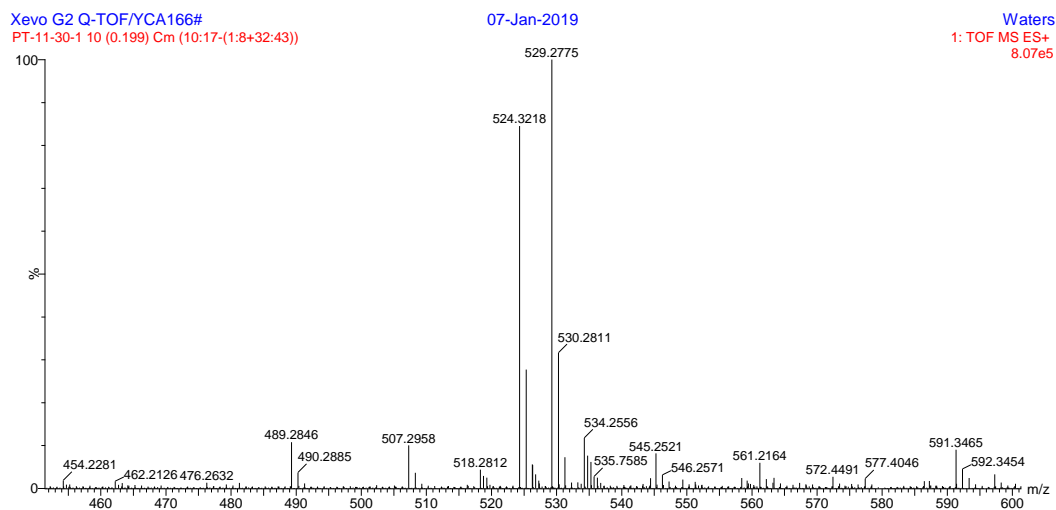


Figure S102. HRESIMS spectrum of **12**



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
507.2958	507.2958	0.0	0.0	7.5	382.4	6.116	0.22	C <sub>28</sub> H <sub>43</sub> O <sub>8</sub>

Figure S103. Part node clusters of EtOAc extract by molecular networking

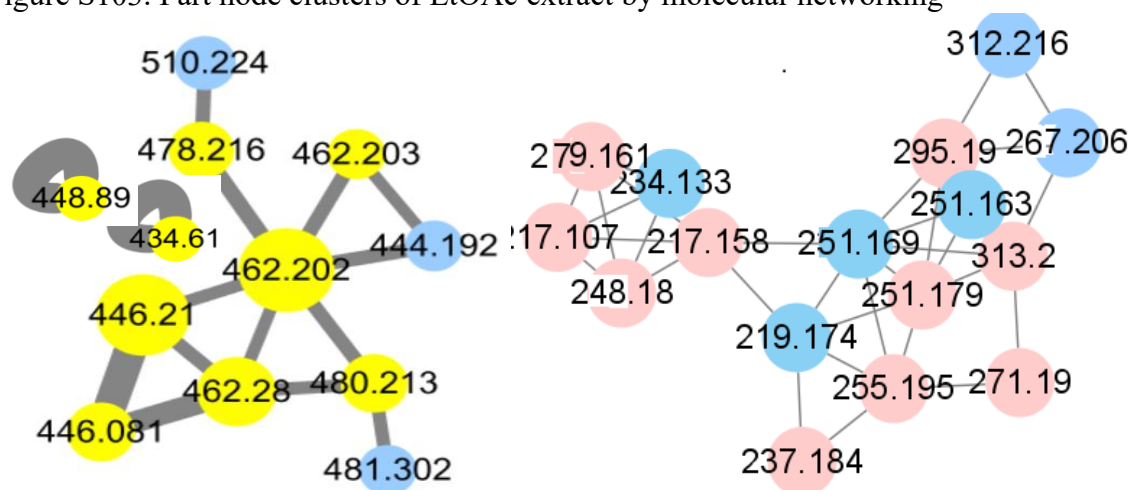


Figure S104. Key HMBC and COSY correlations of **1–10**.

