

## Supporting Information

### Supplementary File

#### **Saccharobisindole, neoasterric methyl ester, and 7-chloro-4(*1H*)-quinolone: three new compounds isolated from the marine bacterium *Saccharomonospora* sp.**

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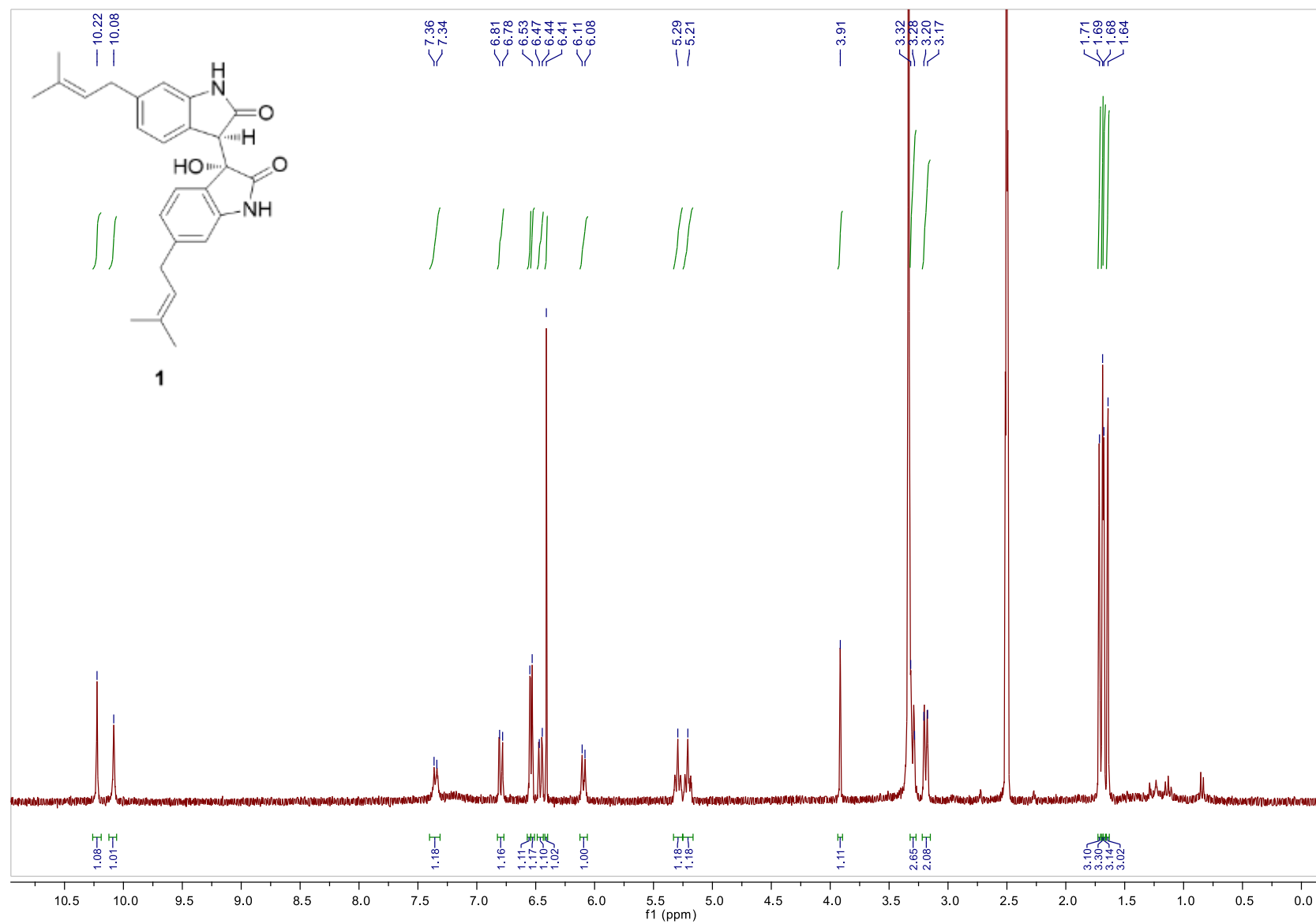
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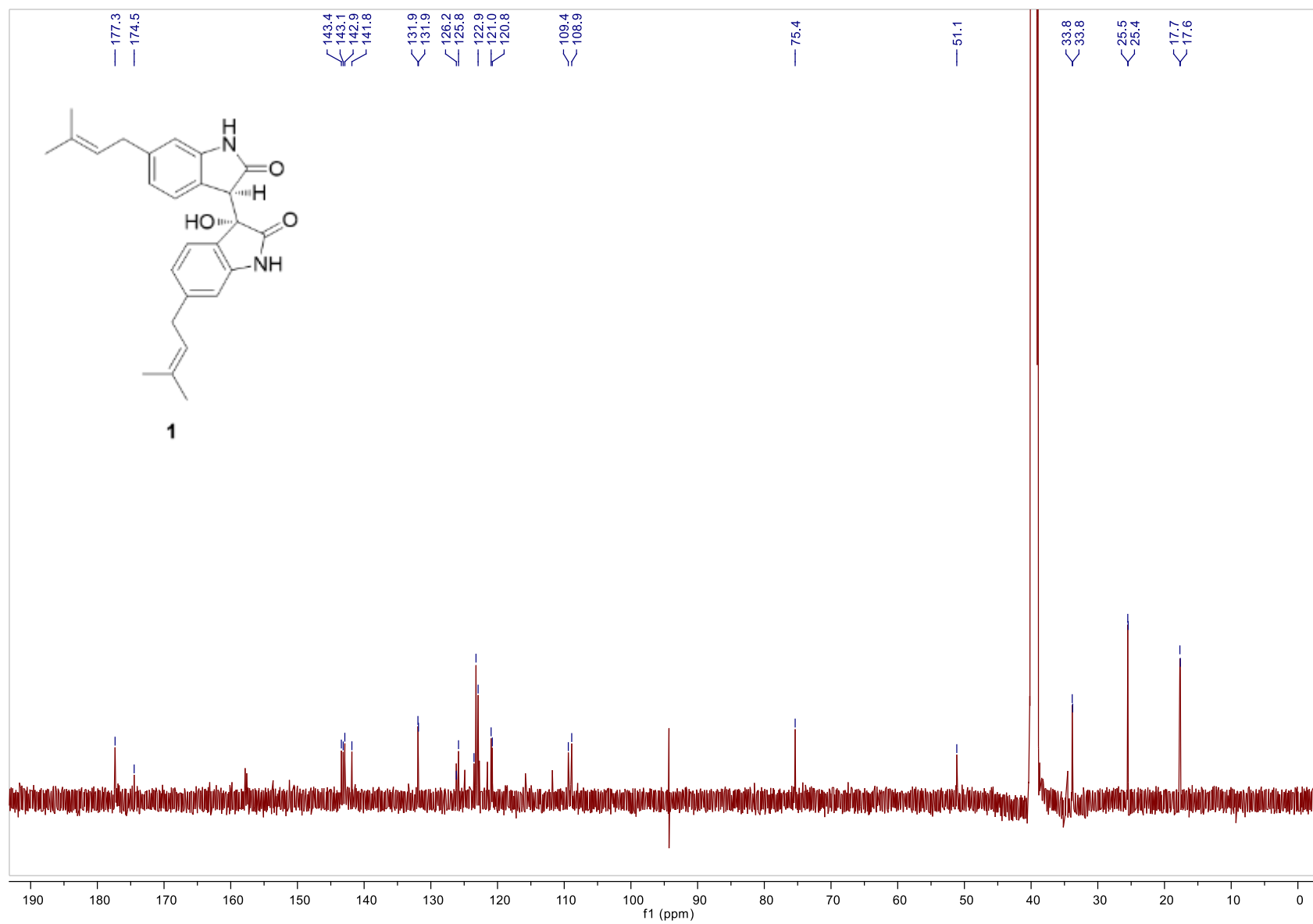
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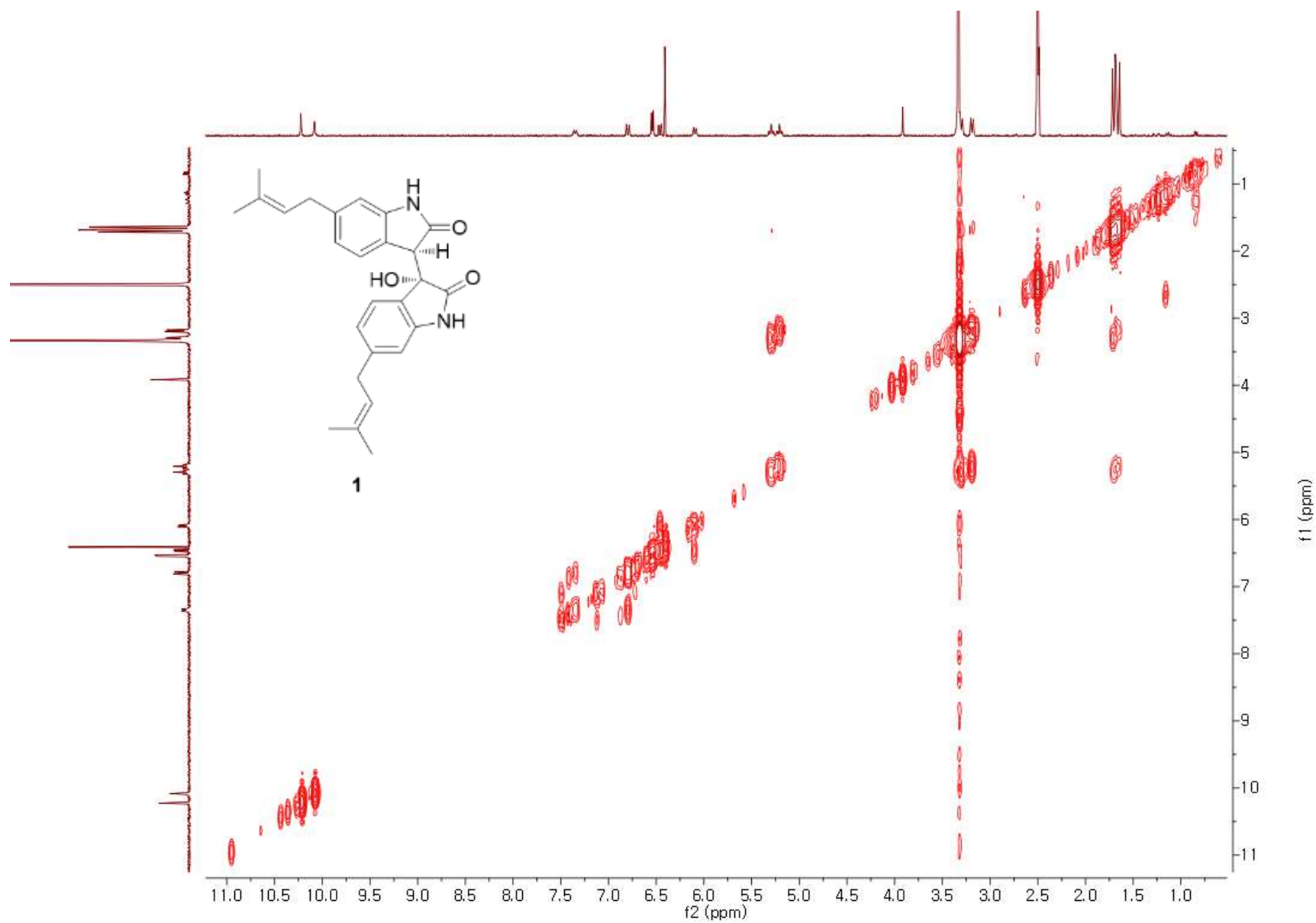
**Figure S1.**  $^1\text{H}$  NMR spectrum (300 MHz) of saccharobisindole (**1**) in  $\text{DMSO}-d_6$



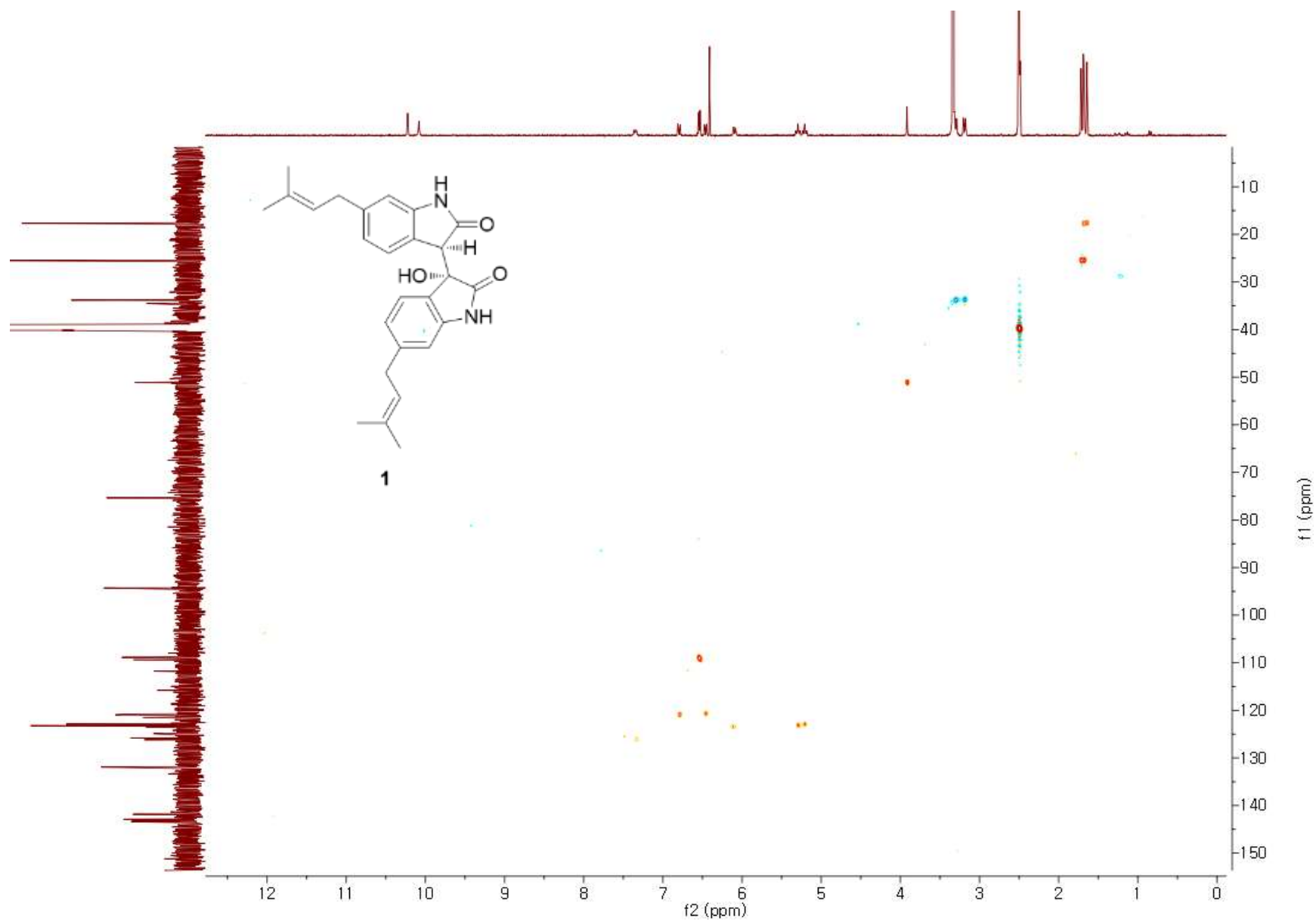
**Figure S2.**  $^{13}\text{C}$  NMR spectrum (75 MHz) of saccharobisindole (**1**) in  $\text{DMSO-}d_6$



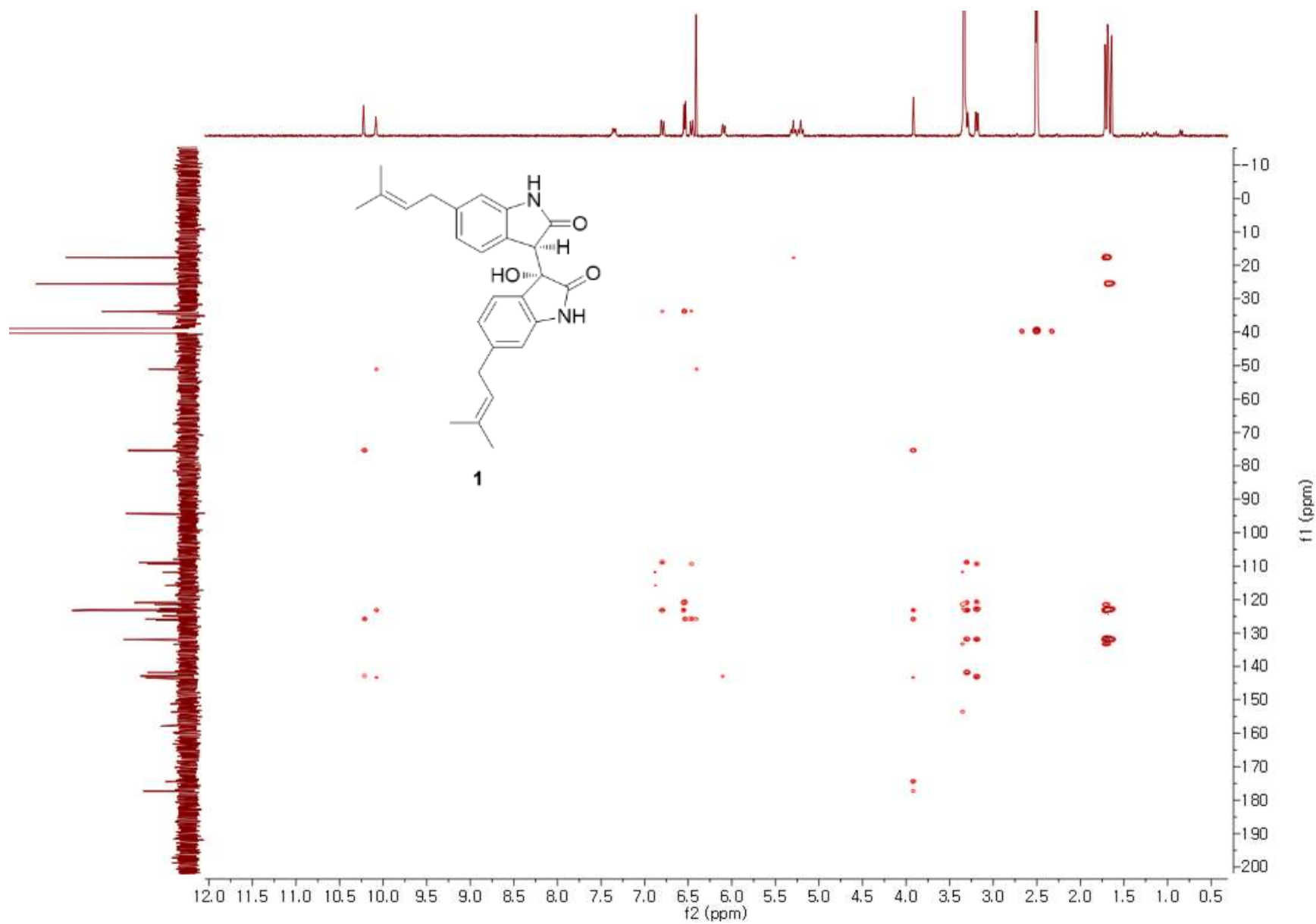
**Figure S3.** COSY spectrum (300 MHz) of saccharobisindole (**1**) in DMSO- $d_6$



**Figure S4.** HSQC spectrum (300 MHz) of saccharobisindole (**1**) in DMSO-*d*<sub>6</sub>

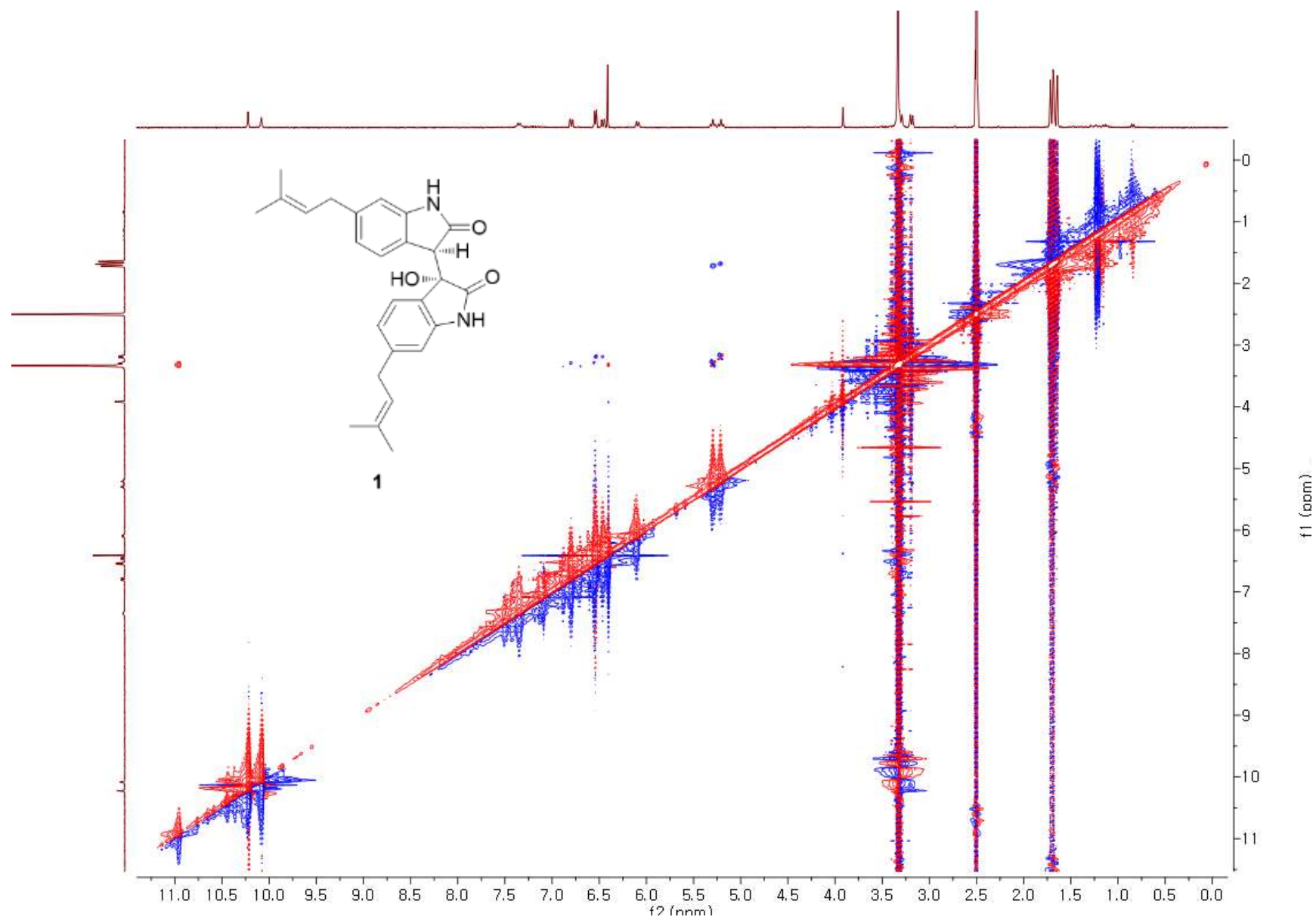


**Figure S5.** HMBC spectrum (300 MHz) of saccharobisindole (**1**) in DMSO- $d_6$





**Figure S6.** NOESY spectrum (300 MHz) of saccharobisindole (**1**) in DMSO- $d_6$



**Figure S7.** High resolution mass data of saccharobisindole (1)

```
[ Elemental Composition ]
Data : FAB-P861                      Date : 29-Sep-2017 17:17
Sample: CNQ490D5-1(C5-1)
Note : m-NBA
Inlet : Direct                       Ion Mode : FAB+
RT : 1.81 min                        Scan#: (81,88)
Elements : C 100/0, H 100/0, N 10/0, O 10/0
Mass Tolerance : 20ppm, 5mmu if m/z < 250, 10mmu if m/z > 500
Unsaturation (U.S.) : -0.5 - 50.0

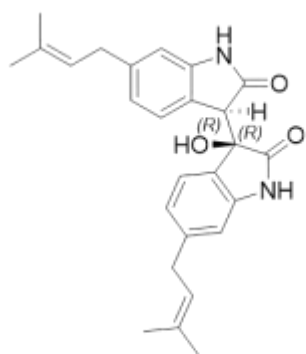
Observed m/z  Int%  Err[ppm / mmu]  U.S.  Composition
417.2181      0.6    -5.7 / -2.4    18.0  C 29 H 27 N 3
               -19.8 / -8.3    14.5  C 21 H 25 N 10
               -8.9 / -3.7    17.5  C 31 H 29 O
               +7.1 / +3.0    14.5  C 22 H 25 N 8 O
               +3.9 / +1.6    14.0  C 24 H 27 N 5 O 2
               +0.7 / +0.3    13.5  C 26 H 29 N 2 O 3
               -13.4 / -5.6    10.0  C 18 H 27 N 9 O 3
               +16.8 / +7.0    10.5  C 17 H 25 N 10 O 3
               -16.6 / -6.9     9.5  C 20 H 29 N 6 O 4
               +13.6 / +5.7    10.0  C 19 H 27 N 7 O 4
               -19.8 / -8.3     9.0  C 22 H 31 N 3 O 5
               +10.3 / +4.3     9.5  C 21 H 29 N 4 O 5
               +7.1 / +3.0     9.0  C 23 H 31 N O 6
               -6.9 / -2.9     5.5  C 15 H 29 N 8 O 6
               -10.2 / -4.2     5.0  C 17 H 31 N 5 O 7
               +20.0 / +8.3     5.5  C 16 H 29 N 6 O 7
               -13.4 / -5.6     4.5  C 19 H 33 N 2 O 8
               +16.8 / +7.0     5.0  C 18 H 31 N 3 O 8
               +2.7 / +1.1     1.5  C 10 H 29 N 10 O 8
               +13.5 / +5.7     4.5  C 20 H 33 O 9
               -0.5 / -0.2     1.0  C 12 H 31 N 7 O 9
               -3.7 / -1.6     0.5  C 14 H 33 N 4 O 10

[ Theoretical Ion Distribution ]
Molecular Formula : C26 H29 N2 O3
(m/z 417.2178, MW 417.5279, U.S. 13.5)
Base Peak : 417.2178, Averaged MW : 417.5252(a), 417.5260(w)

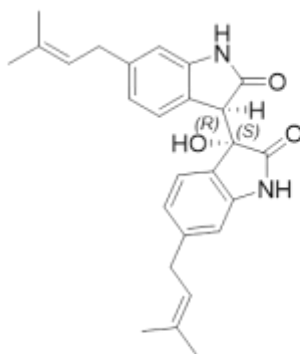
m/z      INT.
417.2178 100.0000 *****
418.2210 29.7671 *****
419.2239 4.8696 ***
420.2267 0.5713
421.2295 0.0528
422.2321 0.0040
423.2348 0.0003
```

**Figure S8.** Alpha-D data and Calculated optical rotation of saccharobisindole (**1**)

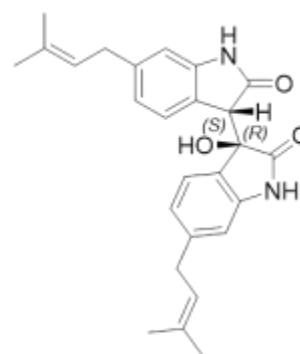
Basis functions	Def-SV(P)	6-31G*	6-31G**
<i>R,R</i> - diastereomer	-798.2	-868.15	-889.46
<i>R,S</i> – diastereomer	-12.43	<b>+40.51</b>	<b>+51.93</b>
<i>S,R</i> – diastereomer	-725.36	-751.83	-764.03
<i>S,S</i> - diastereomer	-252.74	-315.09	-308.47
Experimental optical rotation : <b>+161</b>			



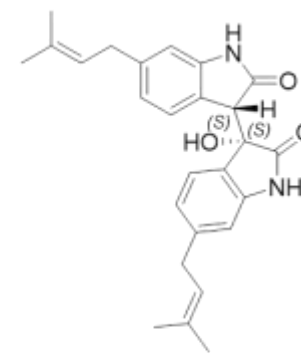
*R,R* - diastereomer



*R,S* - diastereomer

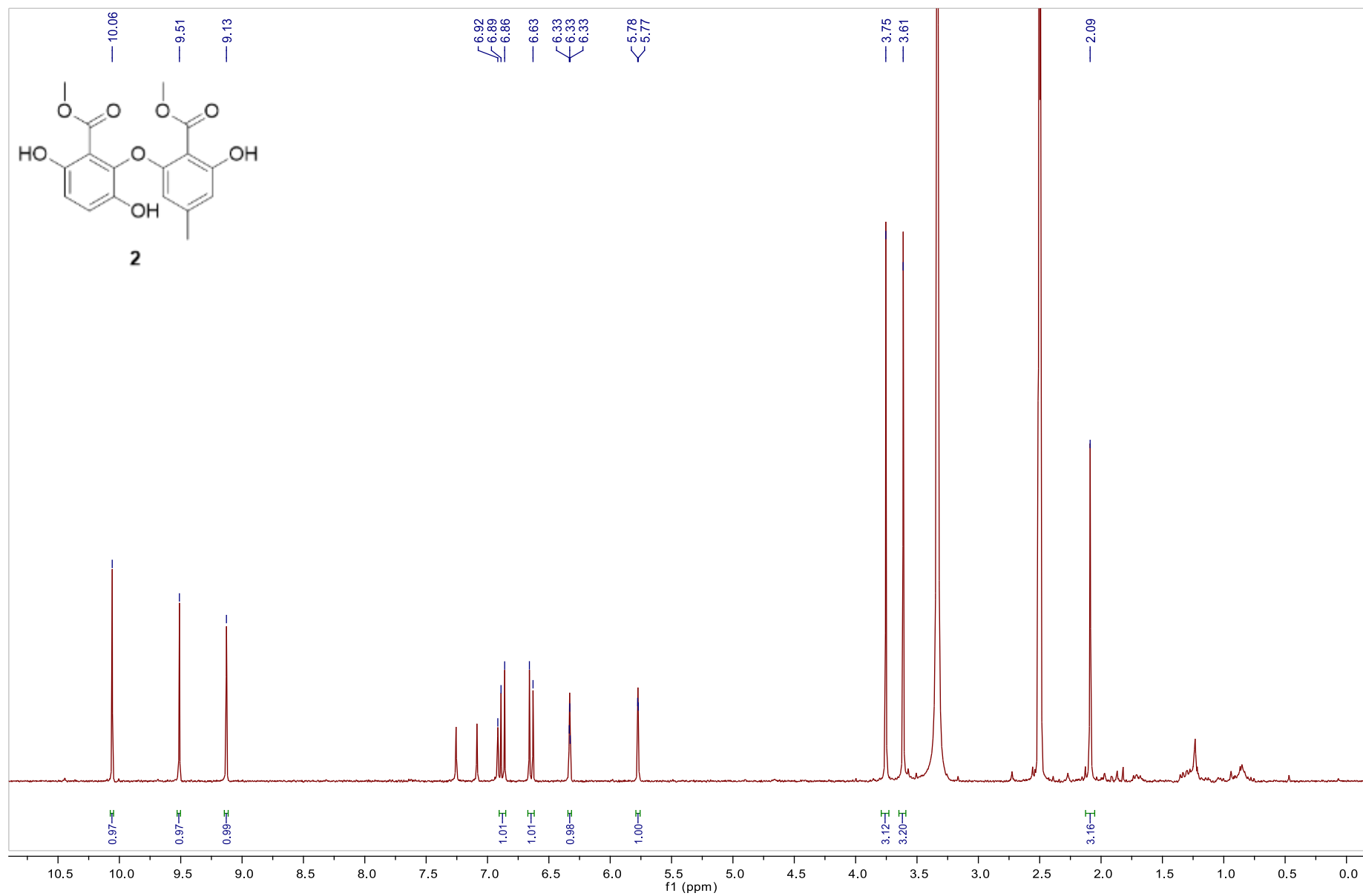


*S,R* - diastereomer

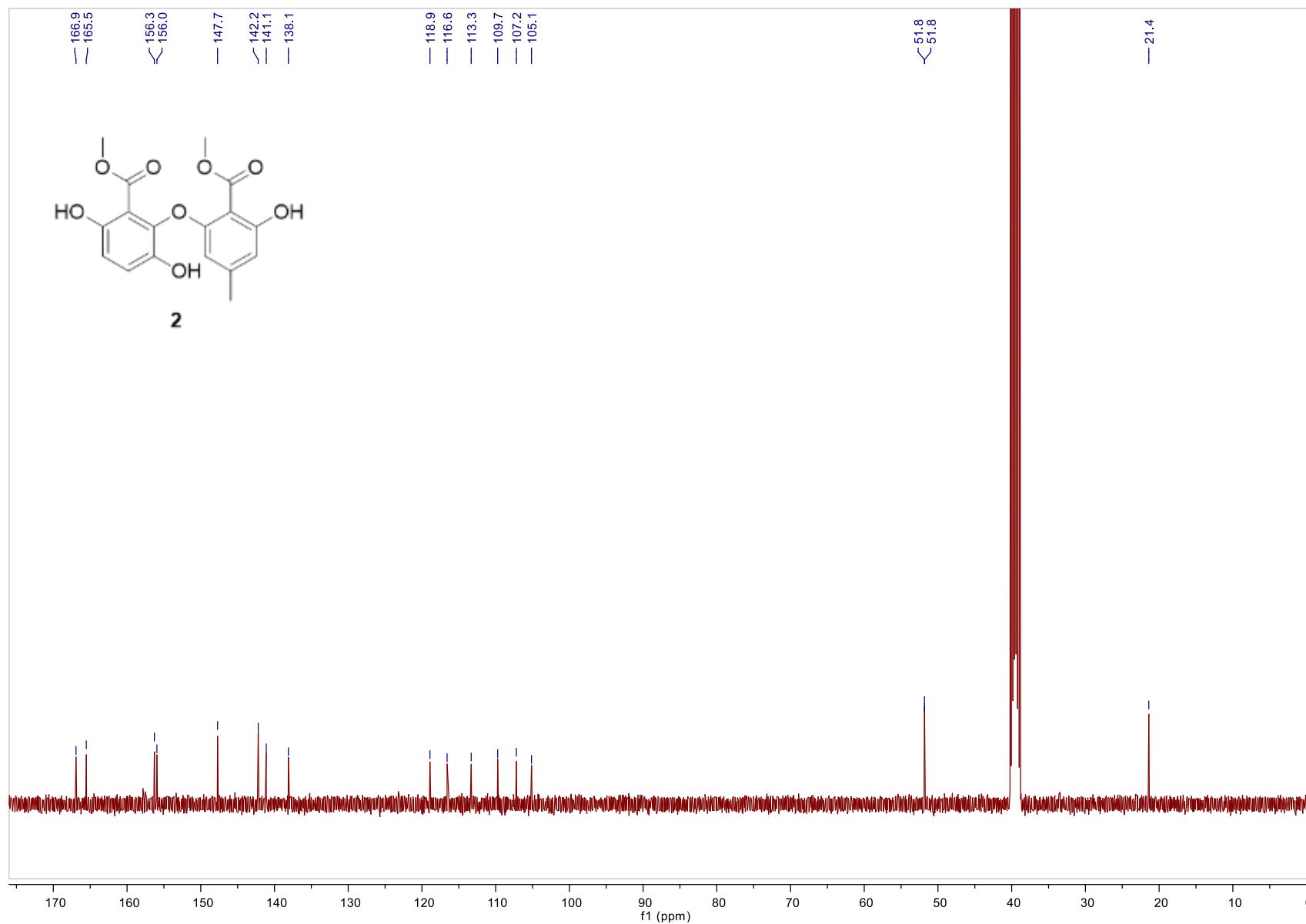


*S,S* - diastereomer

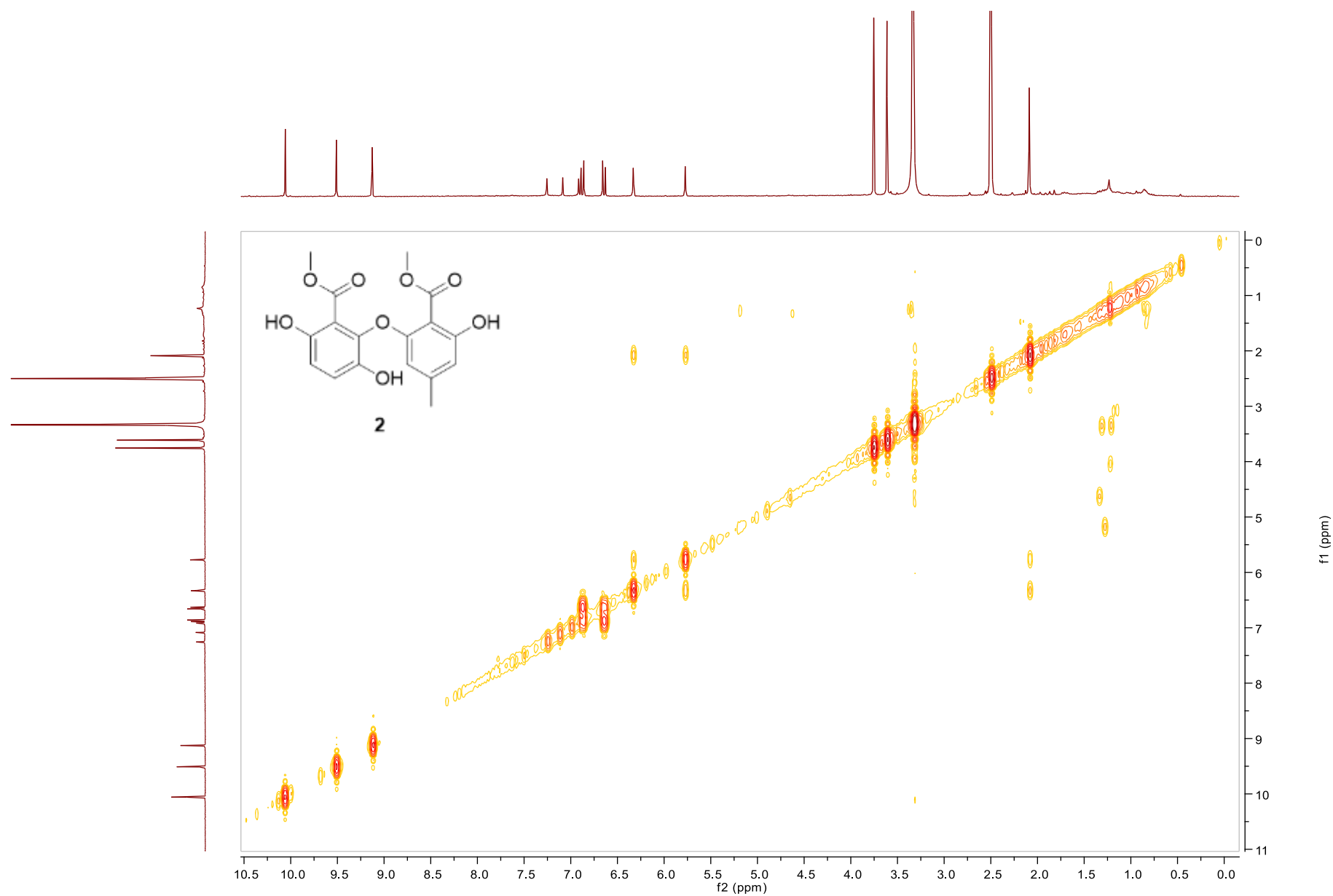
**Figure S9.**  $^1\text{H}$  NMR Spectrum (400 MHz) of neoasterric methyl ester (**2**) in  $\text{DMSO-}d_6$



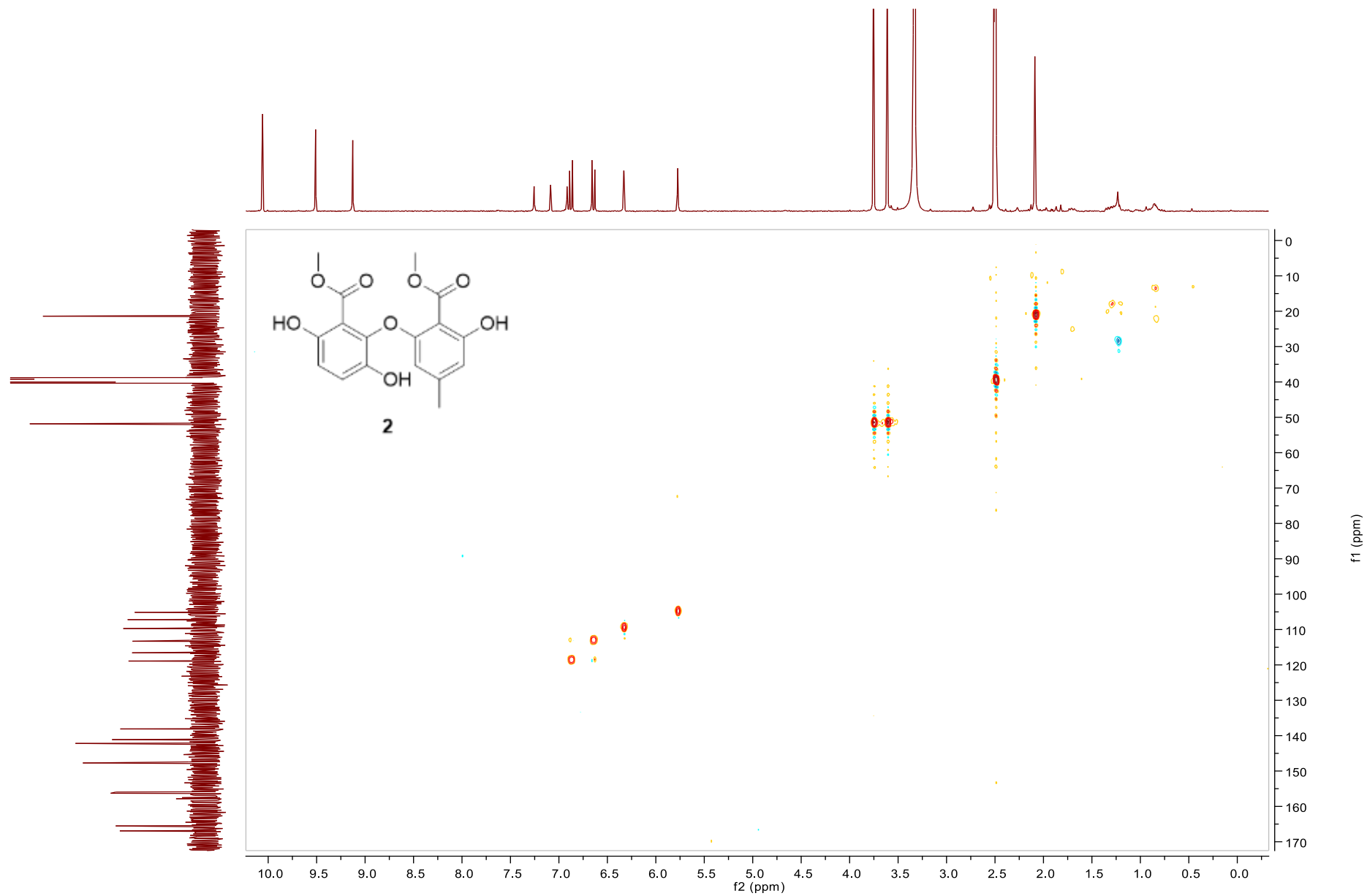
**Figure S10.**  $^{13}\text{C}$  NMR Spectrum (100 MHz) of neoasterric methyl ester (**2**) in  $\text{DMSO-}d_6$



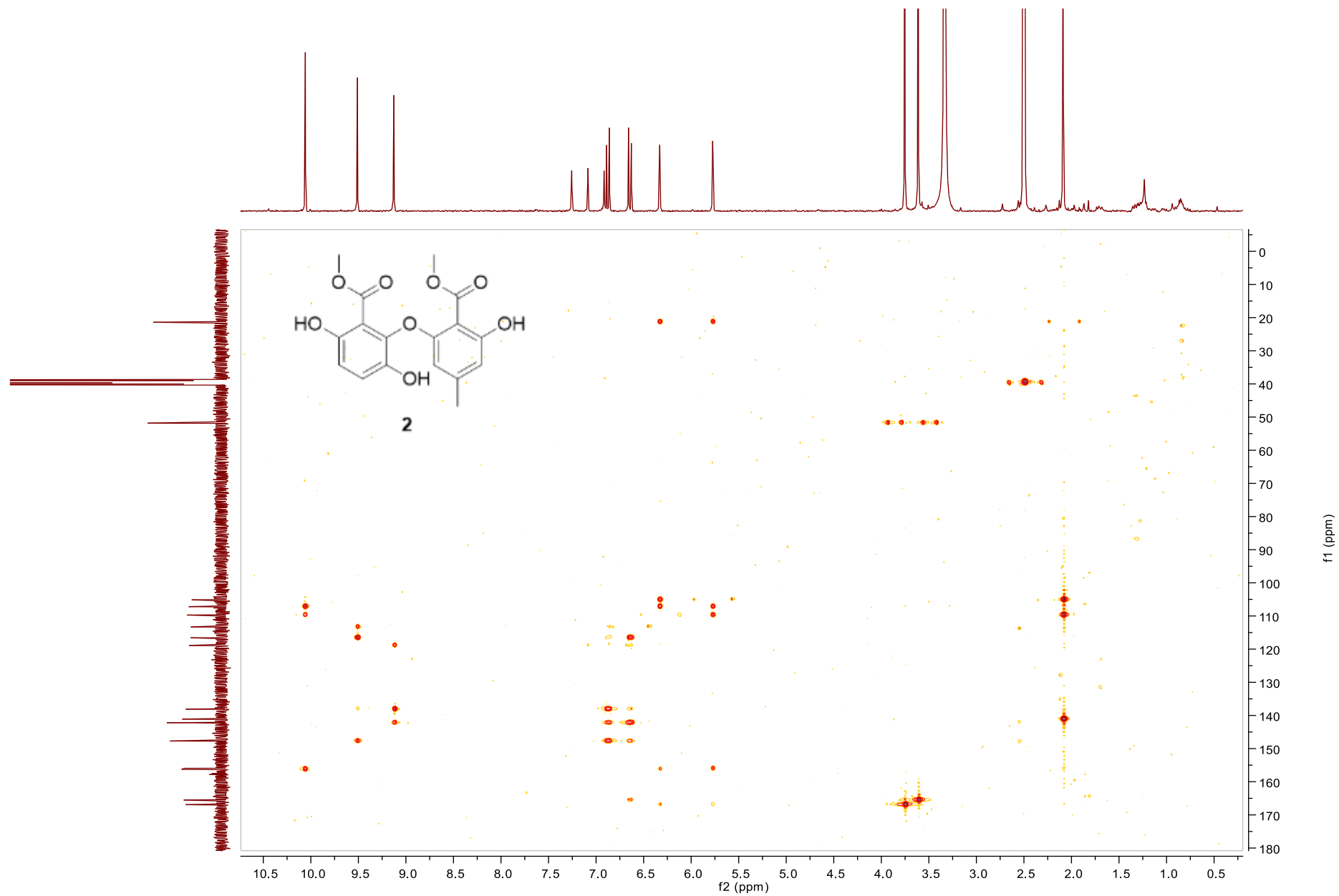
**Figure S11.** COSY Spectra (400 MHz) of neoasterric methyl ester (**2**) in DMSO- $d_6$



**Figure S12.** HSQC Spectra (400 MHz) of neoasterric methyl ester (**2**) in DMSO- $d_6$

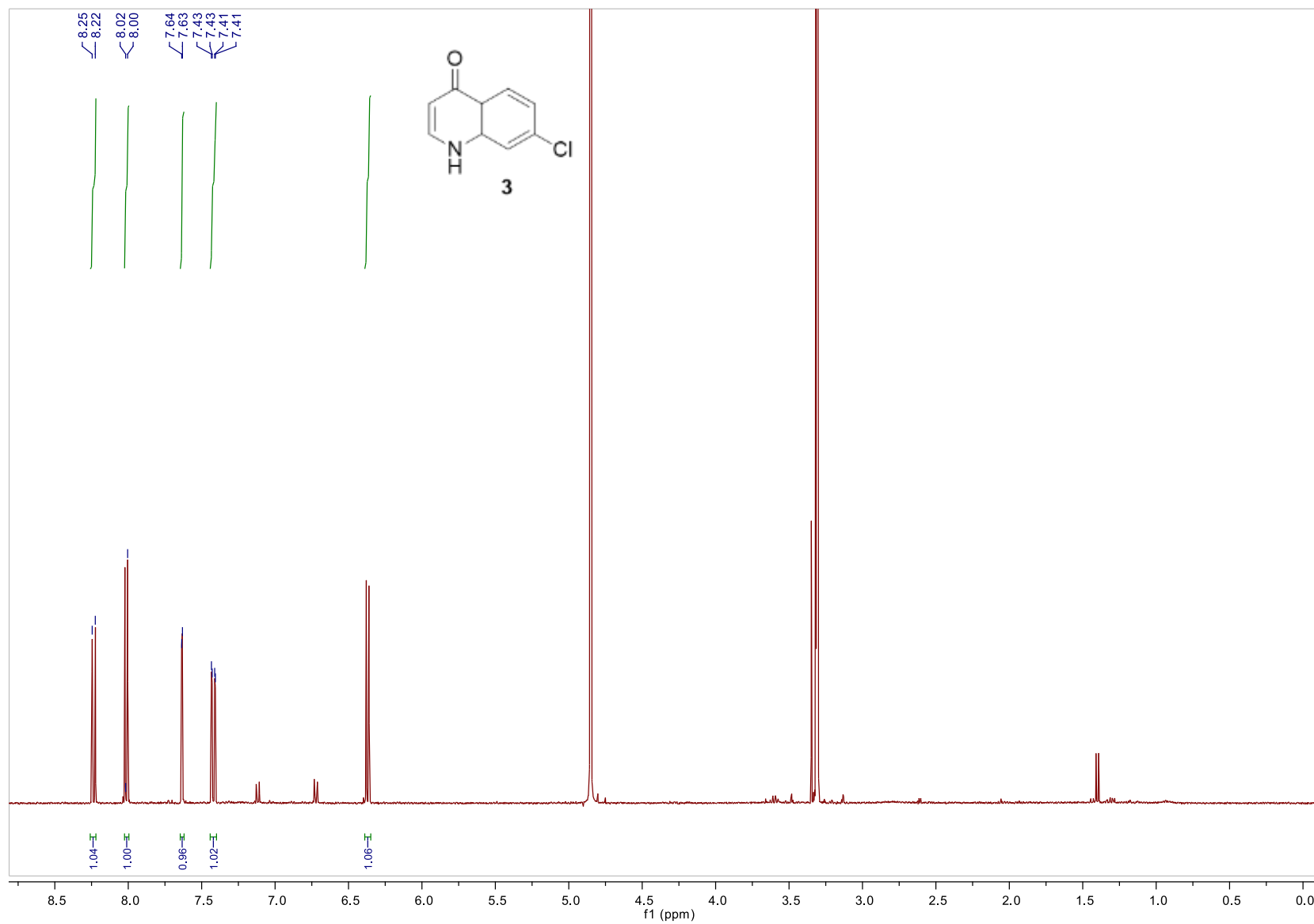


**Figure S13.** HMBC Spectra (400 MHz) of neoasterric methyl ester (**2**) in DMSO- $d_6$

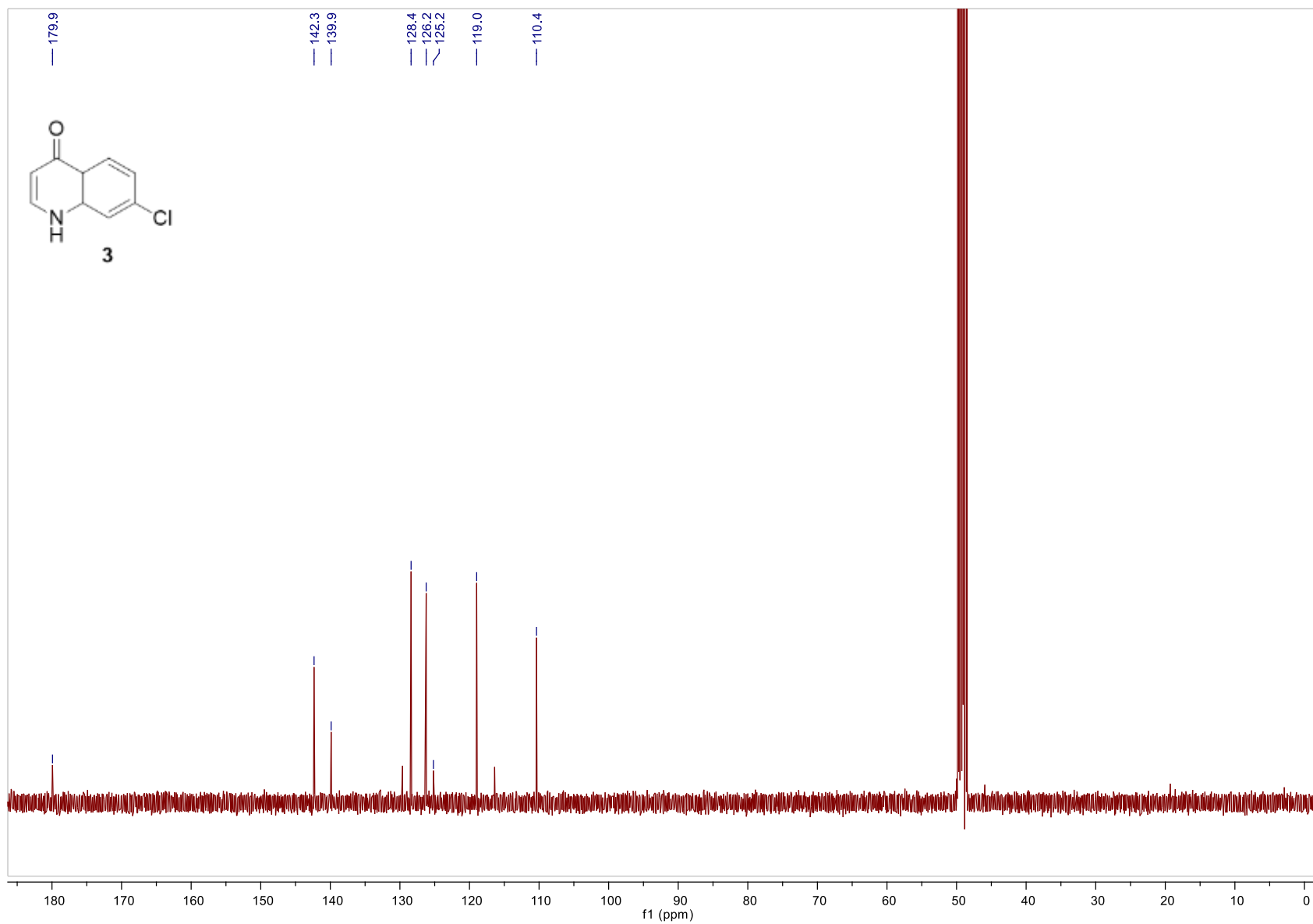




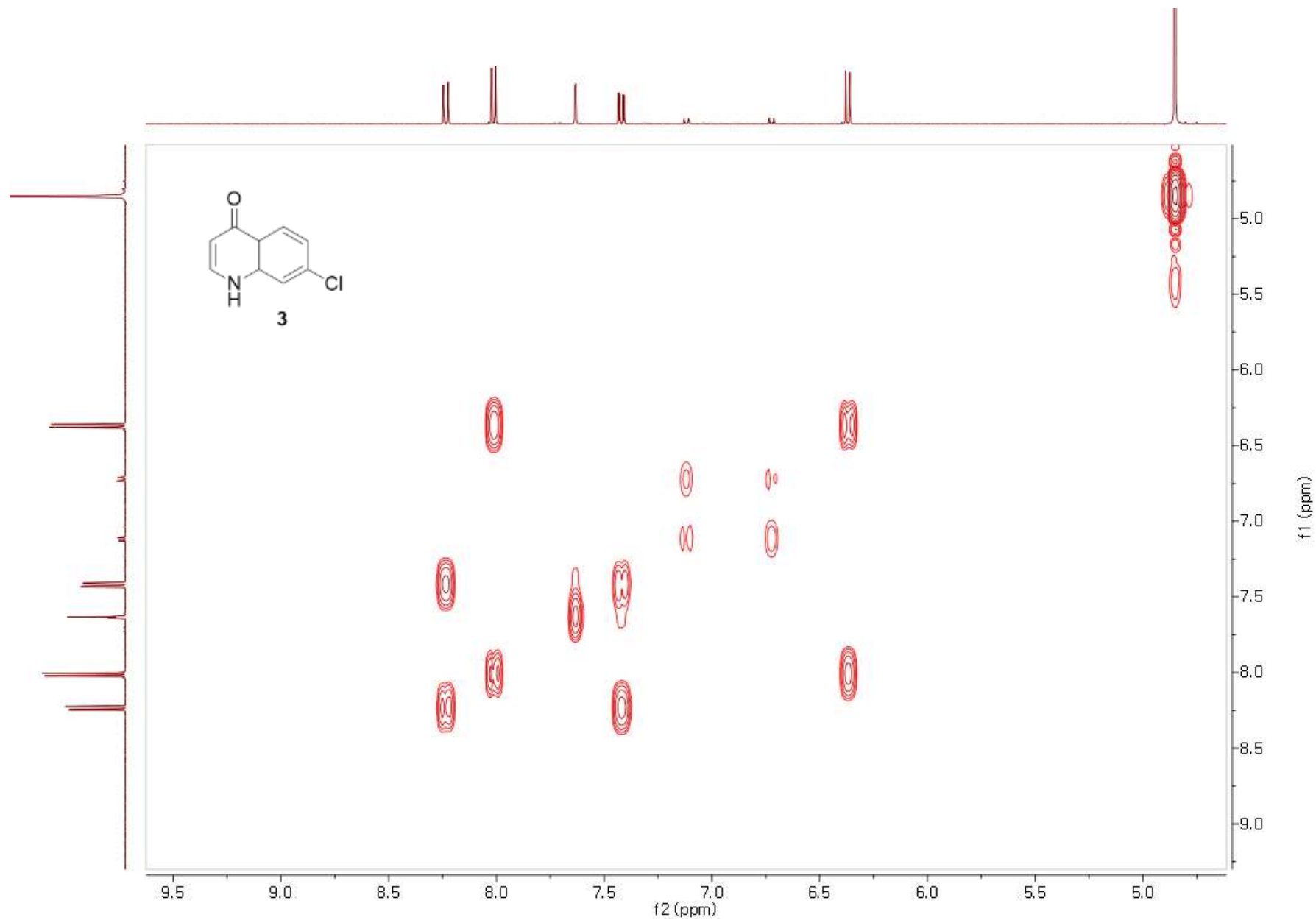
**Figure S14.**  $^1\text{H}$  NMR spectrum (400 MHz) of 7-chloro-4(*1H*)-quinolone (**3**) in  $\text{CD}_3\text{OD}$



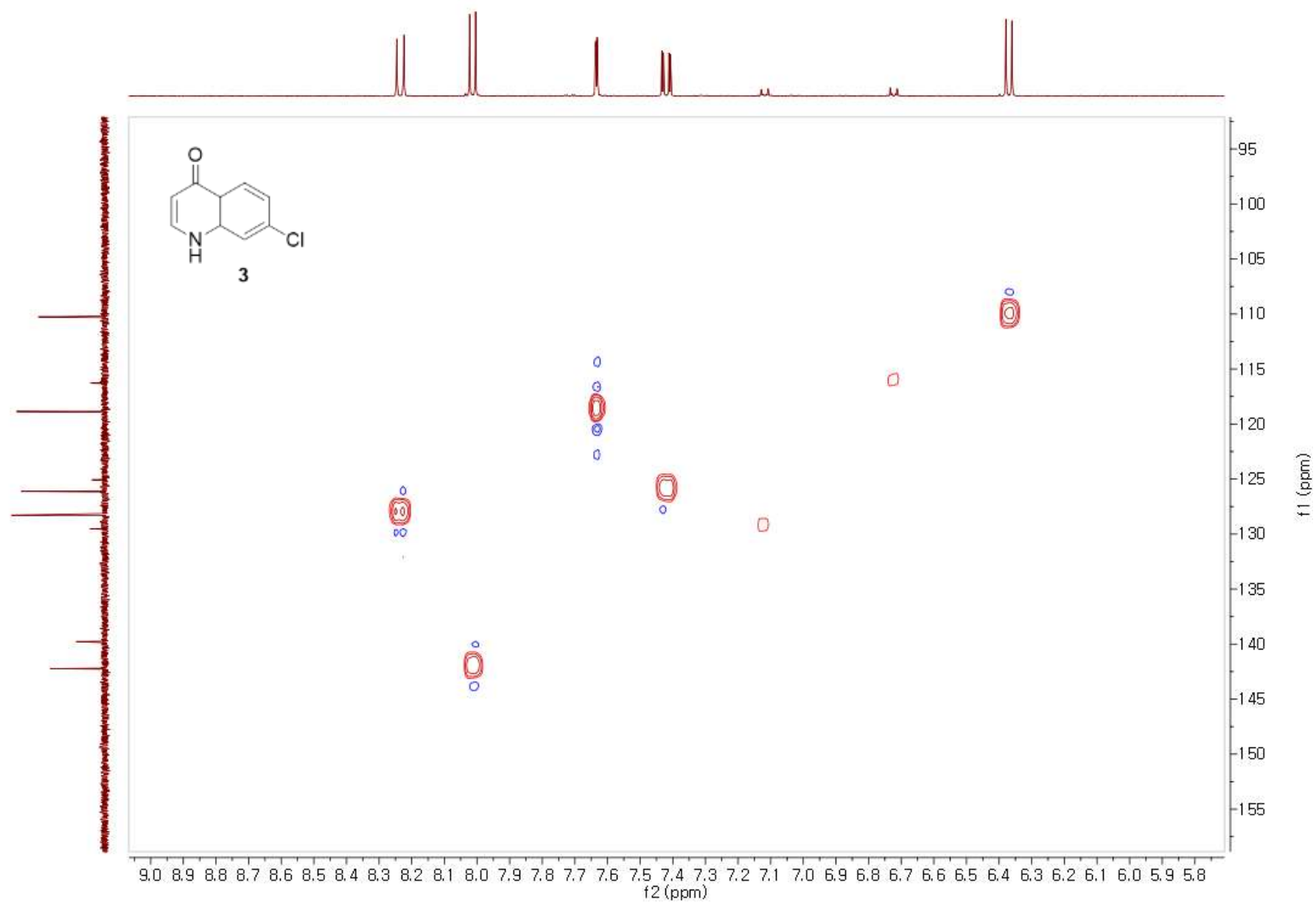
**Figure S15.**  $^{13}\text{C}$  NMR spectrum (100 MHz) of 7-chloro-4(*1H*)-quinolone (**3**) in  $\text{CD}_3\text{OD}$



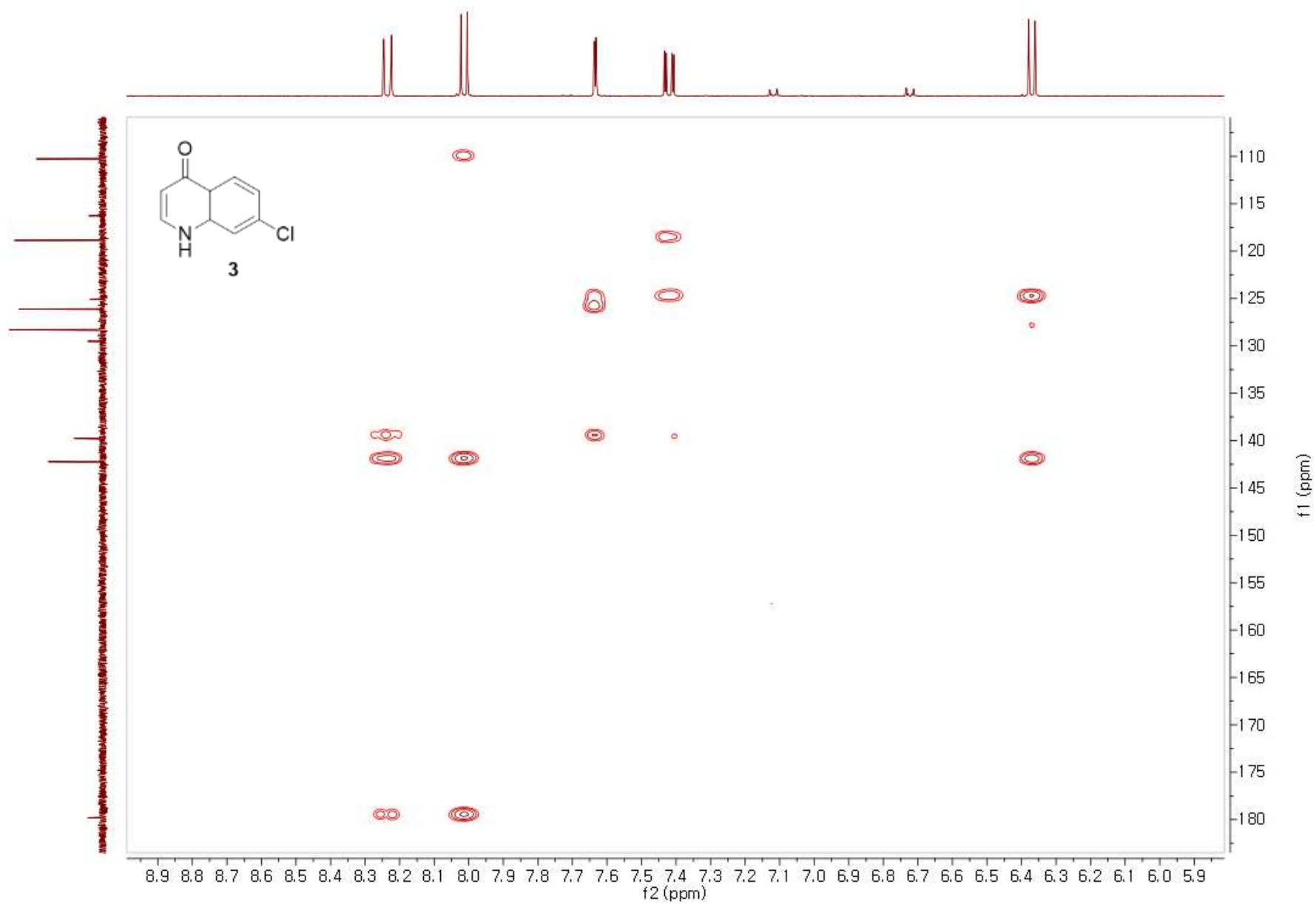
**Figure S16.** COSY spectrum (400 MHz) of 7-chloro-4(1*H*)-quinolone (**3**) in CD<sub>3</sub>OD



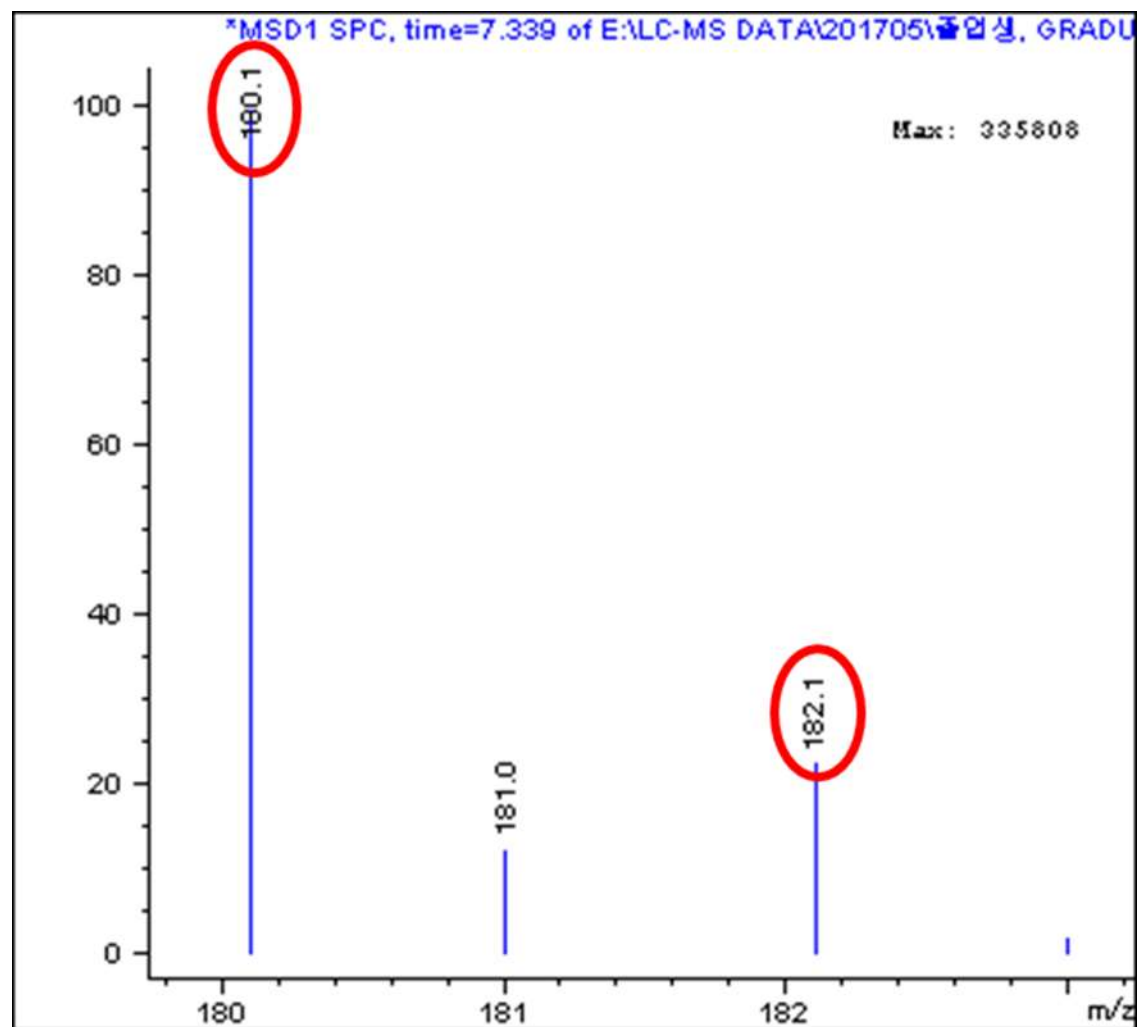
**Figure S17.** HSQC spectrum (400 MHz) of 7-chloro-4(*1H*)-quinolone (**3**) in CD<sub>3</sub>OD



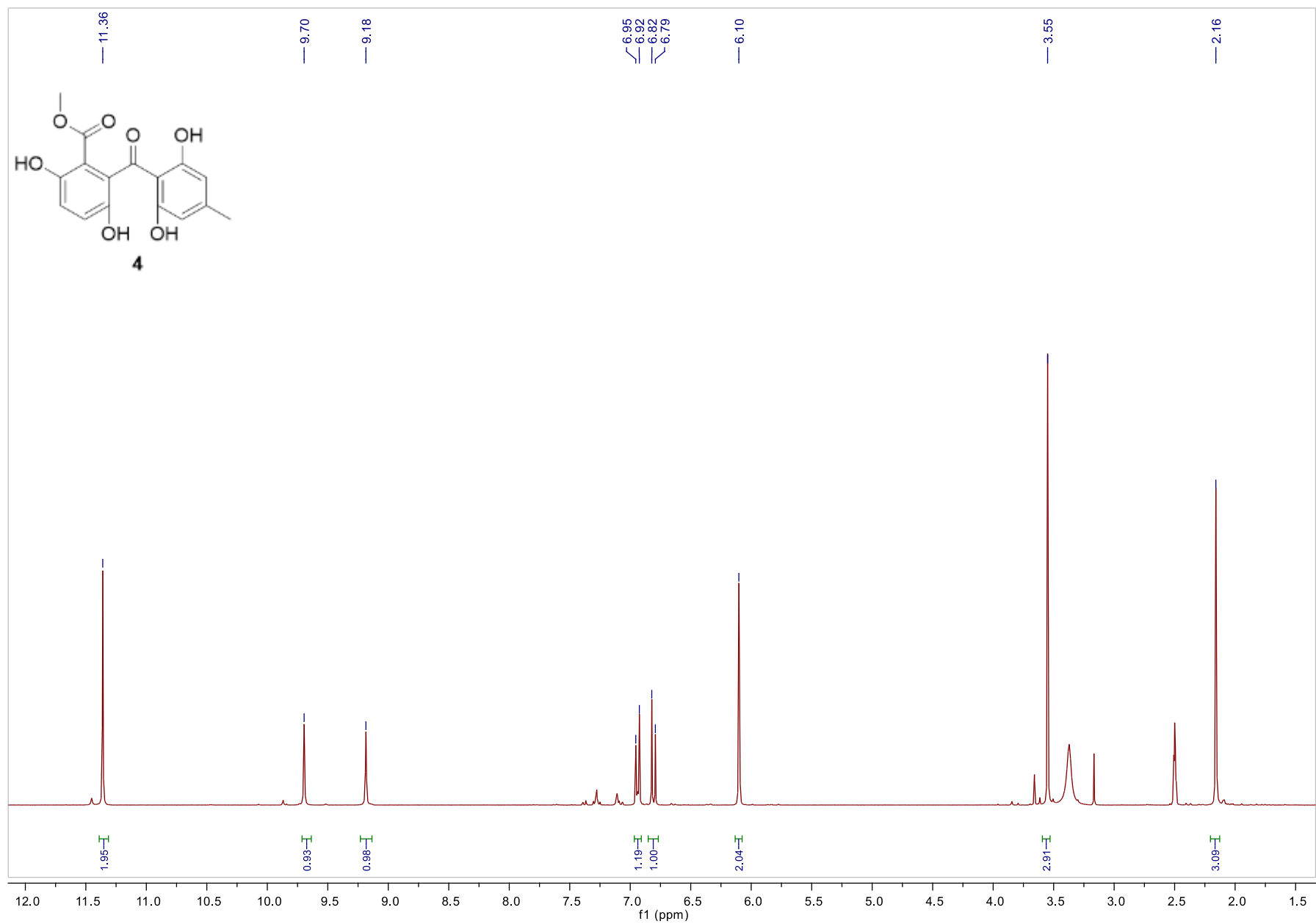
**Figure S18.** HMBC spectrum (400 MHz) of 7-chloro-4(1*H*)-quinolone (**3**) in CD<sub>3</sub>OD



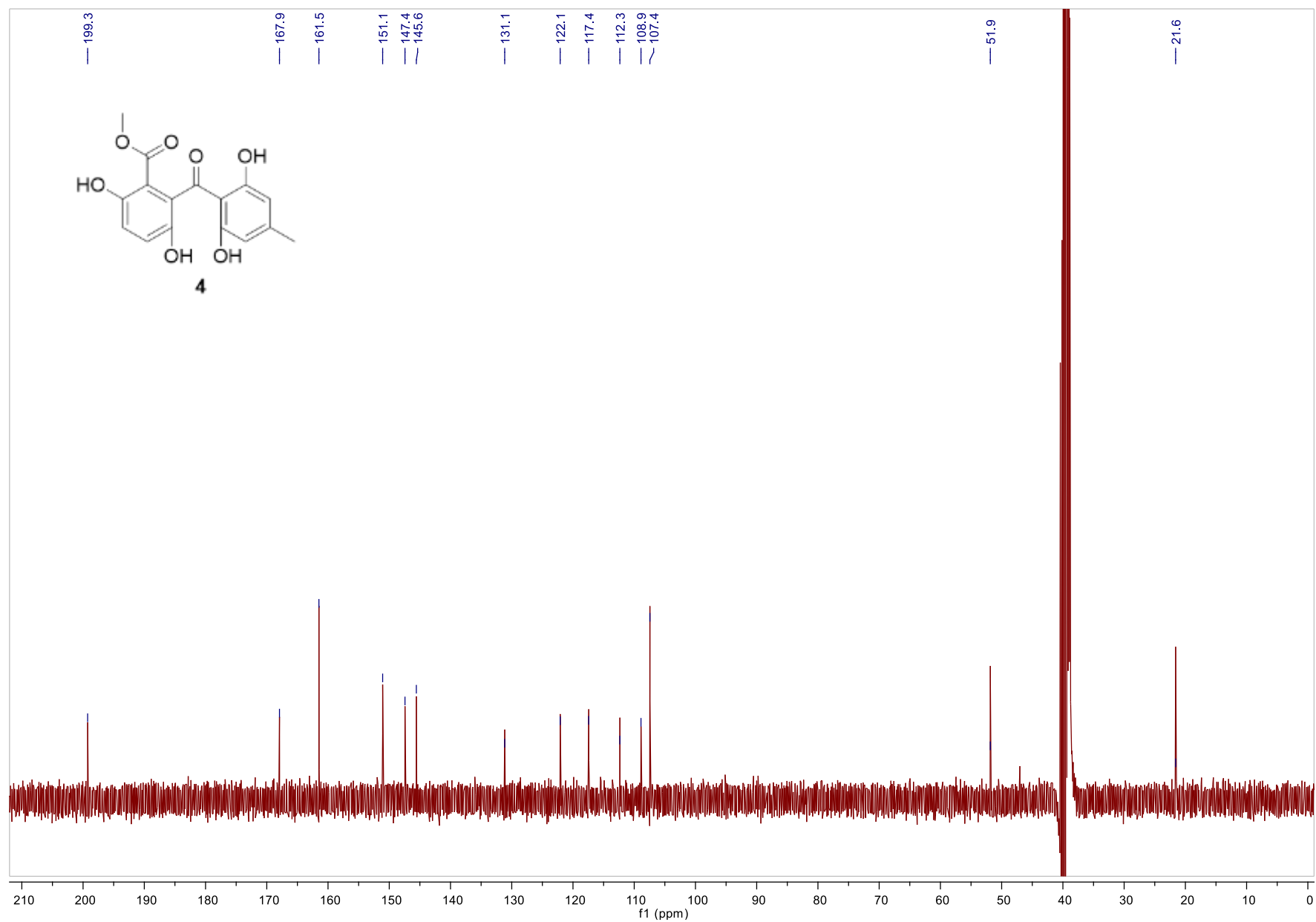
**Figure S19.** LR-ESI-MS spectroscopic data of 7-chloro-4(*1H*)-quinolone (**3**)



**Figure S20.**  $^1\text{H}$  NMR Spectrum (400 MHz) of acremonidine E (**4**) in  $\text{DMSO}-d_6$

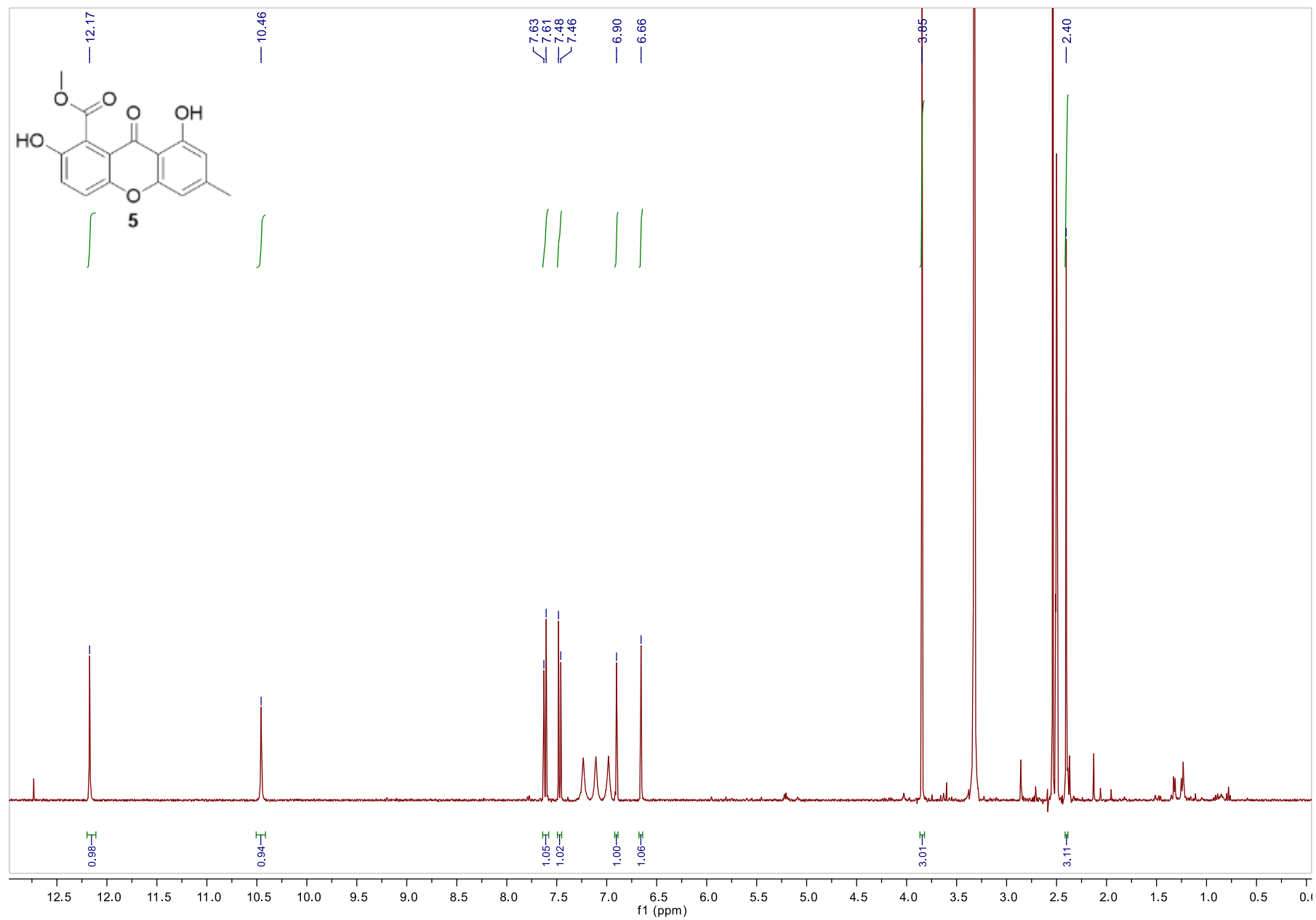


**Figure S21.**  $^{13}\text{C}$  NMR Spectrum (100 MHz) of acremonidine E (**4**) in  $\text{DMSO}-d_6$

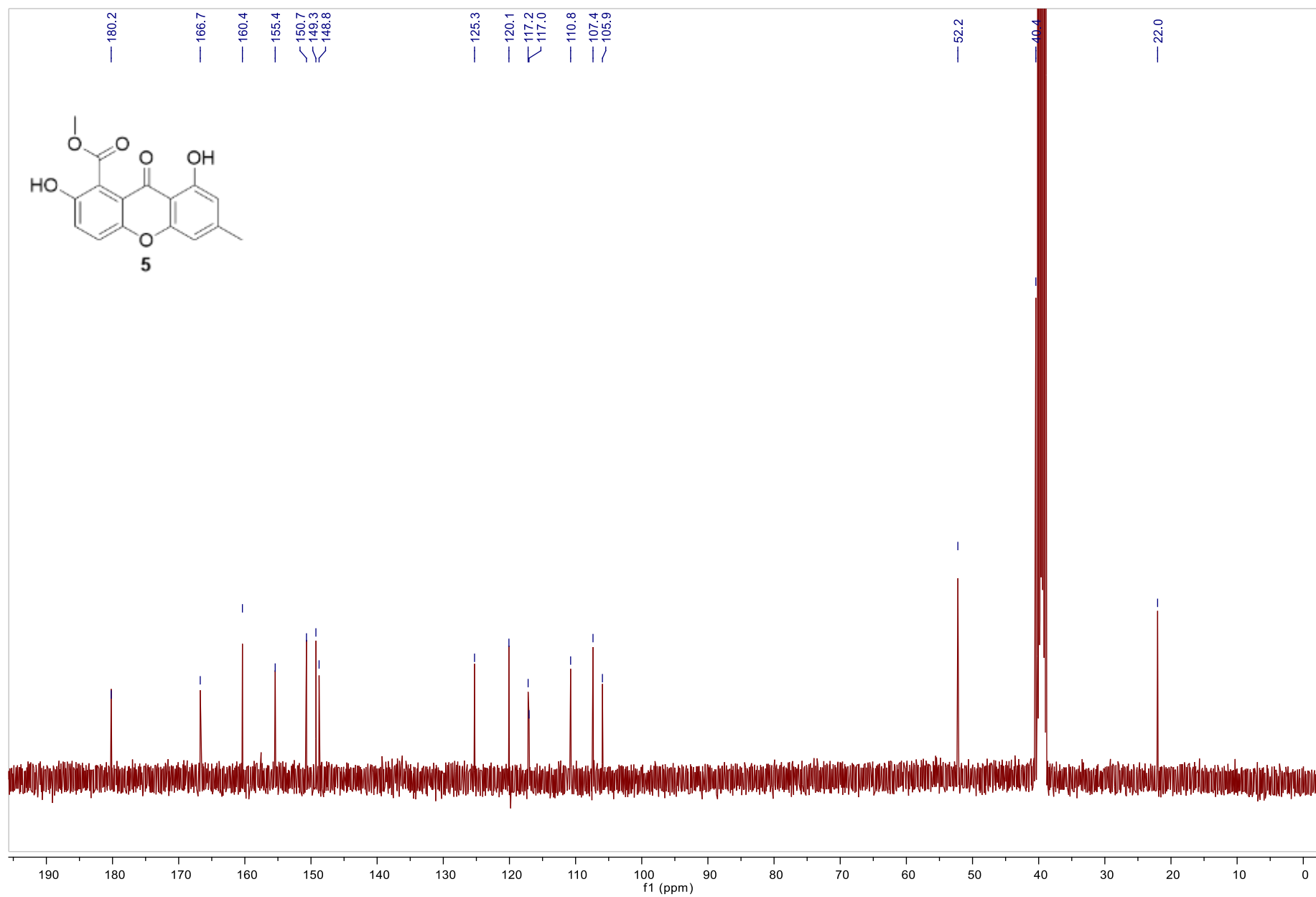




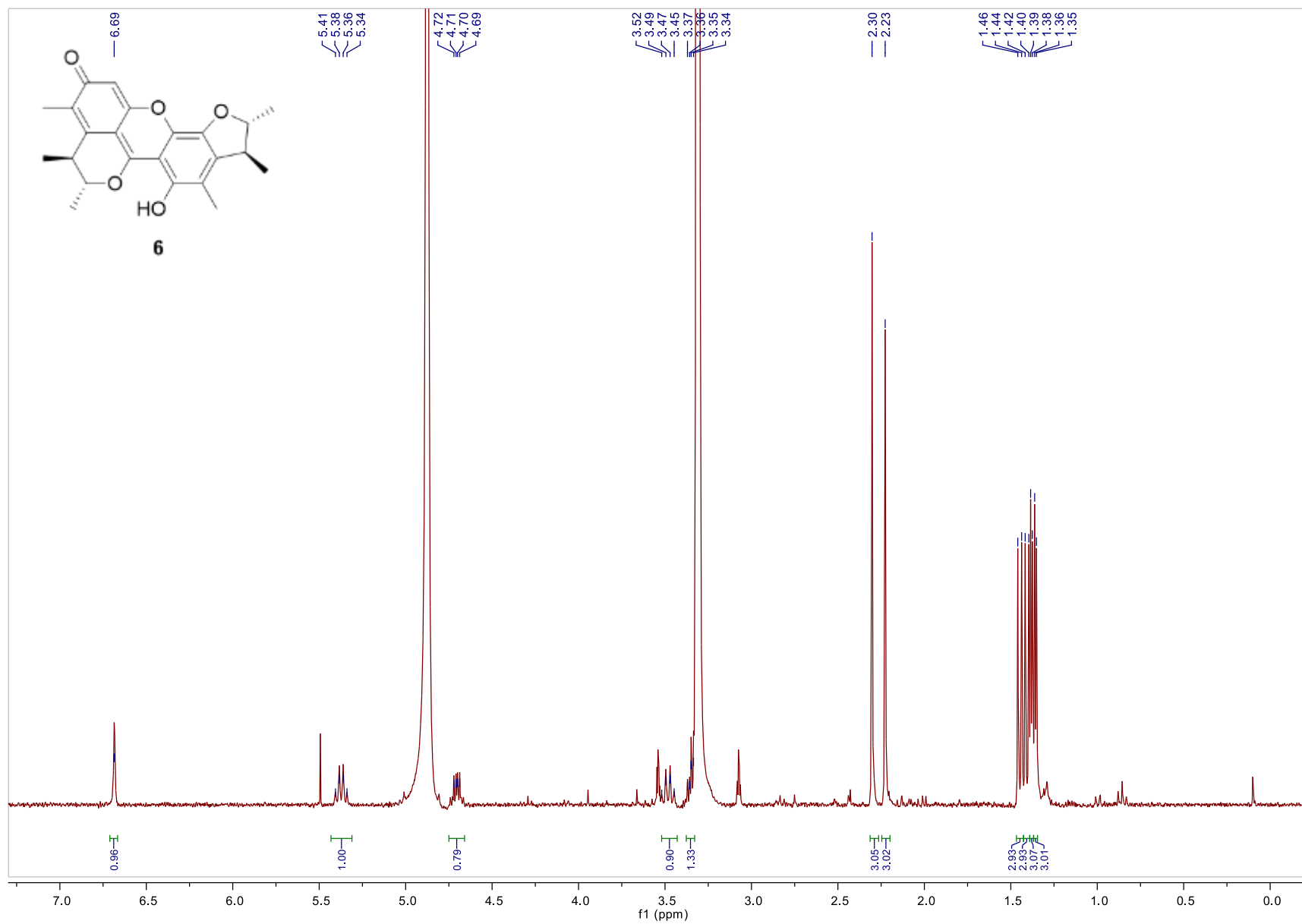
**Figure S22.**  $^1\text{H}$  NMR Spectrum (400 MHz) of pinselin (**5**) in  $\text{DMSO}-d_6$ .



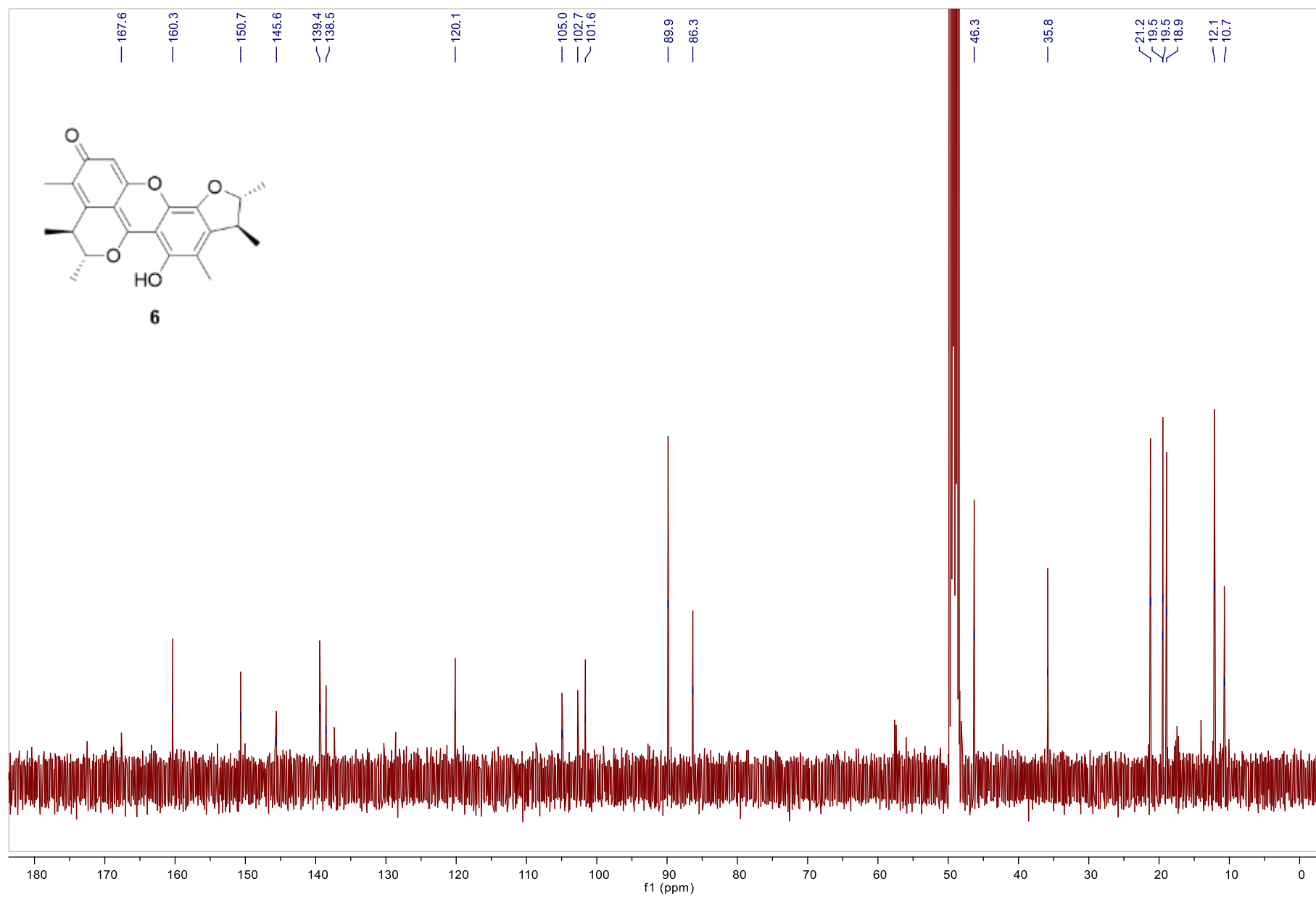
**Figure S23.**  $^{13}\text{C}$  NMR Spectrum (100 MHz) of pinselin (**5**) in  $\text{DMSO}-d_6$ .



**Figure S24.**  $^1\text{H}$  NMR Spectrum (400 MHz) of penicitirinoini A (**6**) in  $\text{CD}_3\text{OD}$



**Figure S25.**  $^{13}\text{C}$  NMR Spectrum (100 MHz) of penicitirinoi A (**6**) in  $\text{CD}_3\text{OD}$



**Figure S26.**  $^1\text{H}$  NMR Spectrum (400 MHz) of penicitirinoini E (**7**) in  $\text{CD}_3\text{OD}$

