

## Supplementary Data

# New $\psi$ -santonin derivatives from *Crossostephium chinense* and their anti- proliferative activities against *Leishmania* *major* and human cancer cells A549

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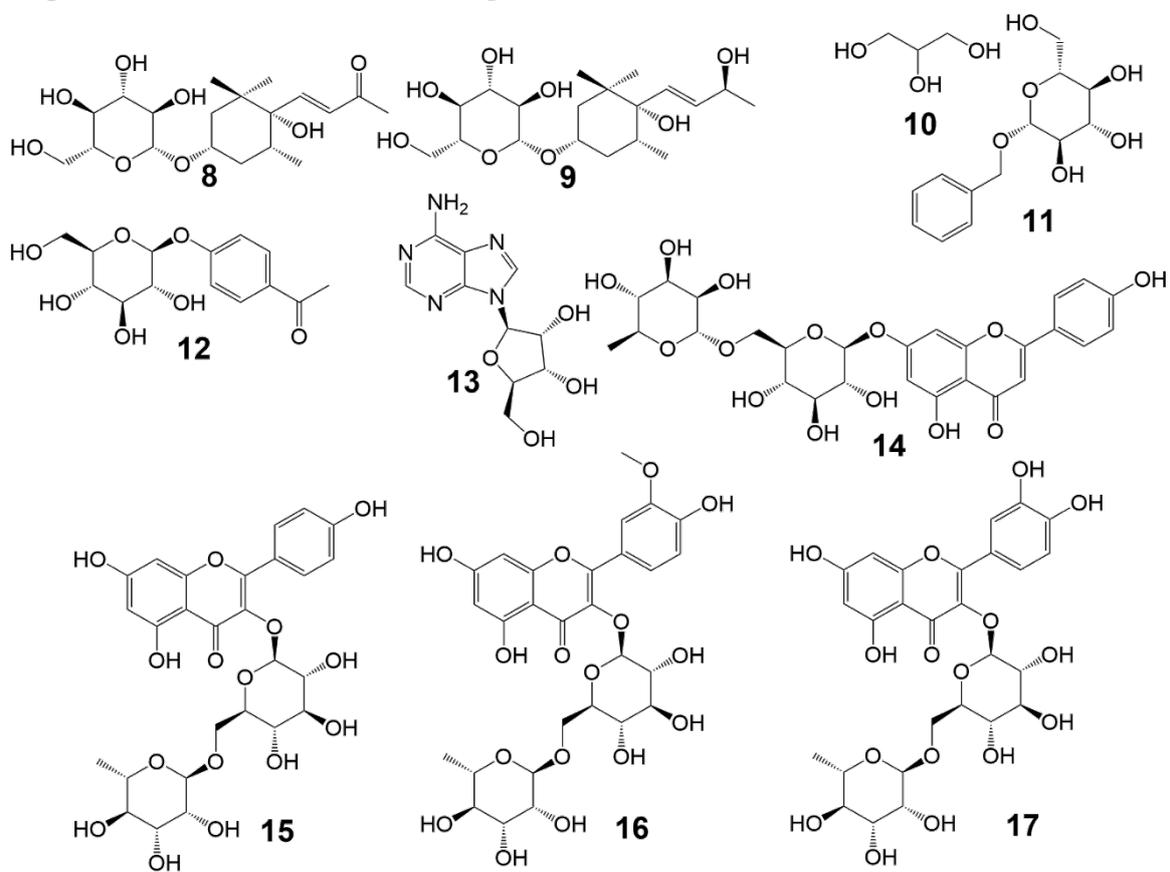
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H-CC-B-1-3-5-P3(1.2mg).010.001.1r.esp

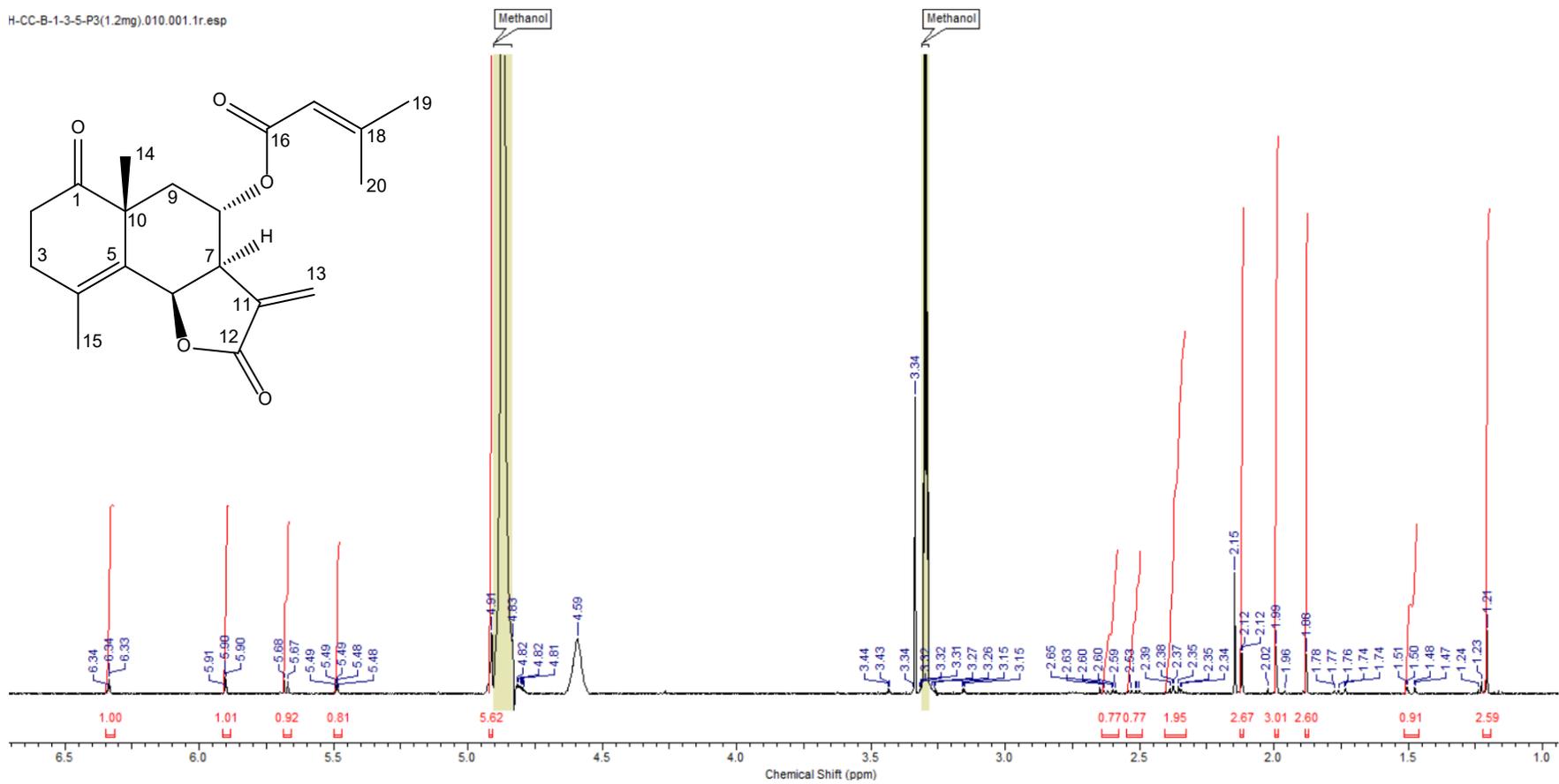
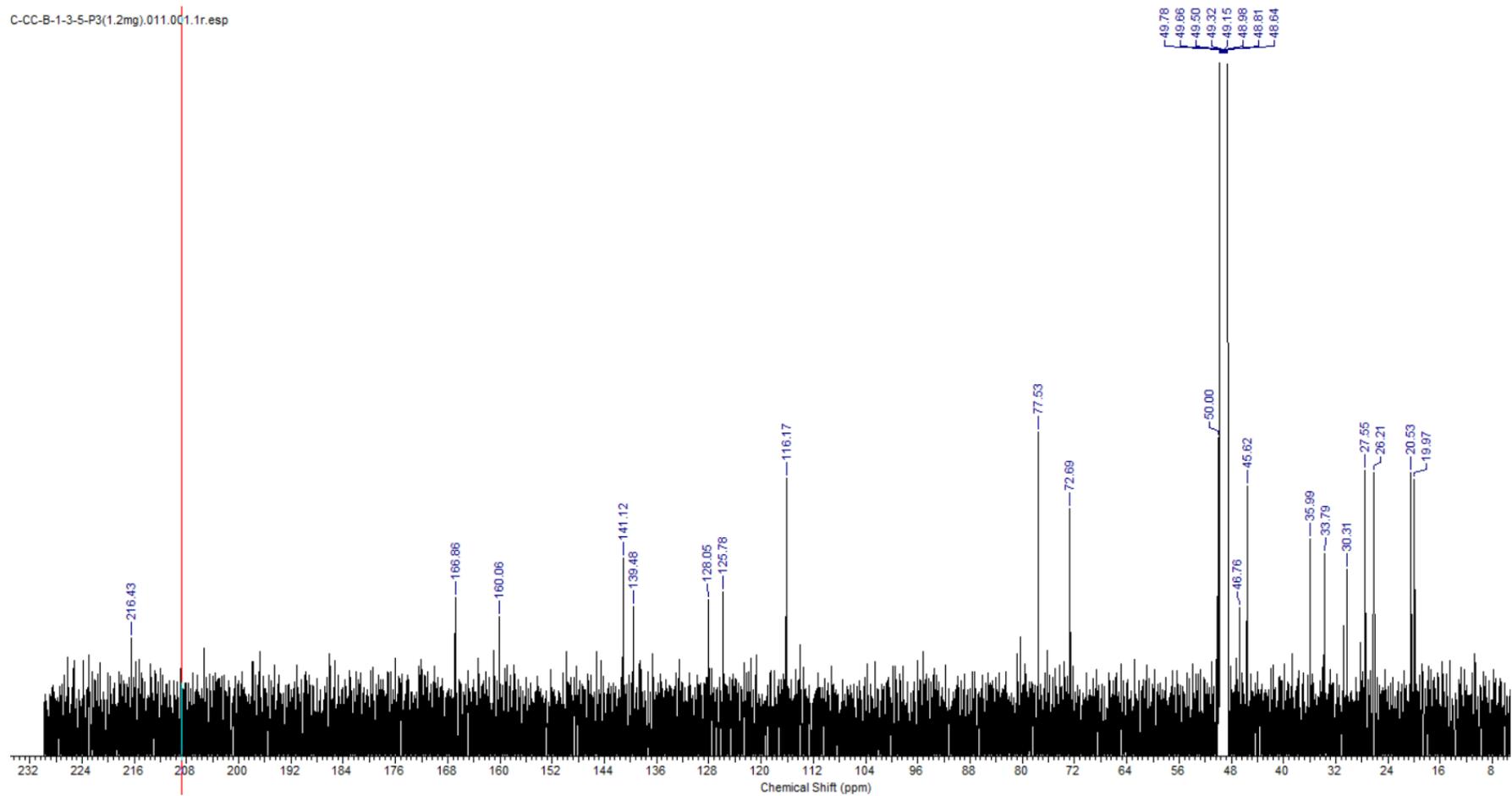
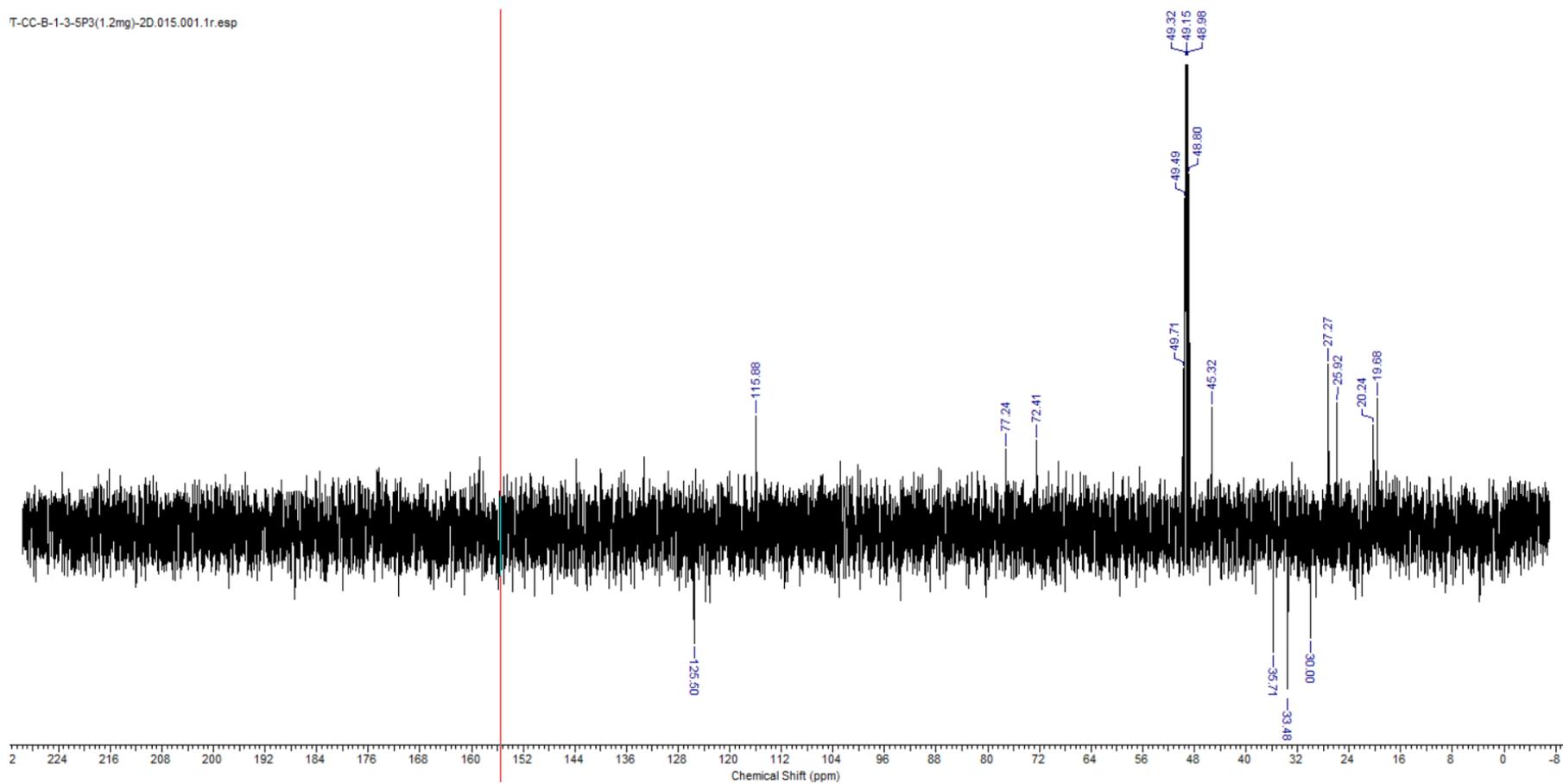


Figure S2. <sup>1</sup>H-NMR spectrum of **1** in MeOD (500 MHz)



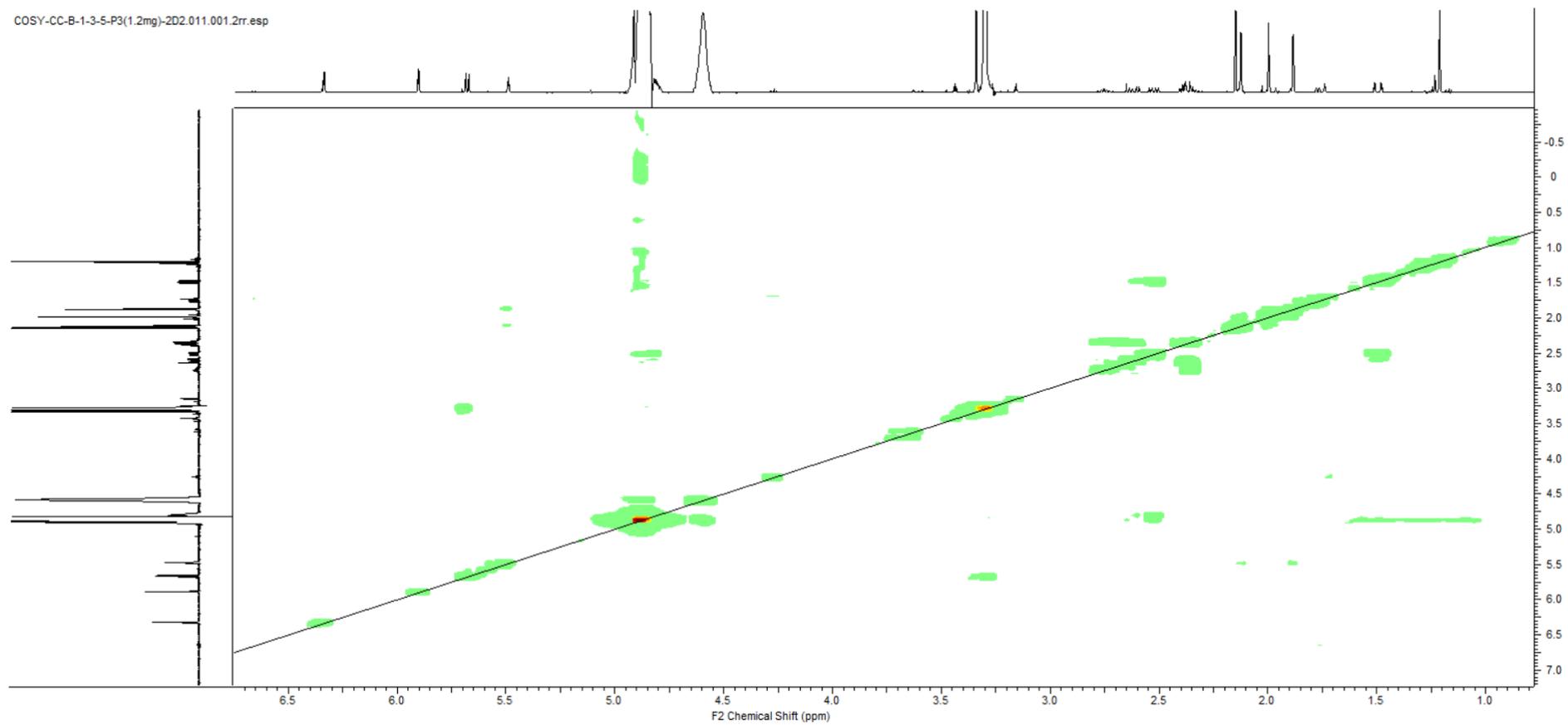
**Figure S3.**  $^{13}\text{C}$ -NMR spectrum of **1** in MeOD (125 MHz)

T-CC-B-1-3-5P3(1.2mg)-2D.015.001.1r.esp



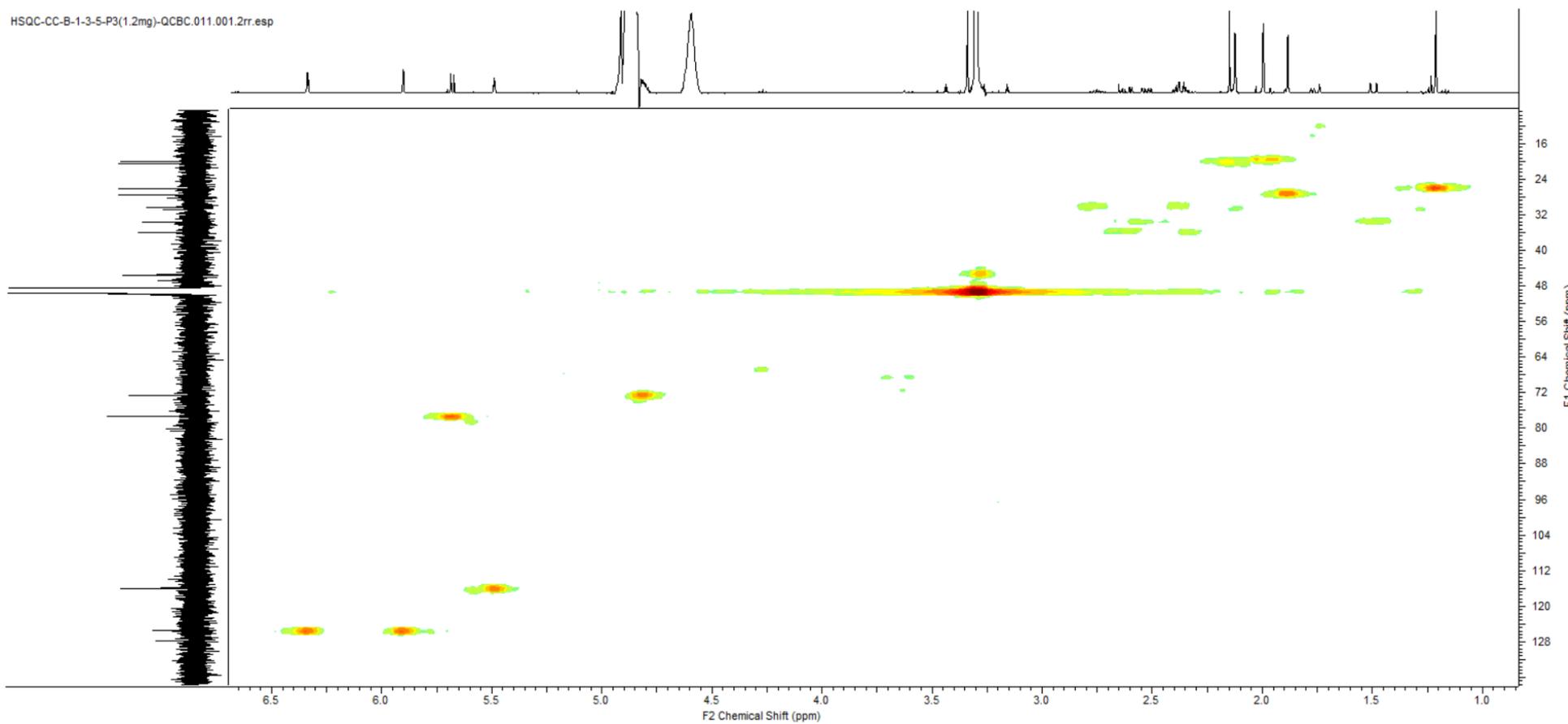
**Figure S4.**  $^{13}\text{C}$  DEPT135 NMR spectrum of **1** in MeOD (125 MHz)

COSY-CC-B-1-3-5-P3(1.2mg)-2D2.011.001.2rr.esp



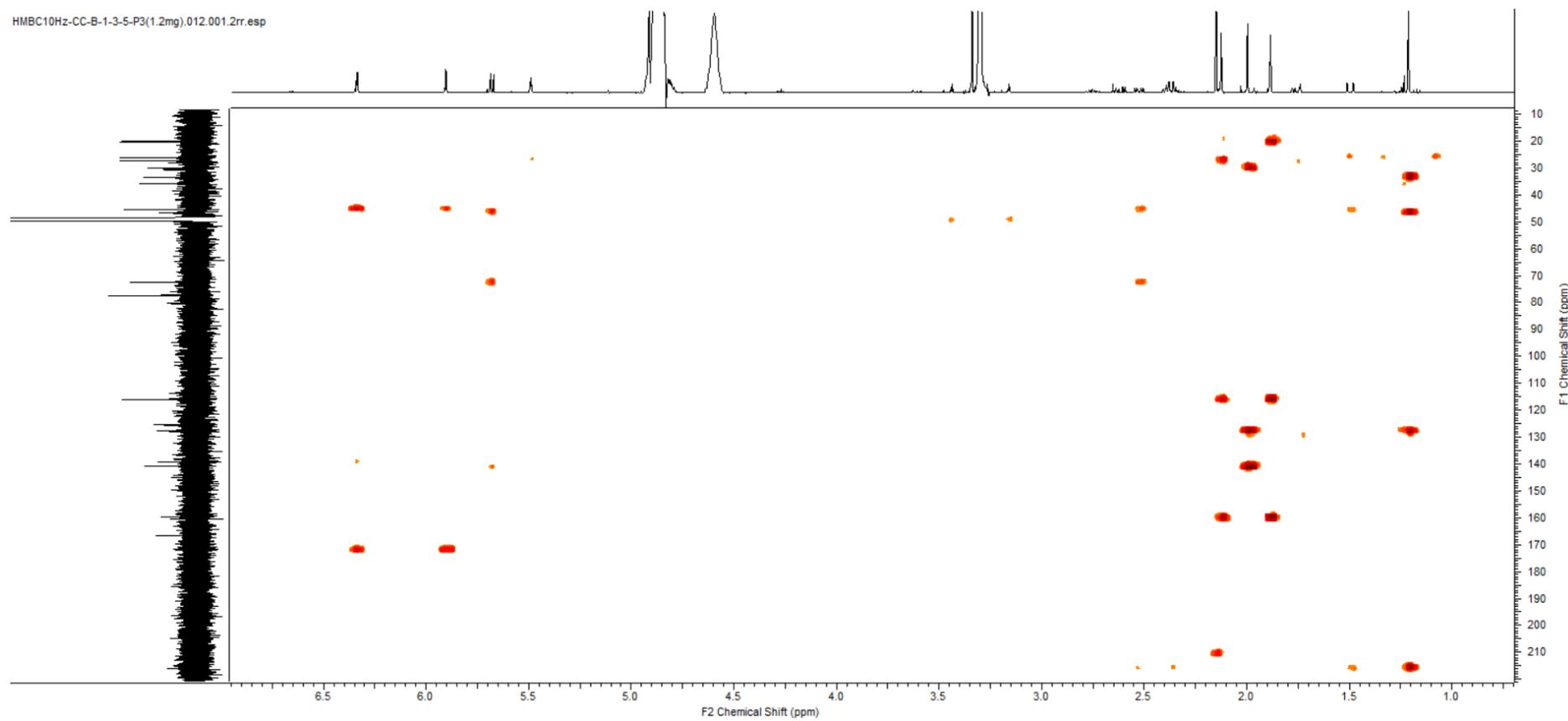
**Figure S5.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **1** in MeOD (500 MHz)

HSQC-CC-B-1-3-5-P3(1.2mg)-QCBC.011.001.2rr.esp



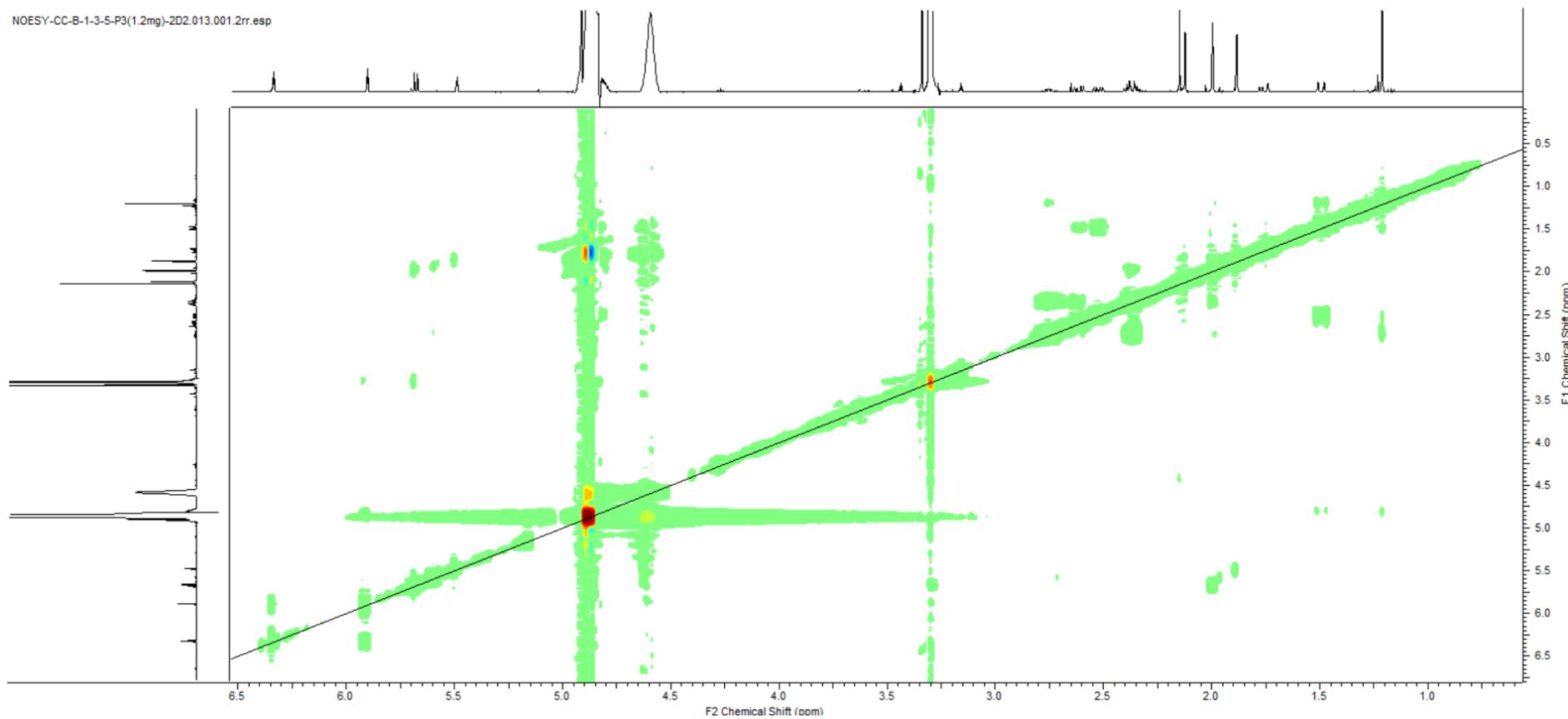
**Figure S6.** HSQC spectrum of **1** in MeOD (500 MHz)

HMBC10Hz-CC-B-1-3-5-P3(1.2mg).012.001.2rr.esp



**Figure S7.** HMBC spectrum of **1** in MeOD (500 MHz)

NOESY-CC-B-1-3-5-P3(1.2mg)-2D2.013.001.2rr.esp



**Figure S8.** PS-NOESY spectrum of **1** in MeOD (500 MHz)

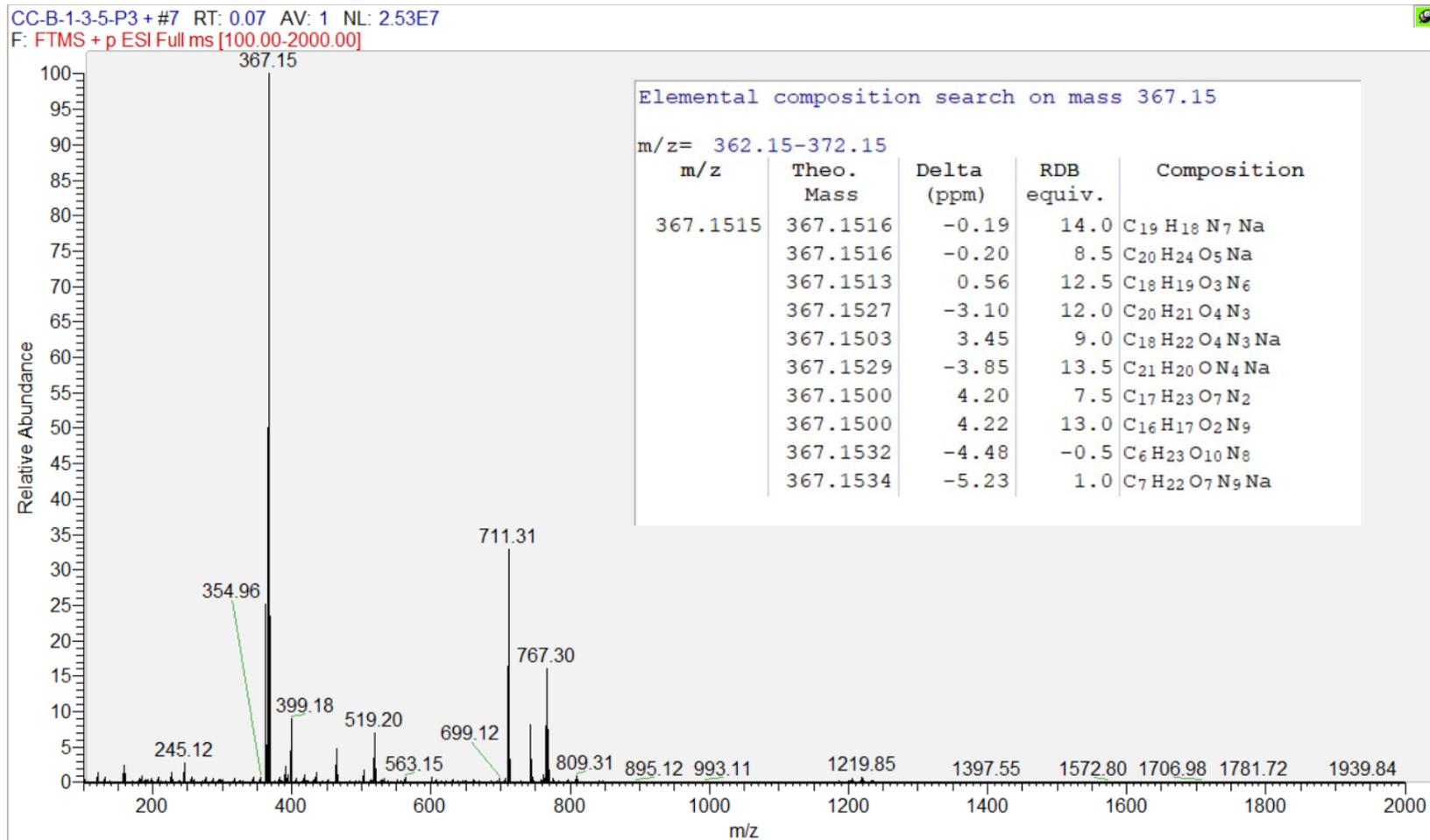


Figure S9. HR-ESI-MS spectrum of **1**

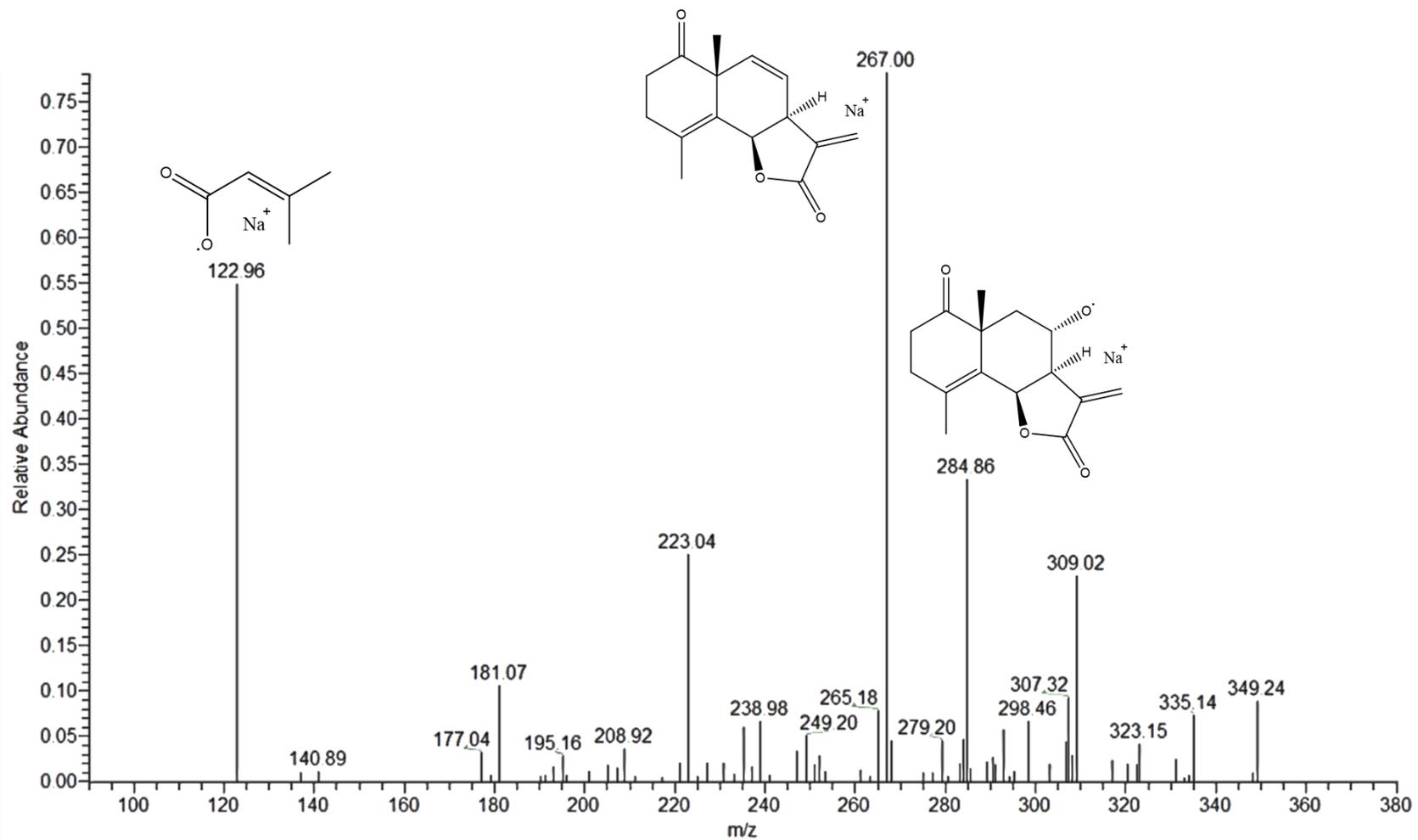


Figure S10. ESI-MS/MS spectrum of 1

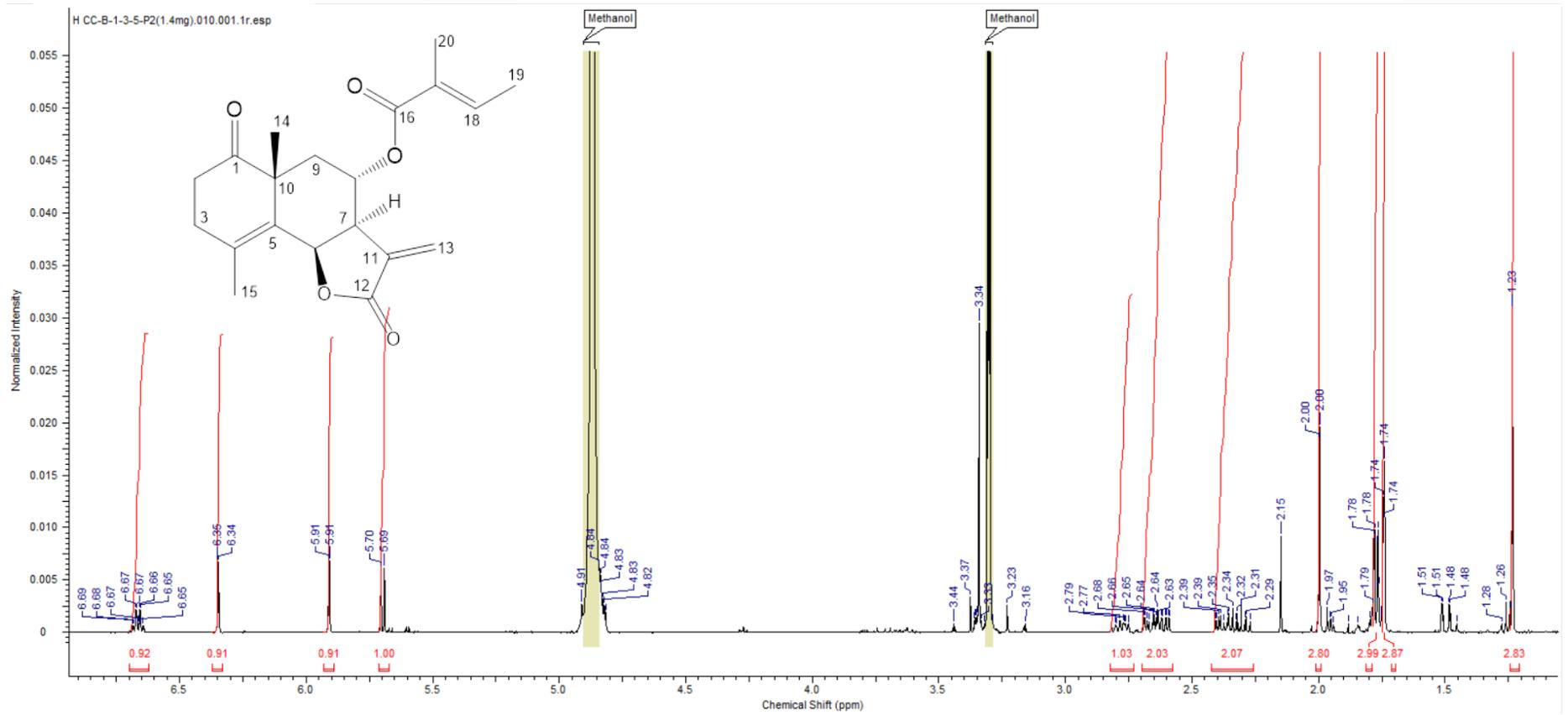


Figure S11.  $^1\text{H}$ -NMR spectrum of 2 in MeOD (500 MHz)

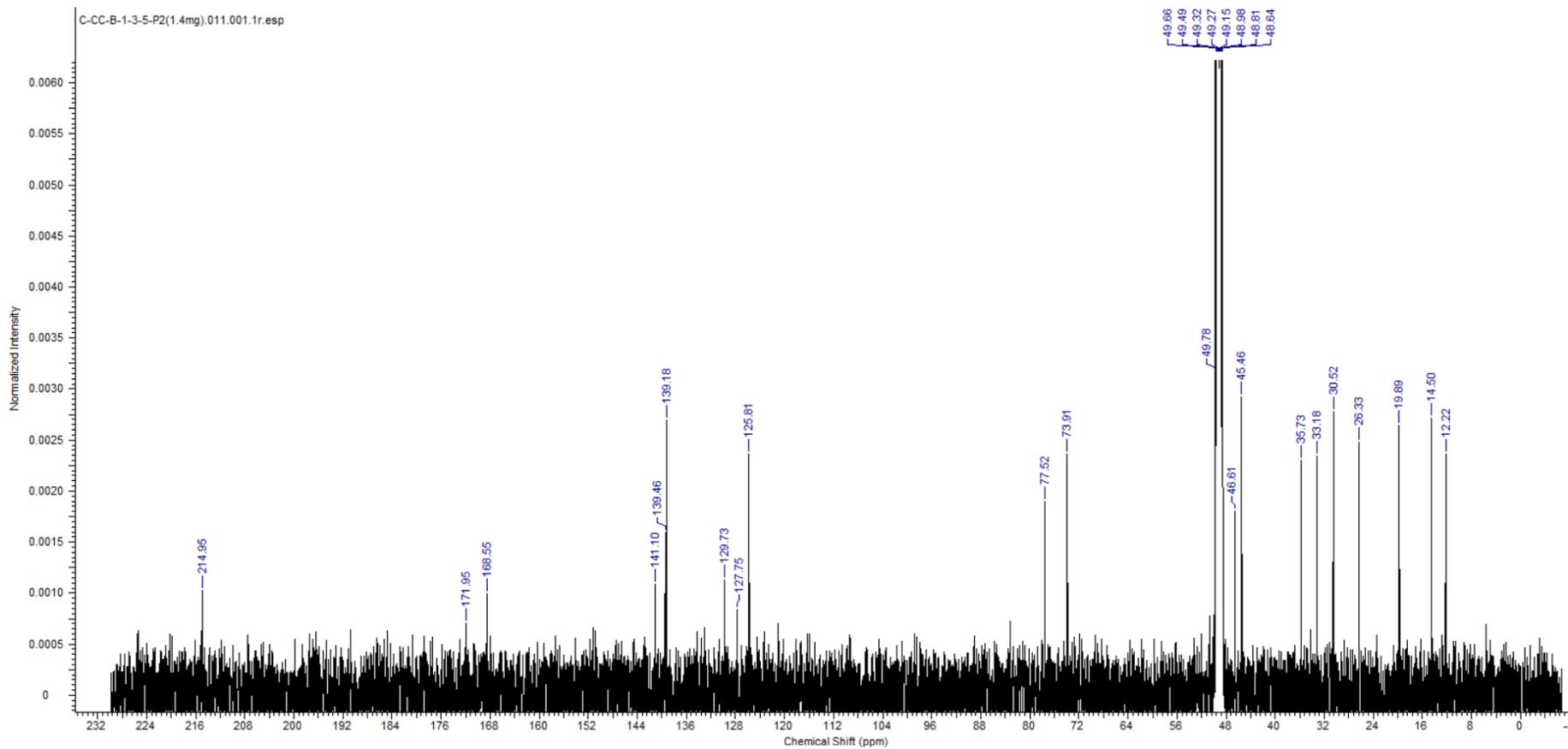
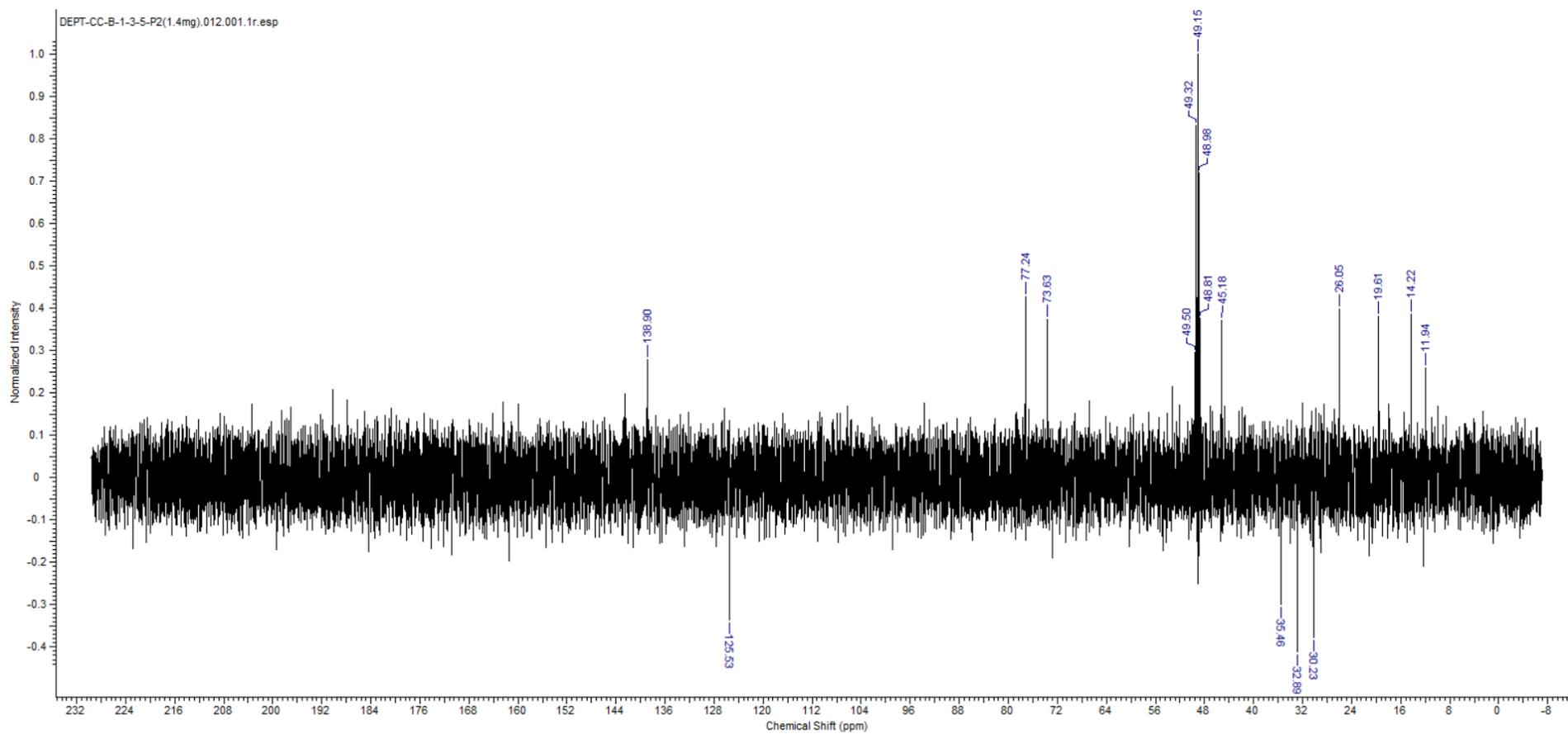
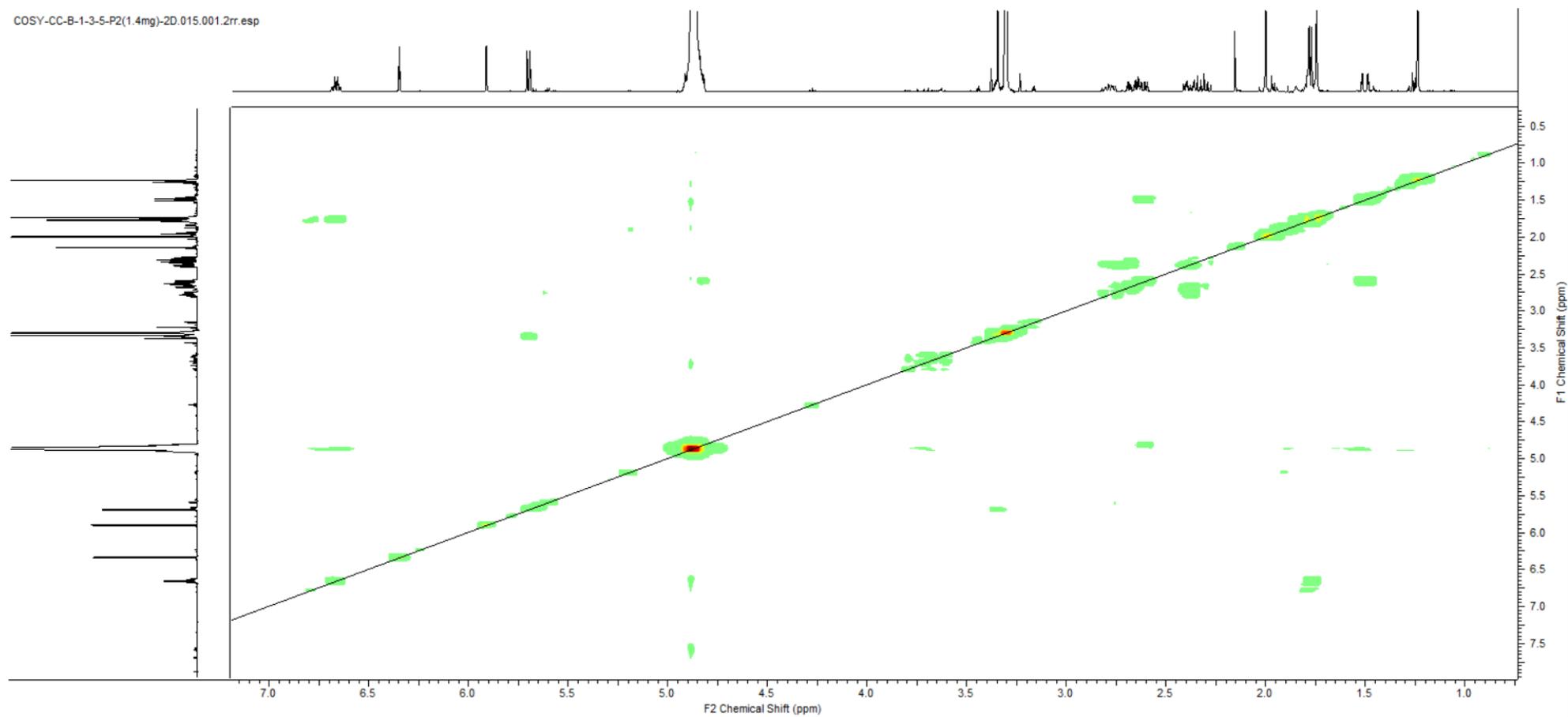


Figure S12.  $^{13}\text{C}$ -NMR spectrum of **2** in MeOD (125 MHz)



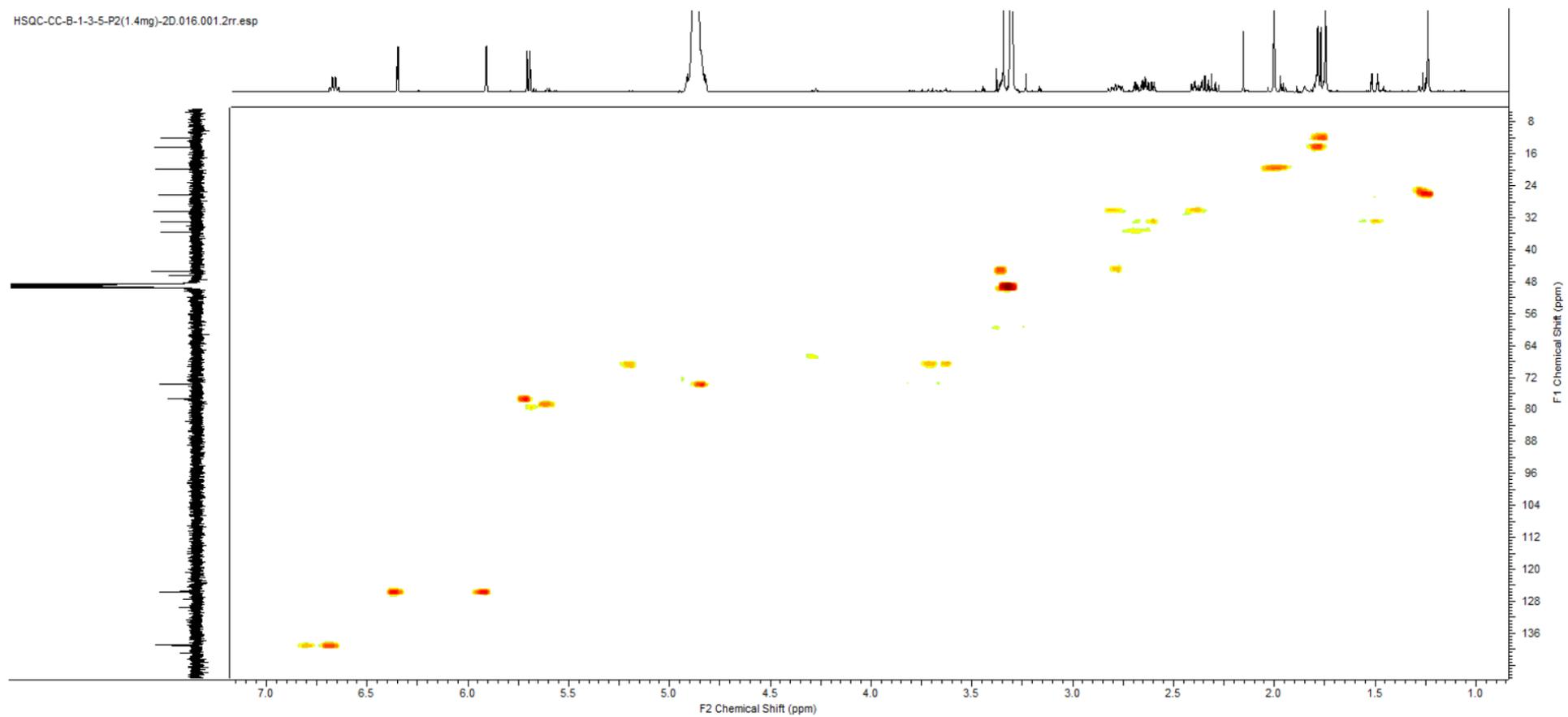
**Figure S13.**  $^{13}\text{C}$  DEPT135 NMR spectrum of **2** in MeOD (125 MHz)

COSY-CC-B-1-3-5-P2(1.4mg)-2D.015.001.2rr.esp



**Figure S14.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **2** in MeOD (500 MHz)

HSQC-CC-B-1-3-5-P2(1.4mg)-2D.016.001.2rr.esp



**Figure S15.** HSQC spectrum of **2** in MeOD (500 MHz)

HMBC-CC-B-1-3-5-P2(1.4mg)-2D.017.001.2rr.esp

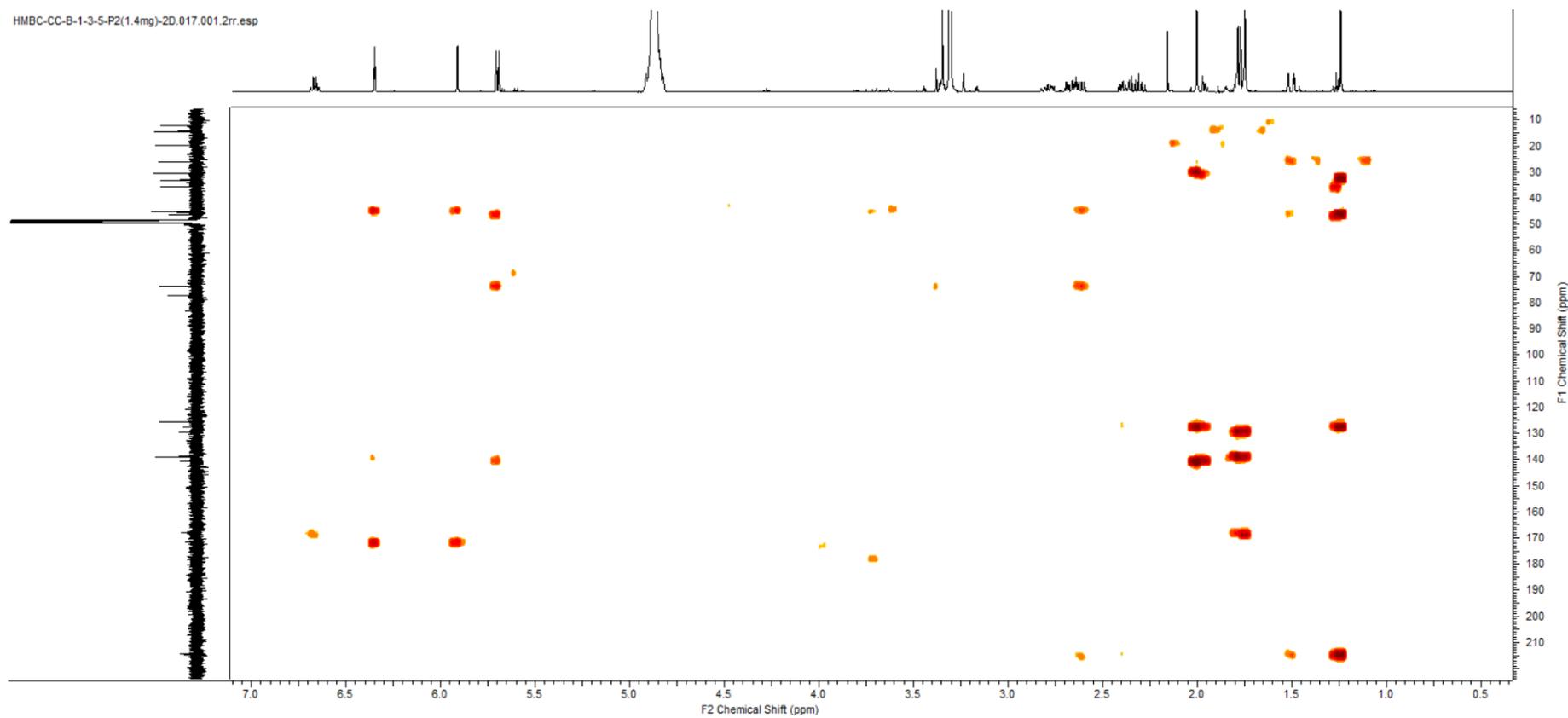
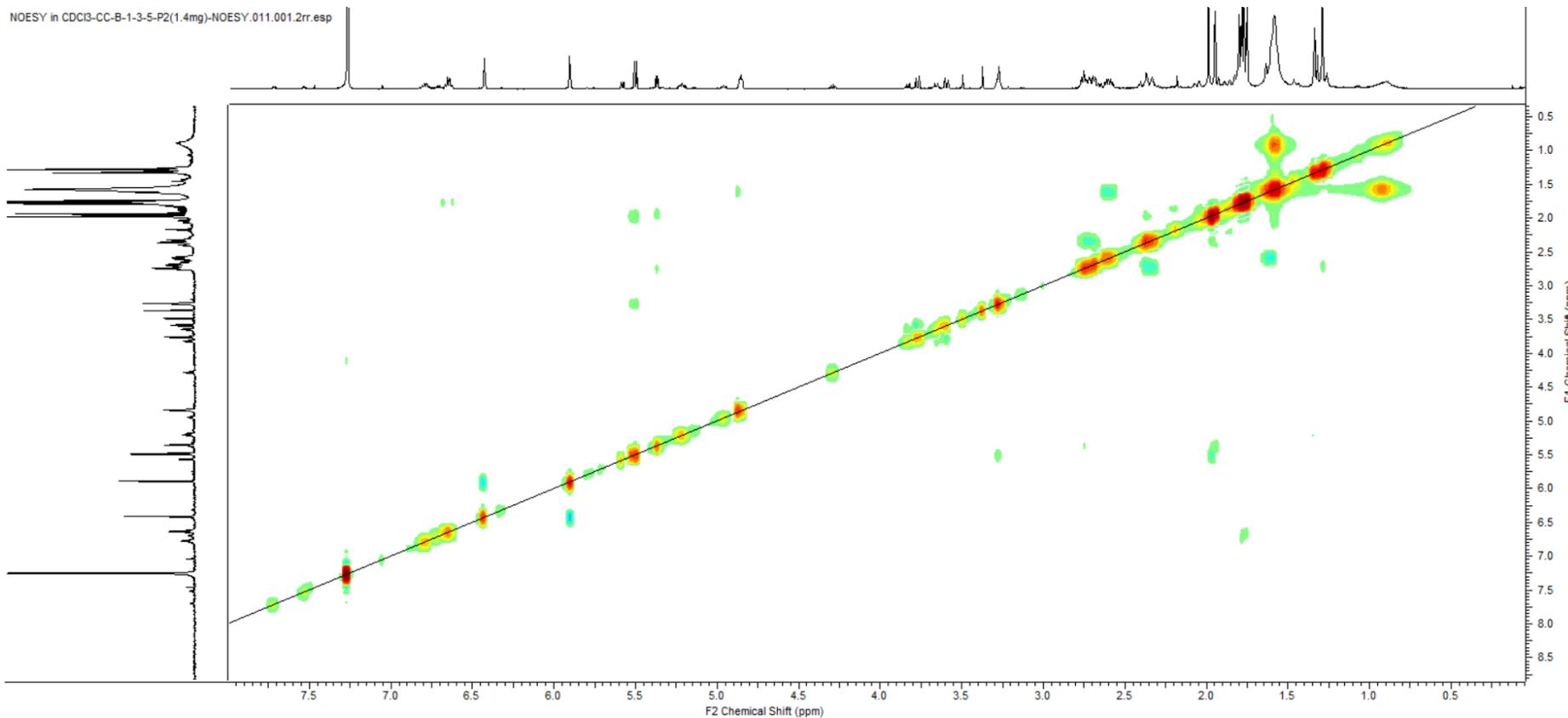


Figure S16. HMBC spectrum of **2** in MeOD (500 MHz)



**Figure S17.** PS-NOESY spectrum of **2** in CDCl<sub>3</sub> (500 MHz)

CC-B-1-3-5-P2+#4 RT: 0.04 AV: 1 NL: 3.17E7  
F: FTMS + p ESI Full ms [100.00-2000.00]

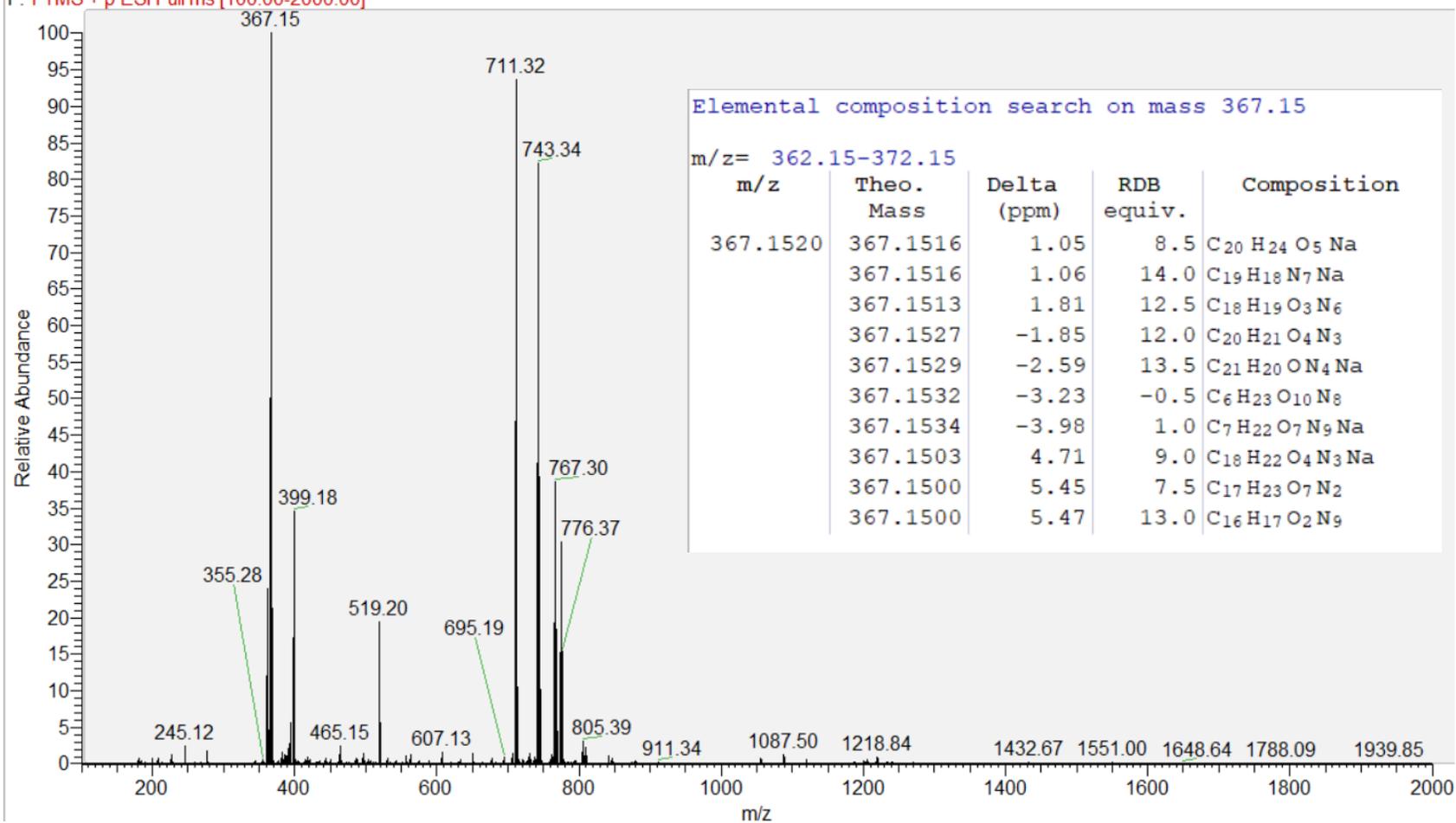


Figure S18. HR-ESI-MS spectrum of **2**

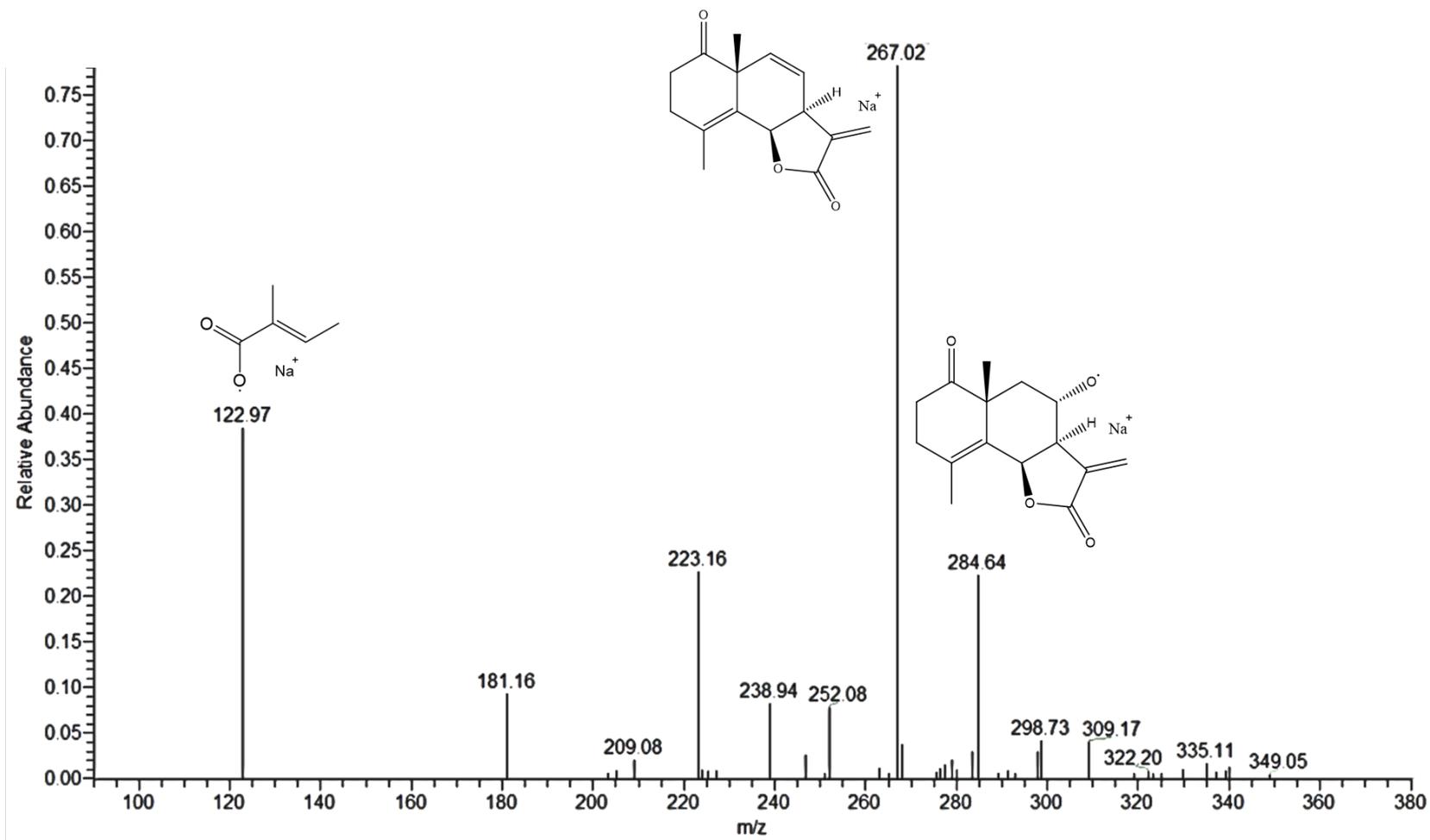
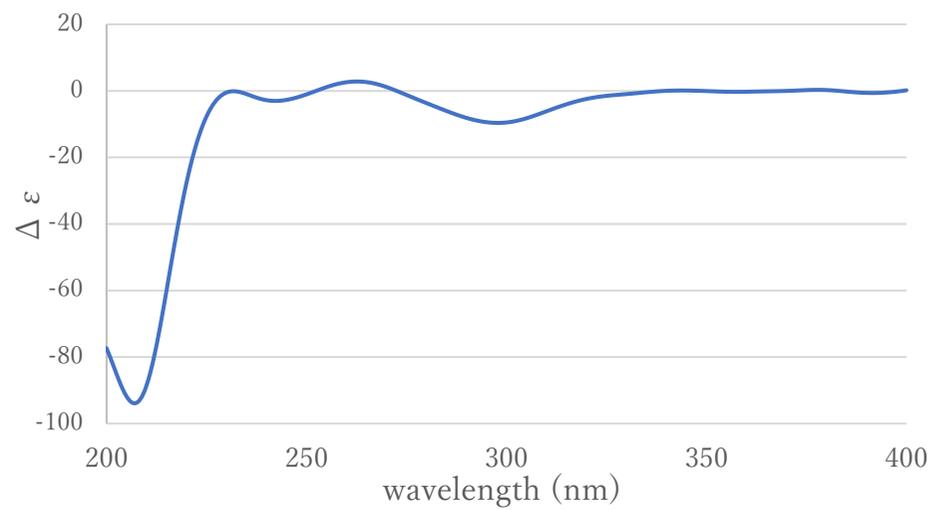


Figure S19. ESI-MS/MS spectrum of 2



**Figure S20.** Experimental CD spectrum of **2** in CH<sub>3</sub>CN

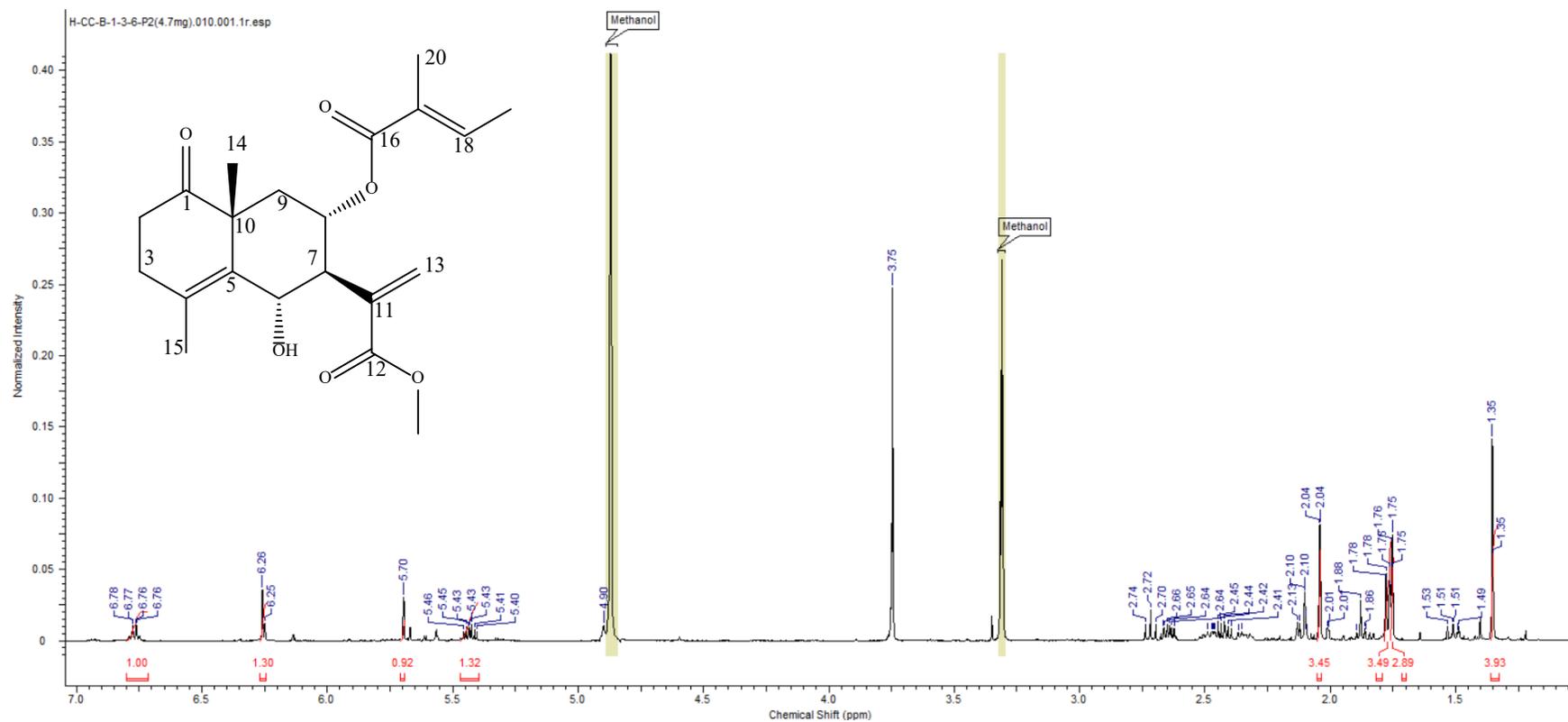


Figure S21.  $^1\text{H-NMR}$  spectrum of **3** in MeOD (500 MHz)

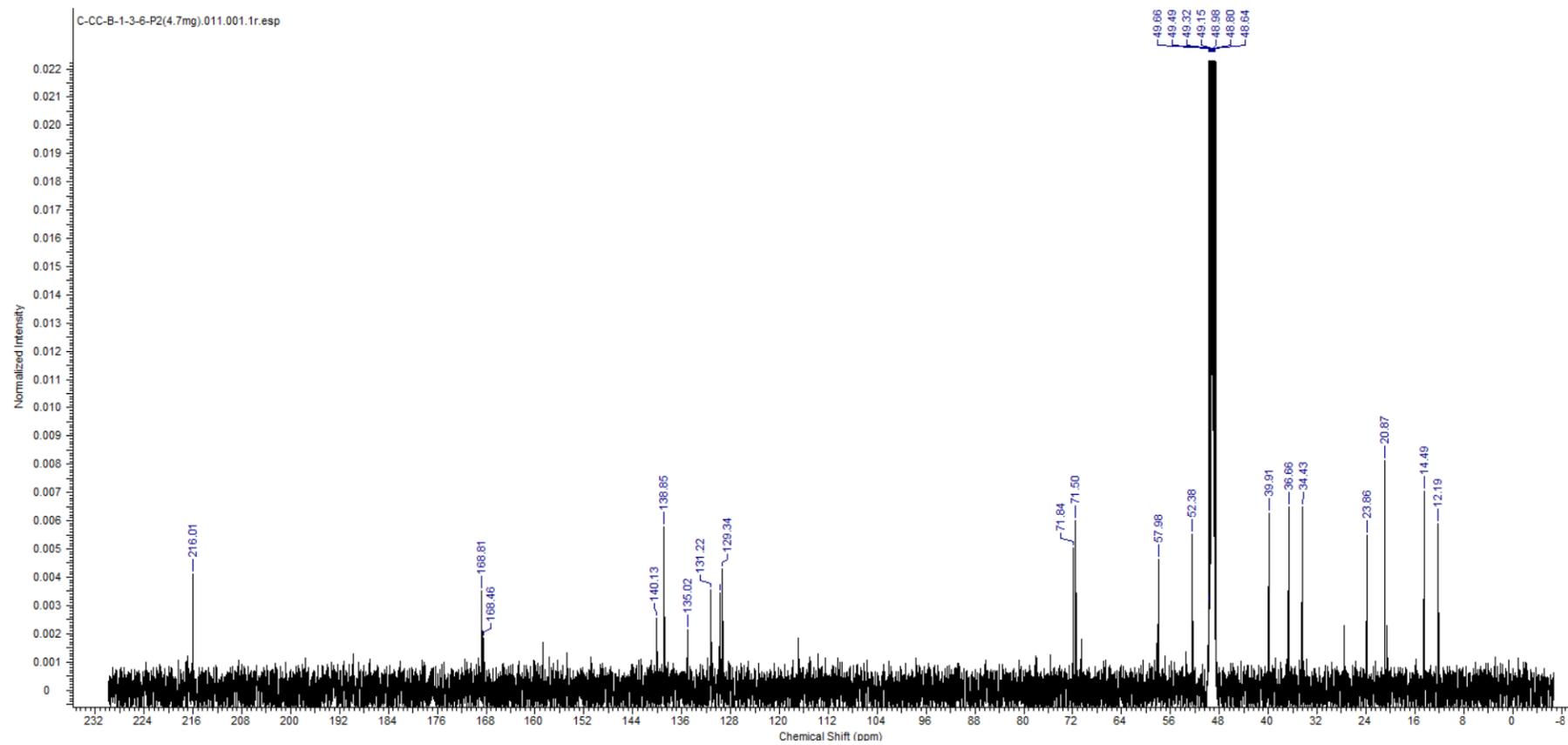


Figure S22.  $^{13}\text{C}$ -NMR spectrum of **3** in MeOD (125 MHz)

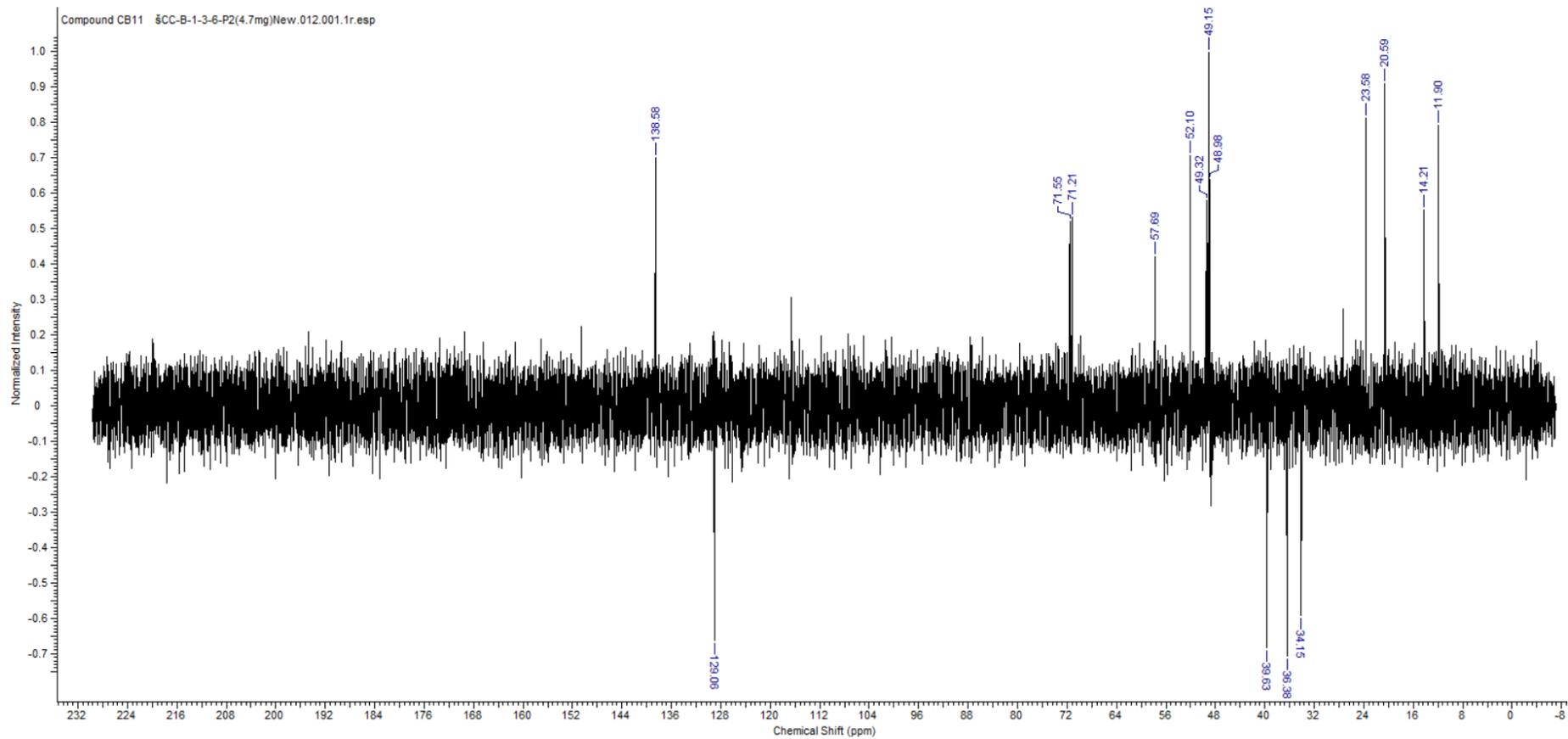
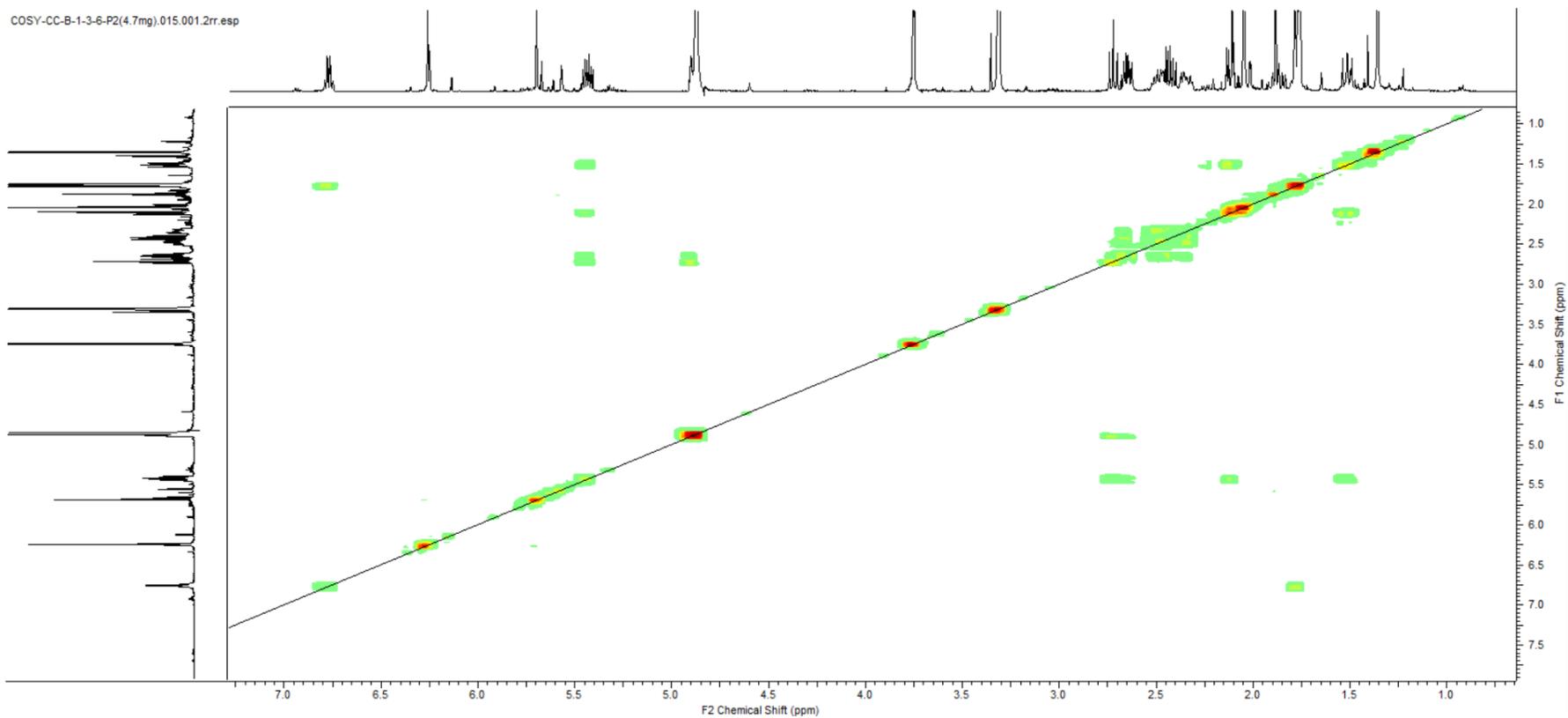


Figure S23.  $^{13}\text{C}$  DEPT135 NMR spectrum of **3** in MeOD (125 MHz)

COSY-CC-B-1-3-6-P2(4.7mg).015.001.2rr.esp



**Figure S24.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **3** in MeOD (500 MHz)

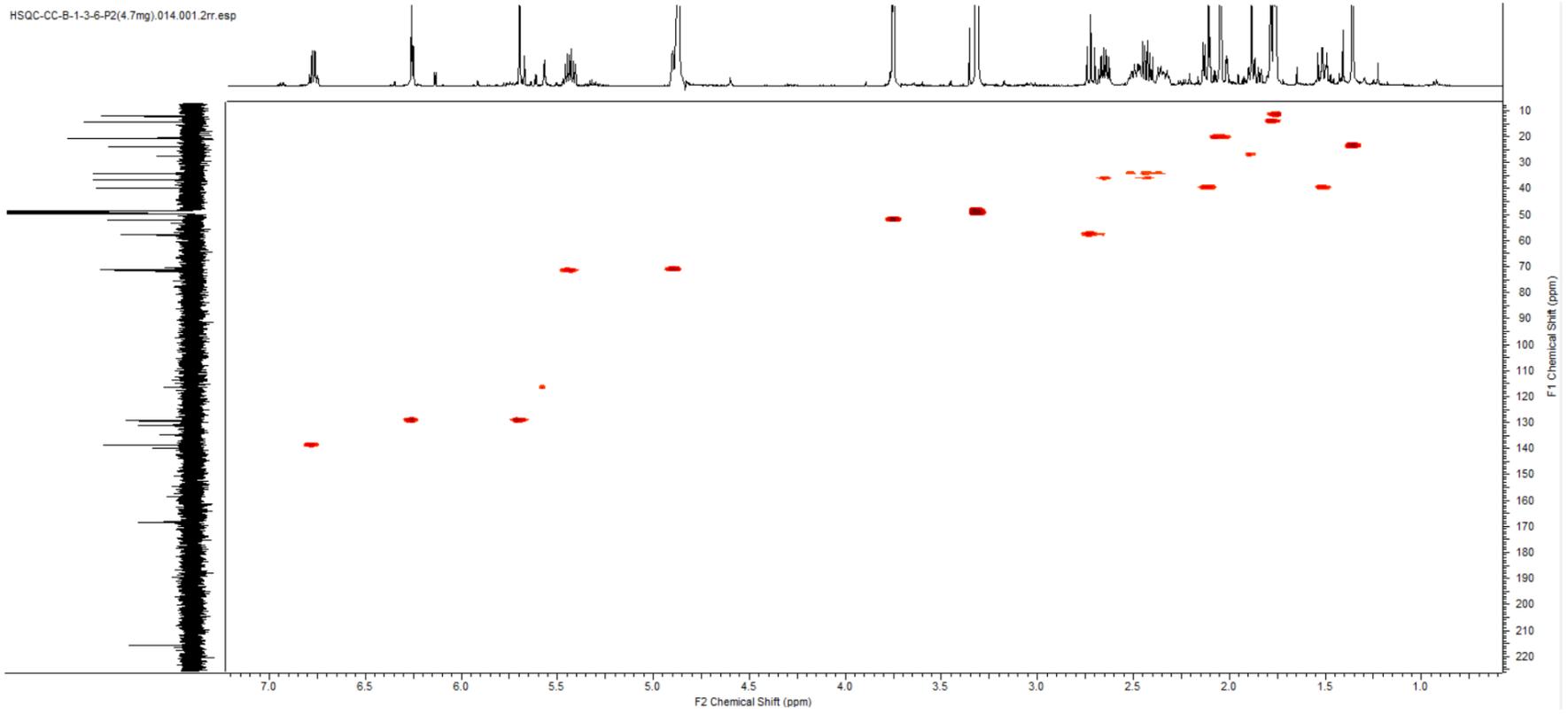


Figure S25. HSQC spectrum of **3** in MeOD (500 MHz)

HMBC-CC-B-1-3-6-P2(4.7mg).016.001.2rr.esp

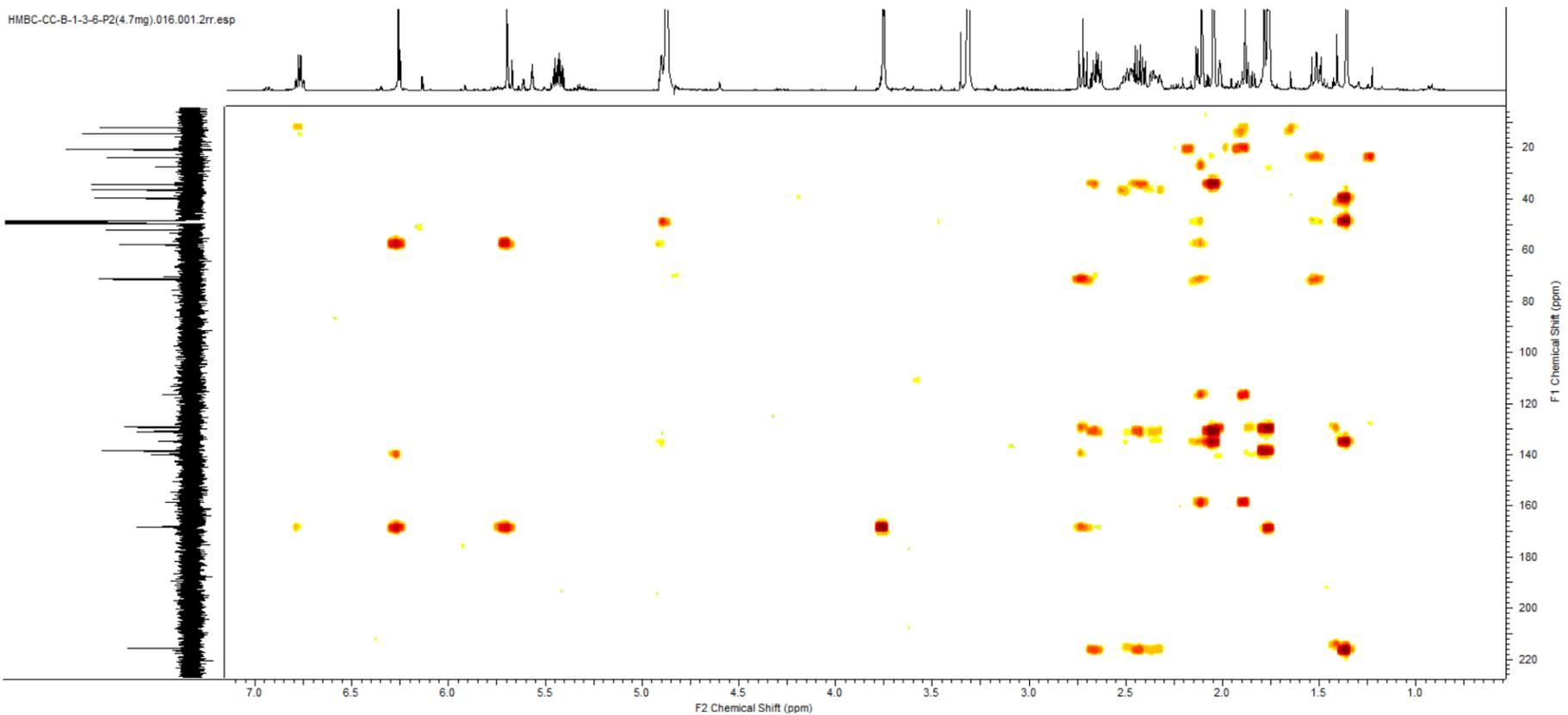
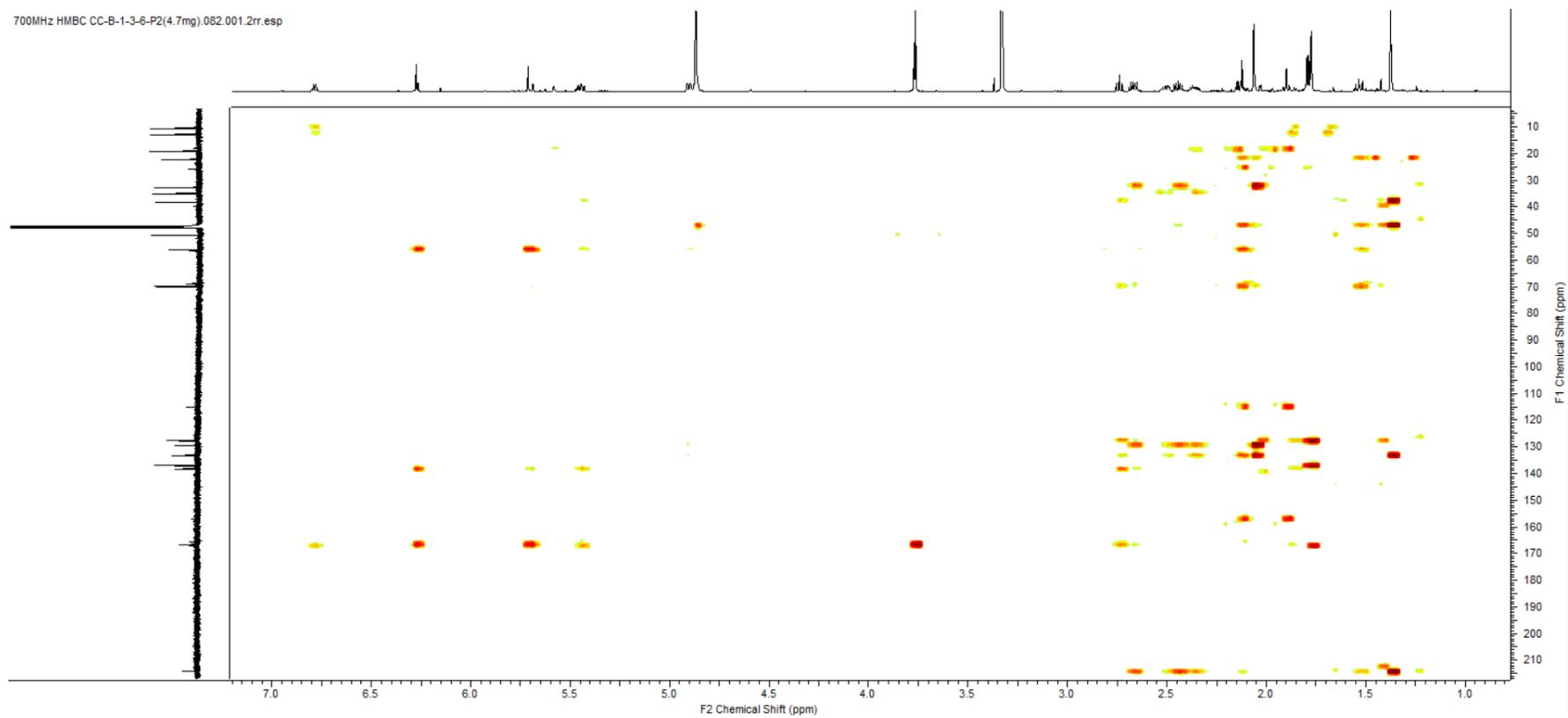


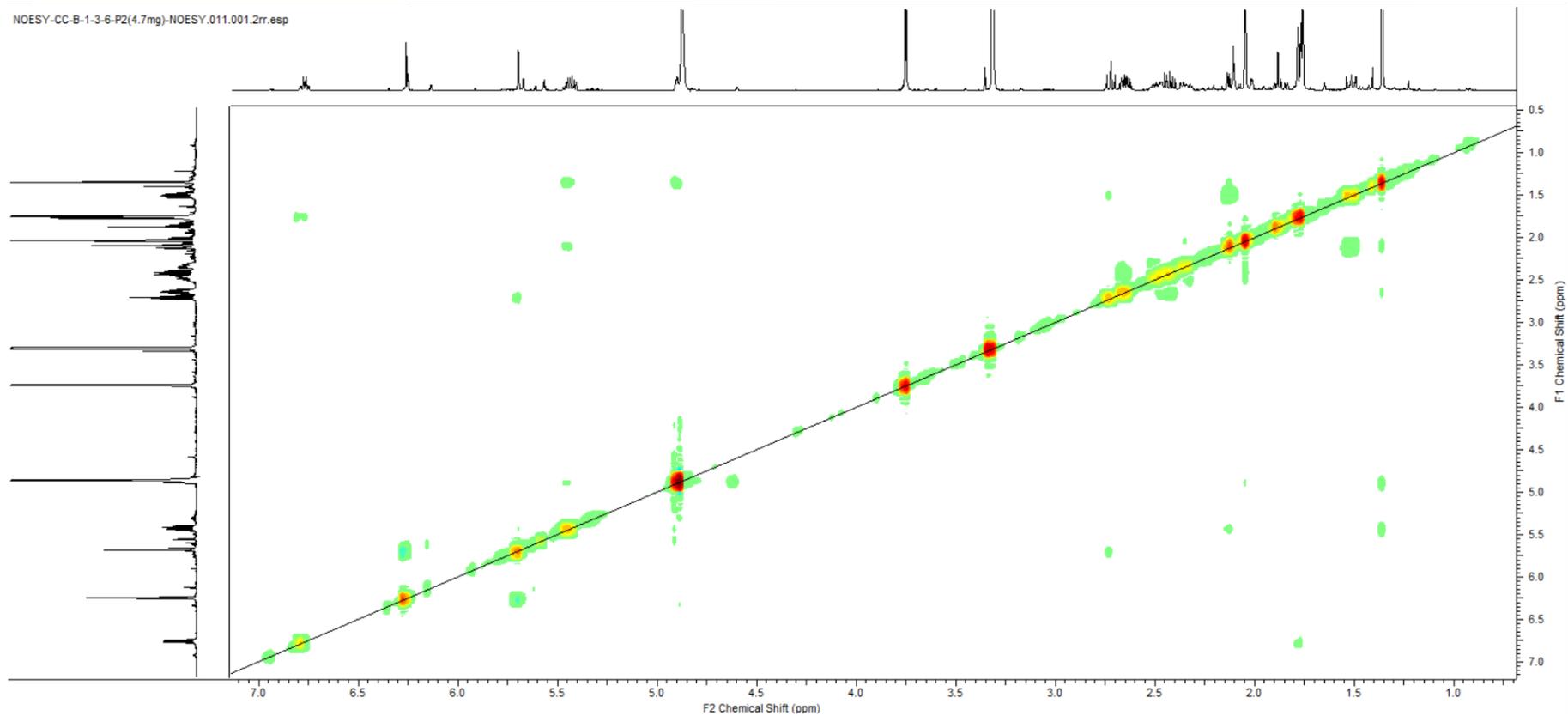
Figure S26. HMBC spectrum of 3 in MeOD (500 MHz)

700MHz HMBC CC-B-1-3-6-P2(4.7mg).082.001.2rr.esp



**Figure S27.** HMBC spectrum of **3** in MeOD (700 MHz)

NOESY-CC-B-1-3-6-P2(4.7mg)-NOESY.011.001.2rr.esp



**Figure S28.** PS-NOESY spectrum of **3** in MeOD (500 MHz)

CC-B-1-3-6 P2 + #7 RT: 0.08 AV: 1 NL: 3.12E6  
F: FTMS + p ESI Full ms [100.00-2000.00]

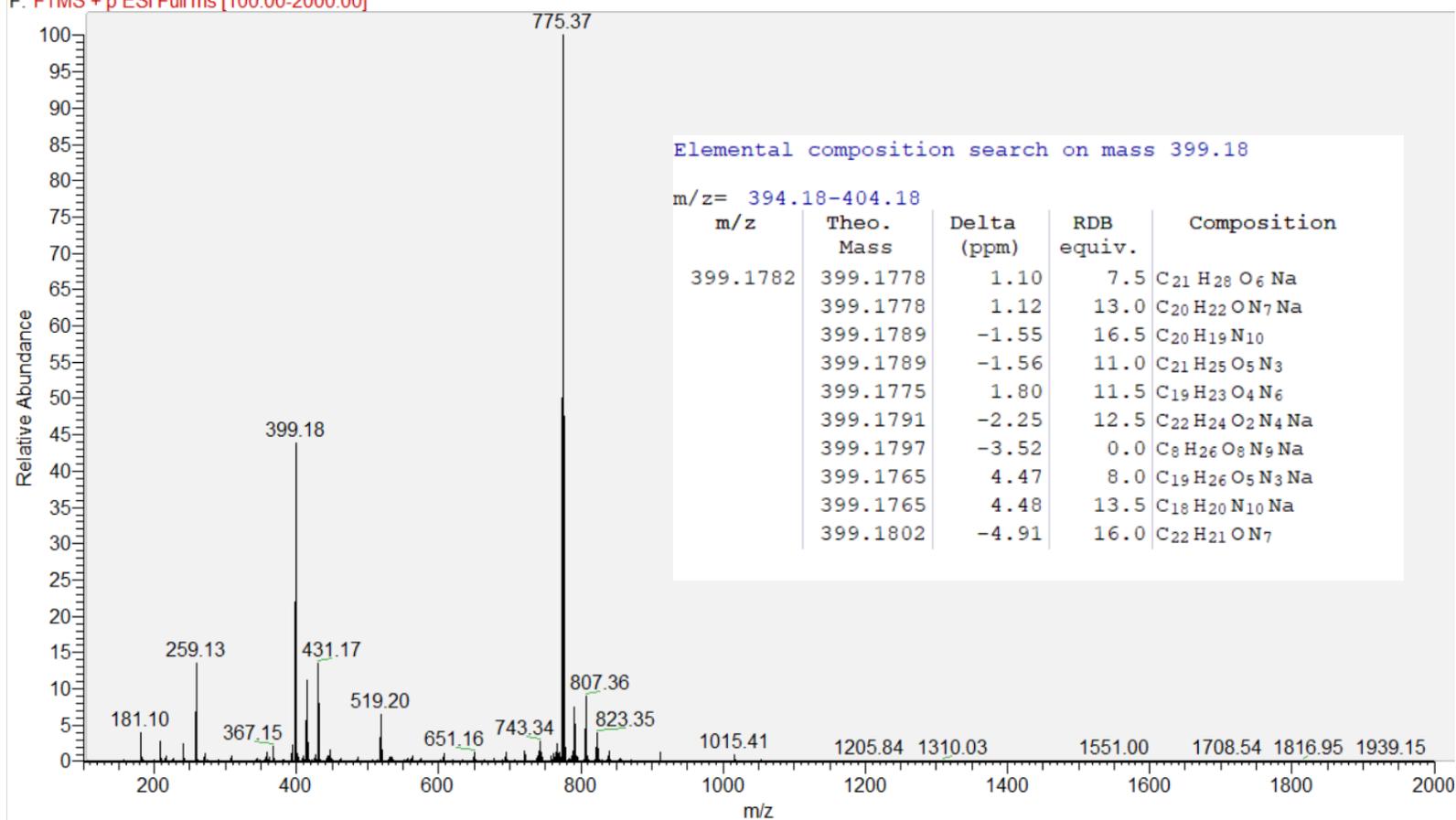


Figure S29. HR-ESI-MS spectrum of **3**

CC-B-1-3-6 P2 + #11 RT: 0.13 AV: 1 NL: 5.25E4  
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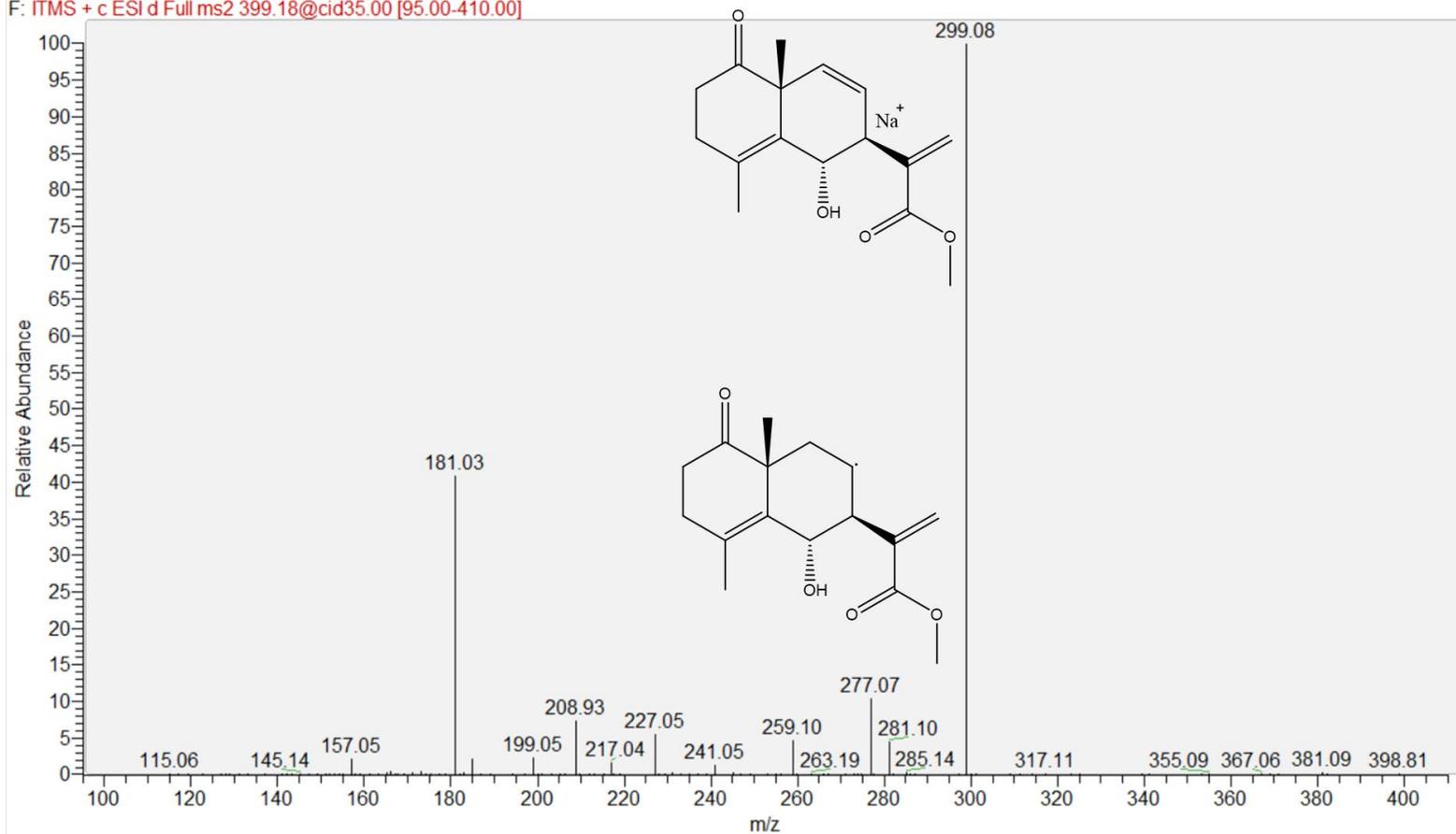


Figure S30. ESI-MS/MS spectrum of **3**

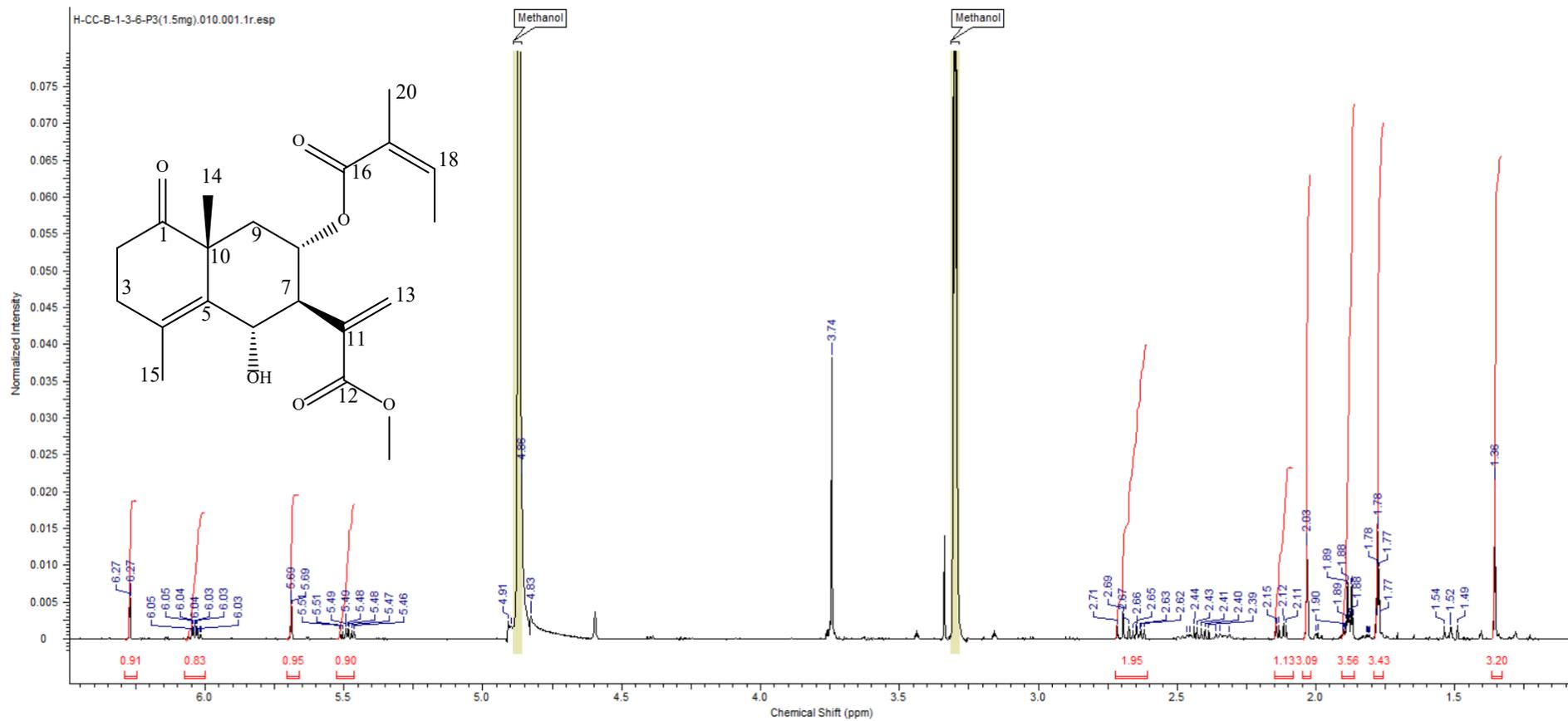


Figure S31. <sup>1</sup>H-NMR spectrum of 4 in MeOD (500 MHz)

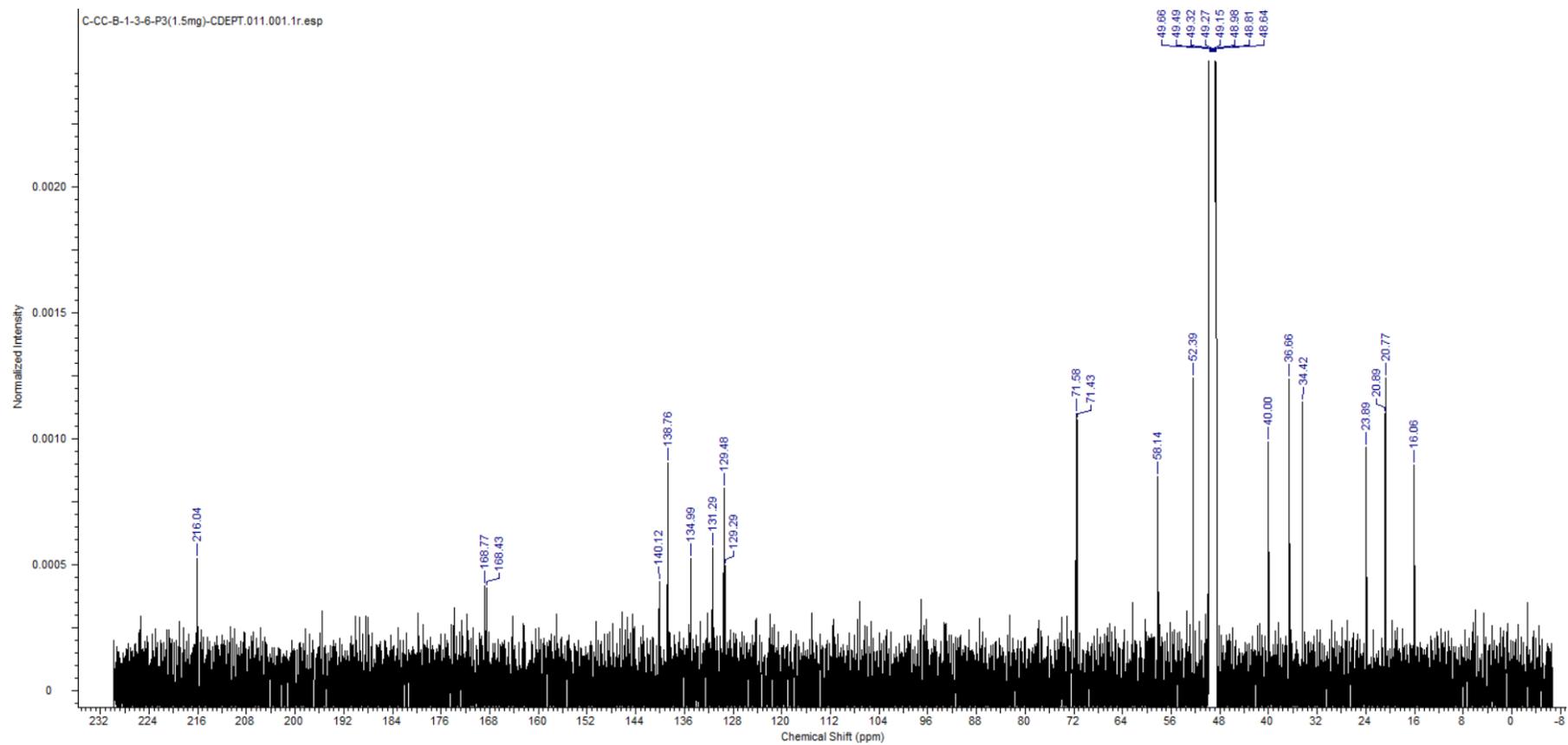


Figure S32.  $^{13}\text{C}$ -NMR spectrum of **4** in MeOD (125 MHz)

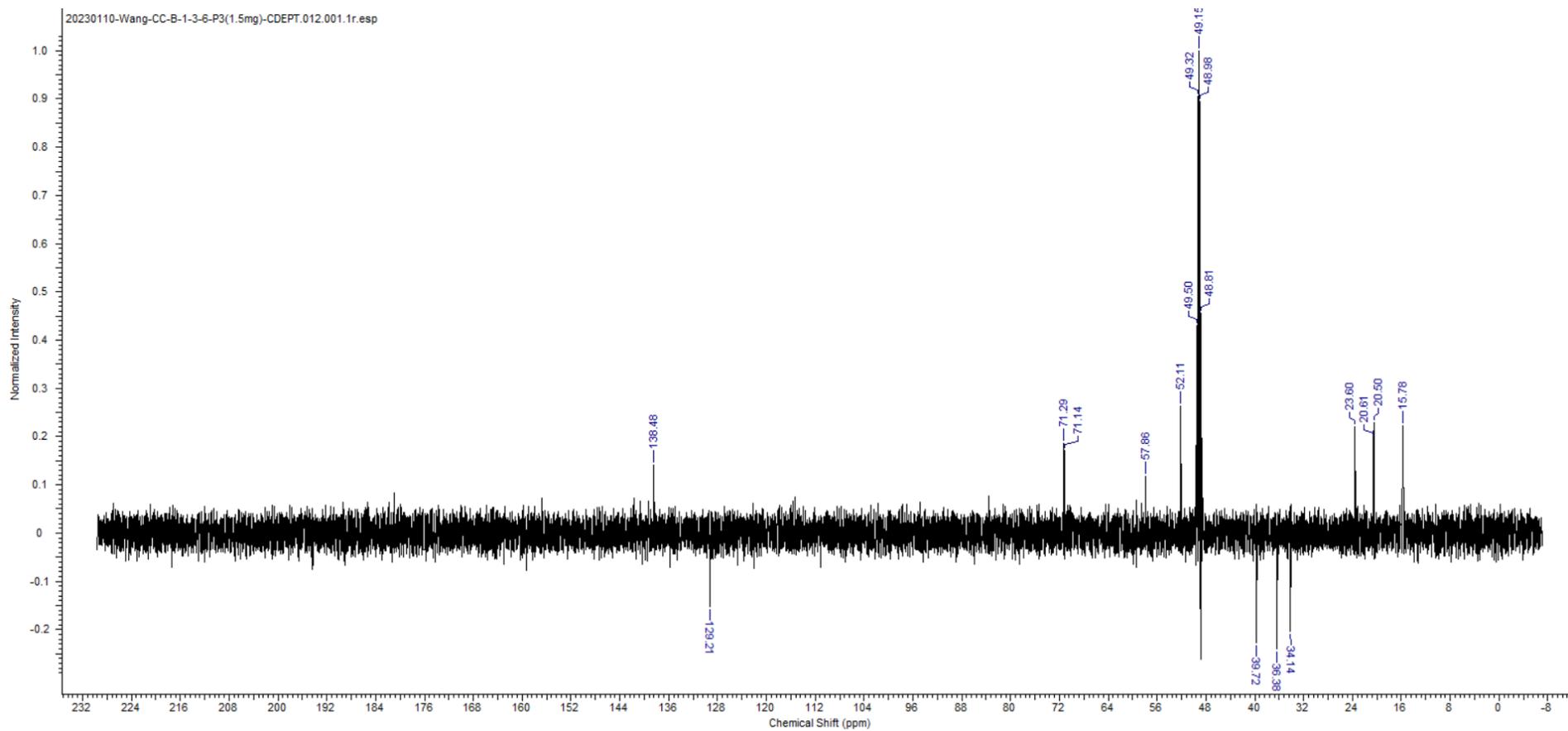
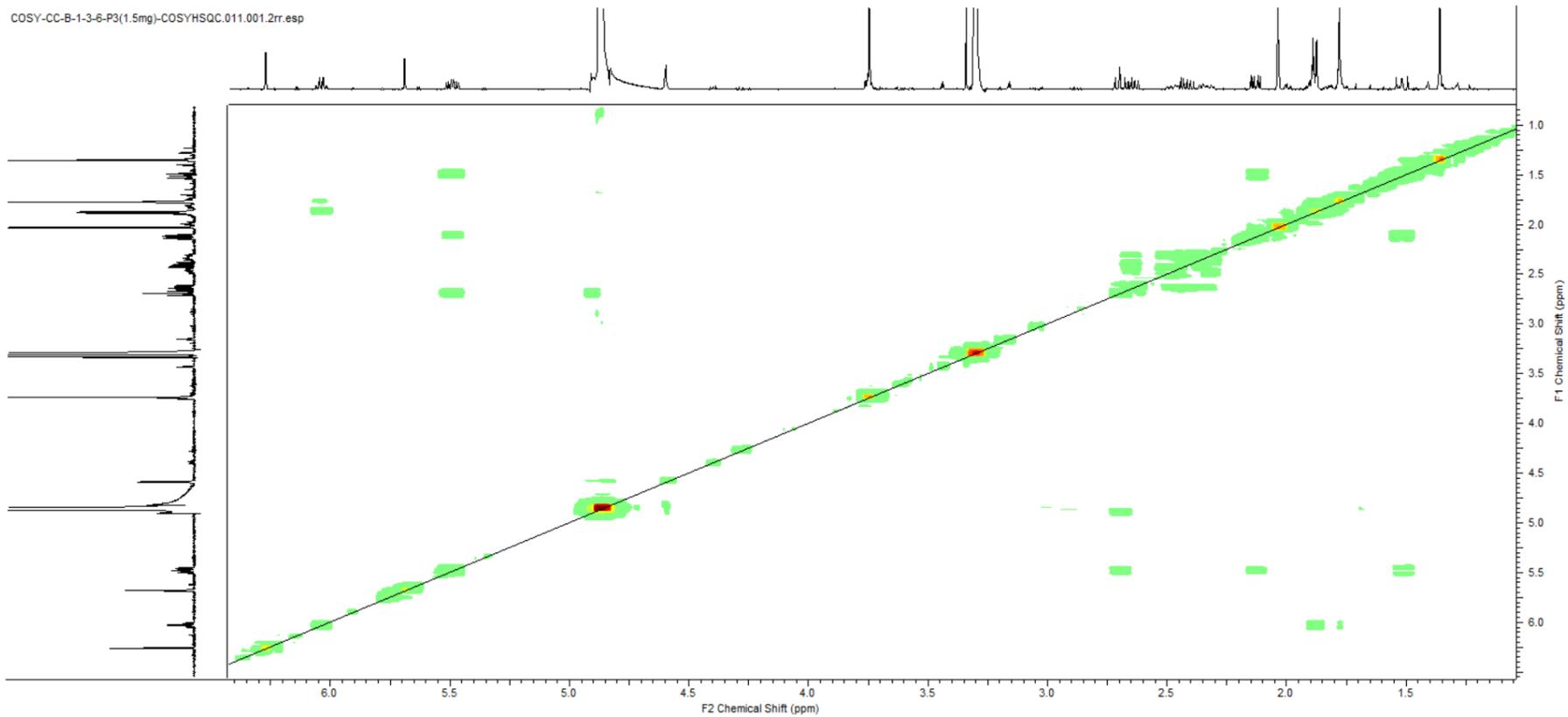
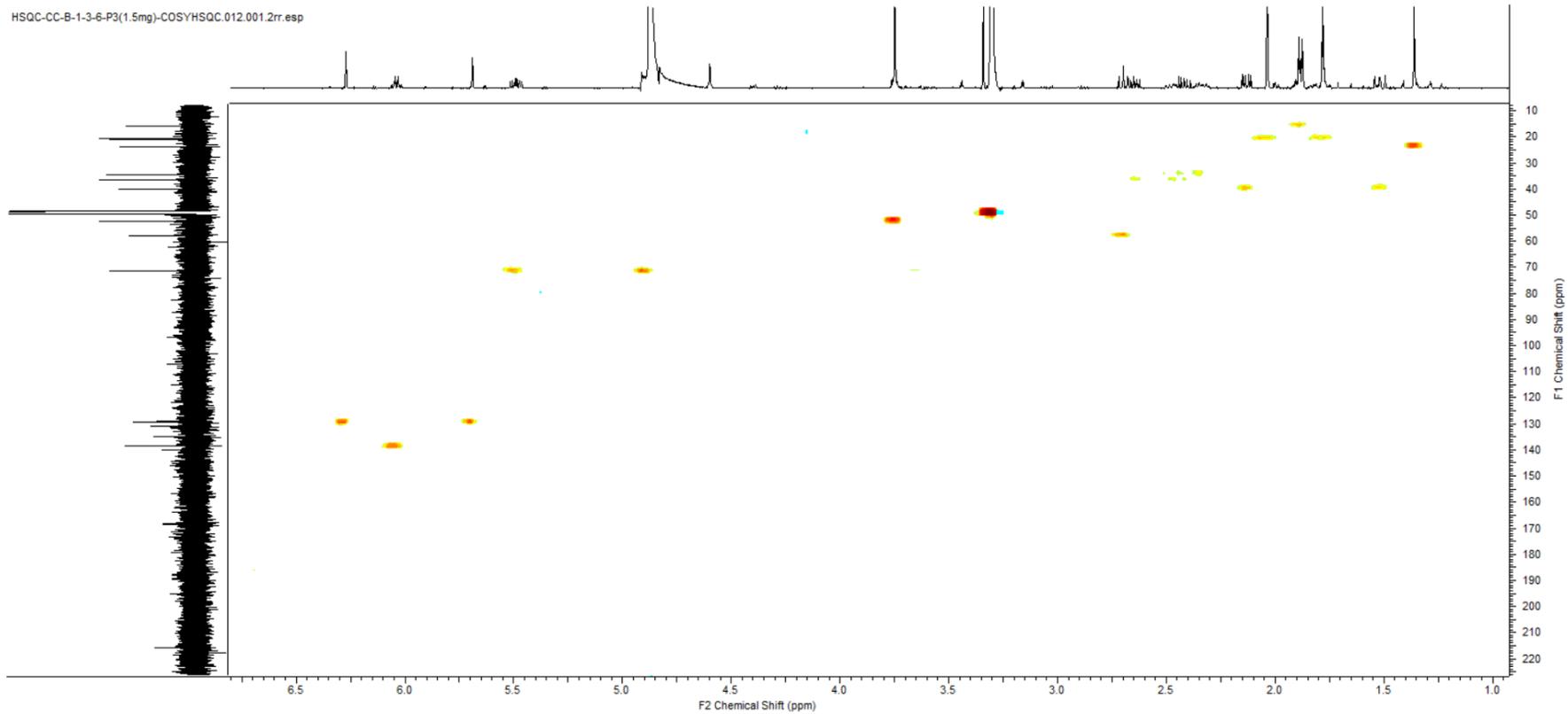


Figure S33.  $^{13}\text{C}$  DEPT135 NMR spectrum of **4** in MeOD (125 MHz)



**Figure S34.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **4** in MeOD (500 MHz)



**Figure S35.** HSQC spectrum of **4** in MeOD (500 MHz)

HMNBC-CC-B-1-3-6-P3(1.5mg)-HMBC.011.001.2rr.esp

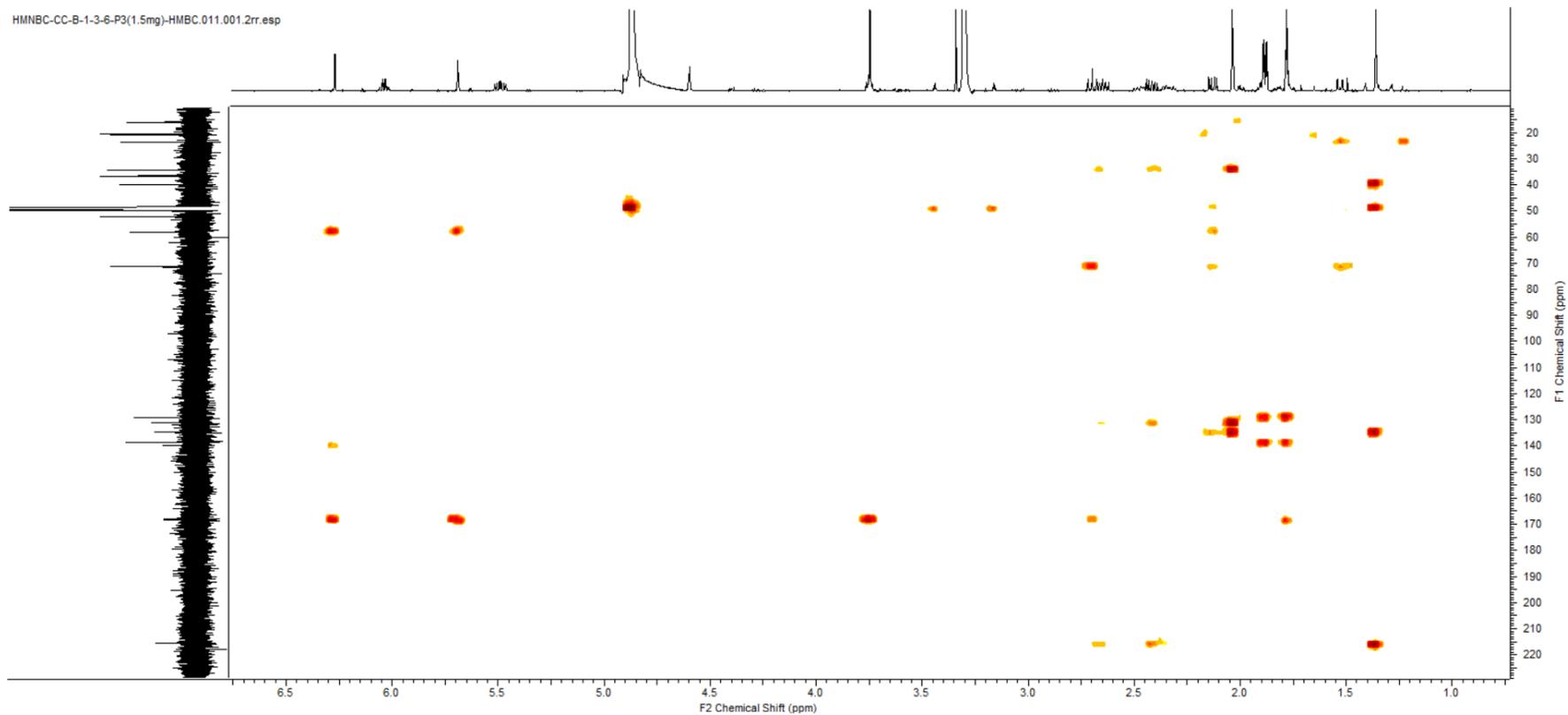
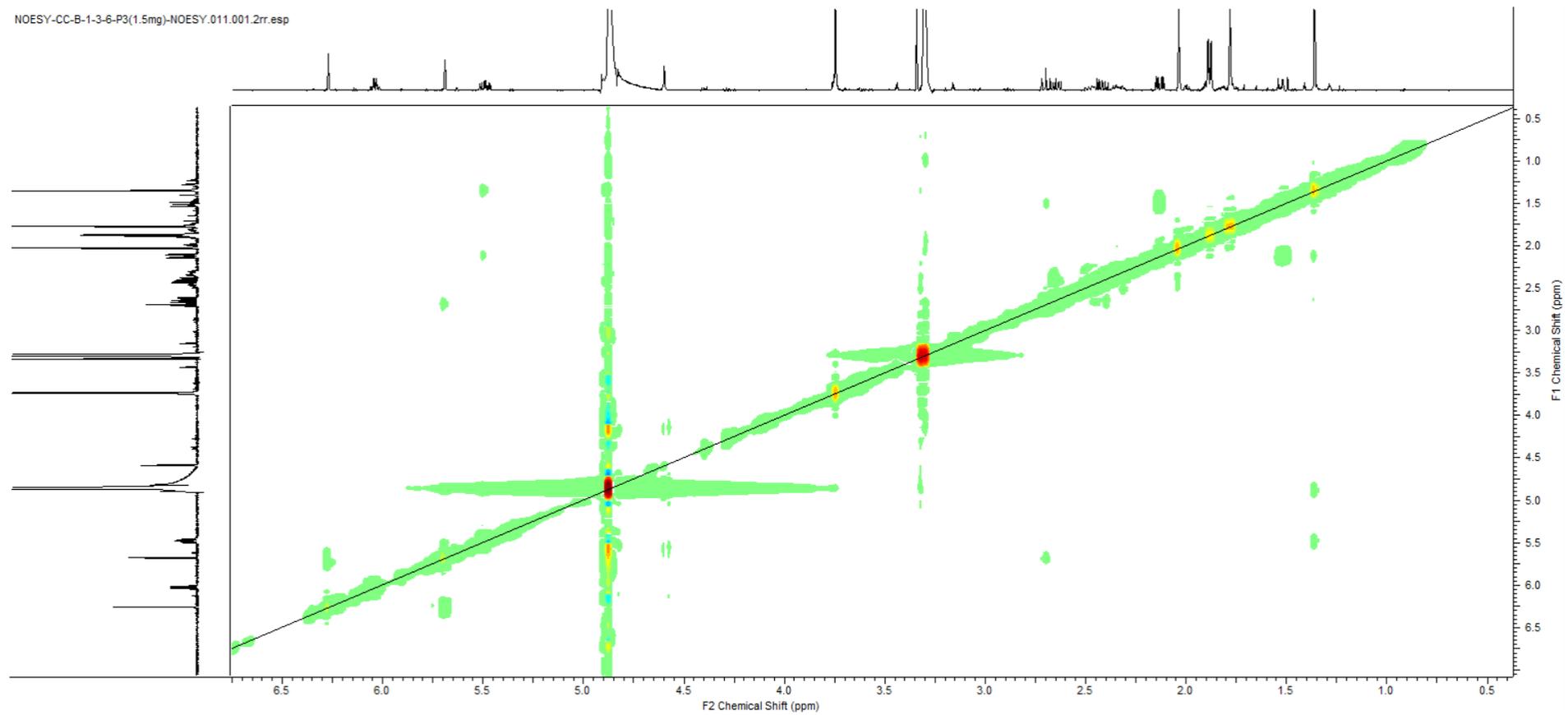


Figure S36. HMBC spectrum of 4 in MeOD (500 MHz)

NOESY-CC-B-1-3-6-P3(1.5mg)-NOESY.011.001.2rr.esp



**Figure S37.** PS-NOESY spectrum of **4** in MeOD (500 MHz)

CC-B-1-3-6 P3 + #7 RT: 0.08 AV: 1 NL: 1.82E6  
F: FTMS + p ESI Full ms [100.00-2000.00]

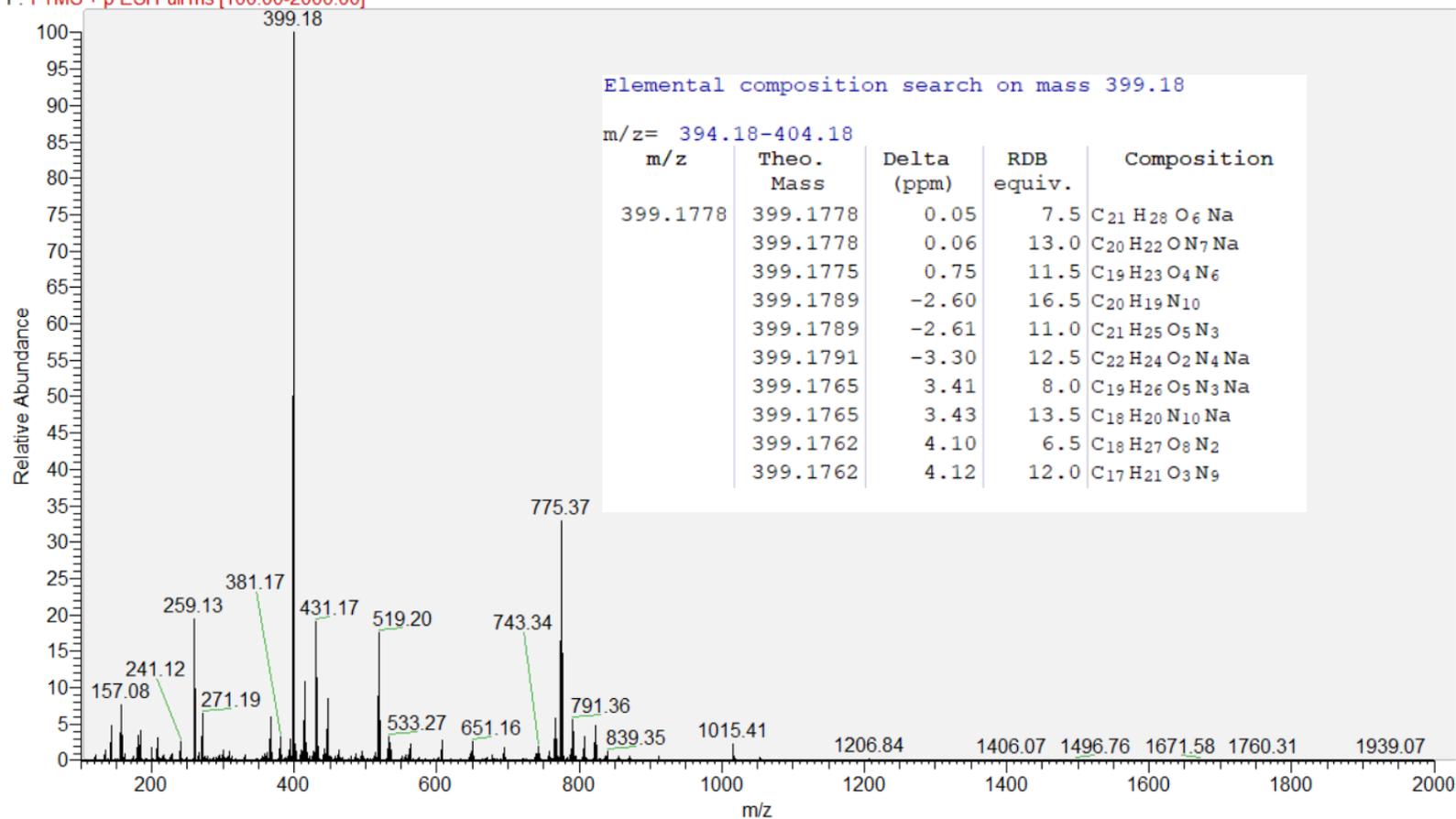


Figure S38. HR-ESI-MS spectrum of 4

CC-B-1-3-6 P3 + #8 RT: 0.09 AV: 1 NL: 2.52E4  
F: ITMS + c ESI d Full ms2 399.18@cid35.00 [95.00-410.00]

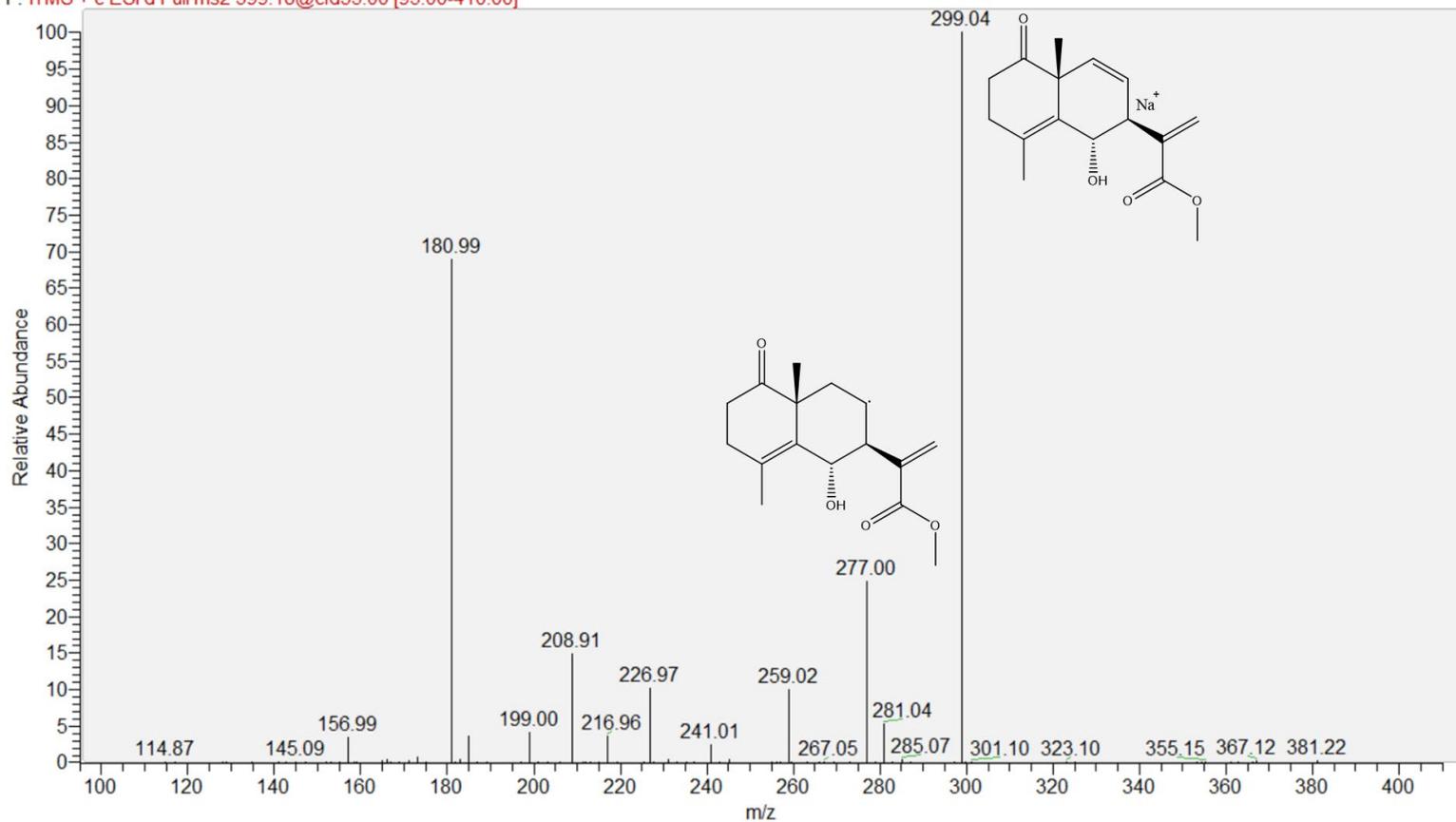


Figure S39. ESI-MS/MS spectrum of 4

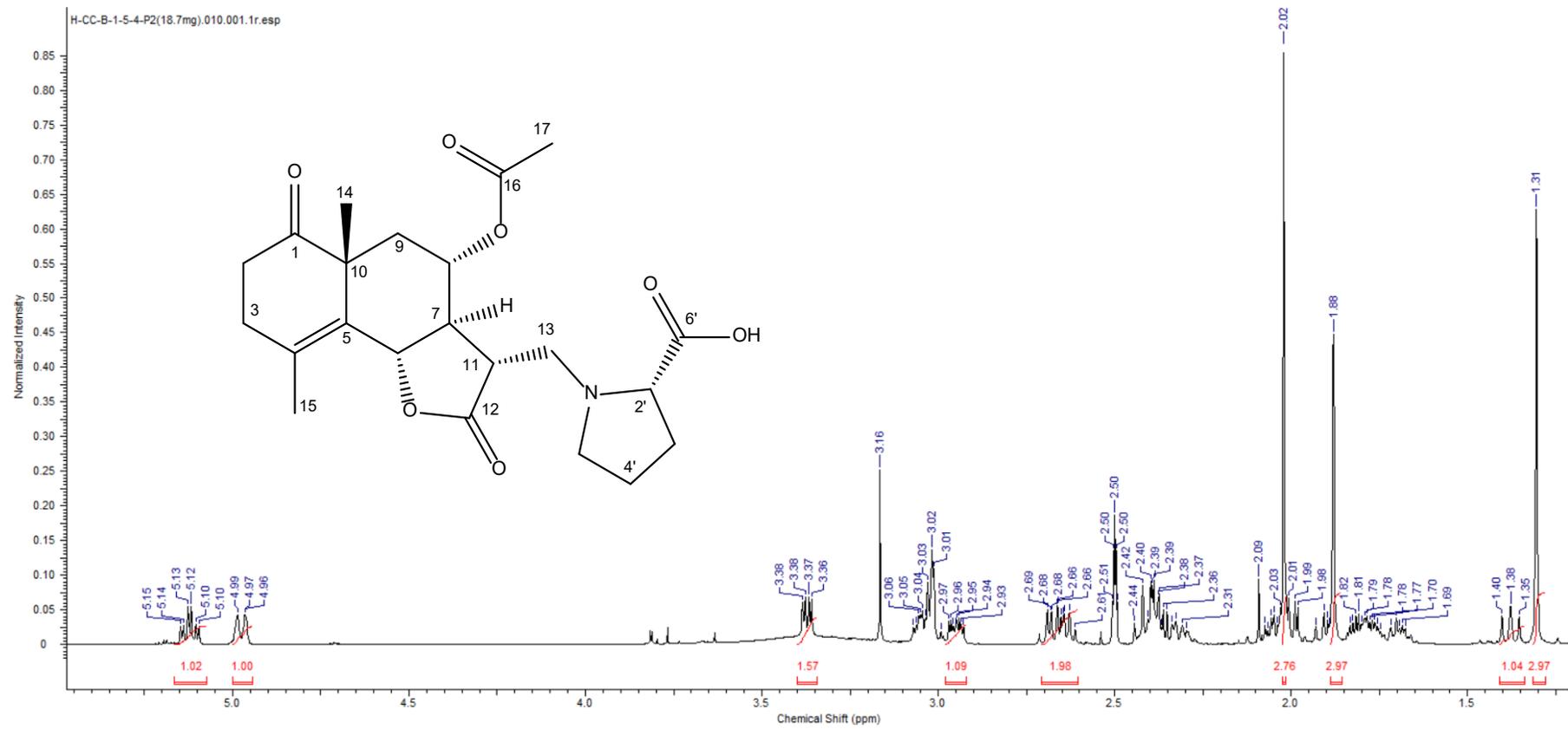


Figure S40.  $^1\text{H-NMR}$  spectrum of **5** in  $\text{DMSO-}d_6$  (500 MHz)

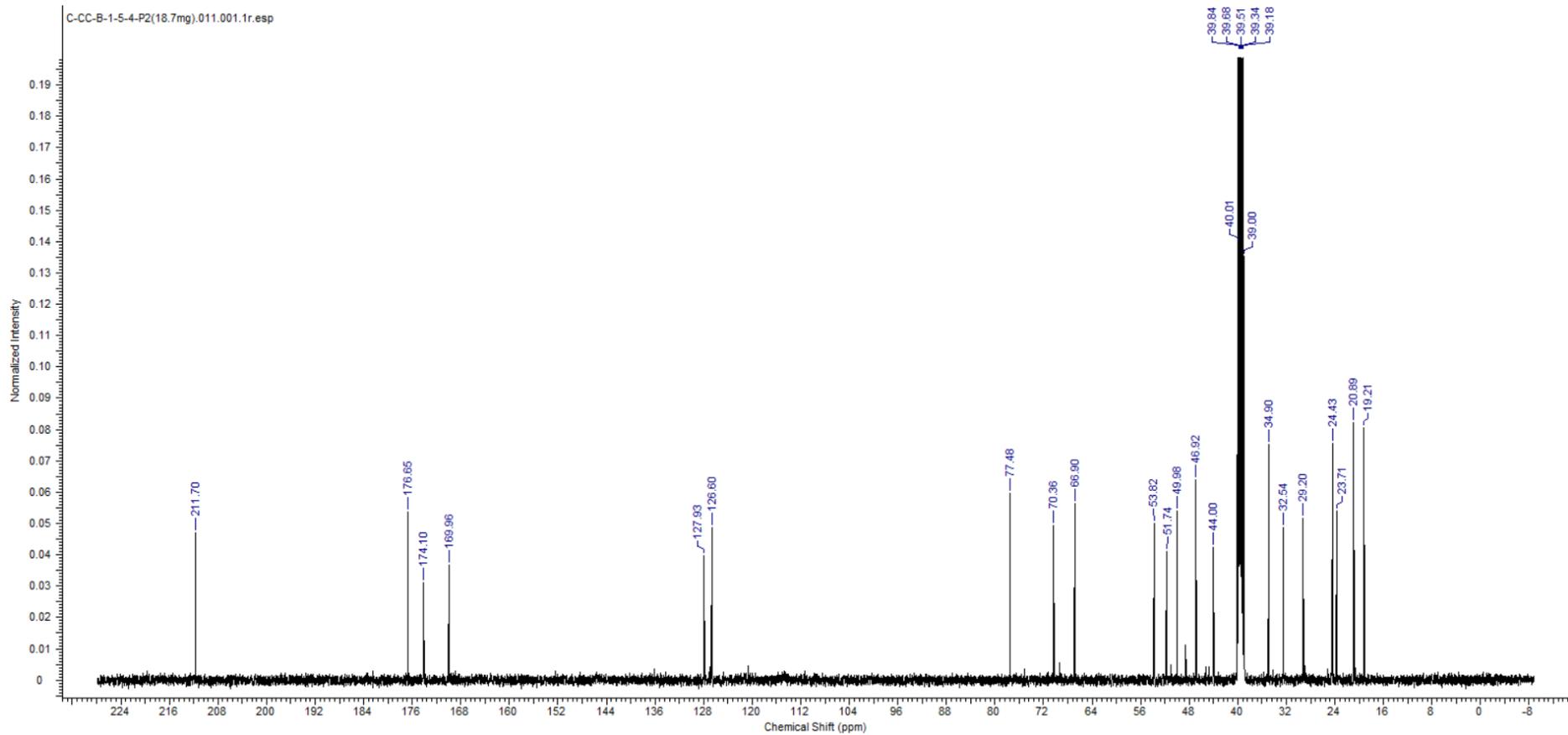
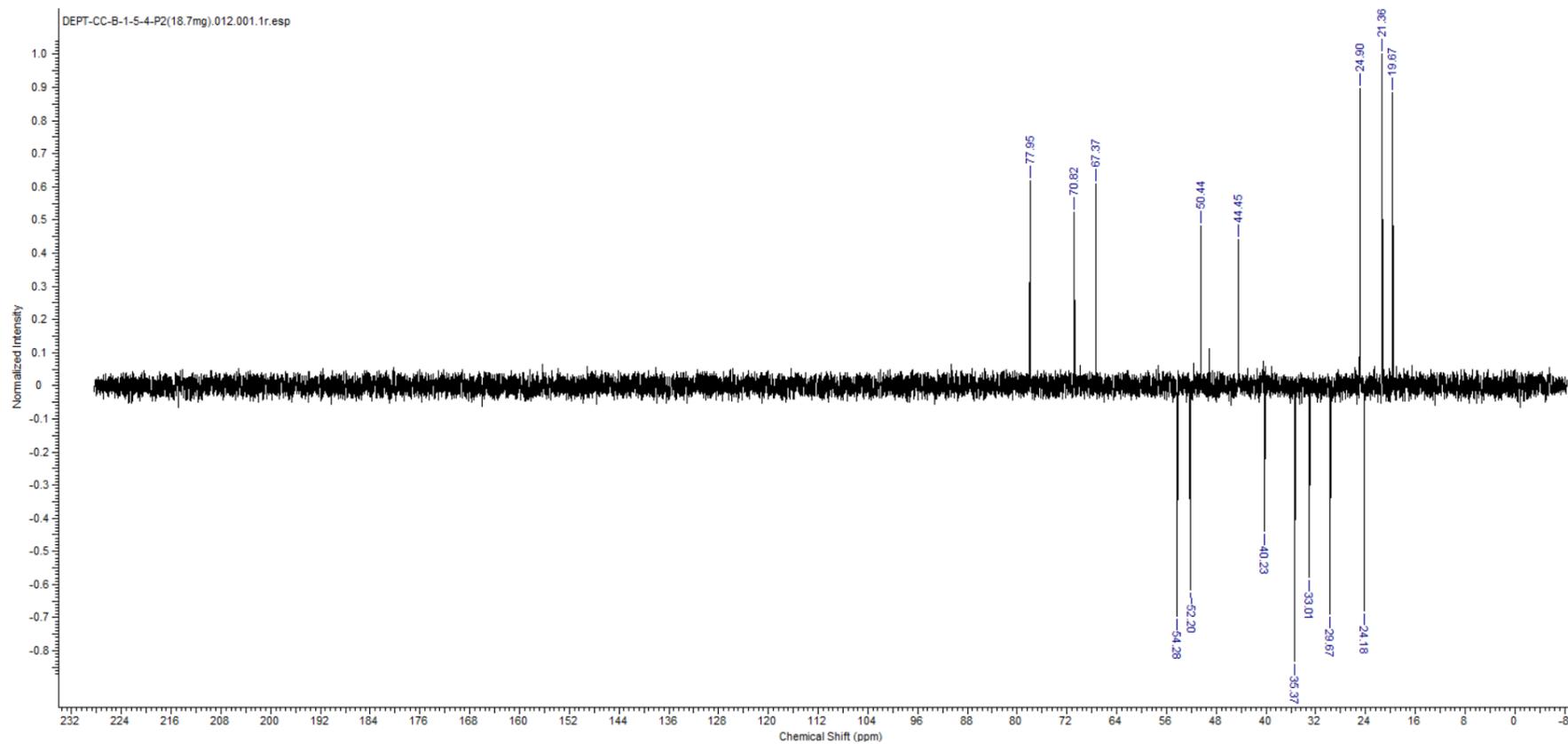
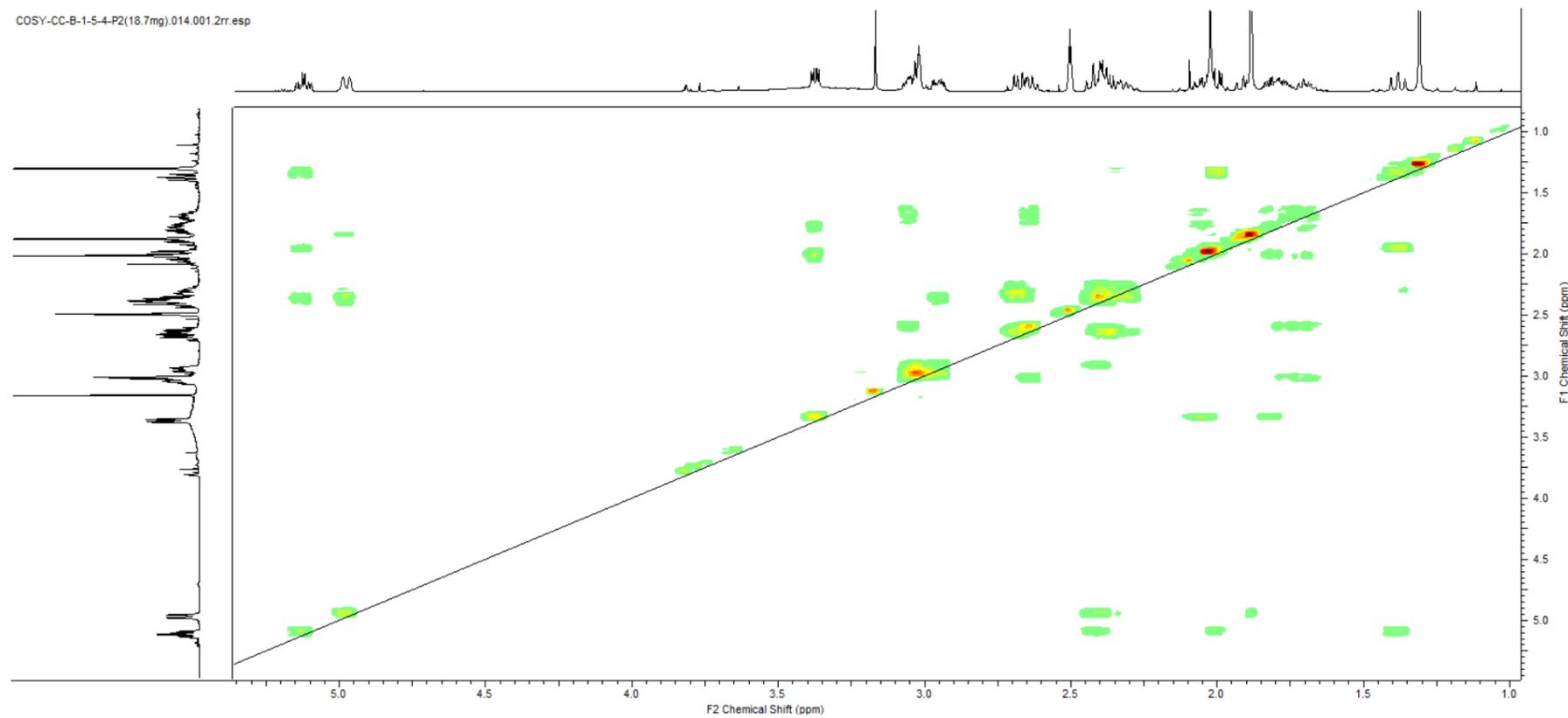


Figure S41.  $^{13}\text{C}$ -NMR spectrum of **5** in  $\text{DMSO-}d_6$  (125 MHz)



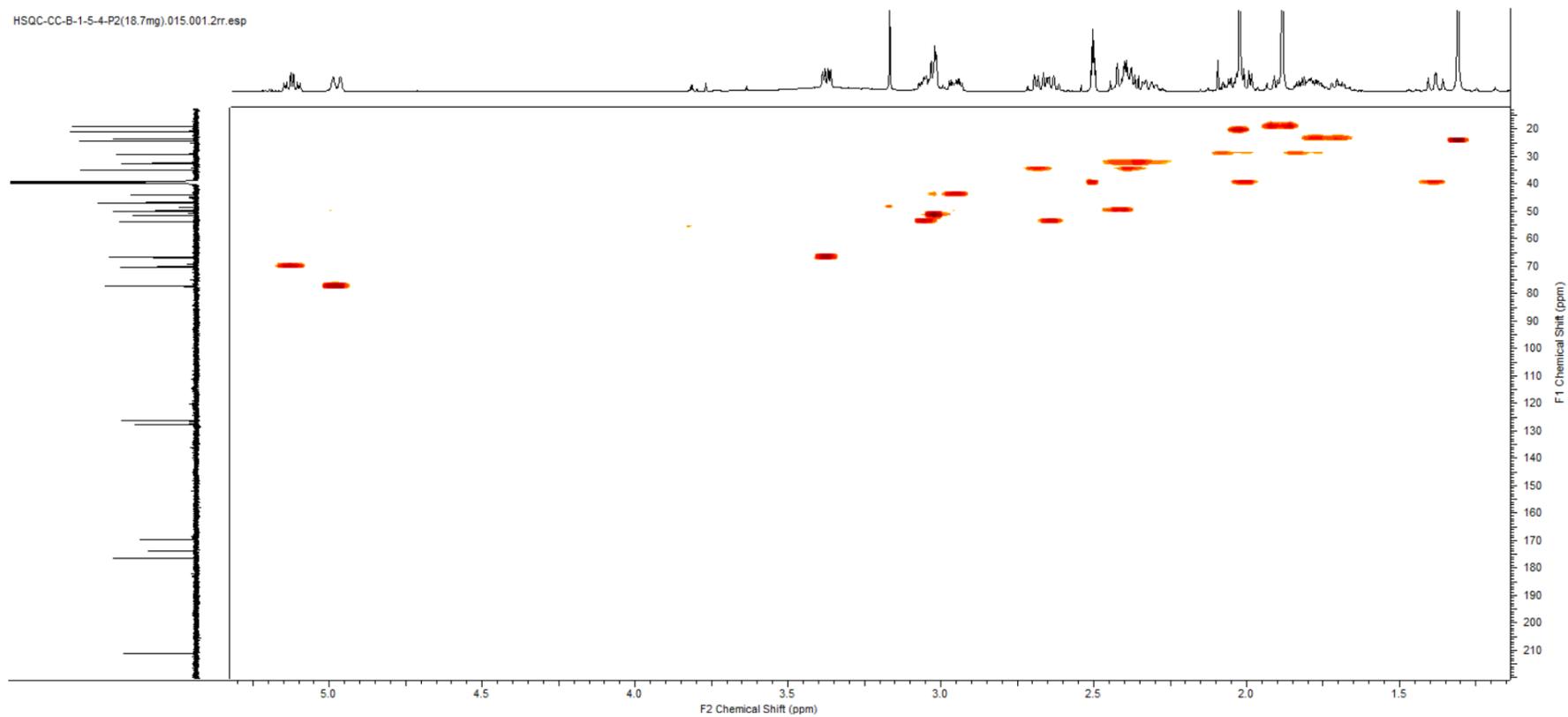
**Figure S42.**  $^{13}\text{C}$  DEPT135 NMR spectrum of **5** in  $\text{DMSO-}d_6$  (125 MHz)

COSY-CC-B-1-5-4-P2(18.7mg).014.001.2rr.esp



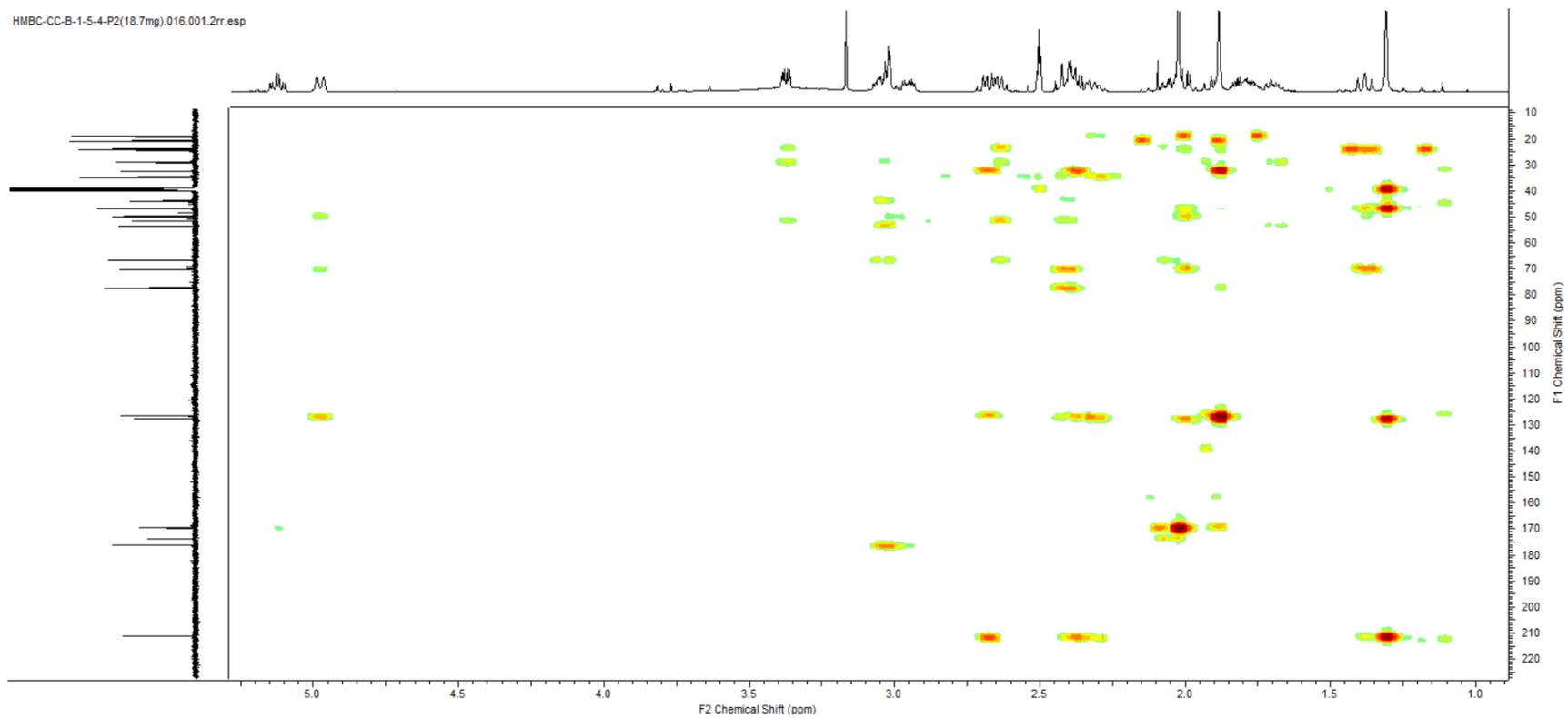
**Figure S43.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **5** in DMSO-*d*<sub>6</sub> (500 MHz)

HSQC-CC-B-1-5-4-F2(18.7mg).015.001.2rr.esp



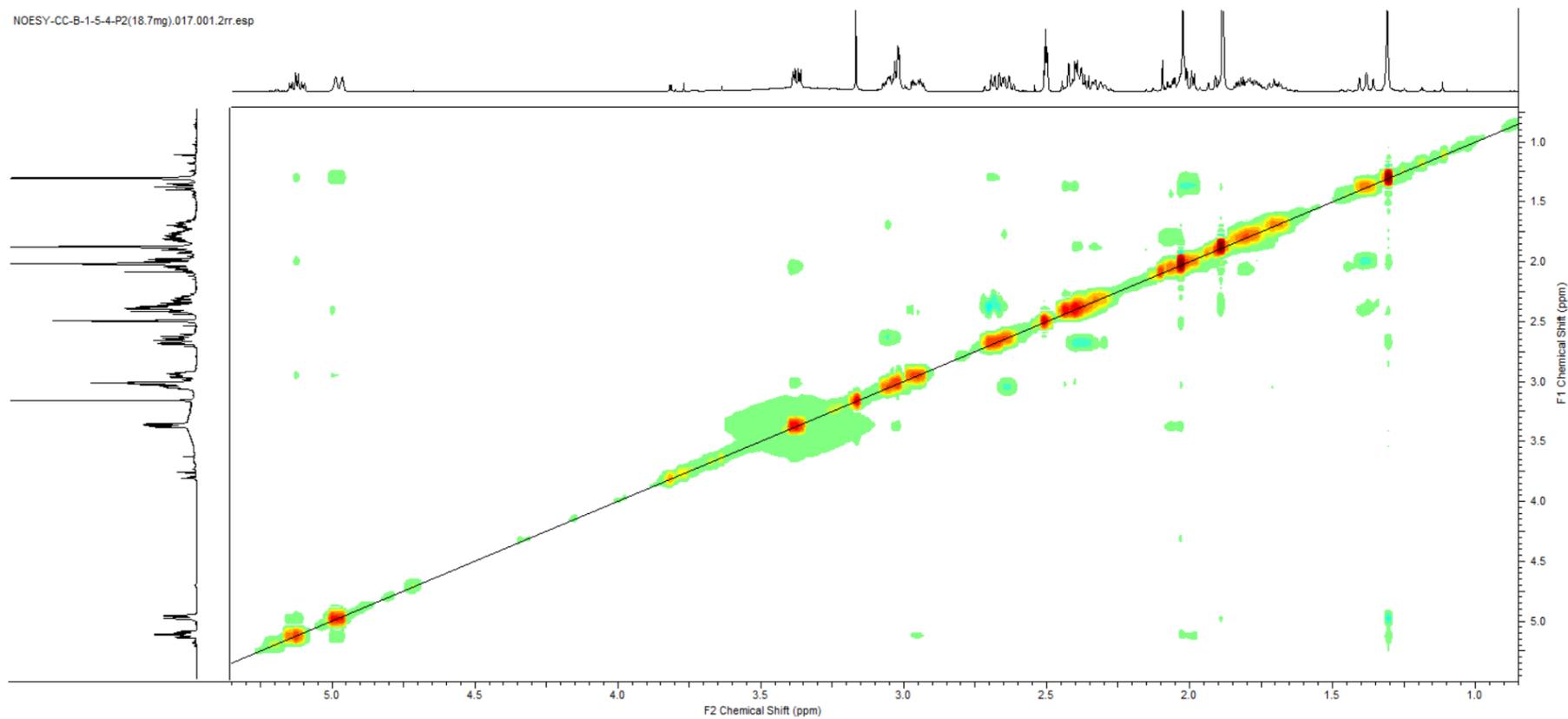
**Figure S44.** HSQC spectrum of **5** in  $\text{DMSO-}d_6$  (500 MHz)

HMBC-CC-B-1-5-4-P2(18.7mg).016.001.2rr.esp



**Figure S45.** HMBC spectrum of **5** in DMSO- $d_6$  (500 MHz)

NOESY-CC-B-1-5-4-P2(18.7mg).017.001.2rr.esp



**Figure S46.** PS-NOESY spectrum of **5** in DMSO-*d*<sub>6</sub> (500 MHz)

CC-B-1-5-4-P2 + #7 RT: 0.08 AV: 1 NL: 1.84E6  
F: FTMS + p ESI Full ms [100.00-2000.00]

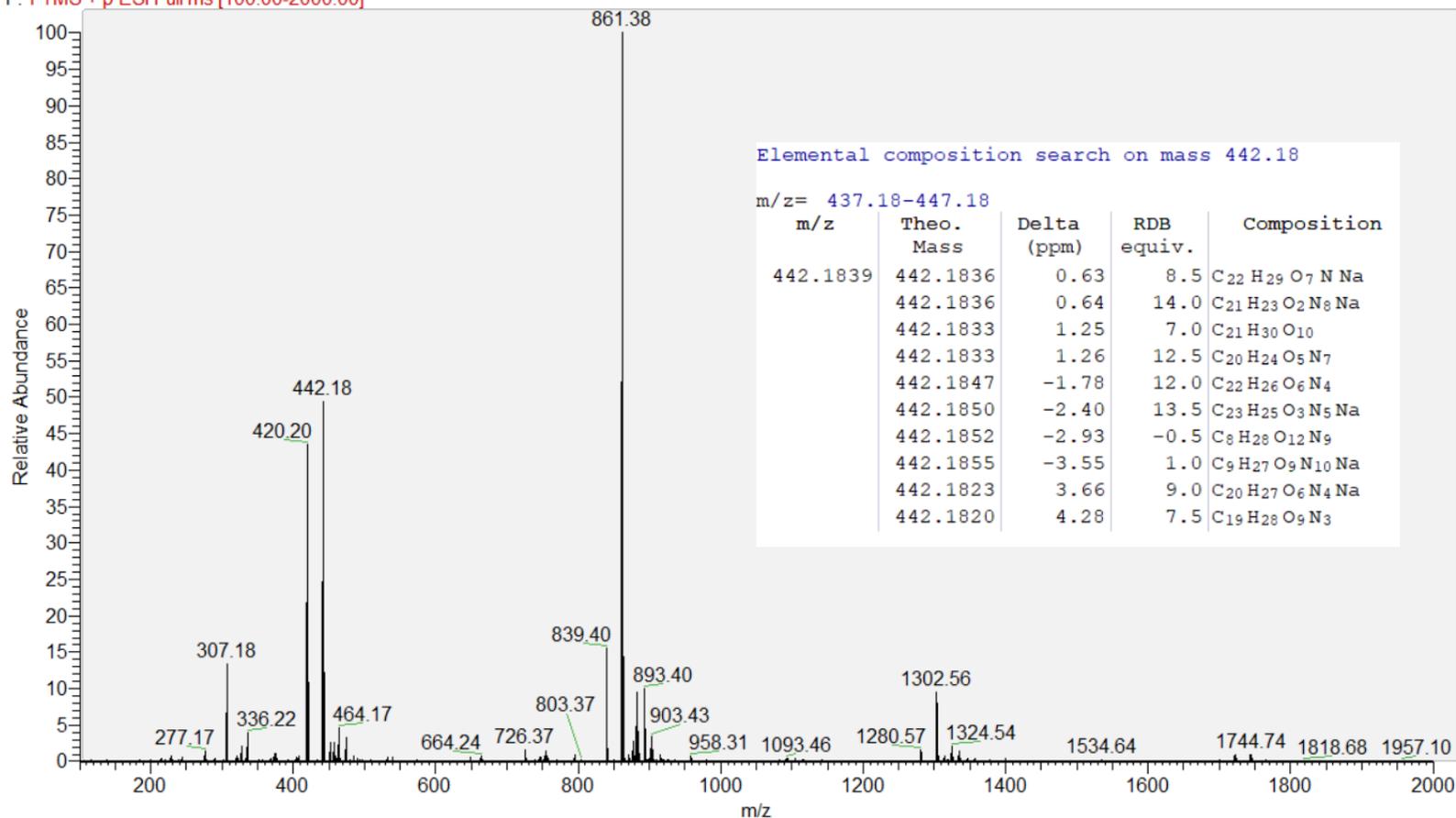


Figure S47. HR-ESI-MS spectrum of 5

CC-B-1-5-4-P2 + #5 RT: 0.06 AV: 1 NL: 3.10E3  
F: ITMS + c ESI d Full ms2 442.18@cid35.00 [110.00-455.00]

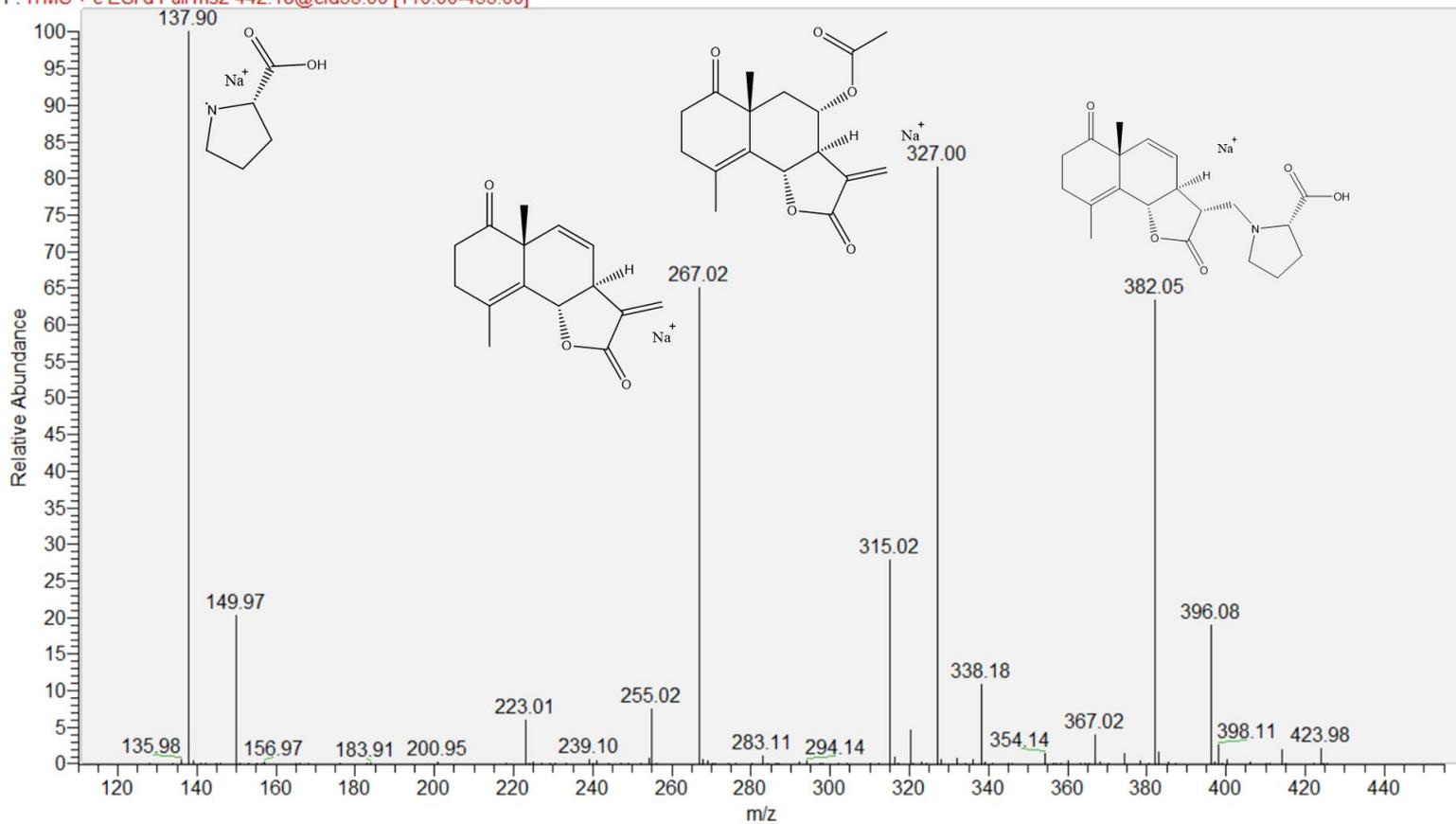


Figure S48. ESI-MS/MS spectrum of 5

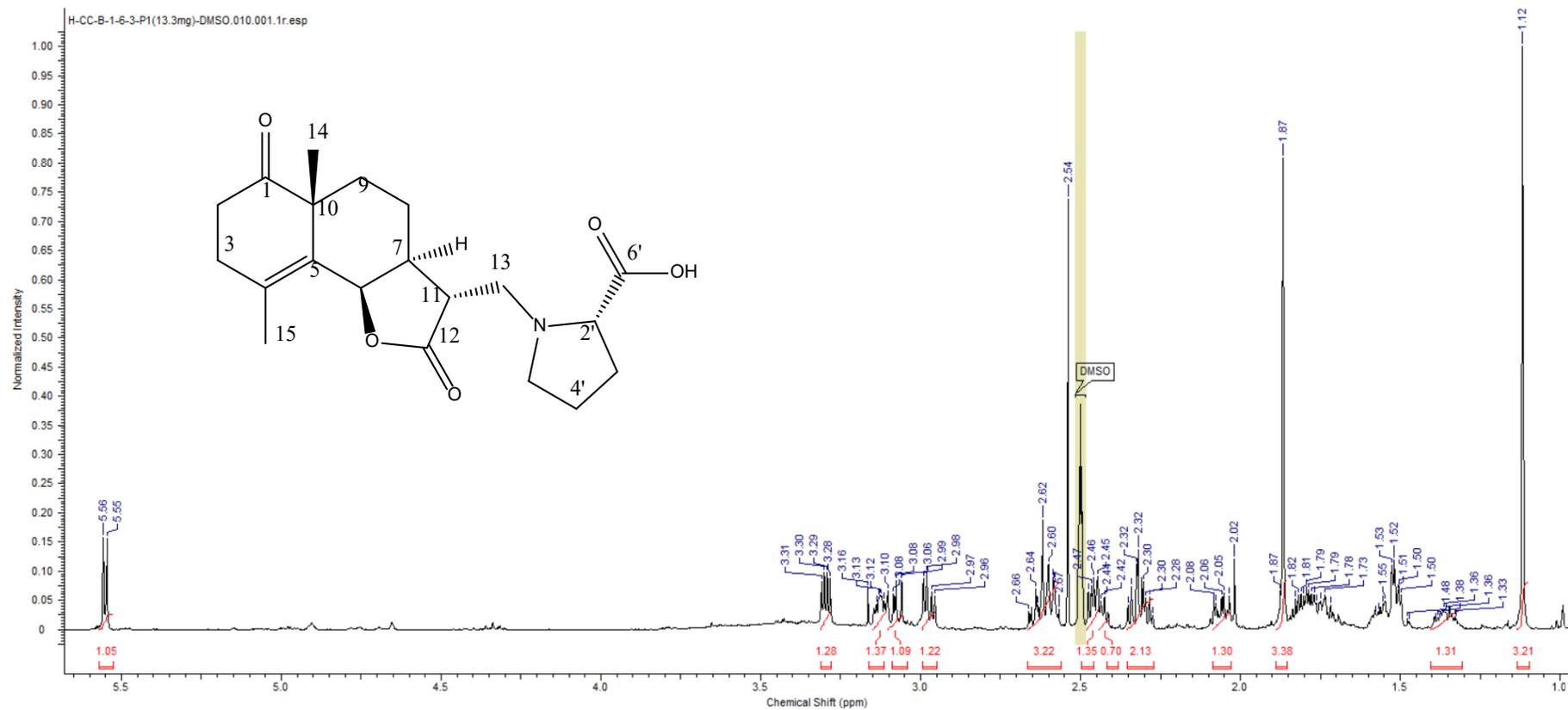


Figure S49.  $^1\text{H-NMR}$  spectrum of **6** in  $\text{DMSO-}d_6$  (500 MHz)

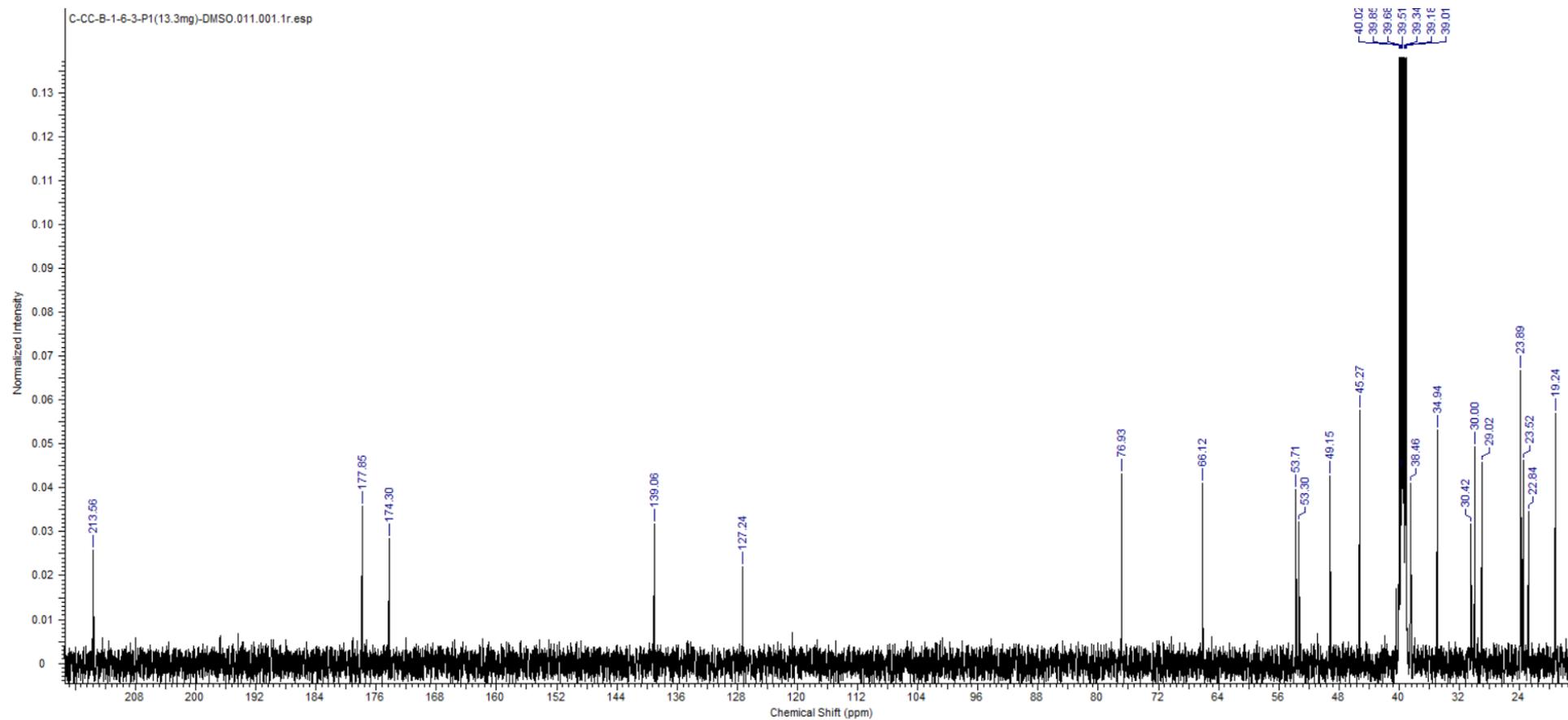
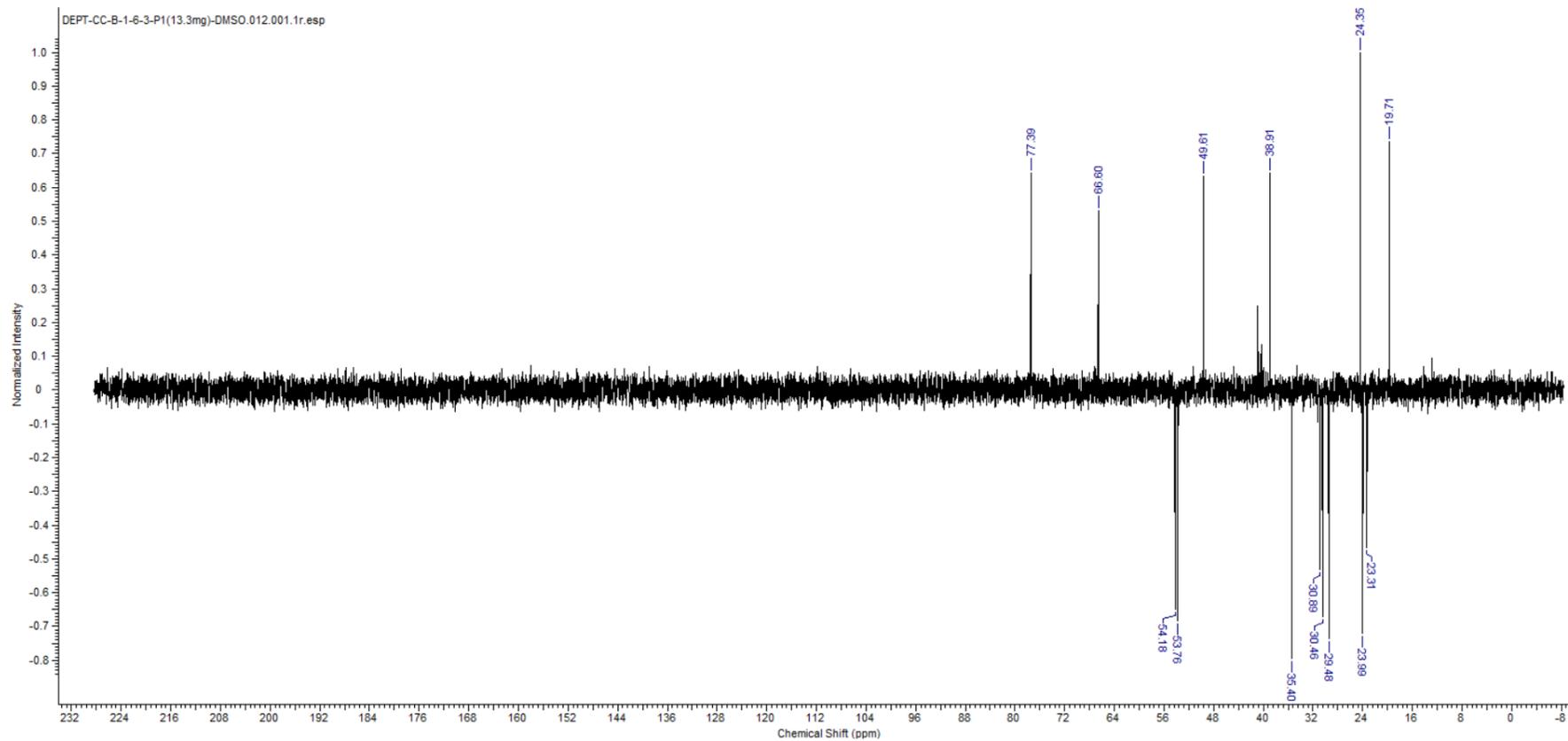
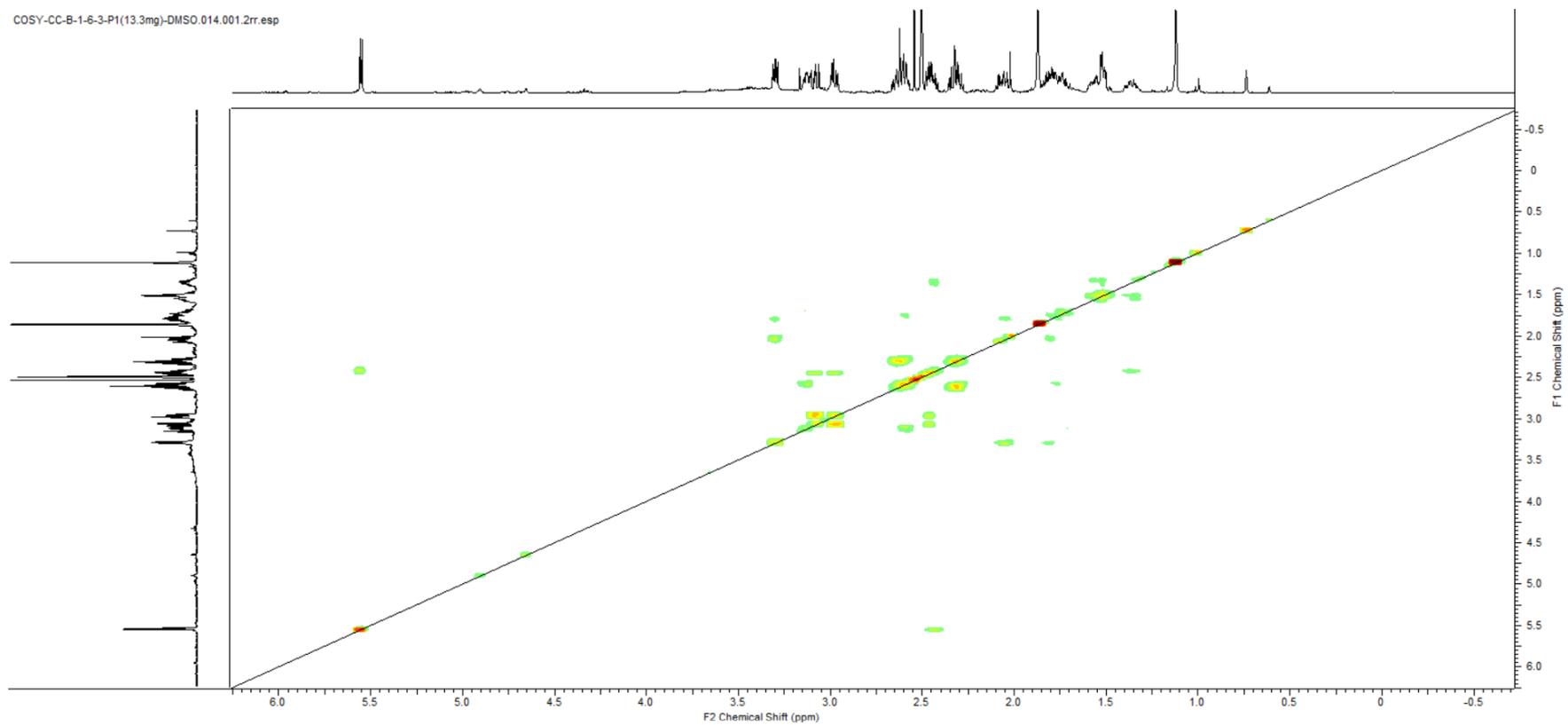


Figure S50.  $^{13}\text{C}$ -NMR spectrum of **6** in  $\text{DMSO-}d_6$  (125 MHz)



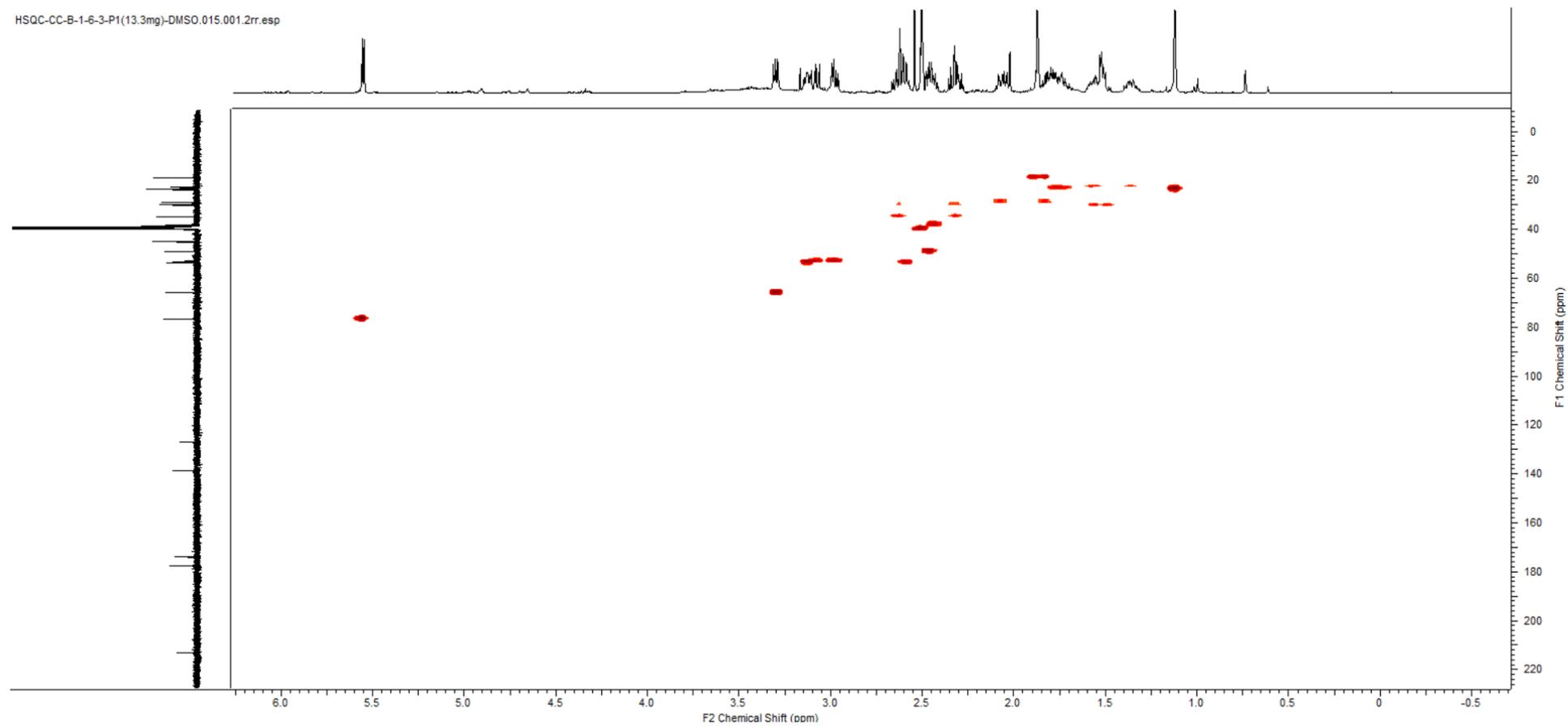
**Figure S51.**  $^{13}\text{C}$  DEPT135 NMR spectrum of **6** in  $\text{DMSO-}d_6$  (125 MHz)

COSY-CC-B-1-6-3-P1(13.3mg)-DMSO.014.001.2rr.esp



**Figure S52.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **6** in DMSO-*d*<sub>6</sub> (500 MHz)

HSQC-CC-B-1-6-3-P1(13.3mg)-DMSO.015.001.2rr.esp



**Figure S53.** HSQC spectrum of **6** in DMSO-*d*<sub>6</sub> (500 MHz)

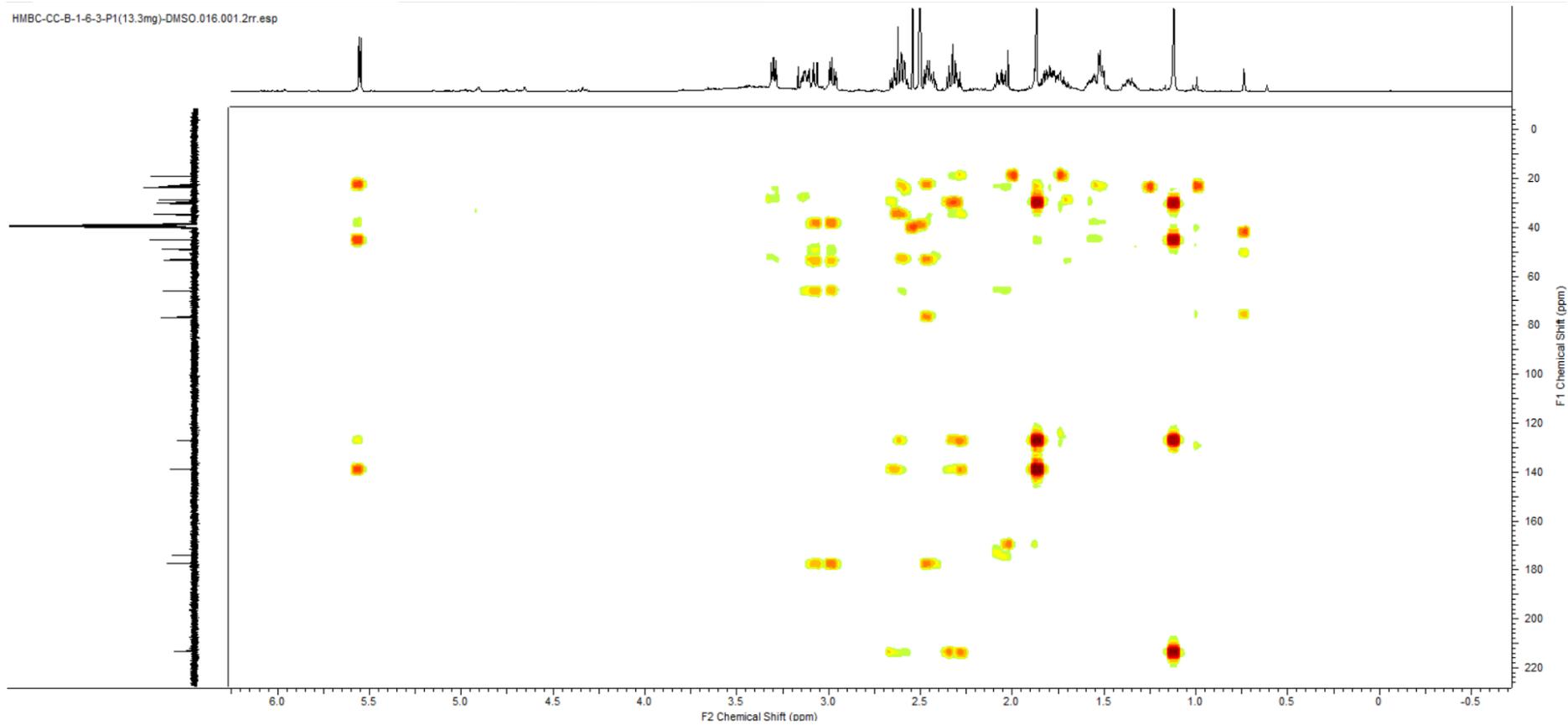
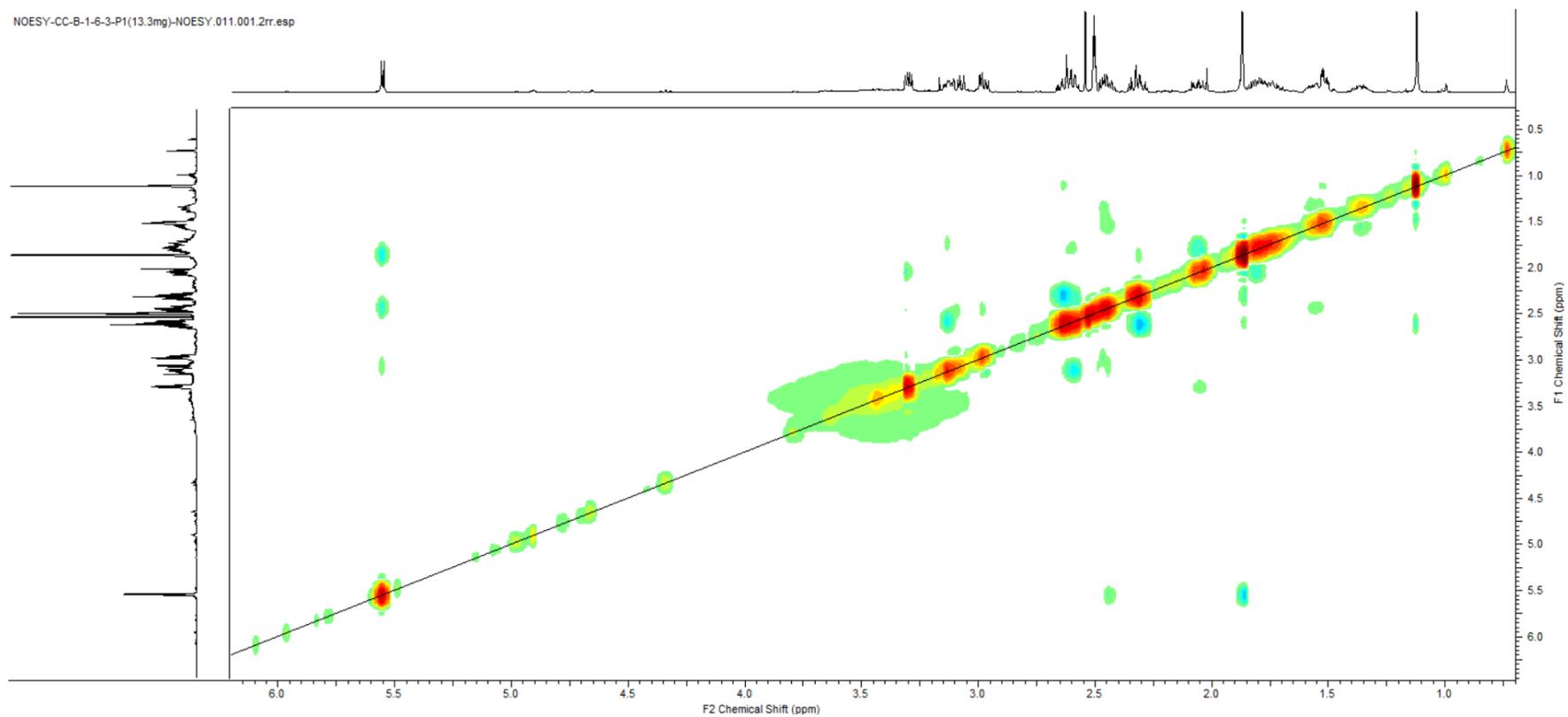


Figure S54. HMBC spectrum of **6** in DMSO-*d*<sub>6</sub> (500 MHz)

NOESY-CC-B-1-6-3-P1(13.3mg)-NOESY.011.001.2rr.esp



**Figure S55.** PS-NOESY spectrum of **6** in DMSO-*d*<sub>6</sub> (500 MHz)

CC-B-1-6-3-P1+#10 RT: 0.13 AV: 1 NL: 1.19E6  
F: FTMS + p ESI Full ms [100.00-2000.00]

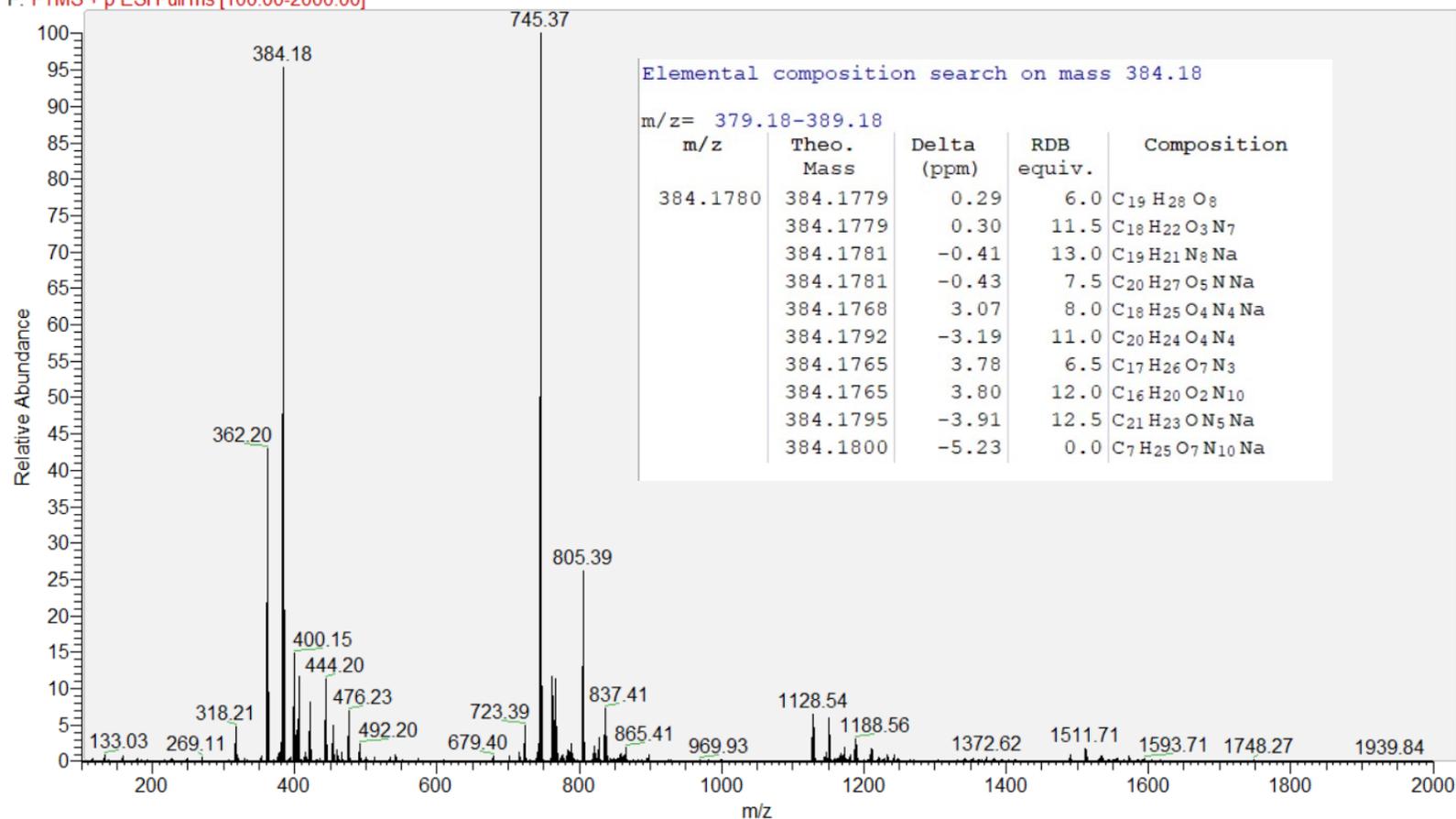


Figure S56. HR-ESI-MS spectrum of **6**

CC-B-1-6-3-P1 + #11 RT: 0.14 AV: 1 NL: 6.52E3  
F: ITMS + c ESI d Full ms2 384.18@cid35.00 [95.00-395.00]

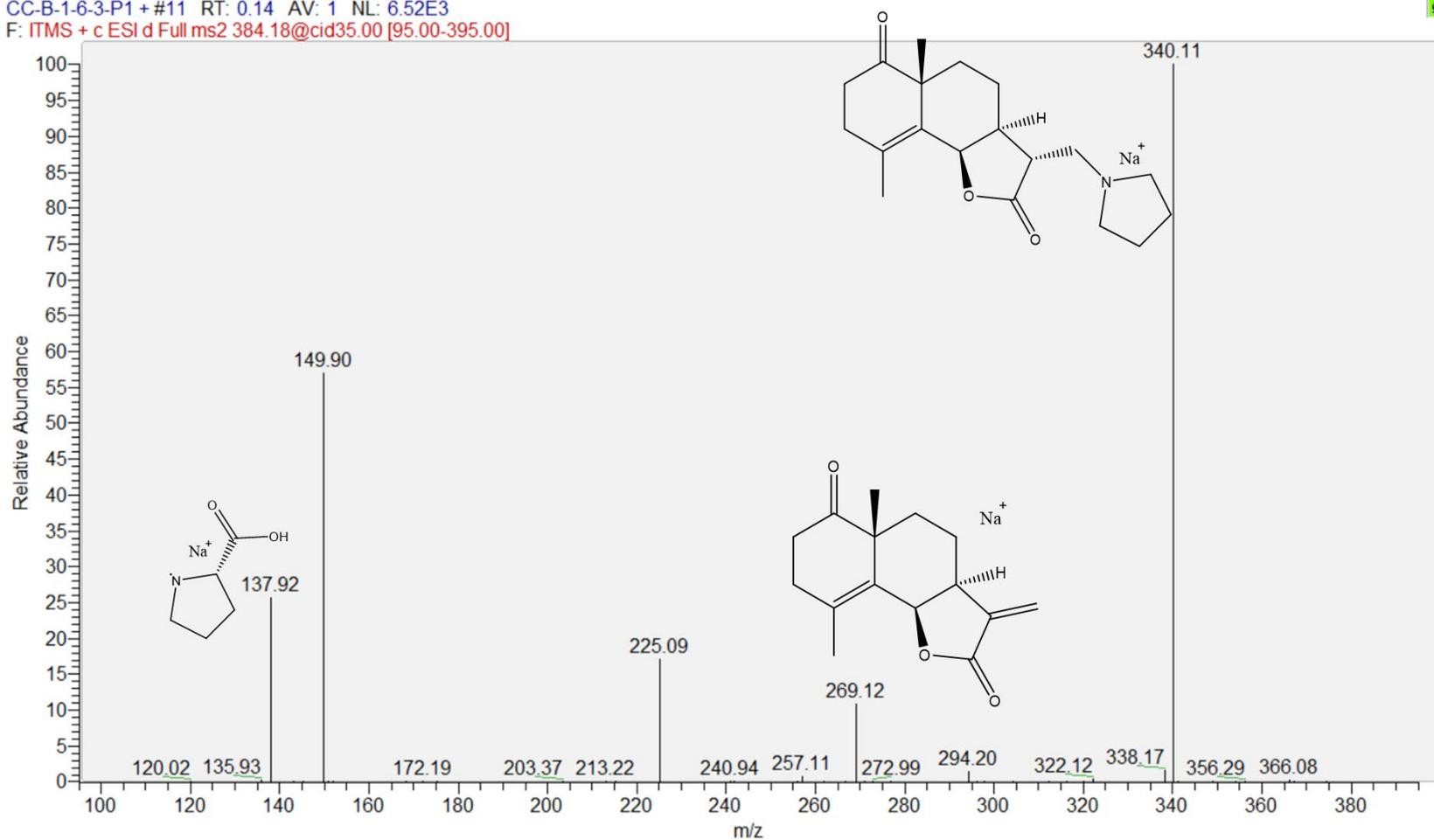


Figure S57. ESI-MS/MS spectrum of 6

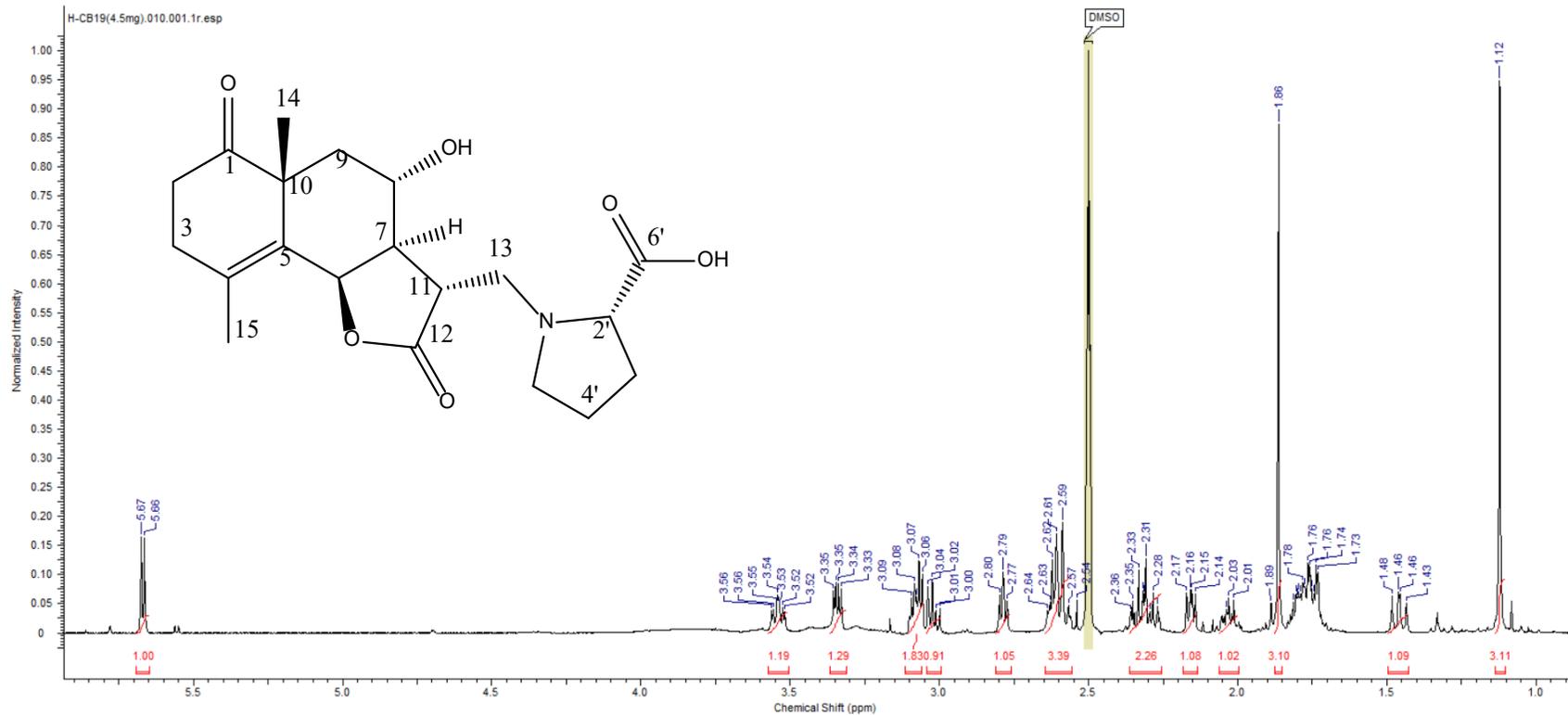


Figure S58.  $^1\text{H-NMR}$  spectrum of **7** in  $\text{DMSO-}d_6$  (500 MHz)

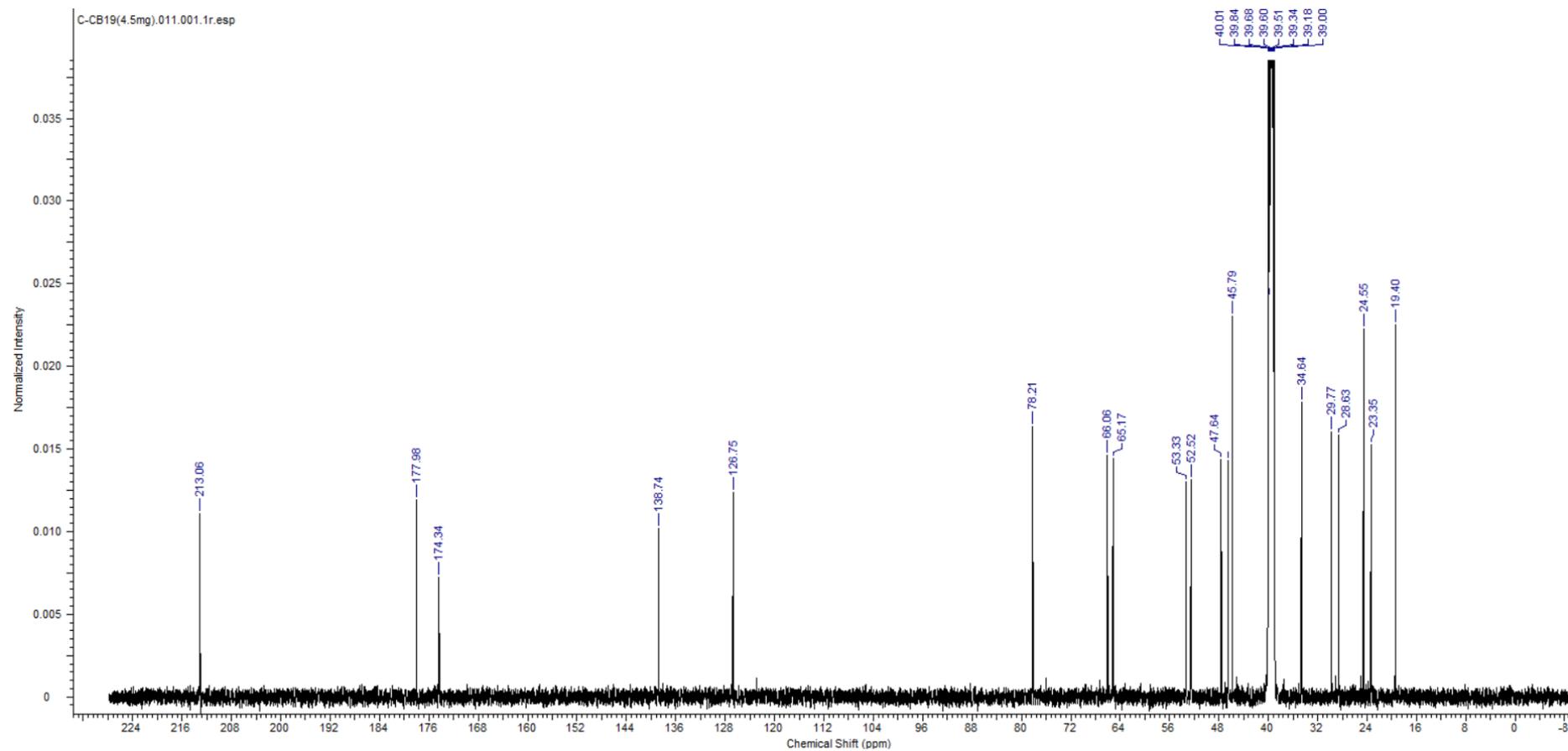
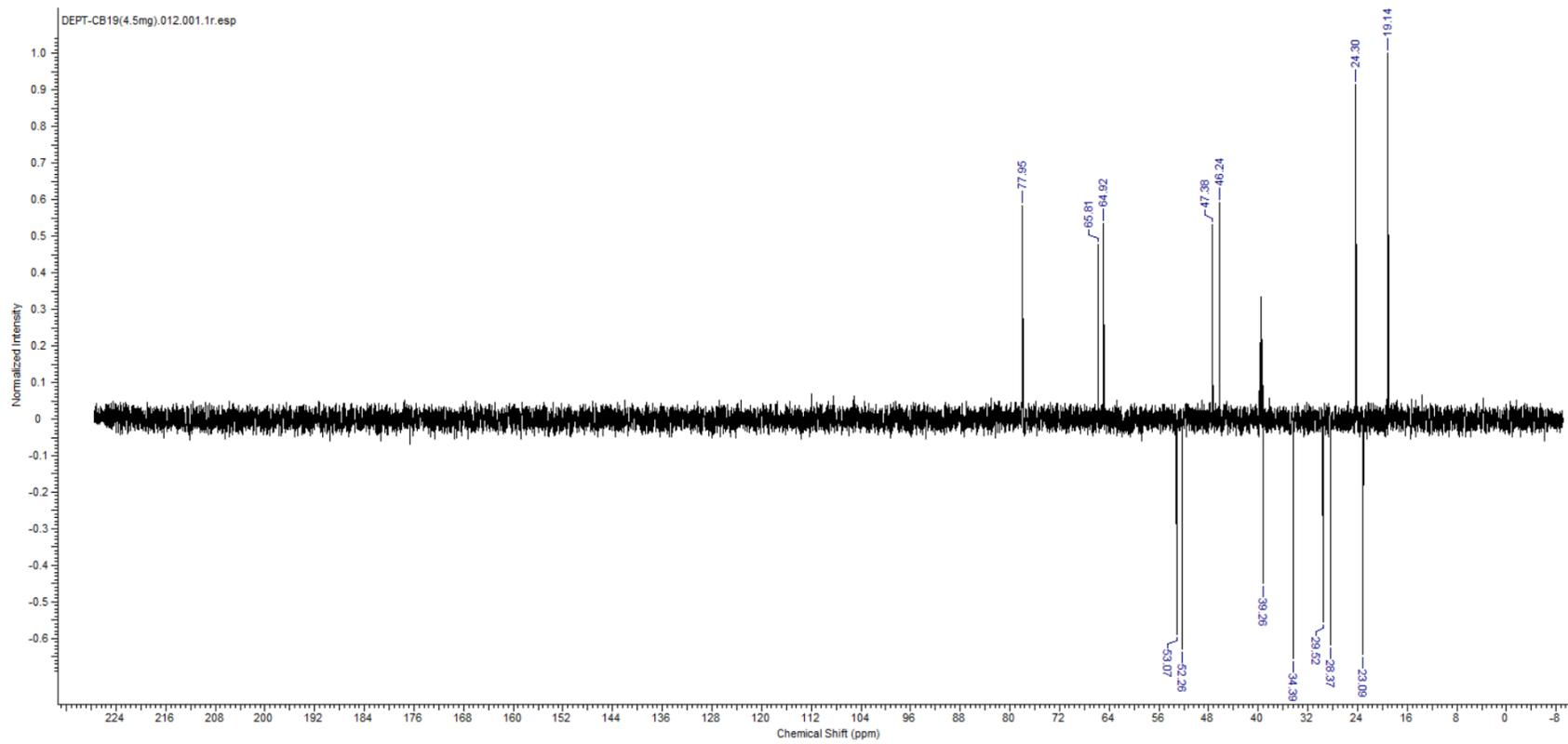
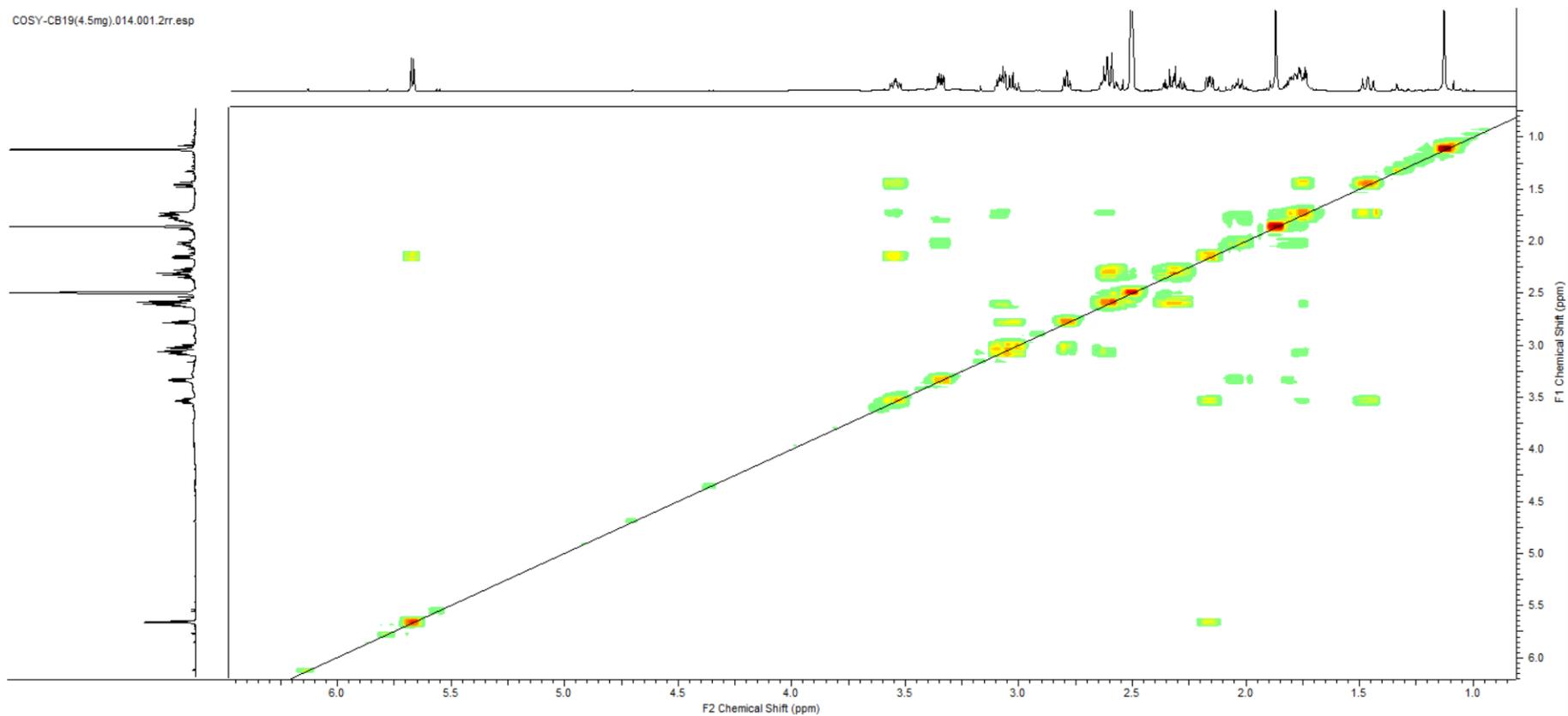


Figure S59.  $^{13}\text{C}$ -NMR spectrum of **7** in  $\text{DMSO-}d_6$  (125 MHz)



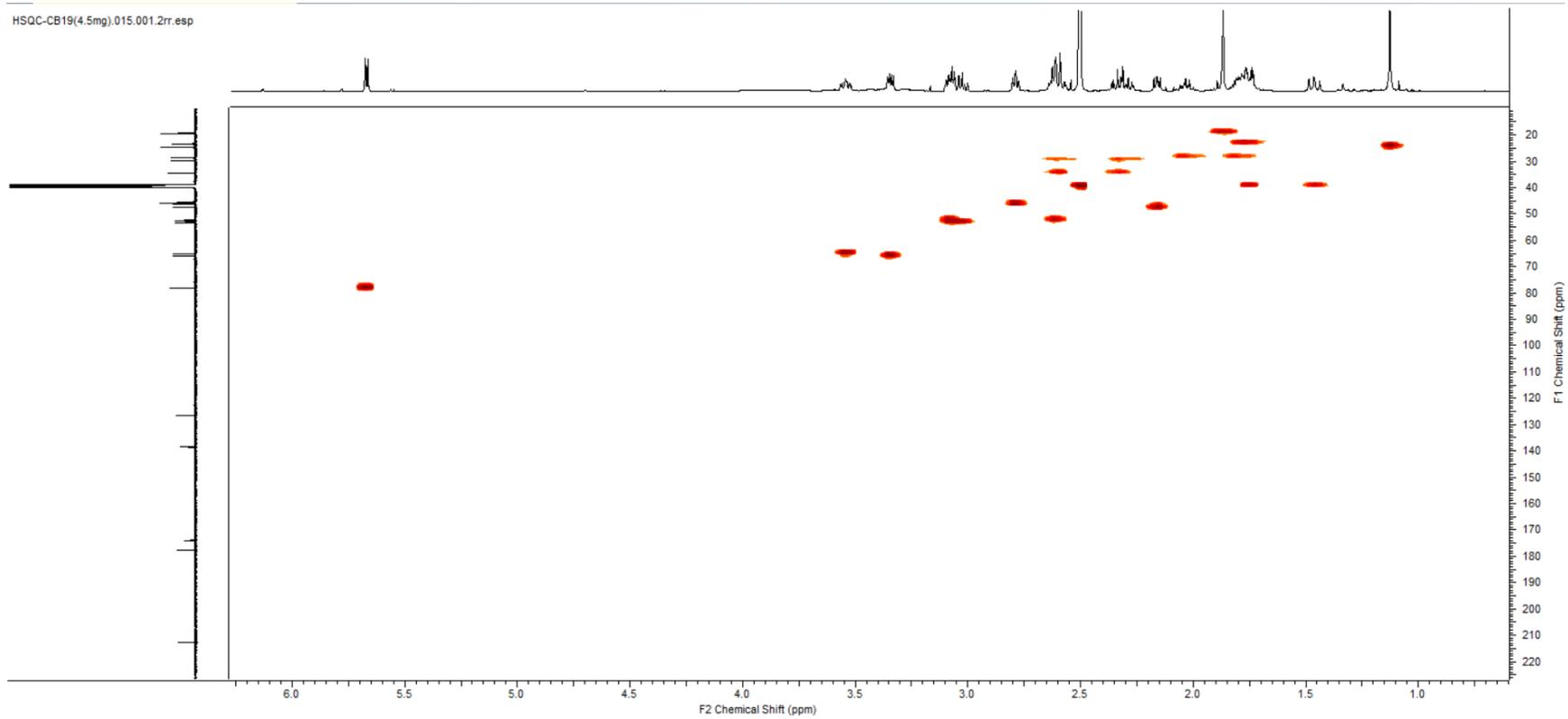
**Figure S60.**  $^{13}\text{C}$  DEPT135 NMR spectrum of **7** in  $\text{DMSO-}d_6$  (125 MHz)

COSY-CB19(4.5mg),014.001.2rr.esp



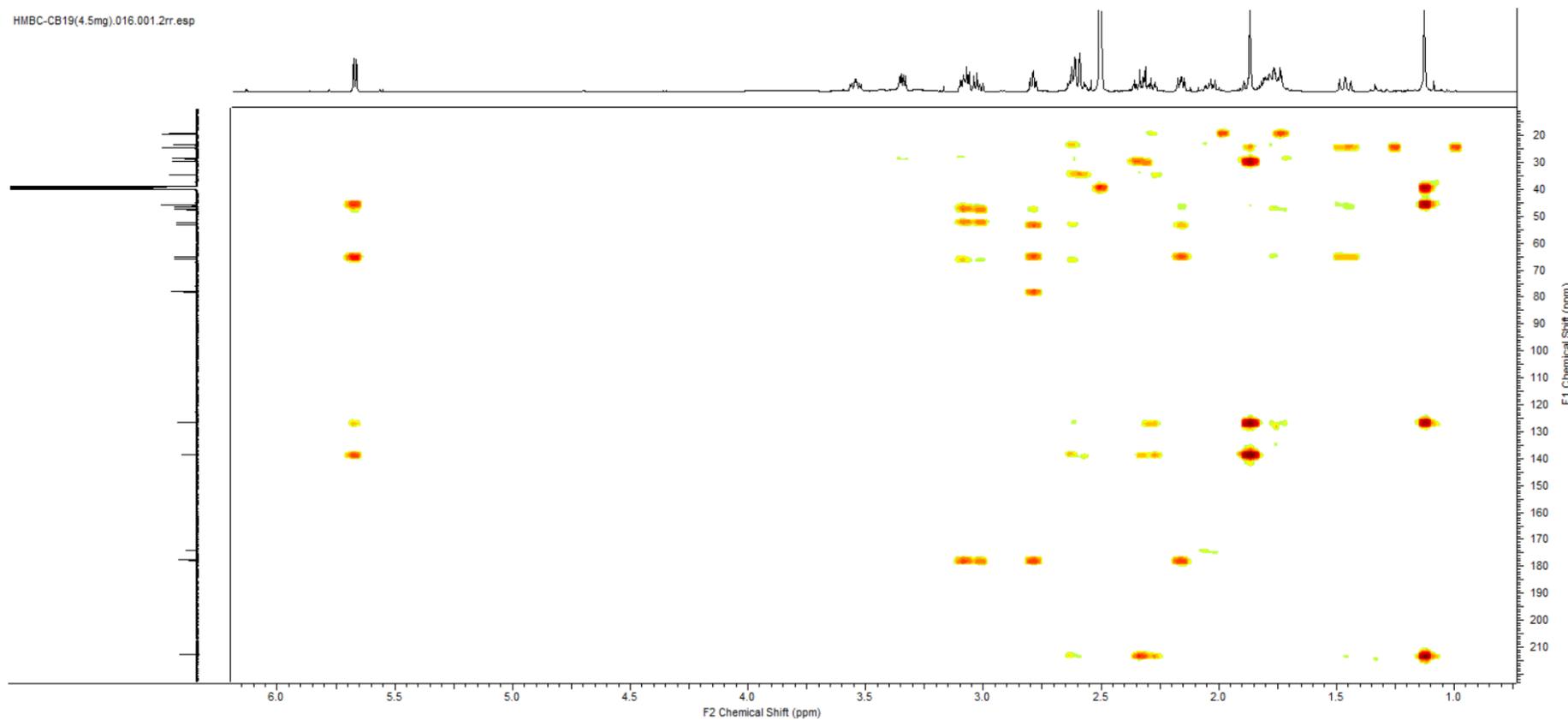
**Figure S61.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **7** in  $\text{DMSO-}d_6$  (500 MHz)

HSQC-CB19(4.5mg).015.001.2rr.esp

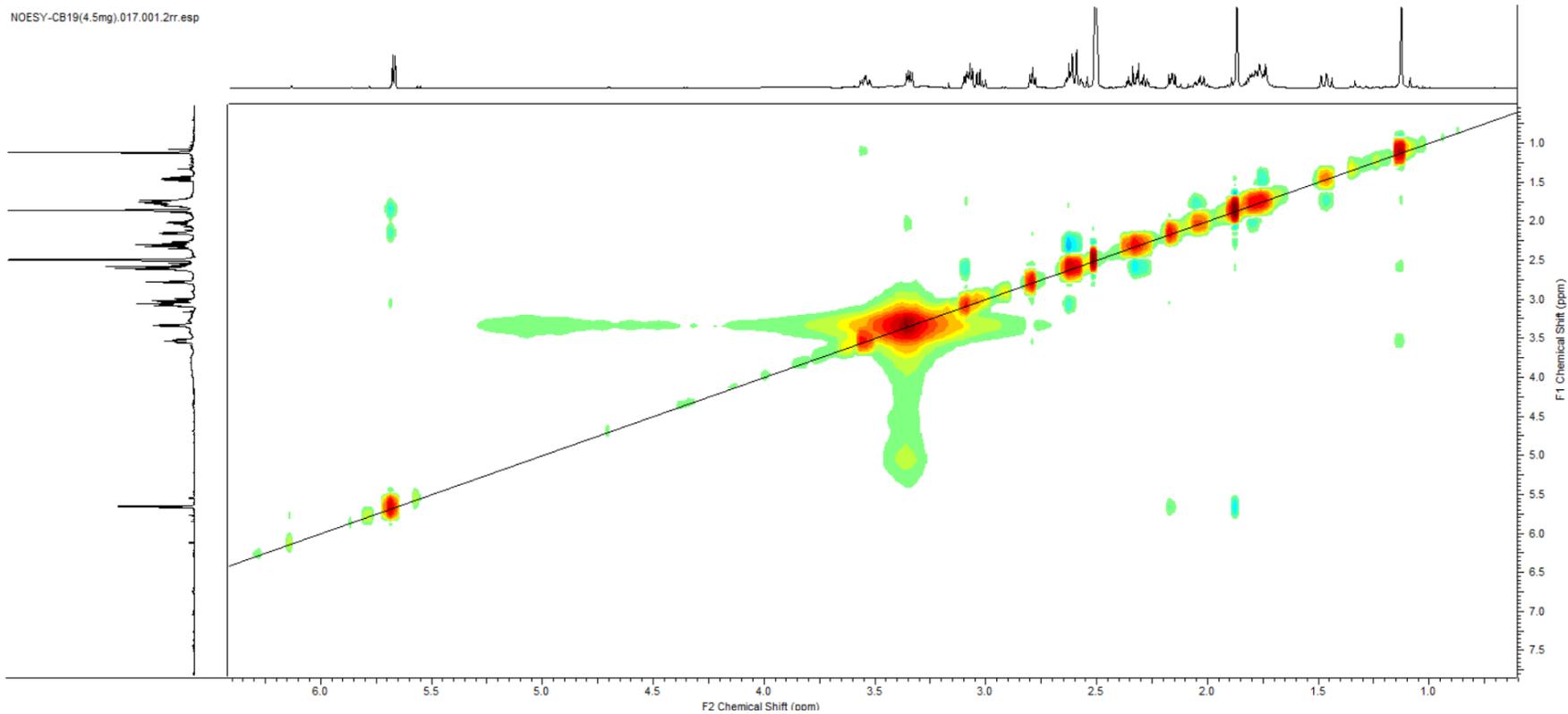


**Figure S62.** HSQC spectrum of **7** in DMSO-*d*<sub>6</sub> (500 MHz)

HMBC-CB19(4.5mg).016.001.2rr.esp

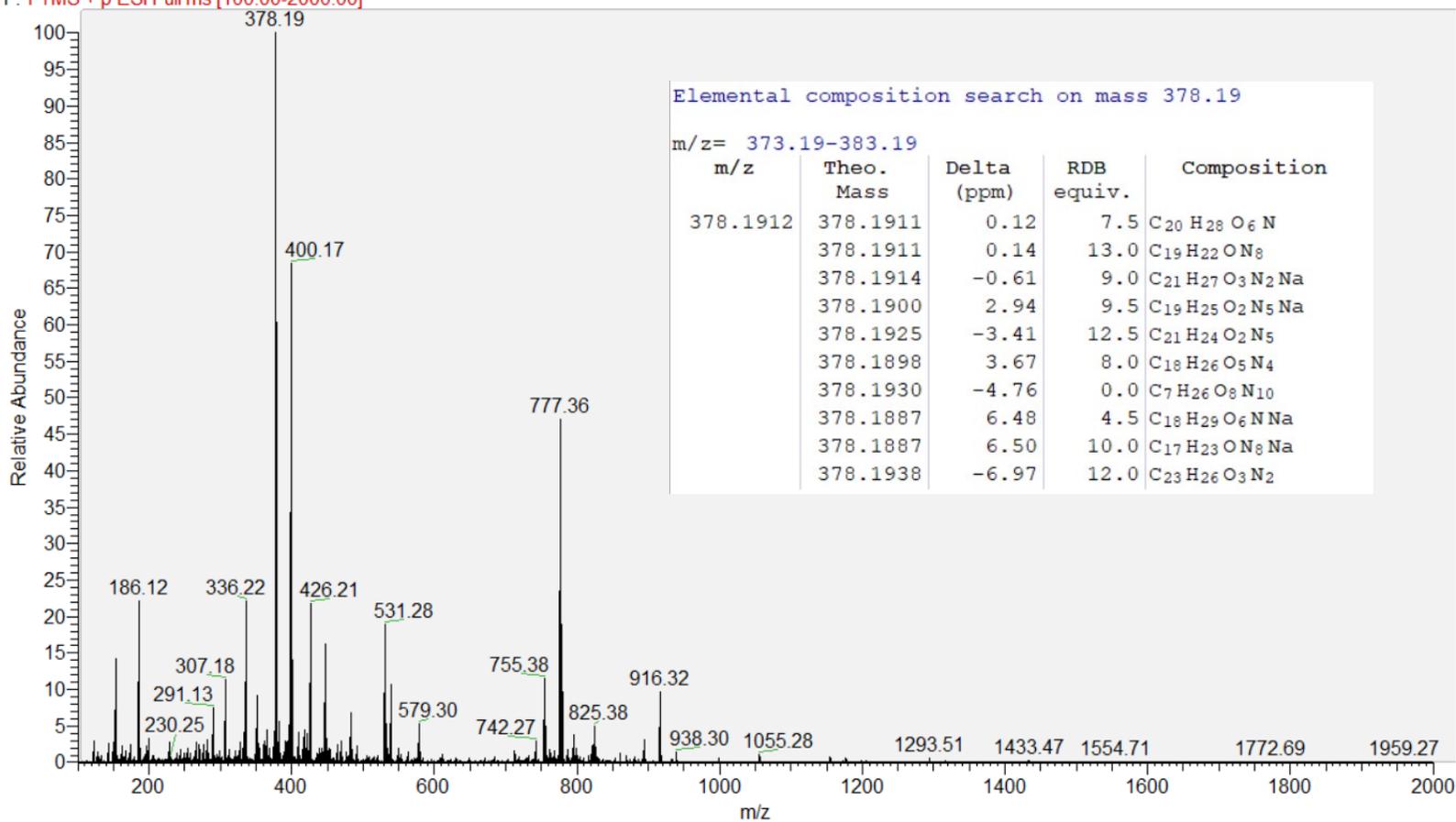


**Figure S63.** HMBC spectrum of **7** in  $\text{DMSO-}d_6$  (500 MHz)



**Figure S64.** PS-NOESY spectrum of **7** in DMSO-*d*<sub>6</sub> (500 MHz)

CC-B-1-5-3-P1 + #7 RT: 0.08 AV: 1 NL: 7.81E5  
F: FTMS + p ESI Full ms [100.00-2000.00]



CC-B-1-5-3-P1 + #8 RT: 0.09 AV: 1 NL: 2.49E4  
F: ITMS + c ESI d Full ms2 378.19@cid35.00 [90.00-390.00]

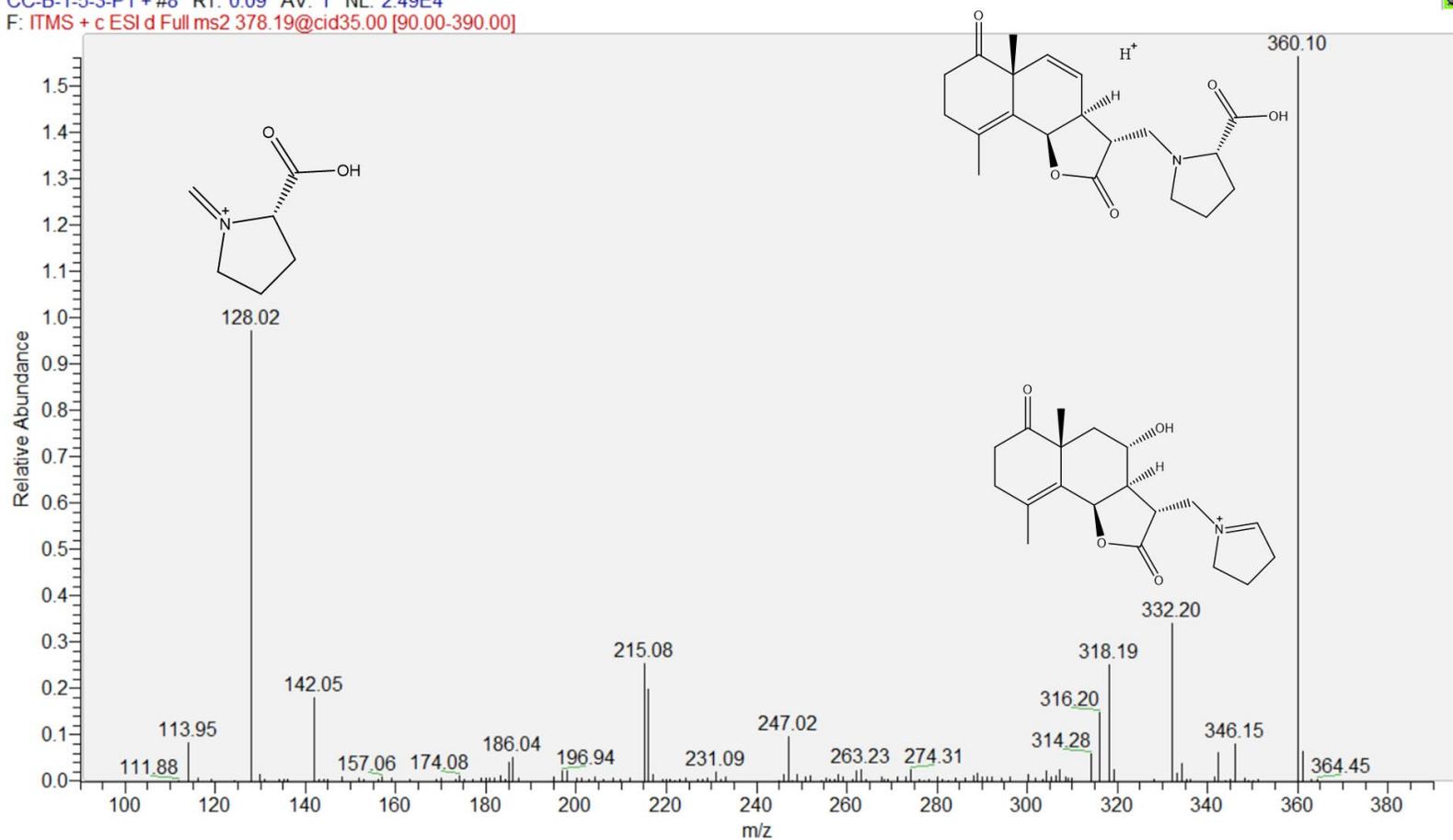


Figure S66. ESI-MS/MS spectrum of 7

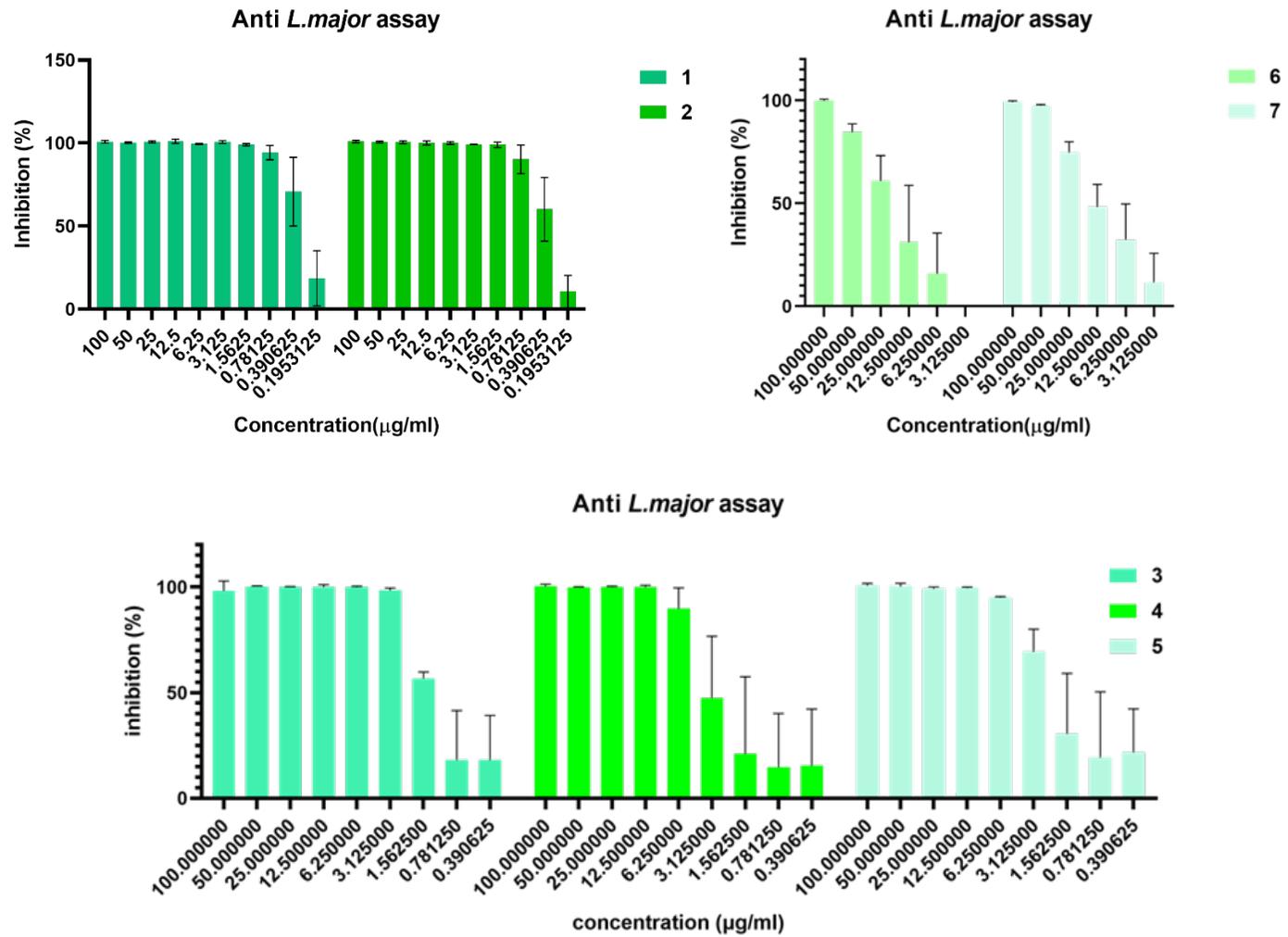


Figure S67. Anti-*L. major* data of 1-7

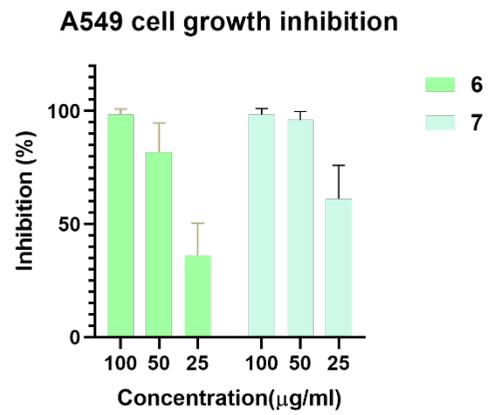
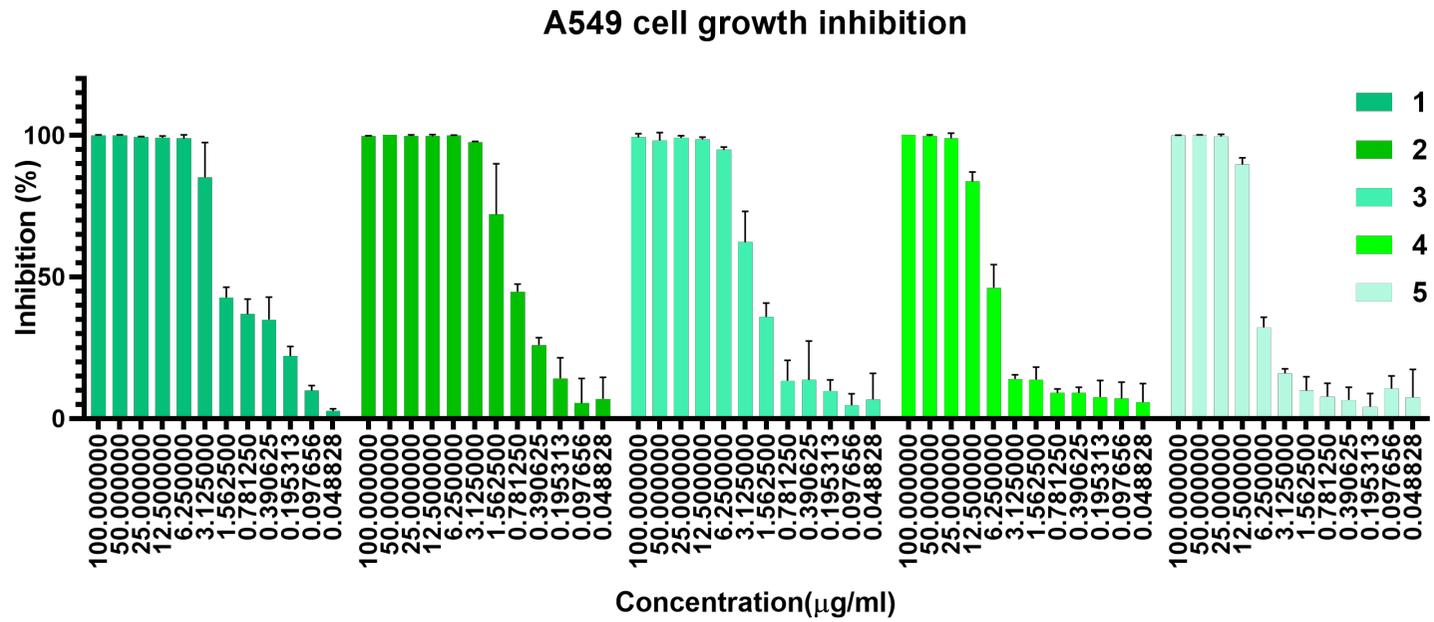


Figure S68. Anti-A549 data of 1-7

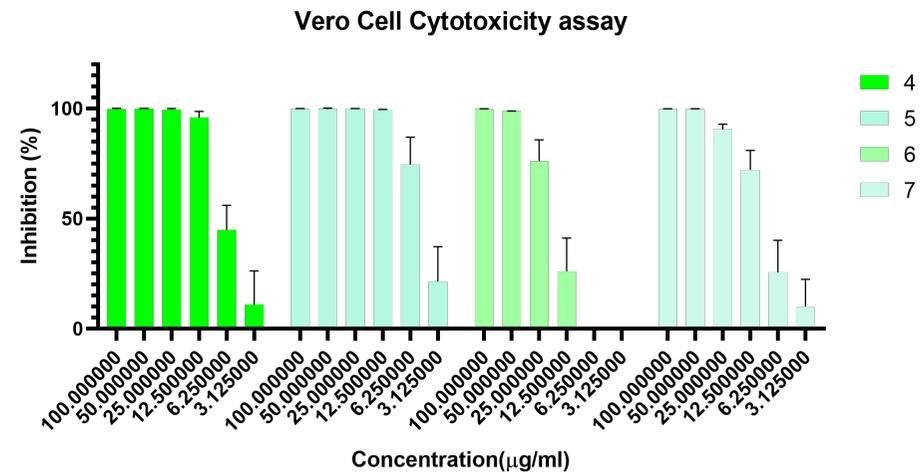
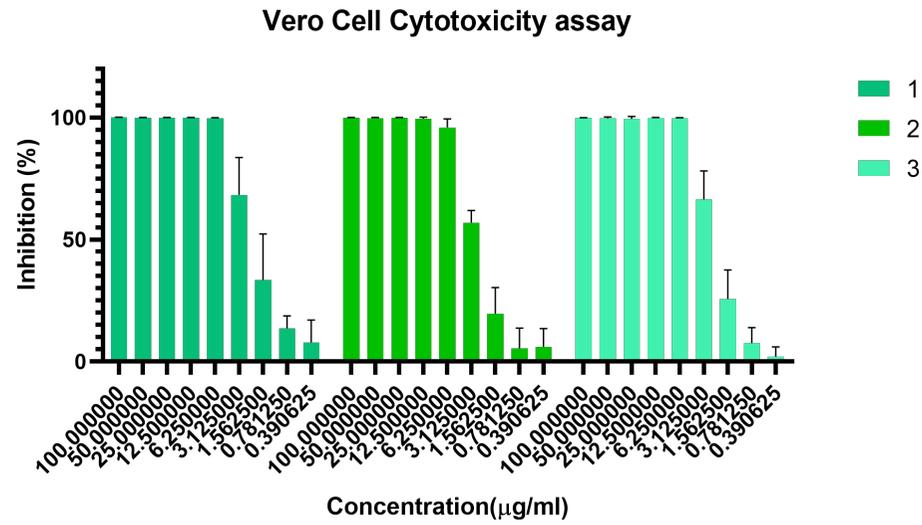


Figure S69. Vero cell cytotoxicity data of 1-7