

Supplementary Information

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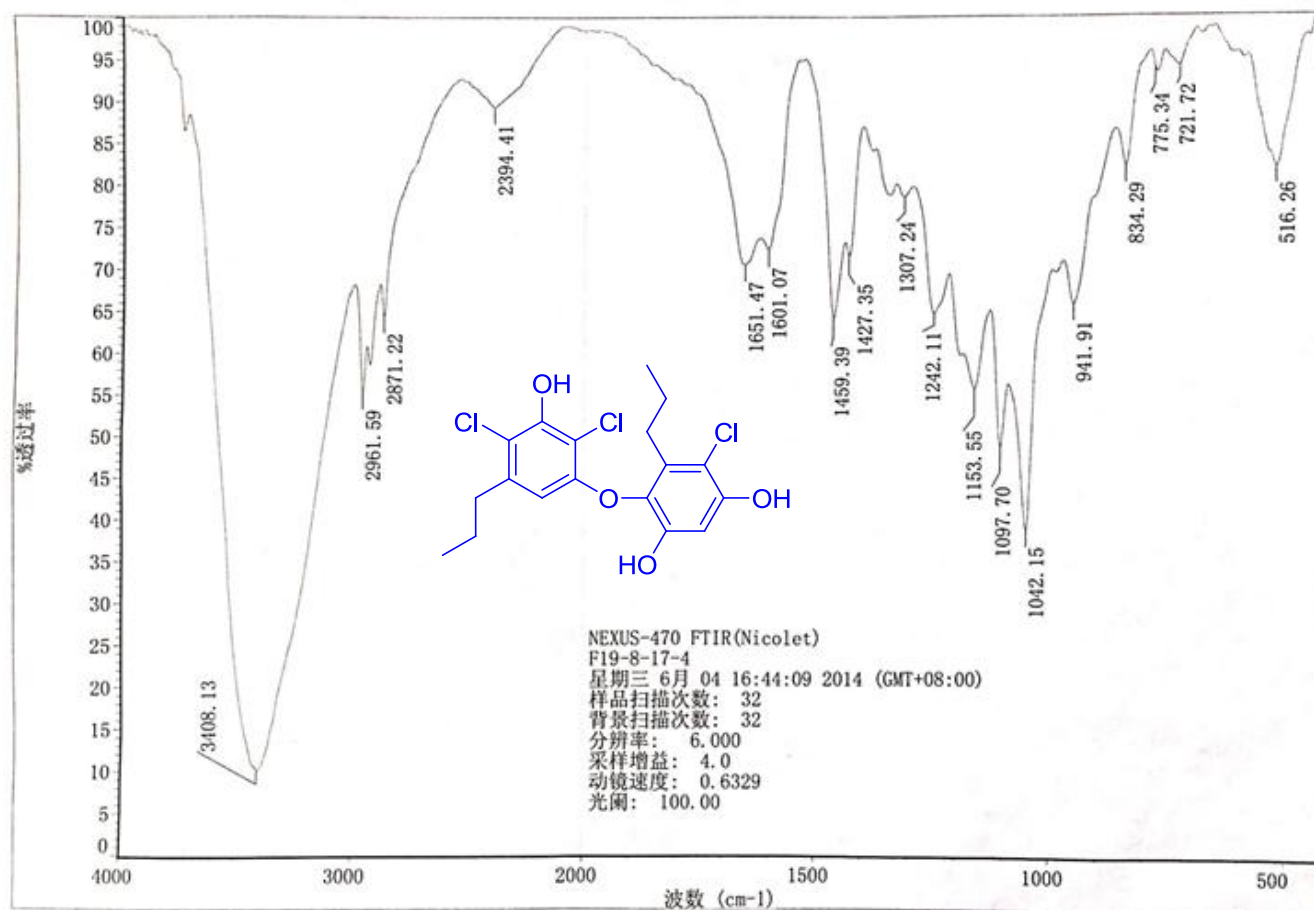


Figure S1. IR spectrum of compound 1.

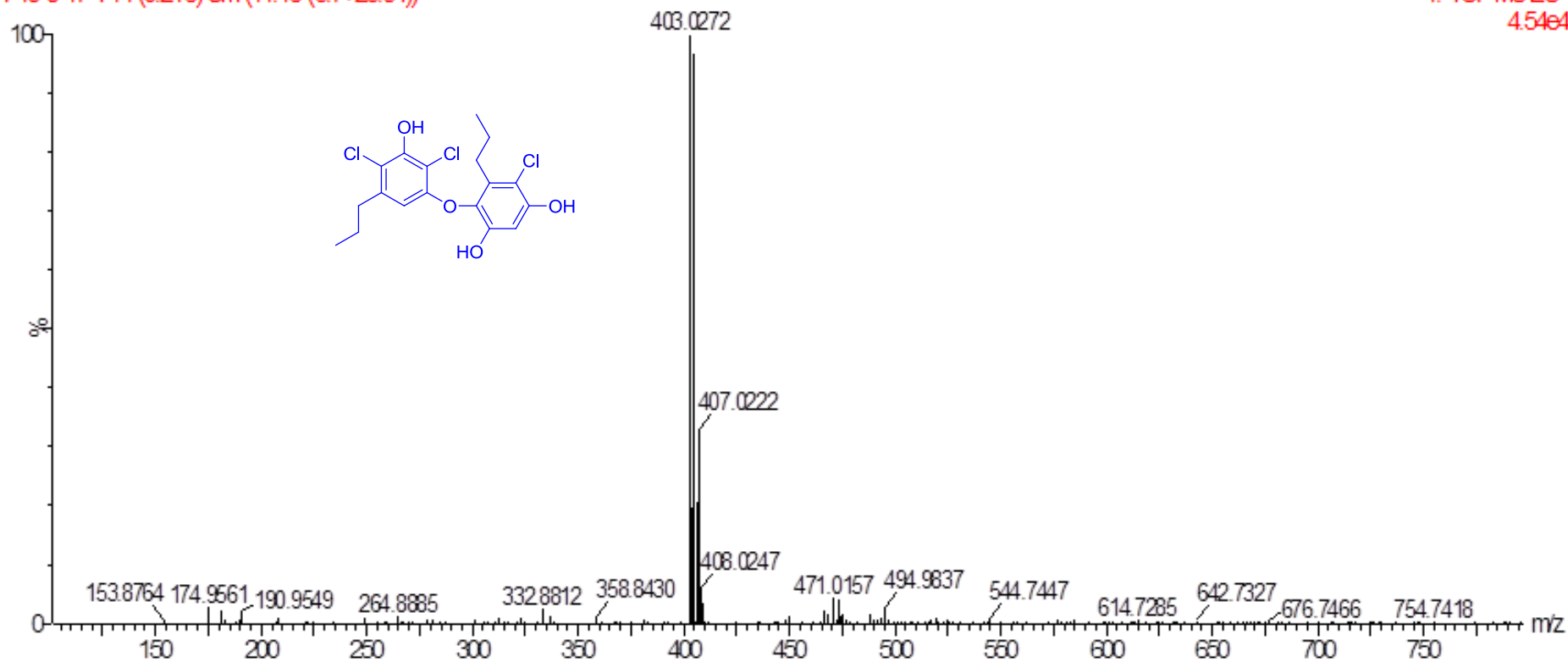
Xevo G2 Q.TOF/YCA166#

07-Jul-2014

Waters

1: TOF MSES-
4.54e4

F19-8-174 11 (0.216) Cm (11:16-(3:7+23:54))

**Figure S2.** Negative mode HRESIMS data of compound 1.

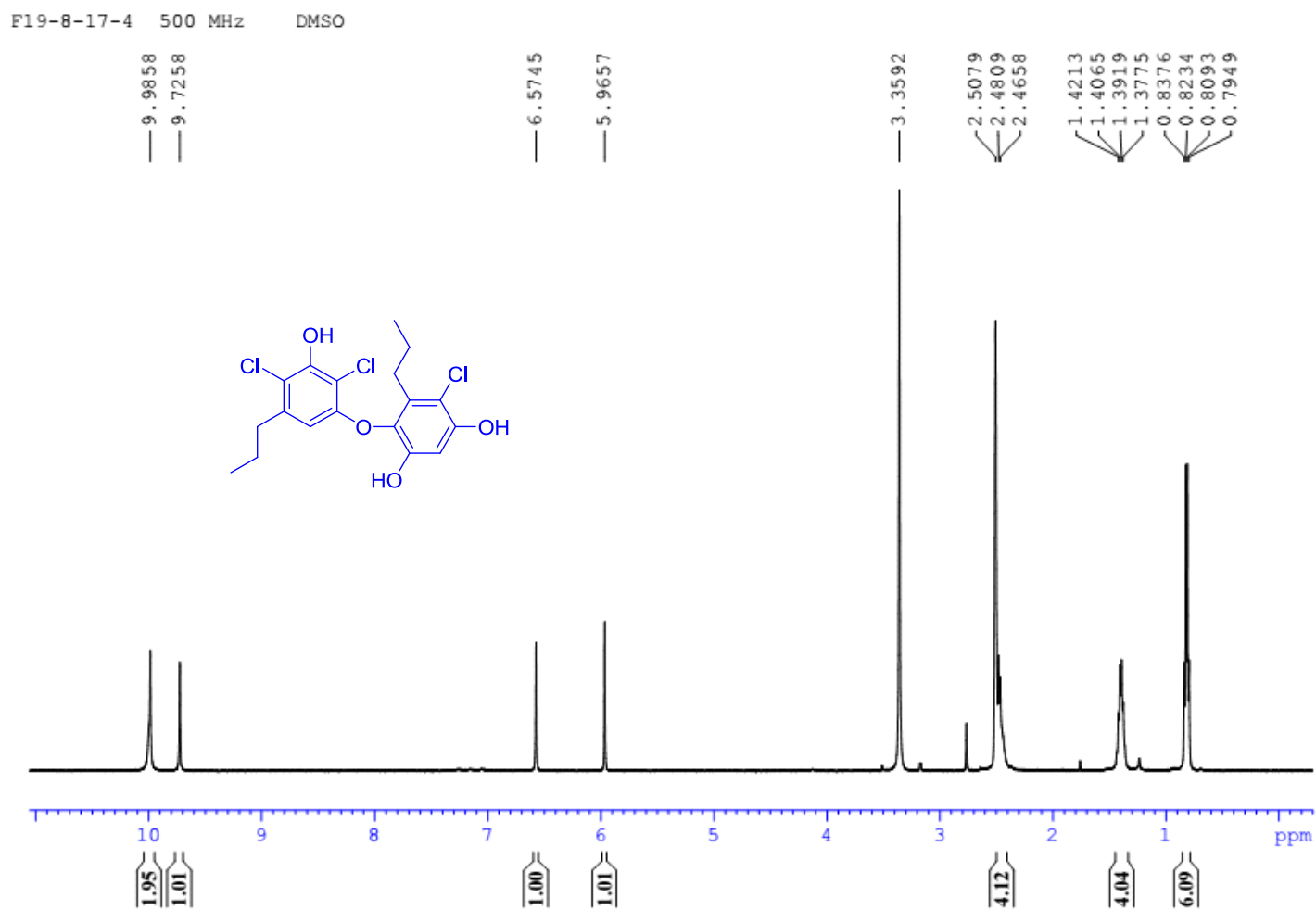


Figure S3. ^1H NMR spectrum of compound **1** in DMSO- d_6 (500 MHz).

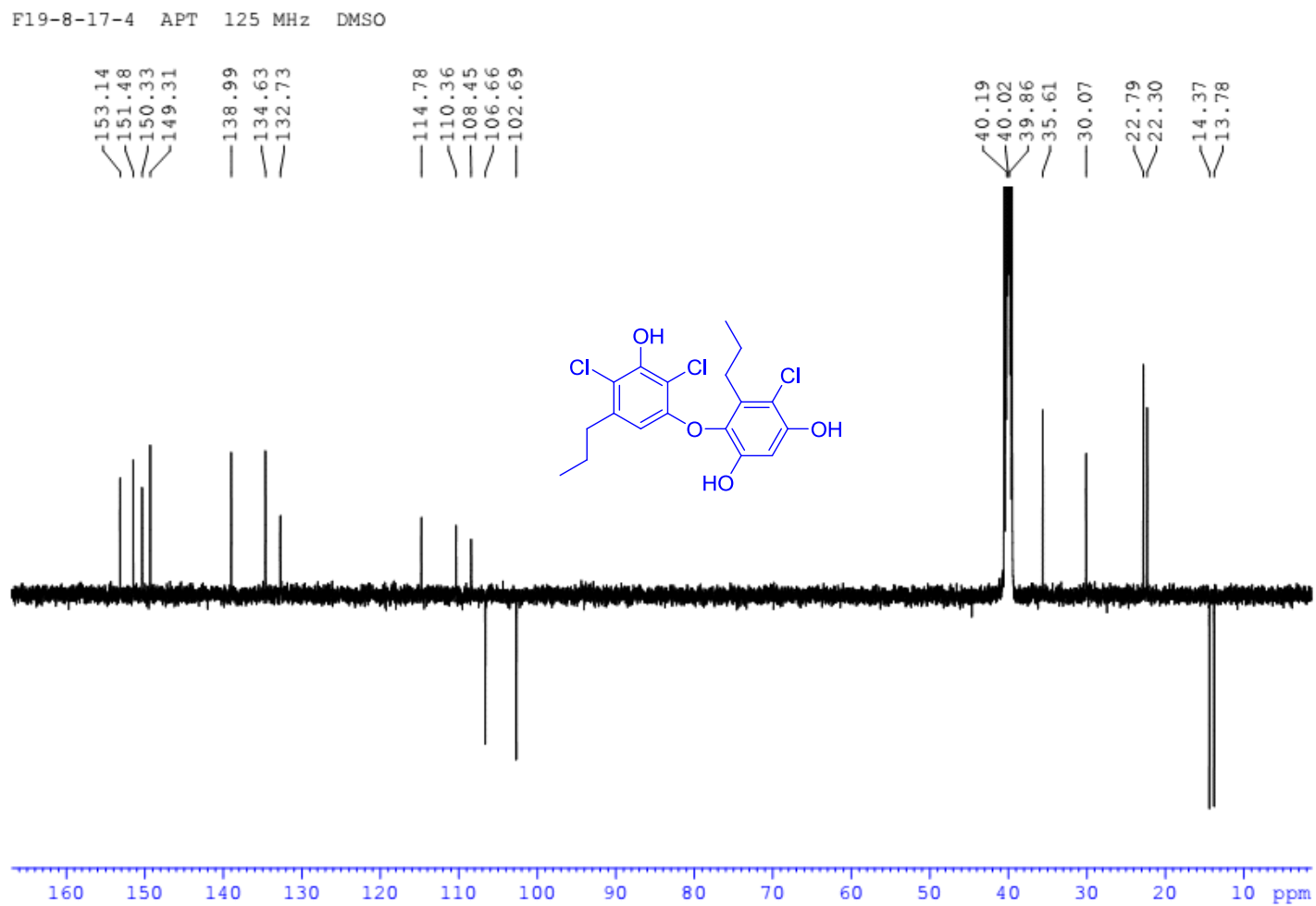


Figure S4. ^{13}C NMR spectrum of compound **1** in DMSO- d_6 (125 MHz).

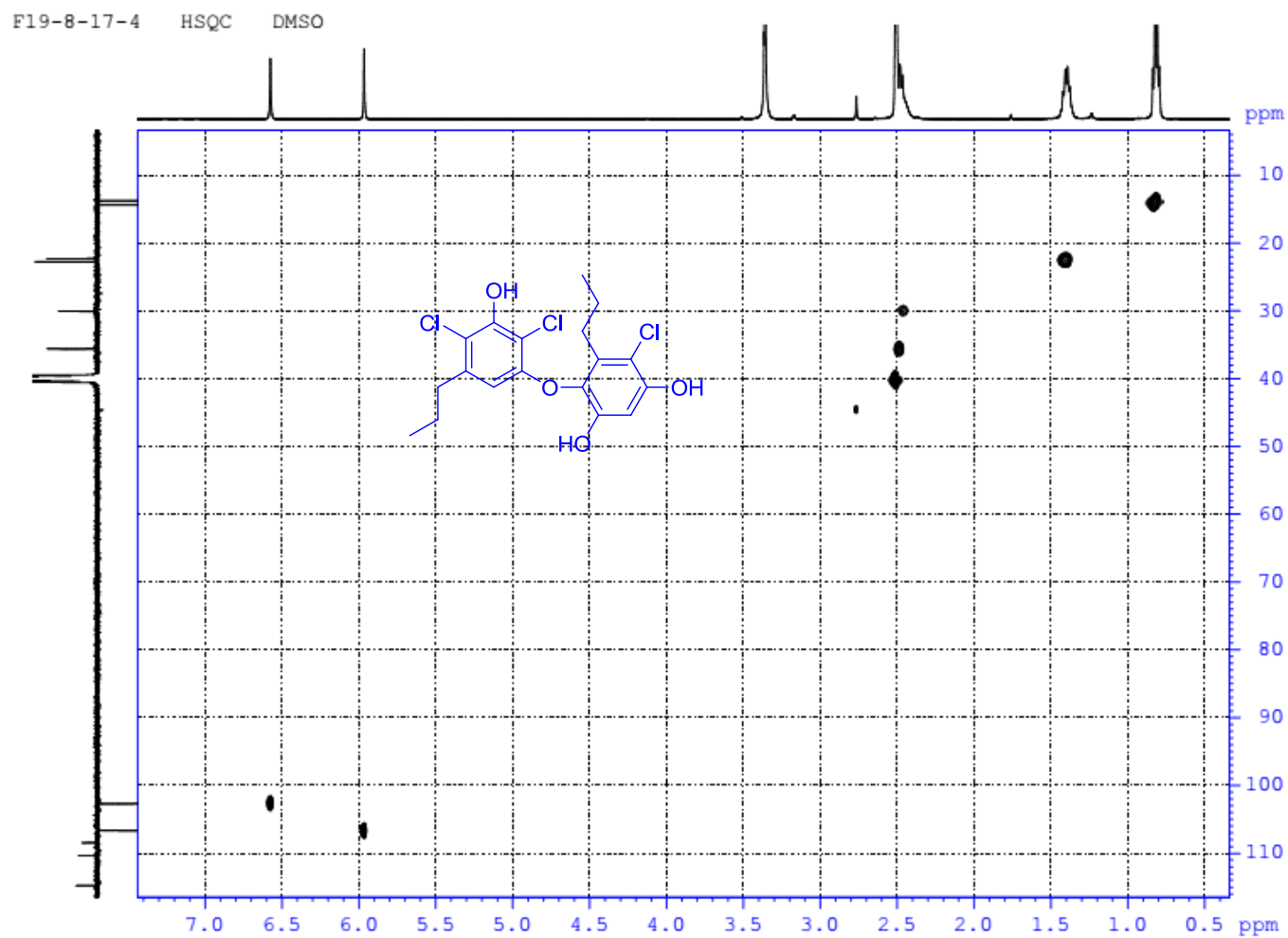


Figure S5. HSQC spectrum of compound 1 in DMSO-d6.

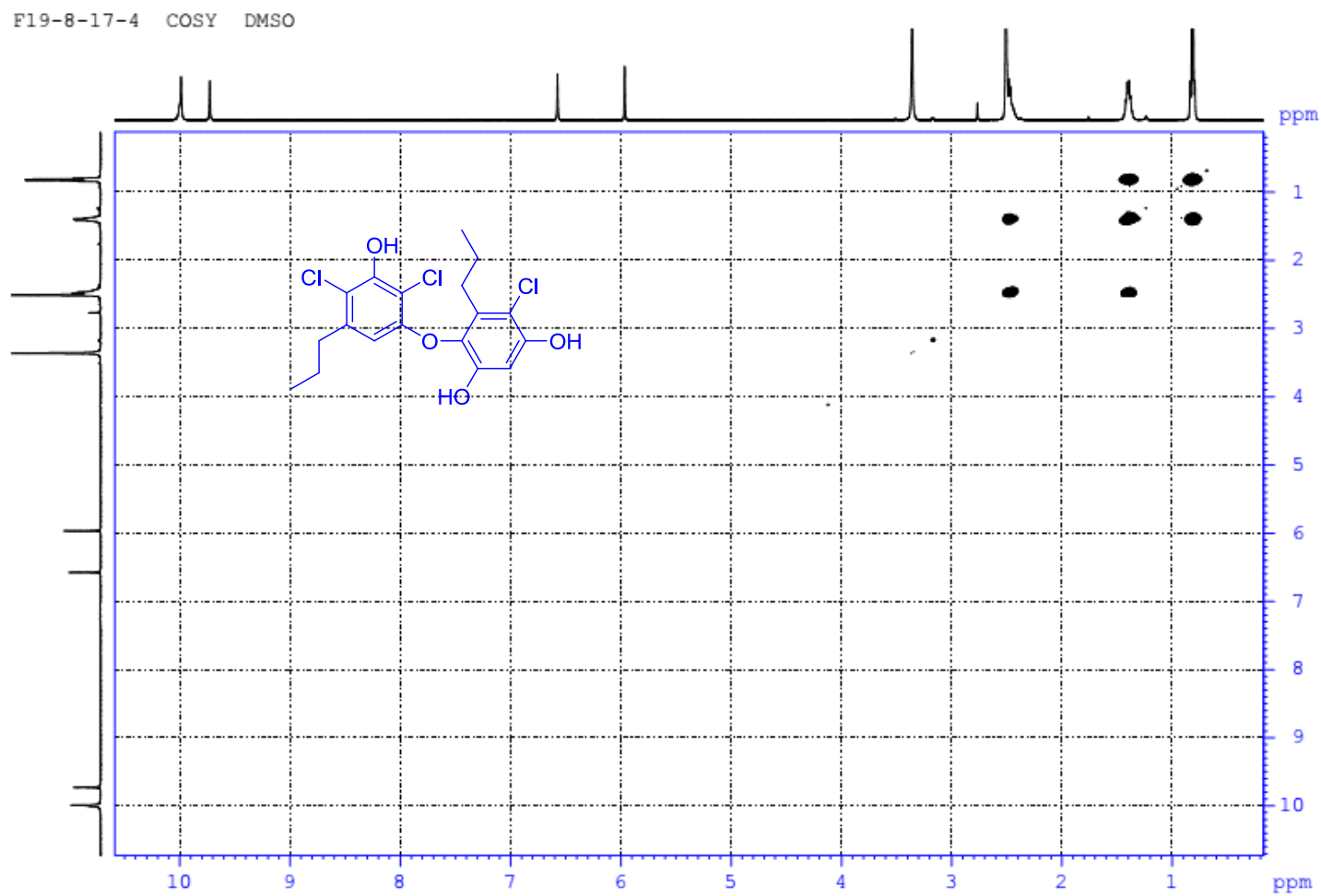


Figure S6. ^1H - ^1H COSY spectrum of compound **1** in DMSO- d_6 .

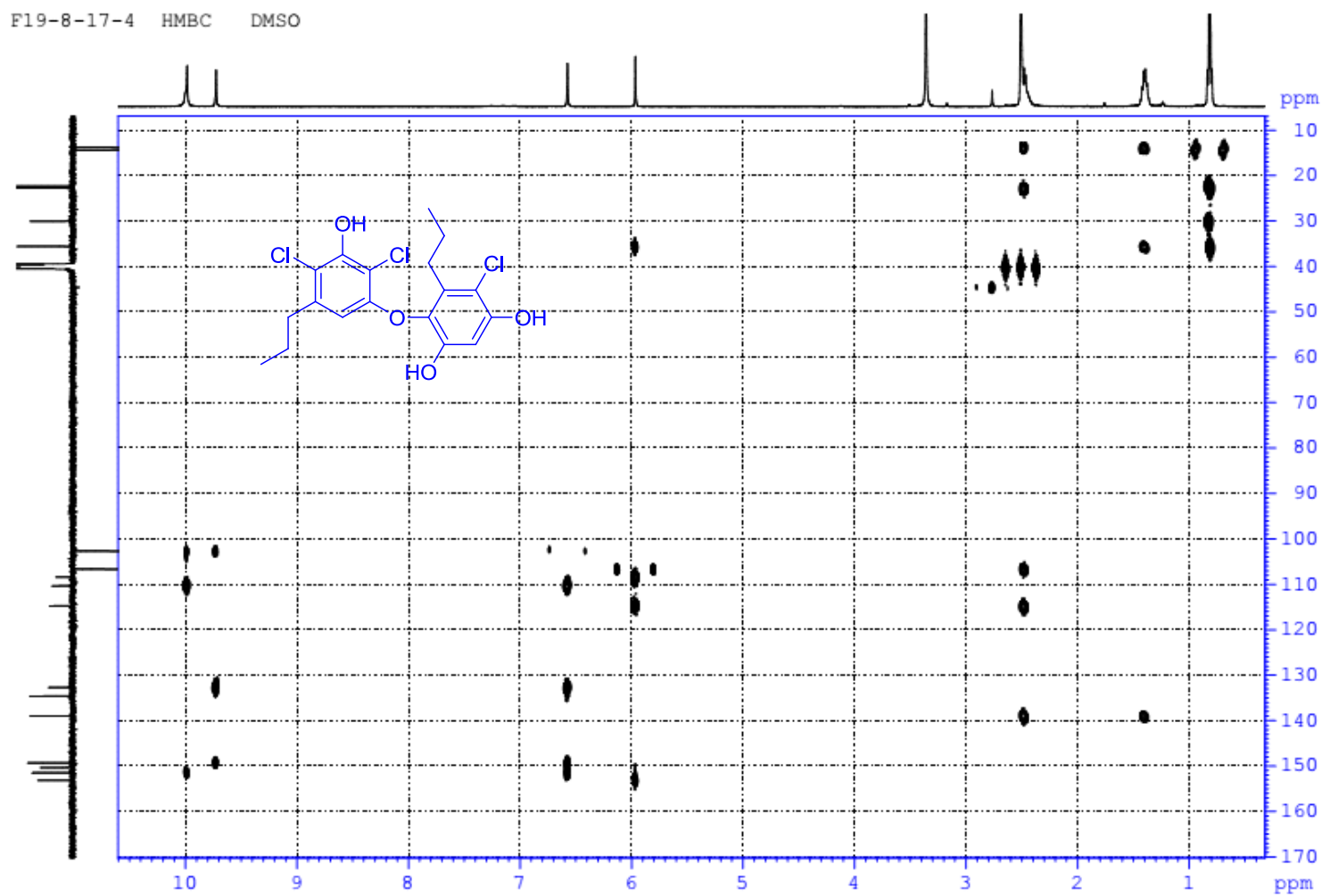


Figure S7. HMBC spectrum of compound **1** in DMSO-d₆.

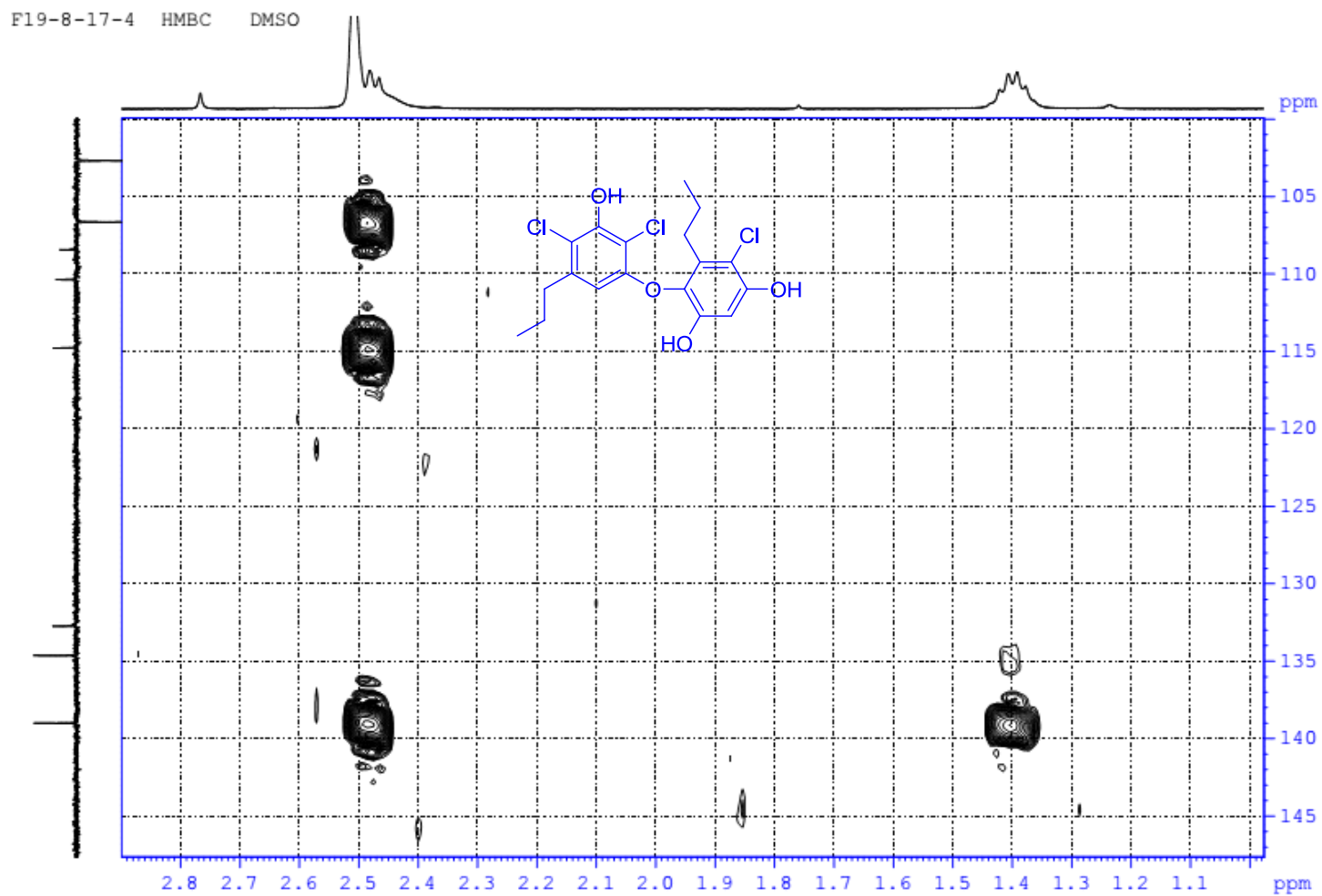


Figure S7-1. HMBC spectrum of compound **1** in DMSO-d₆ (part amplification).

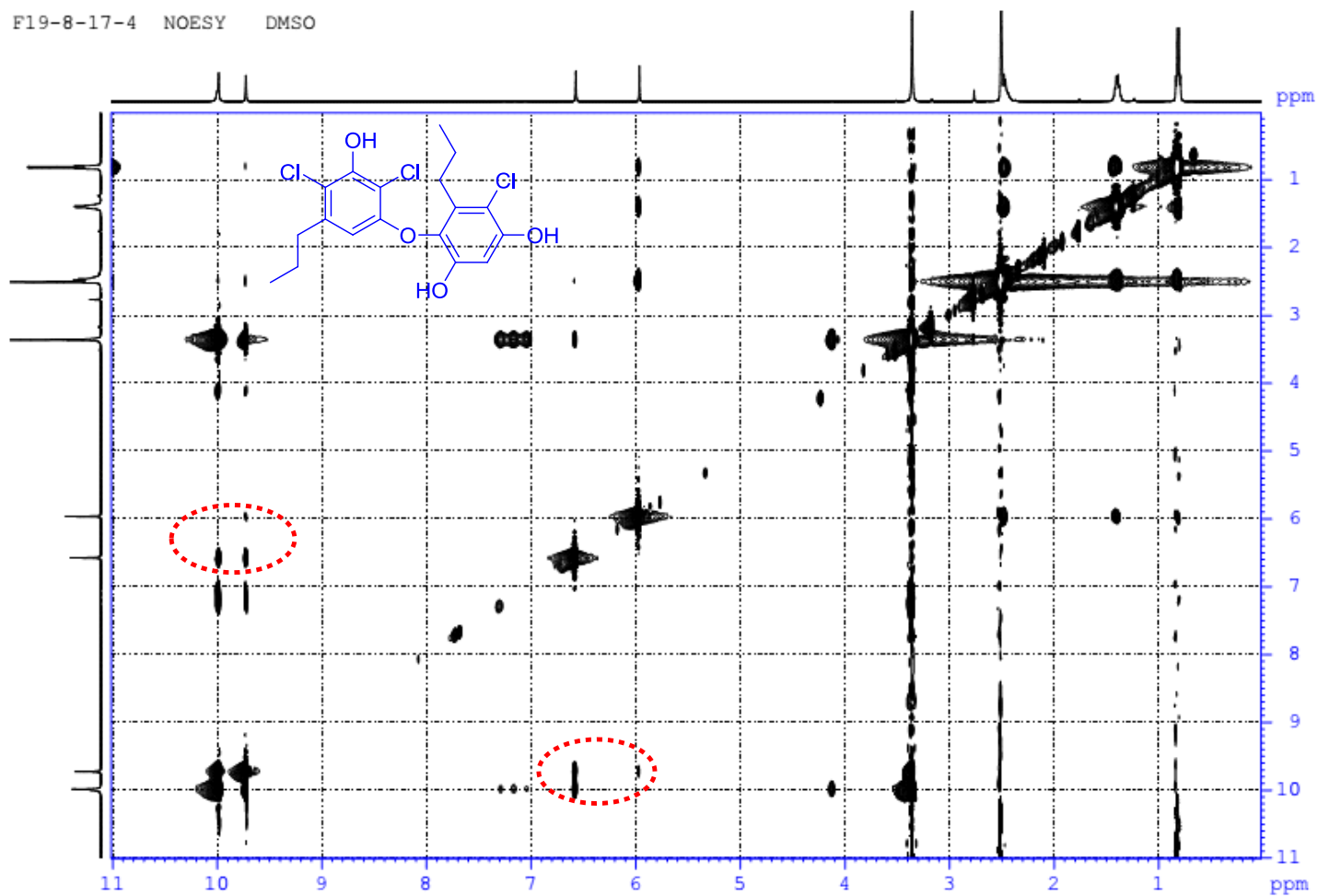


Figure S8. NOESY spectrum of compound 1 in DMSO-d6.

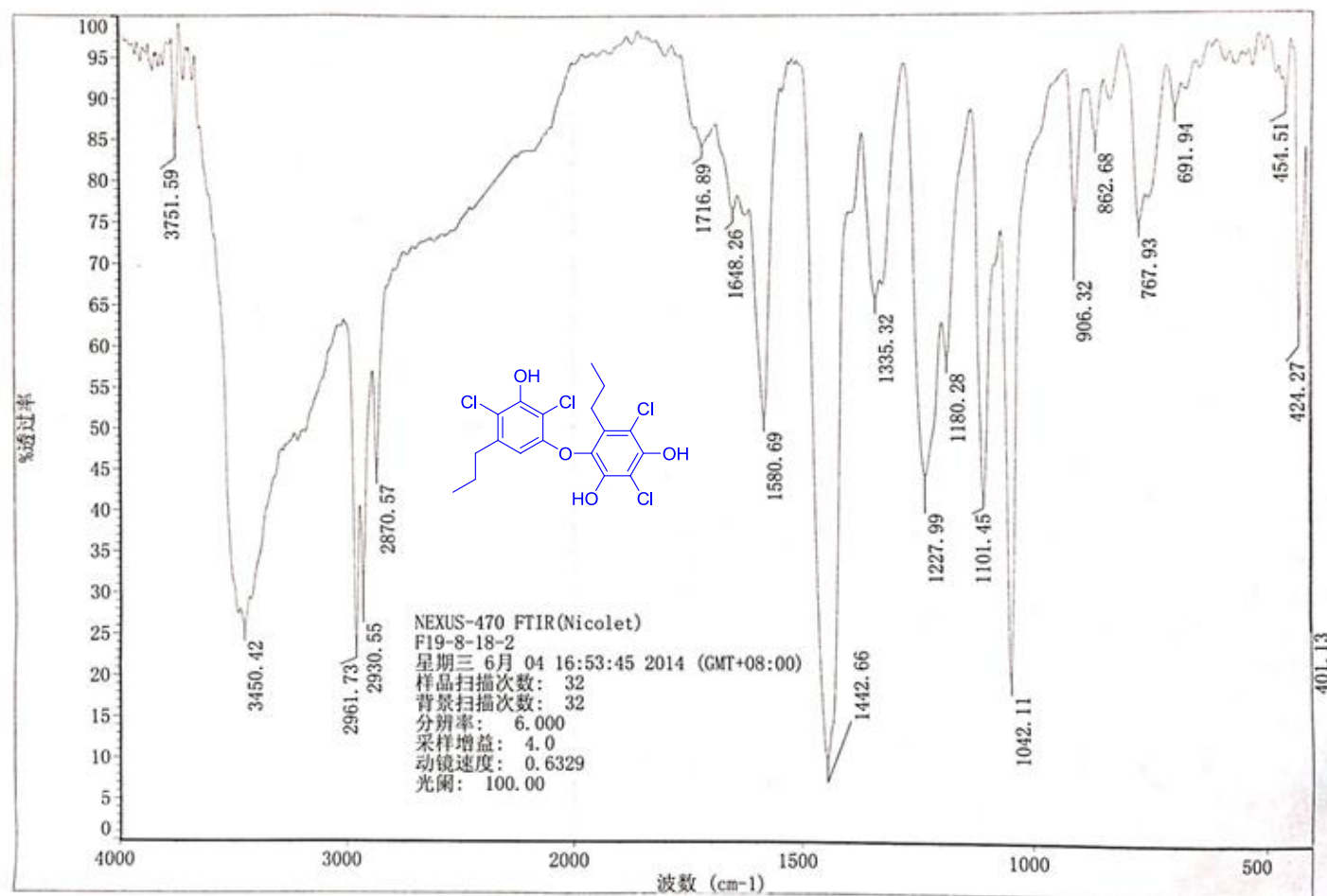


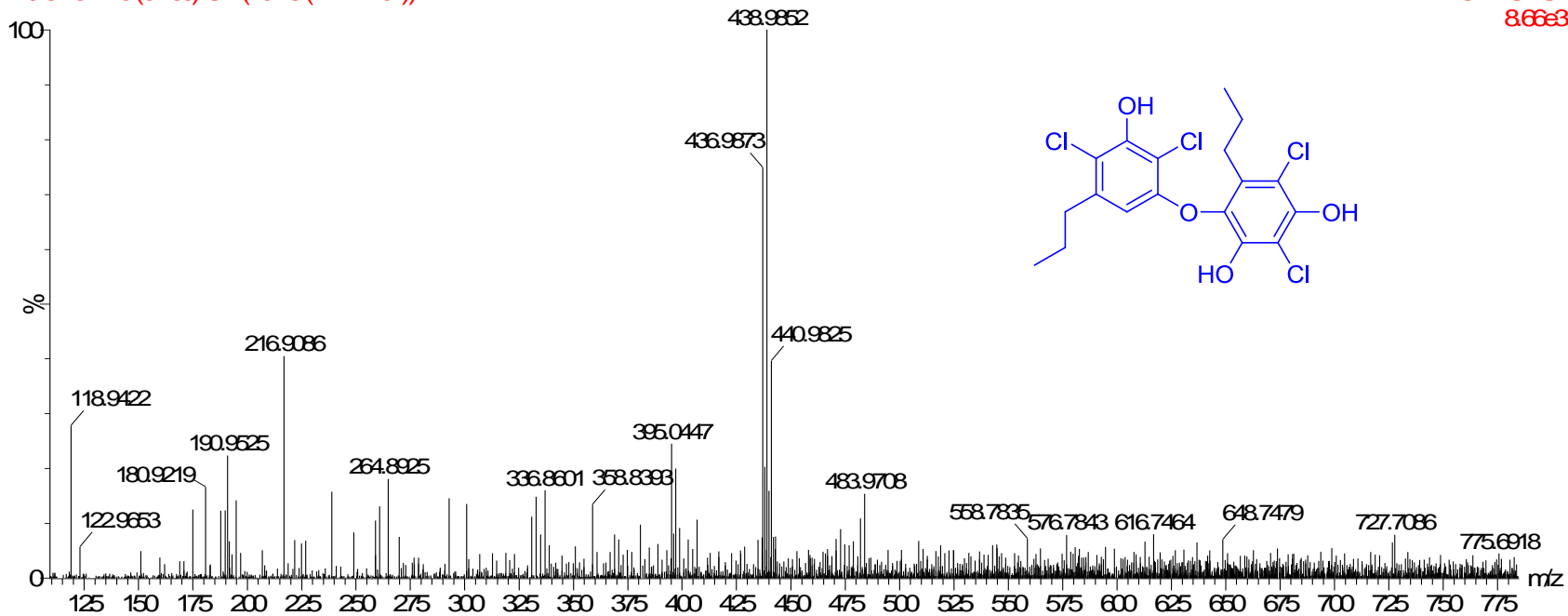
Figure S9. IR spectrum of compound 2.

Xevo G2 Q.TOF YCA166#

F198-18-210 (0.199) Cm (10.16-(27+2251))

07-Jul-2014

Waters

1: TOFMS ES-
8.66e3**Figure S10.** Negative mode HRESIMS data of compound 2.

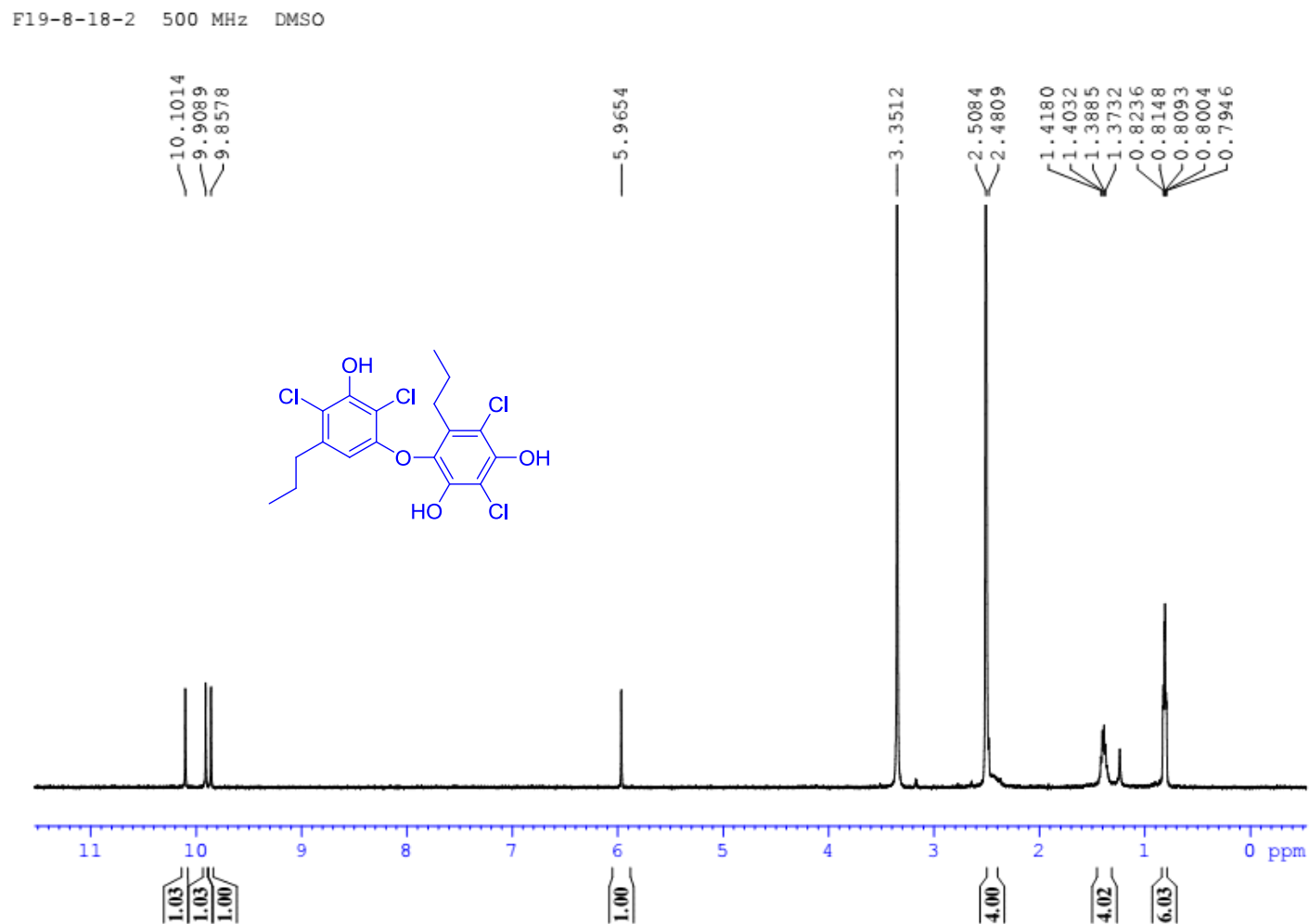


Figure S11. ¹H NMR spectrum of compound 2 in DMSO-d₆ (500 MHz).

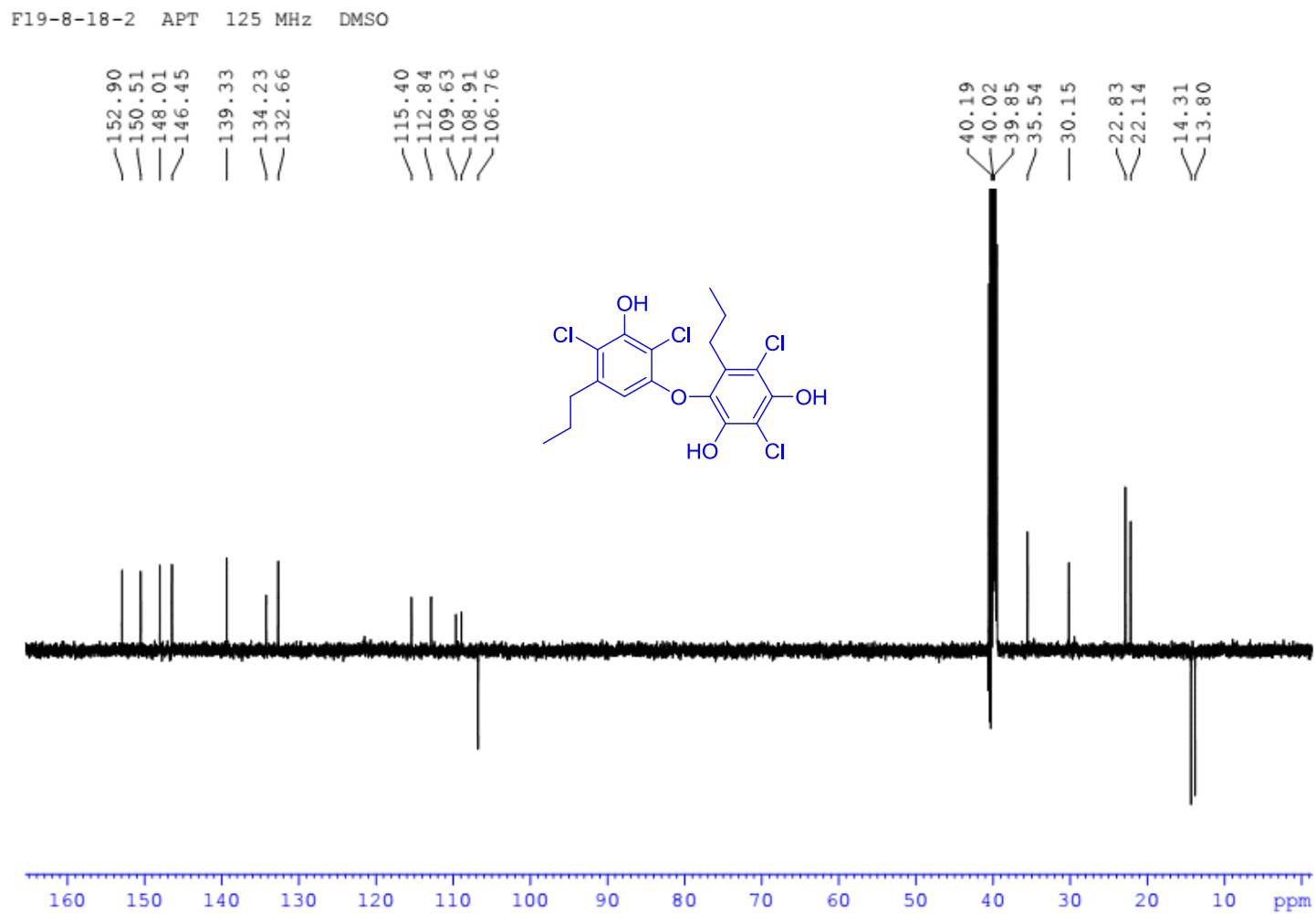


Figure S12. ^{13}C NMR spectrum of compound **2** in DMSO- d_6 (125 MHz).

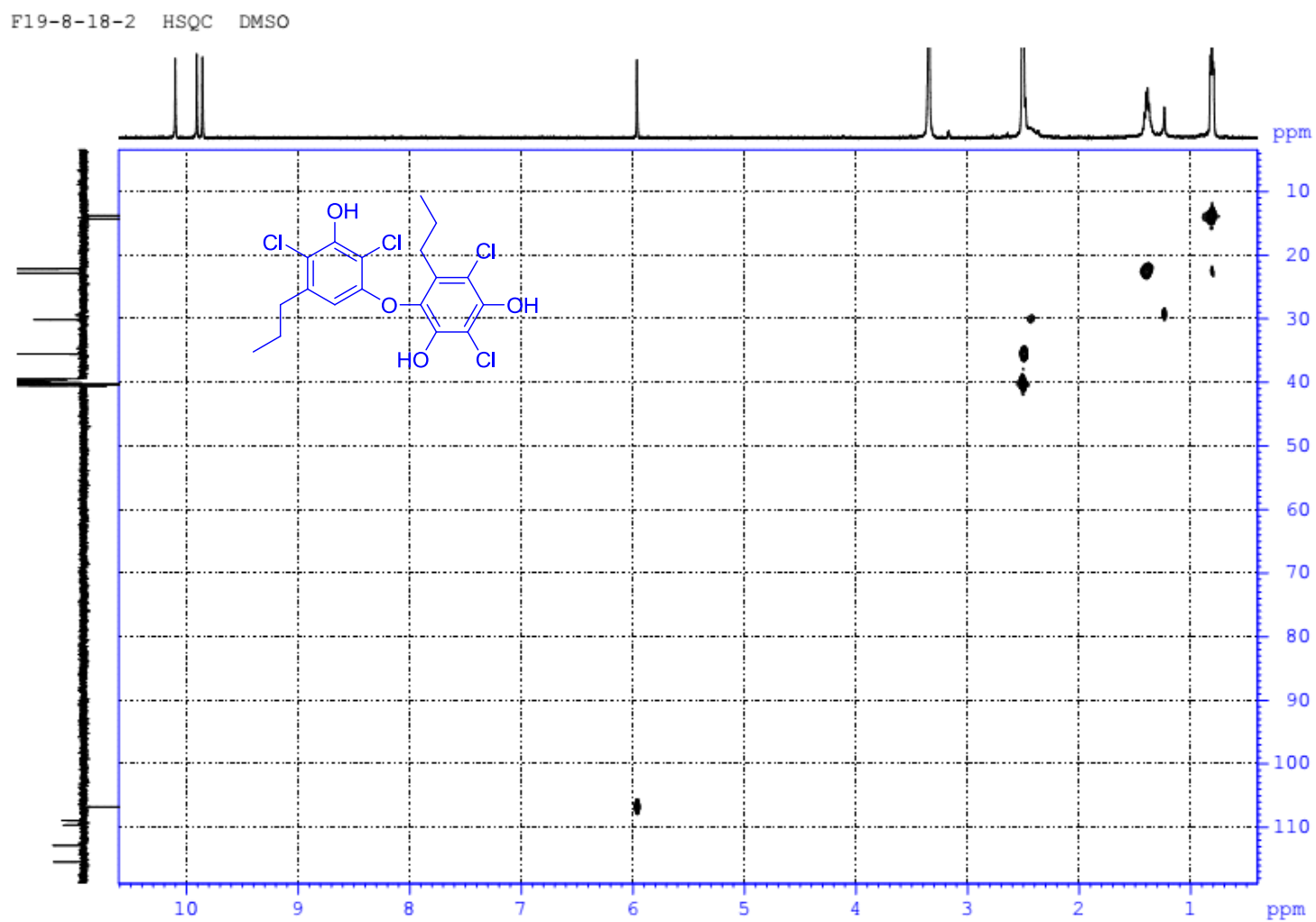


Figure S13. HSQC spectrum of compound 2 in DMSO-d₆.

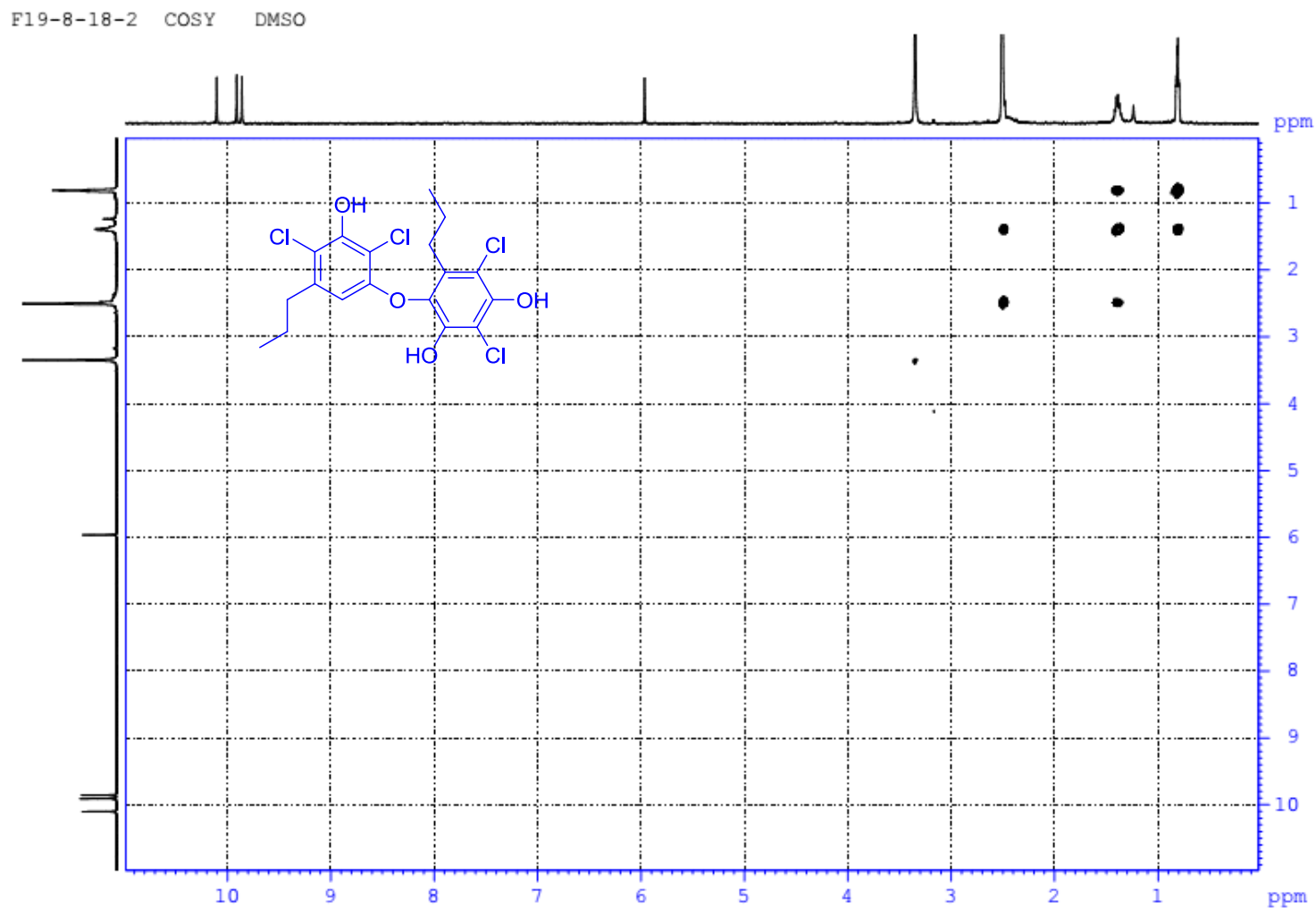


Figure S14. ^1H - ^1H COSY spectrum of compound **2** in DMSO- d_6 .

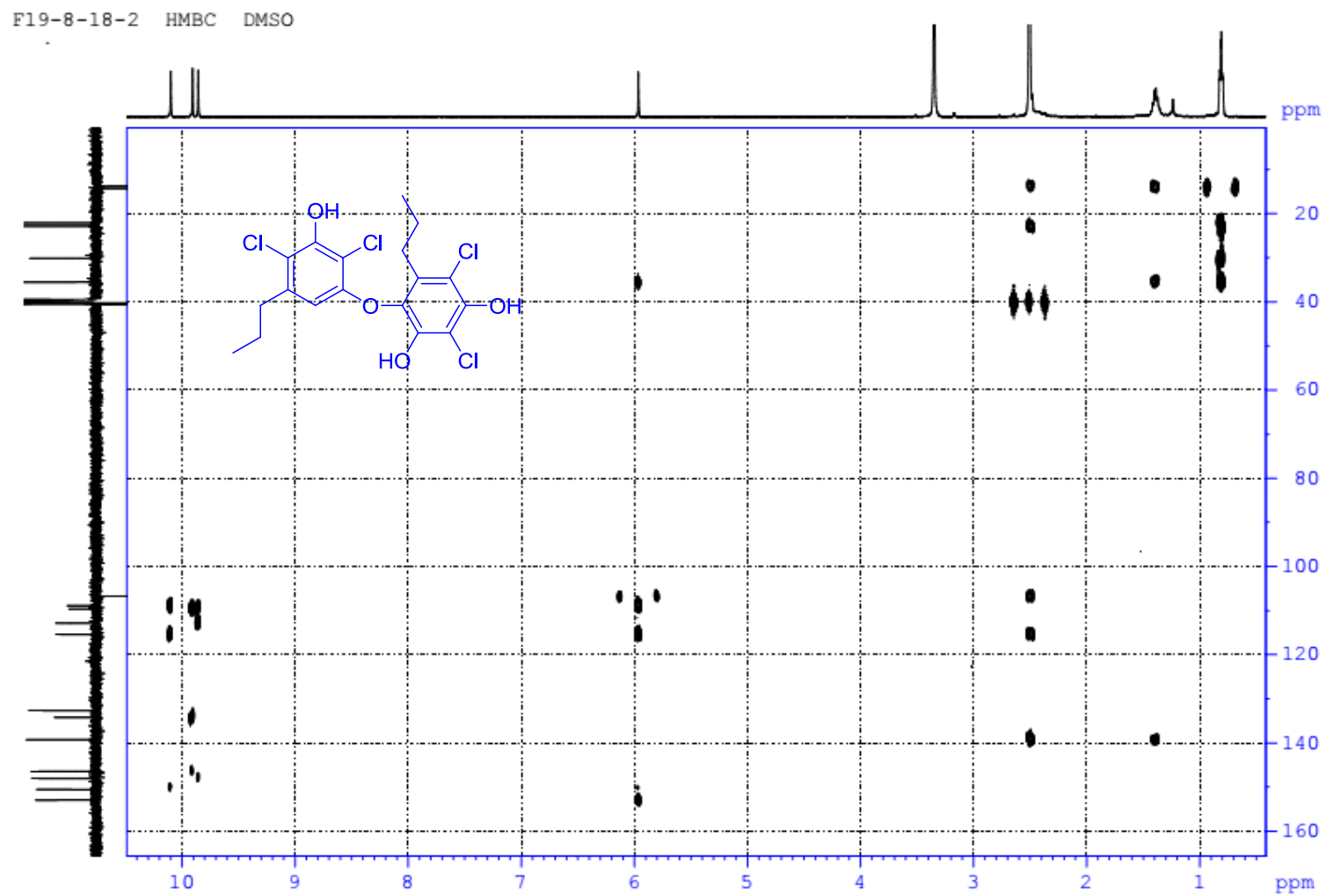


Figure S15. HMBC spectrum of compound 2 in DMSO-d₆.

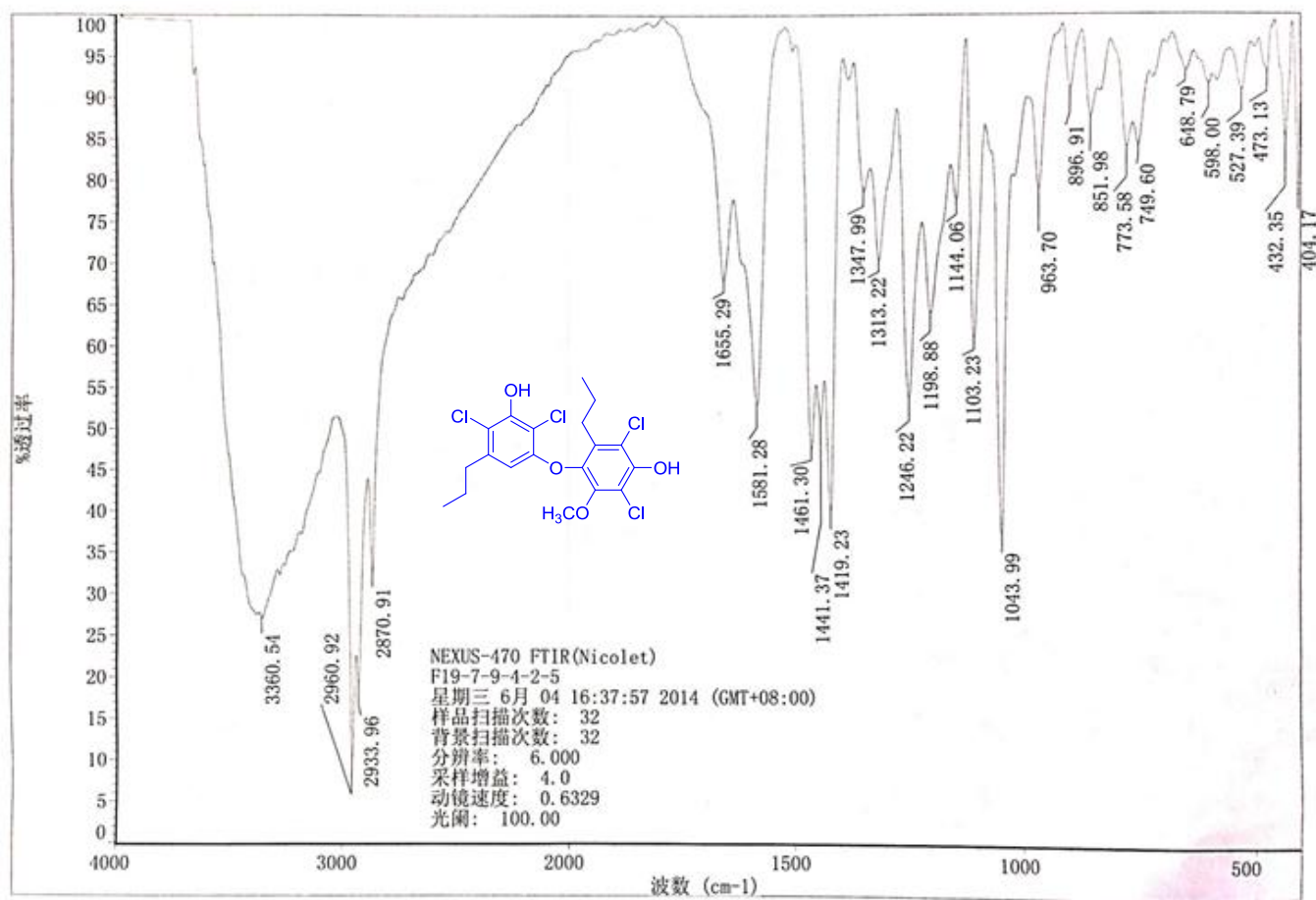


Figure S16. IR spectrum of compound 3.

Xevo G2 Q-TOF/CA166#

07-Jul-2014

Waters

F19-7-94+25 10(0.199) Cm(10:15-(36+23:52))

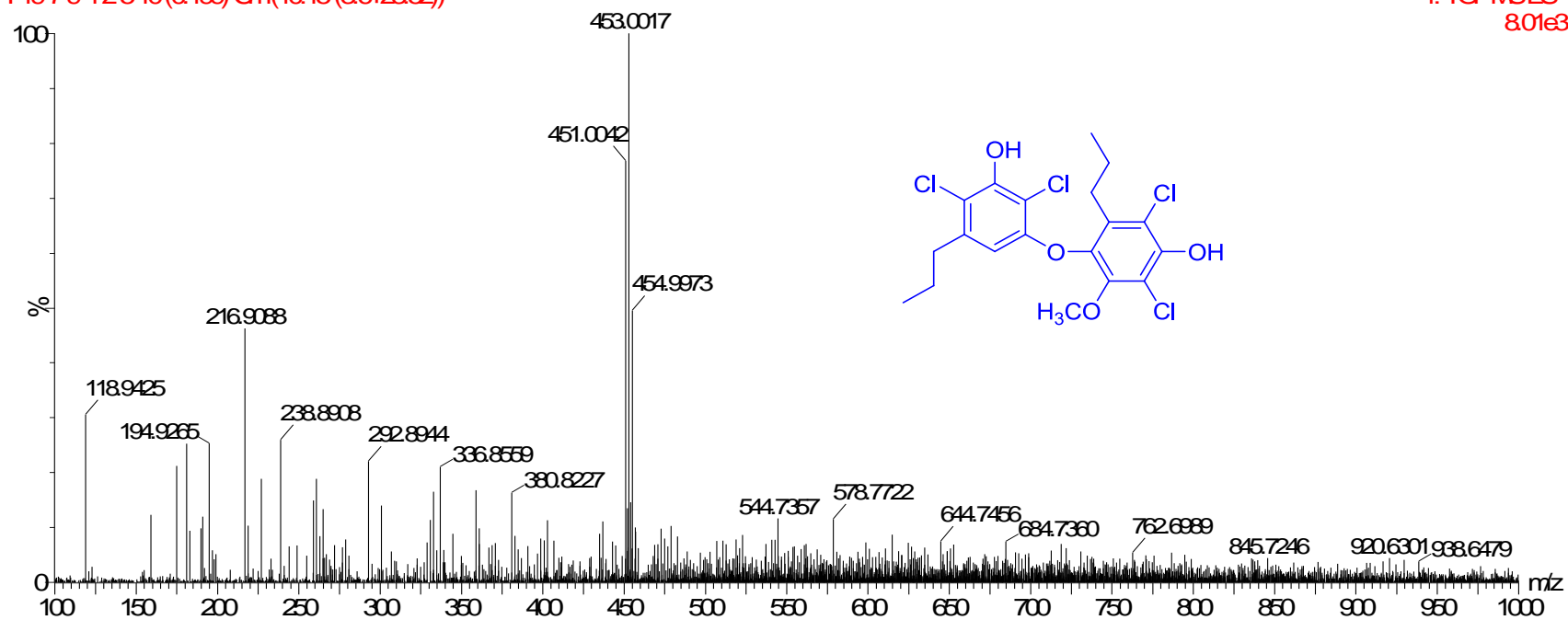
1: TOFMS ES-
8.01e3

Figure S17. Negative mode HRESIMS data of compound 3.

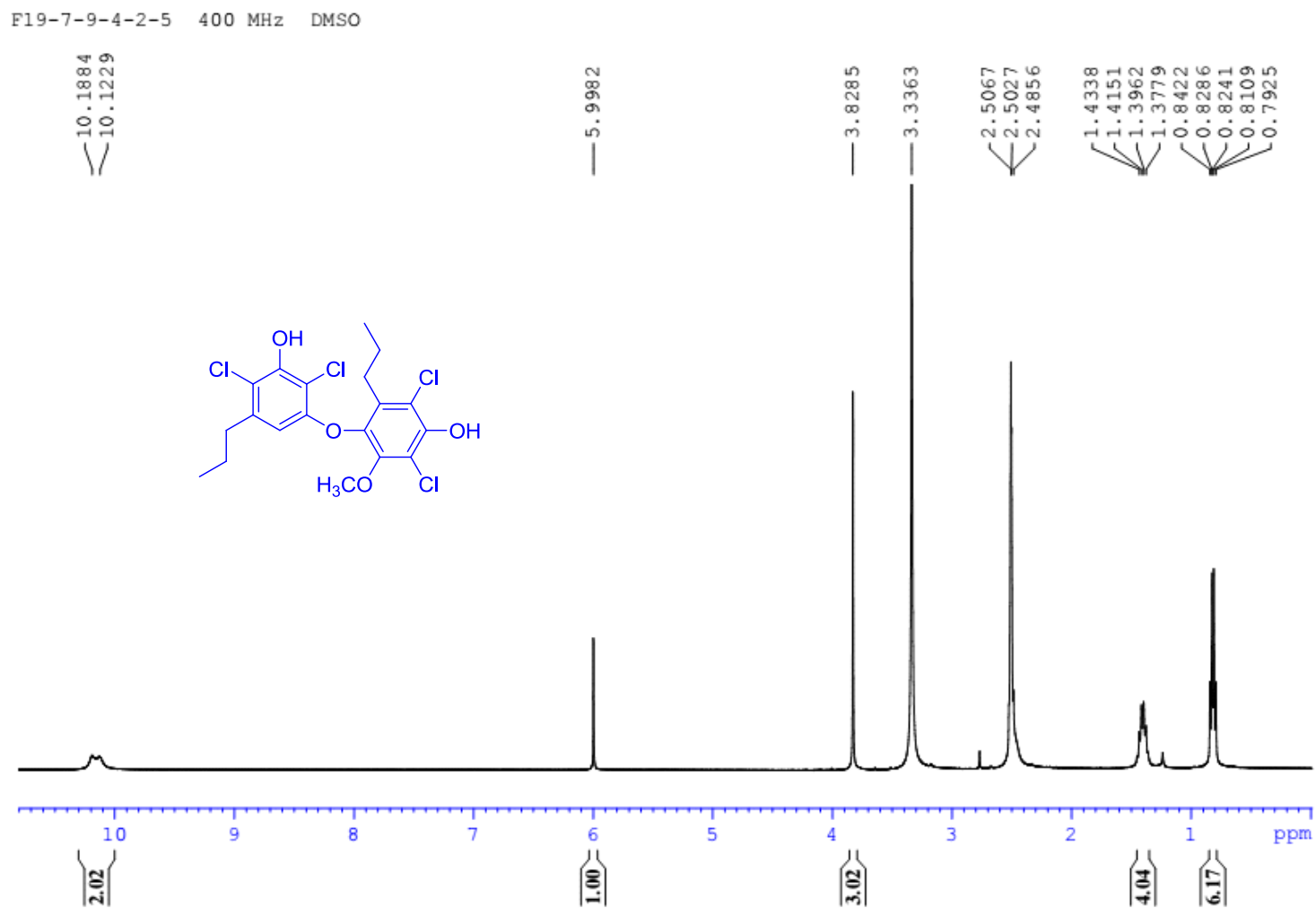


Figure S18. ^1H NMR spectrum of compound **3** in DMSO- d_6 (400 MHz).

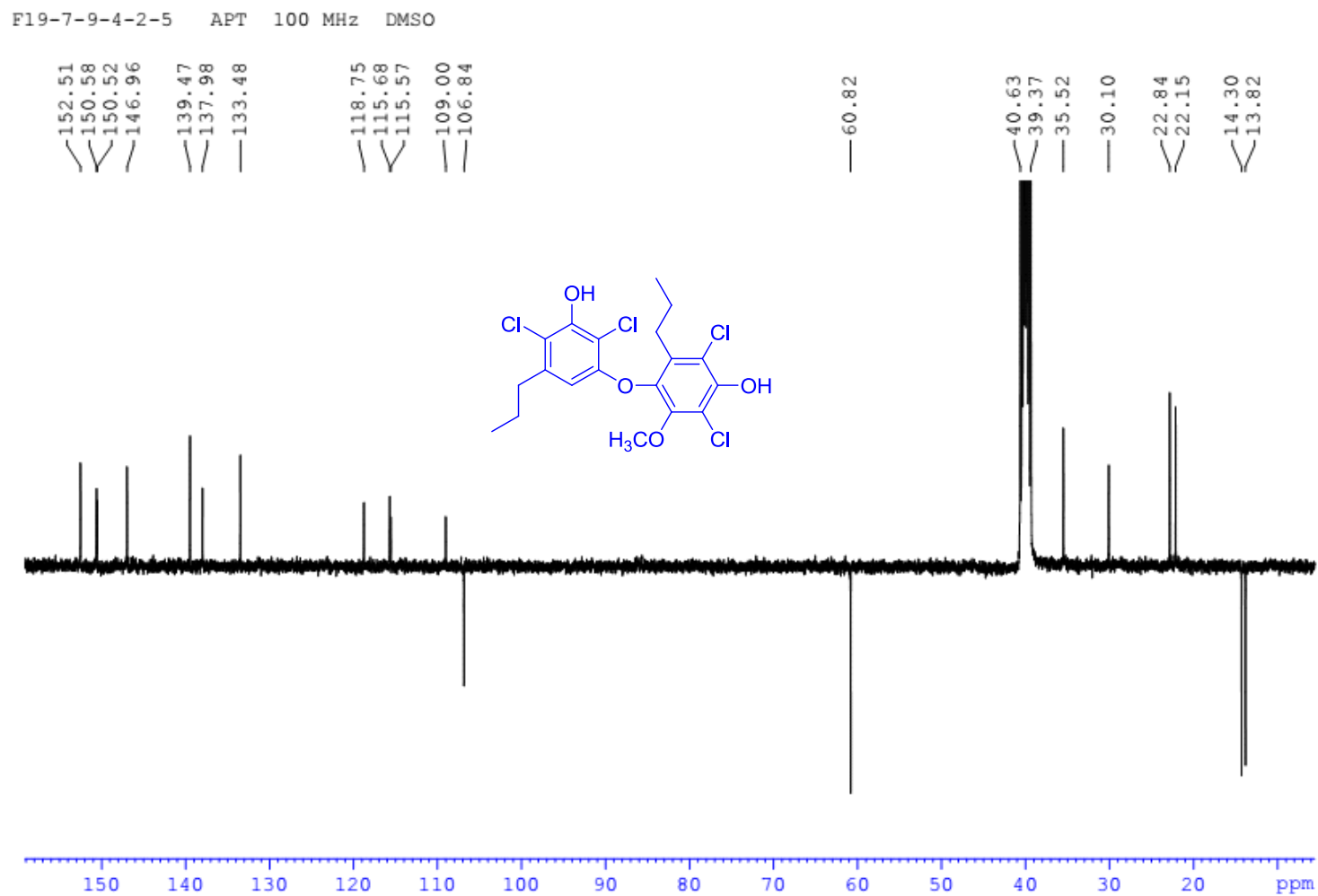


Figure S19. ^{13}C NMR spectrum of compound **3** in DMSO- d_6 (100 MHz).

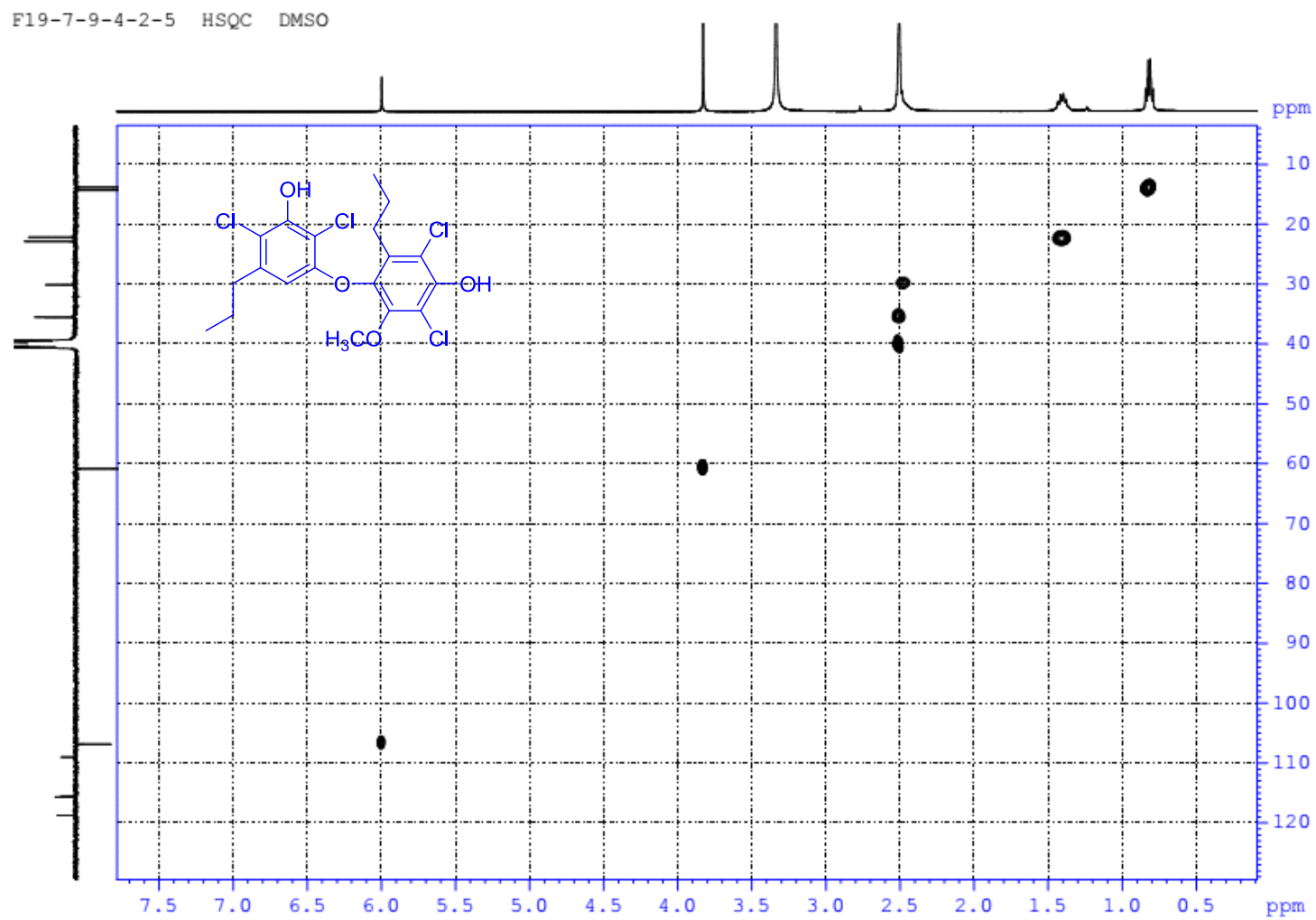


Figure S20. HSQC spectrum of compound 3 in DMSO-d6.

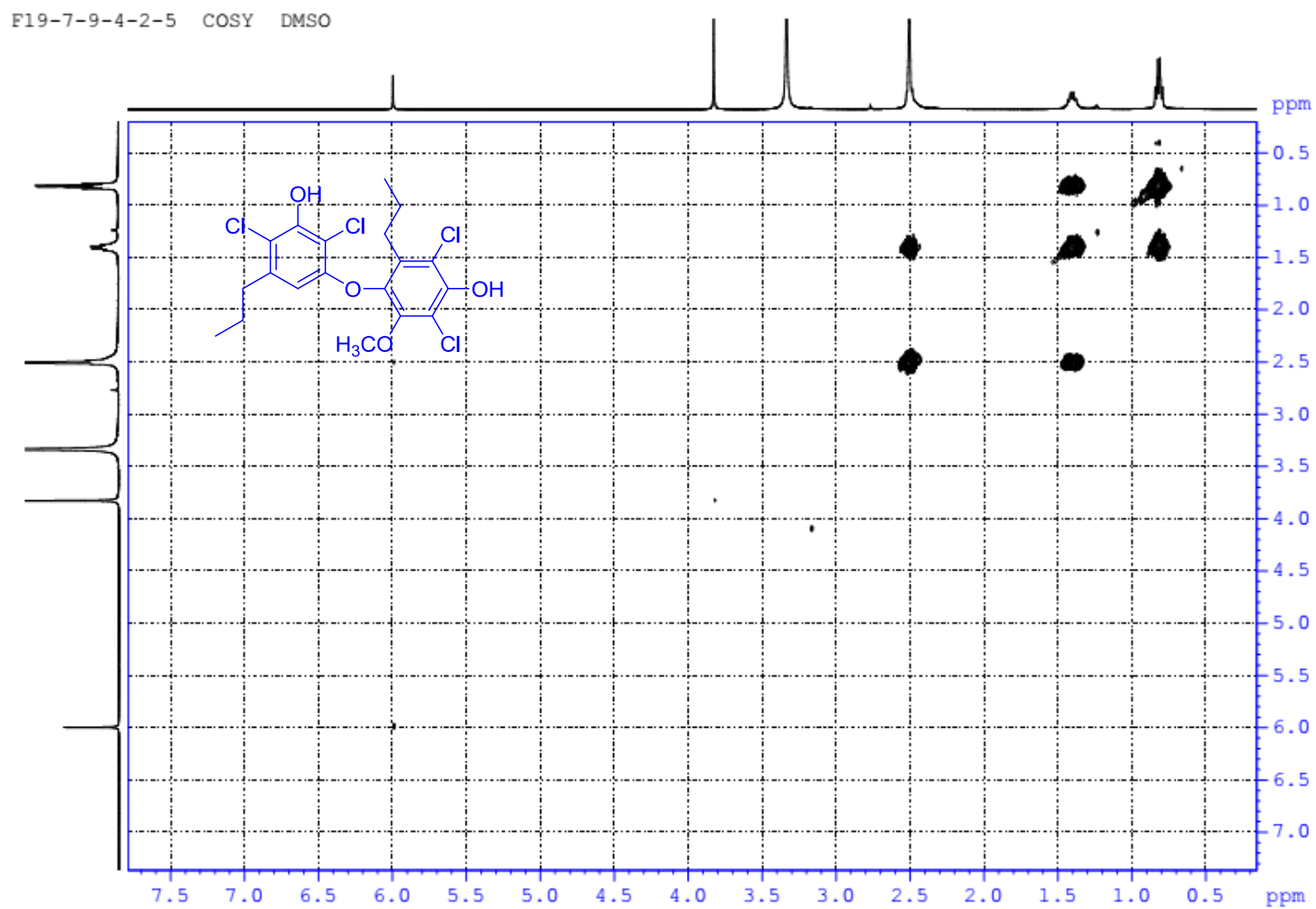


Figure S21. ^1H - ^1H COSY spectrum of compound 3 in DMSO-d₆.

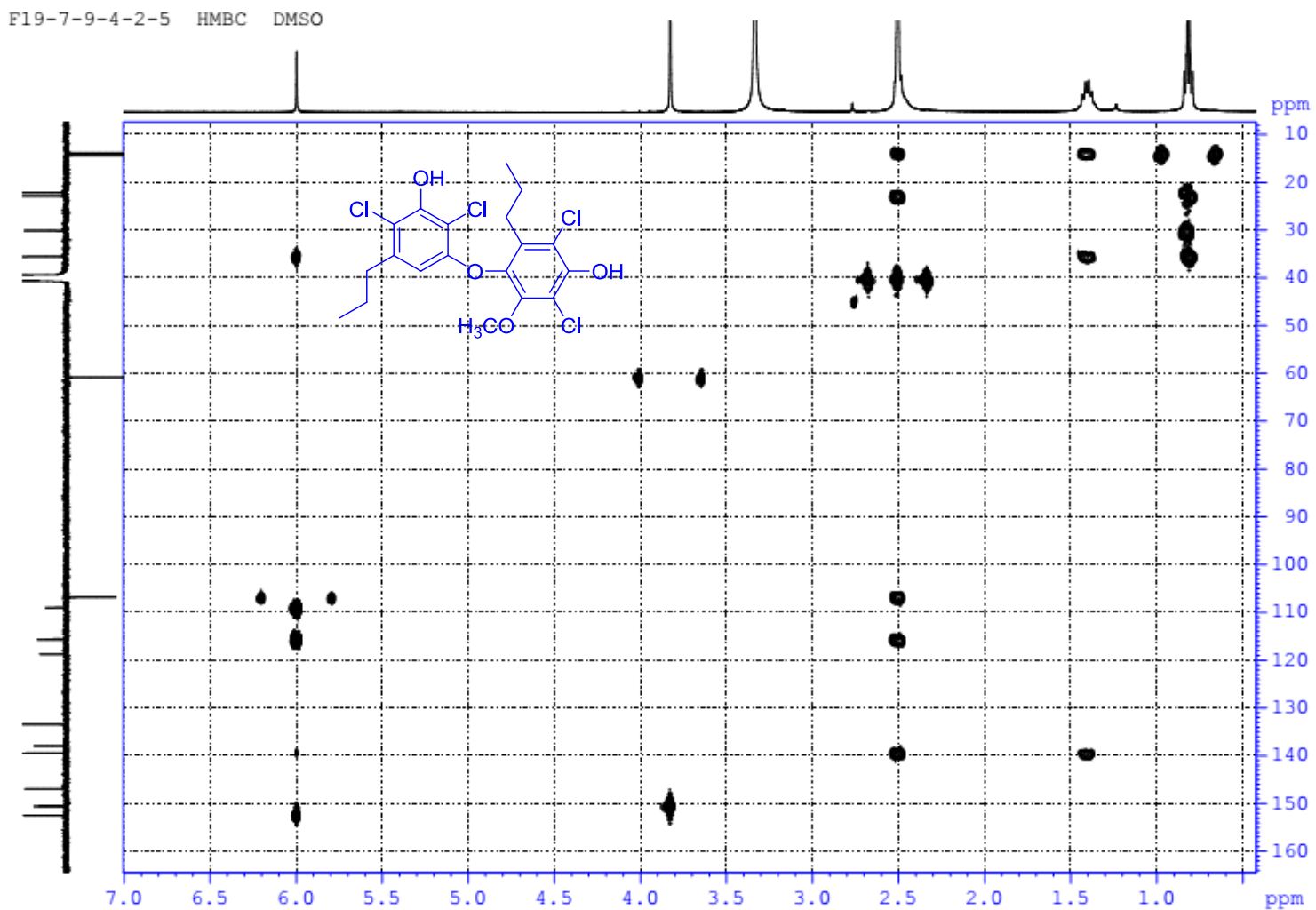


Figure S22. HMBC spectrum of compound 3 in DMSO-d6.

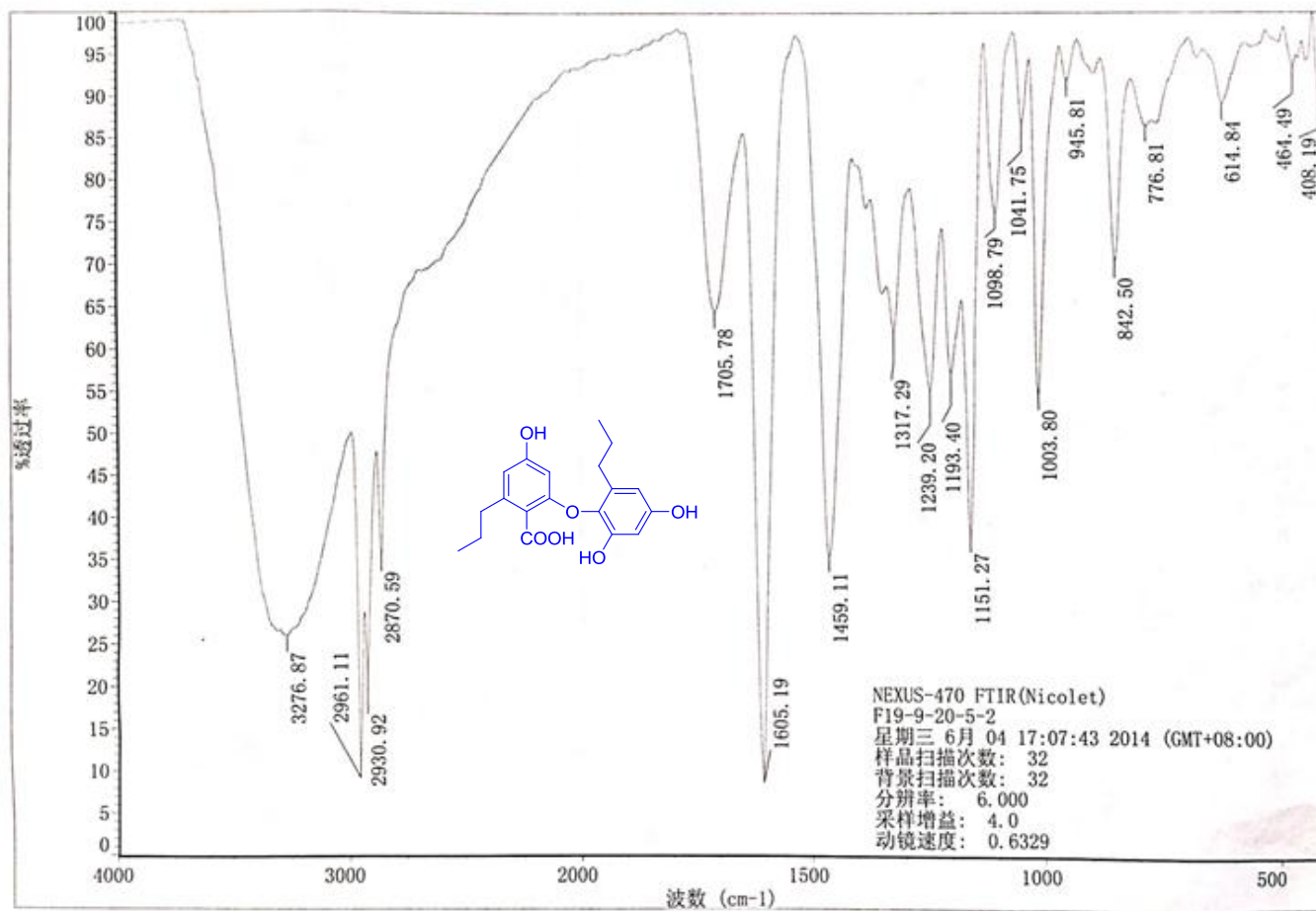


Figure S23. IR spectrum of compound 4.

Xevo G2 Q-TOF/YCA166#

07-Jul-2014

Waters

F19-9-20-5-2 11 (0.216) Cm(10:16-(37+20:53))

1: TOFMS-ES-
2.16e5

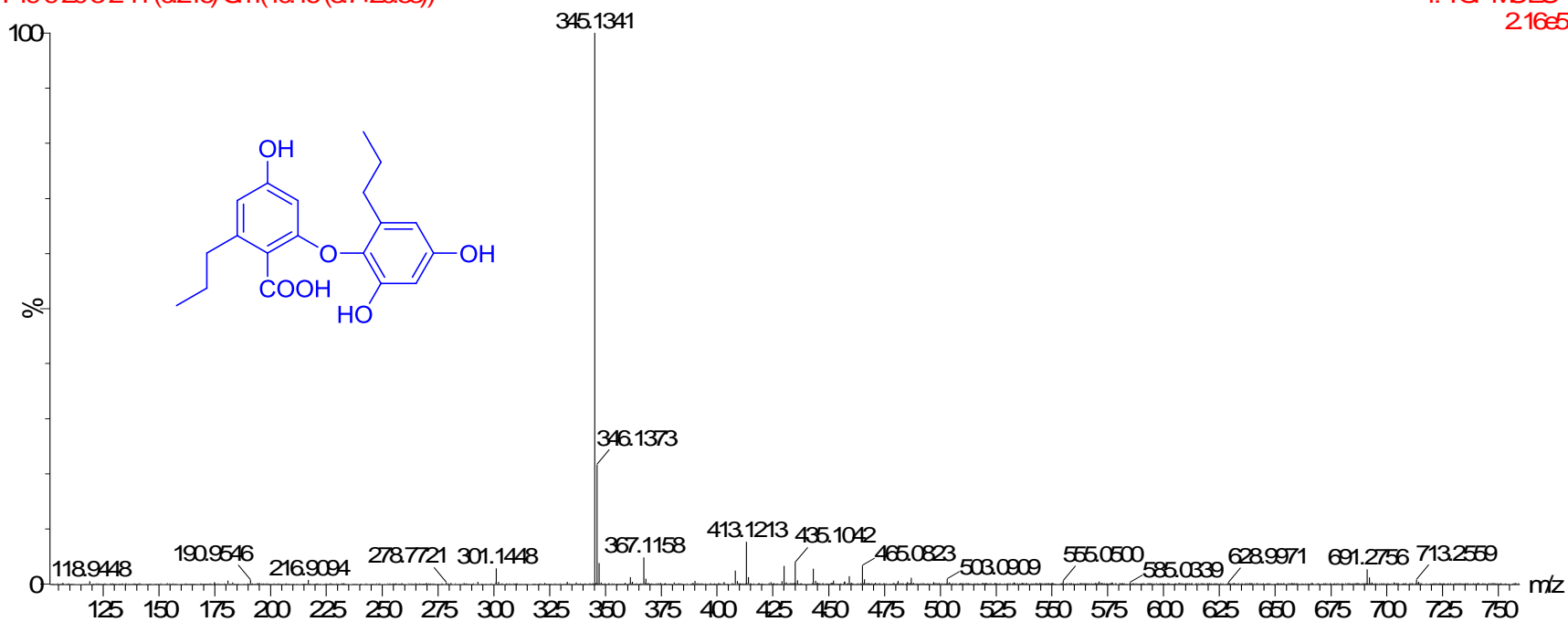


Figure S24. Negative mode HRESIMS data of compound 4.

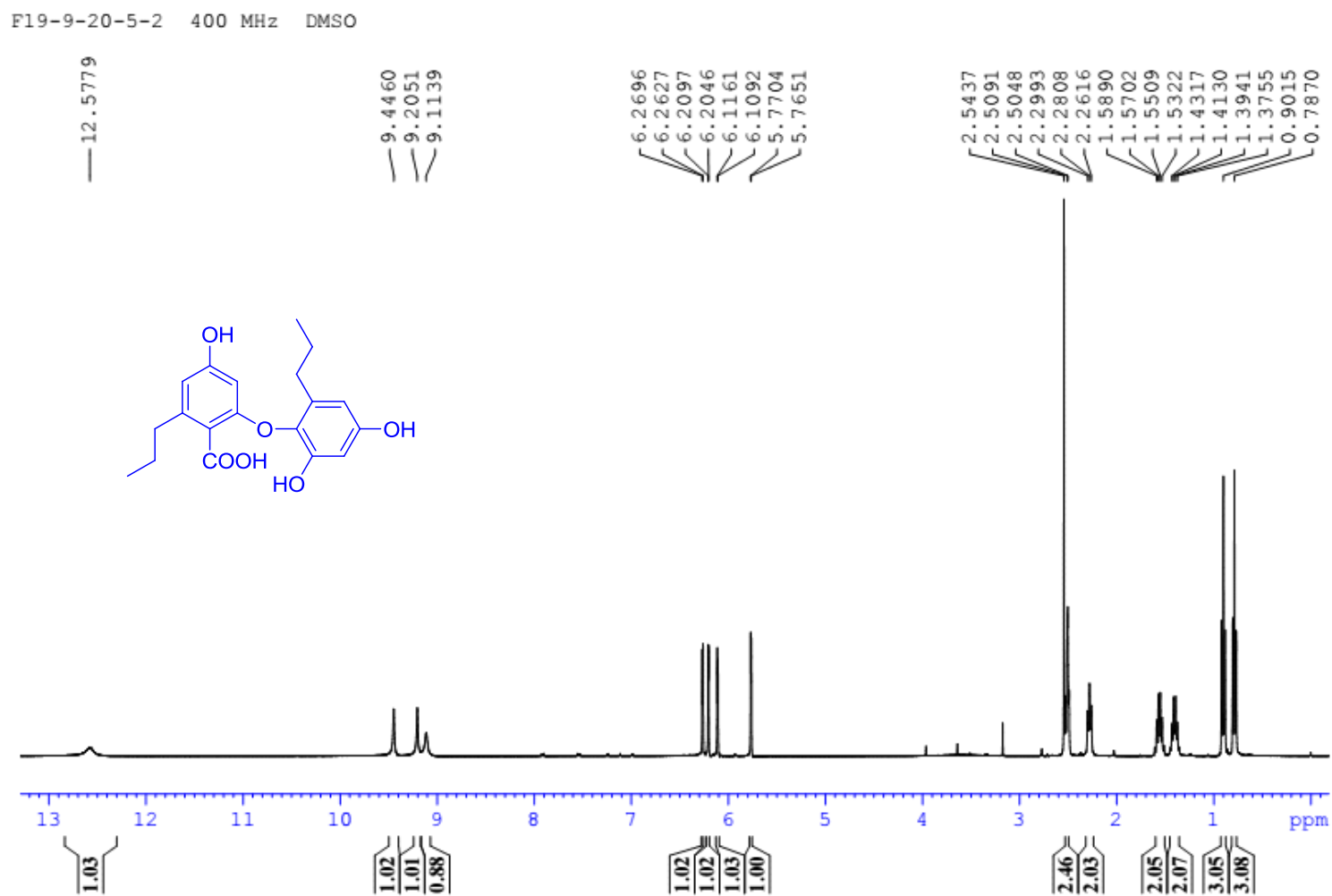


Figure S25. ^1H NMR spectrum of compound 4 in DMSO- d_6 (400 MHz).

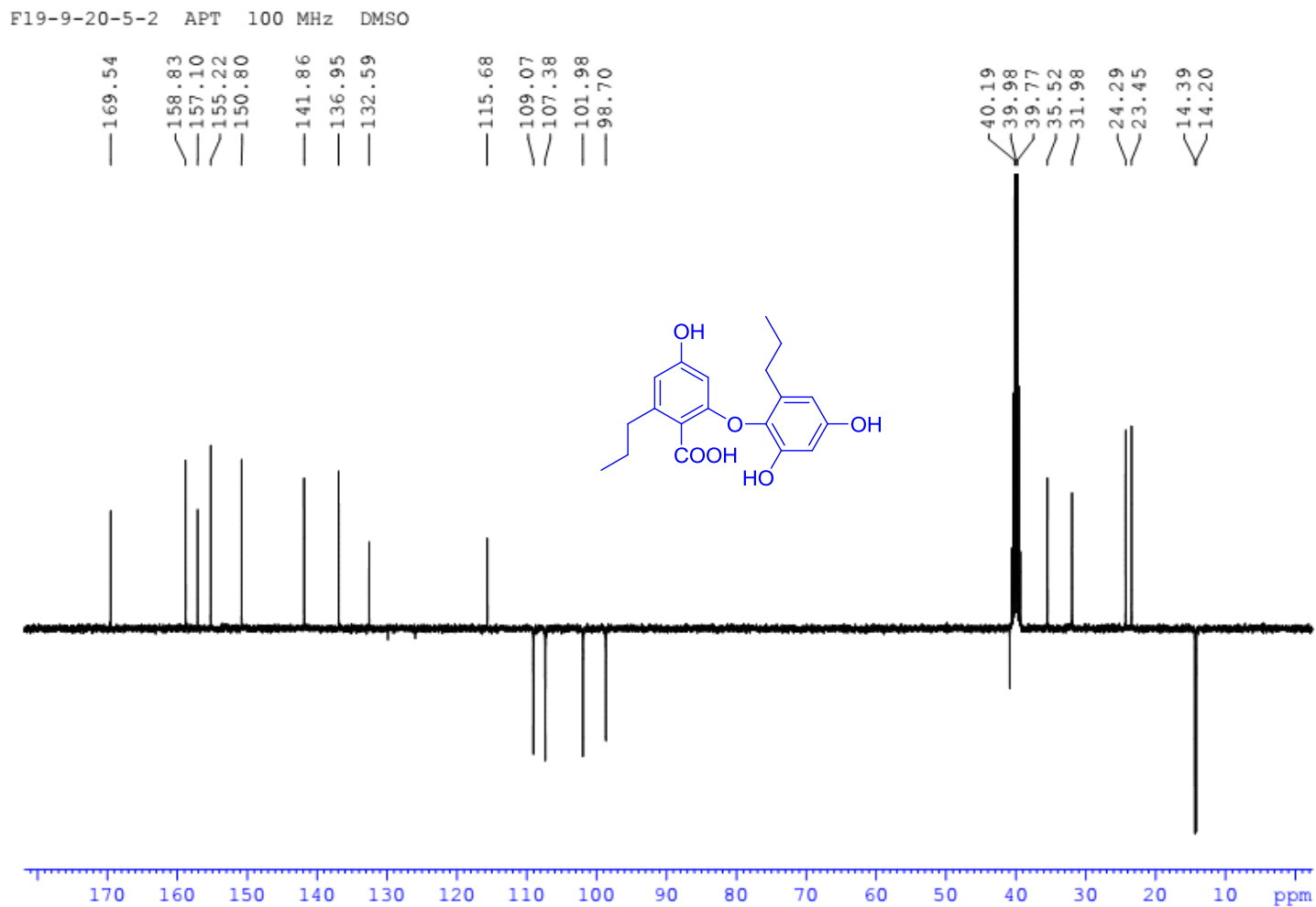


Figure S26. ^{13}C NMR spectrum of compound 4 in DMSO- d_6 (100 MHz).

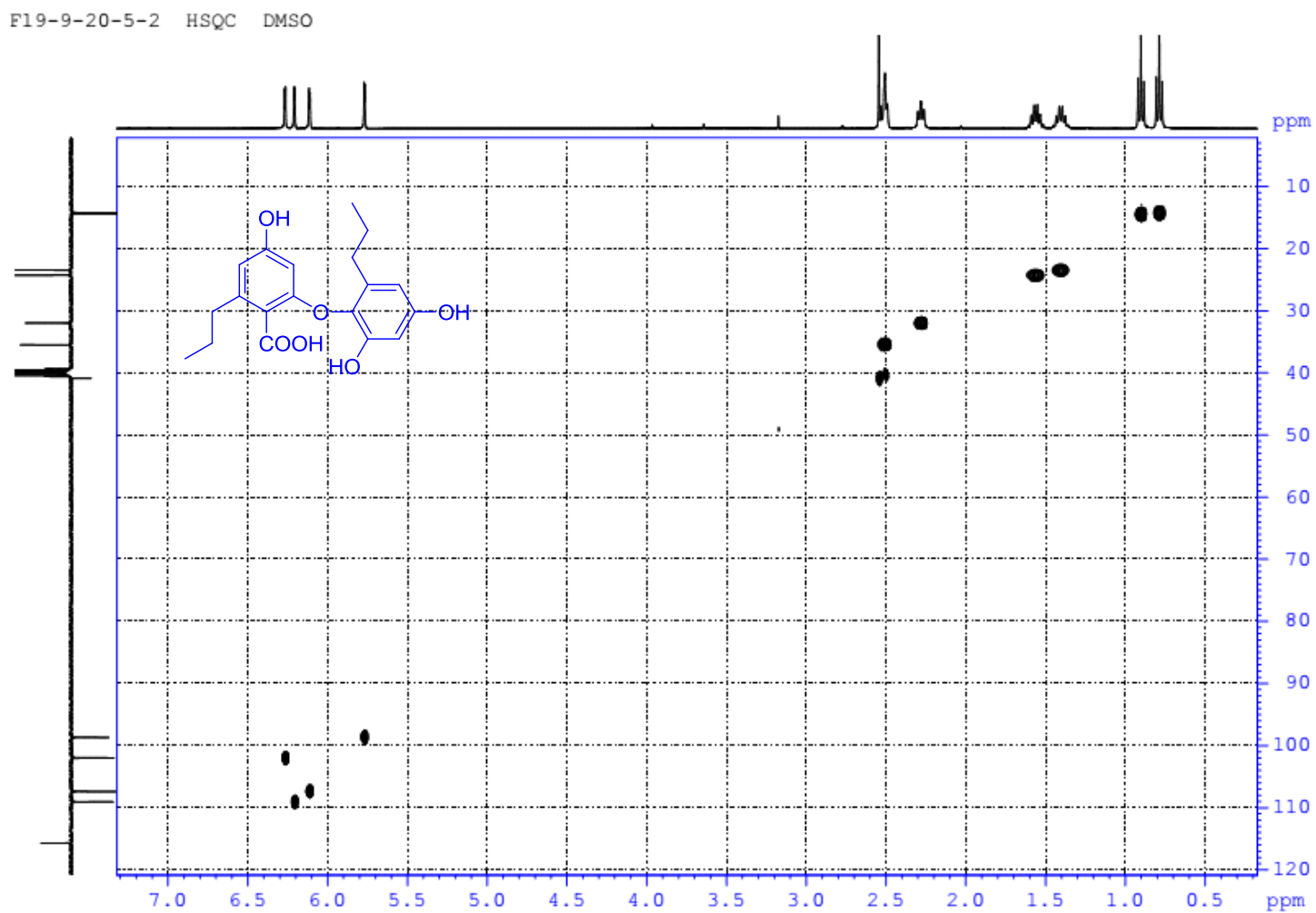


Figure S27. HSQC spectrum of compound 4 in DMSO-d₆.

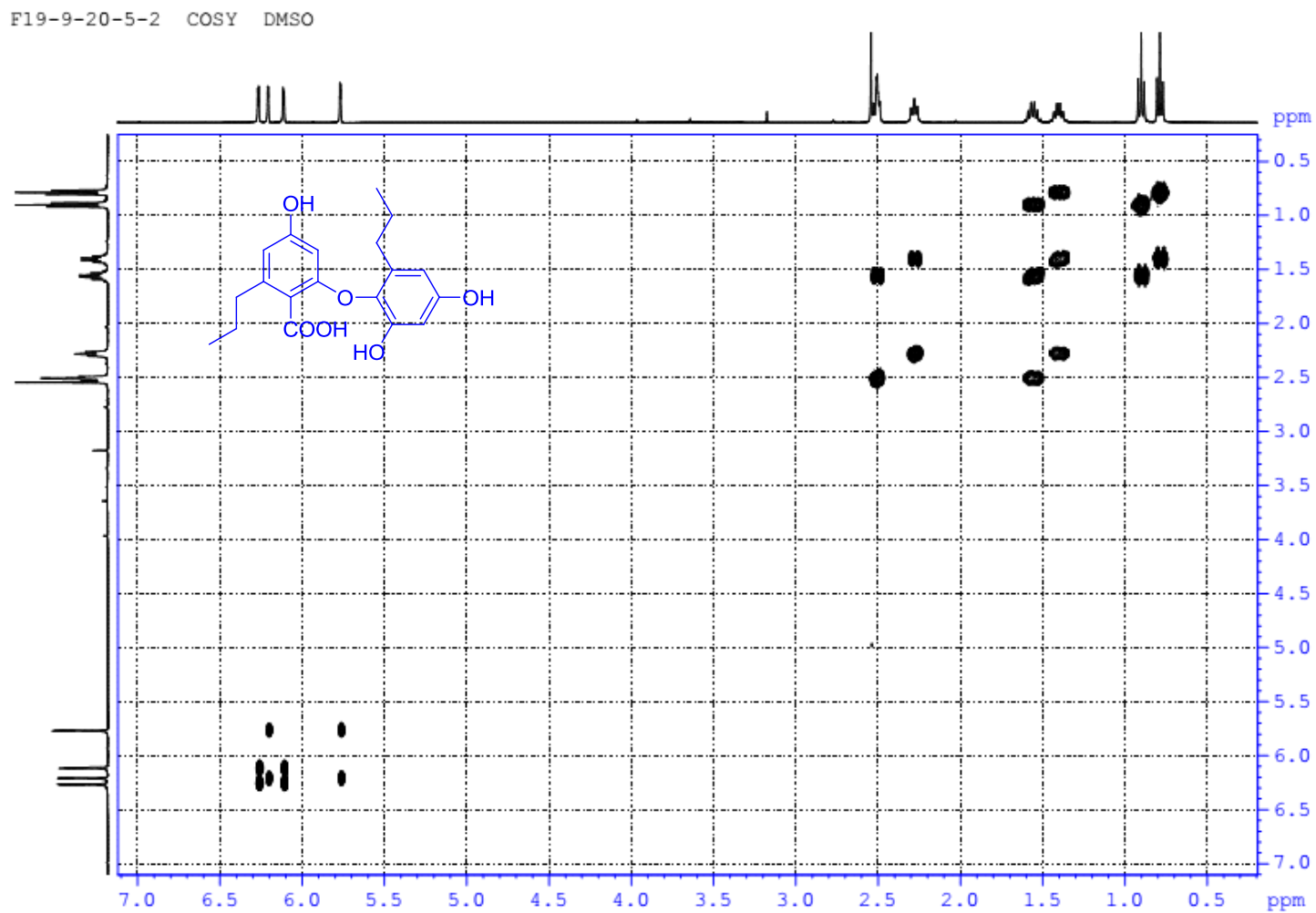


Figure S28. ^1H - ^1H COSY spectrum of compound 4 in DMSO- d_6 .

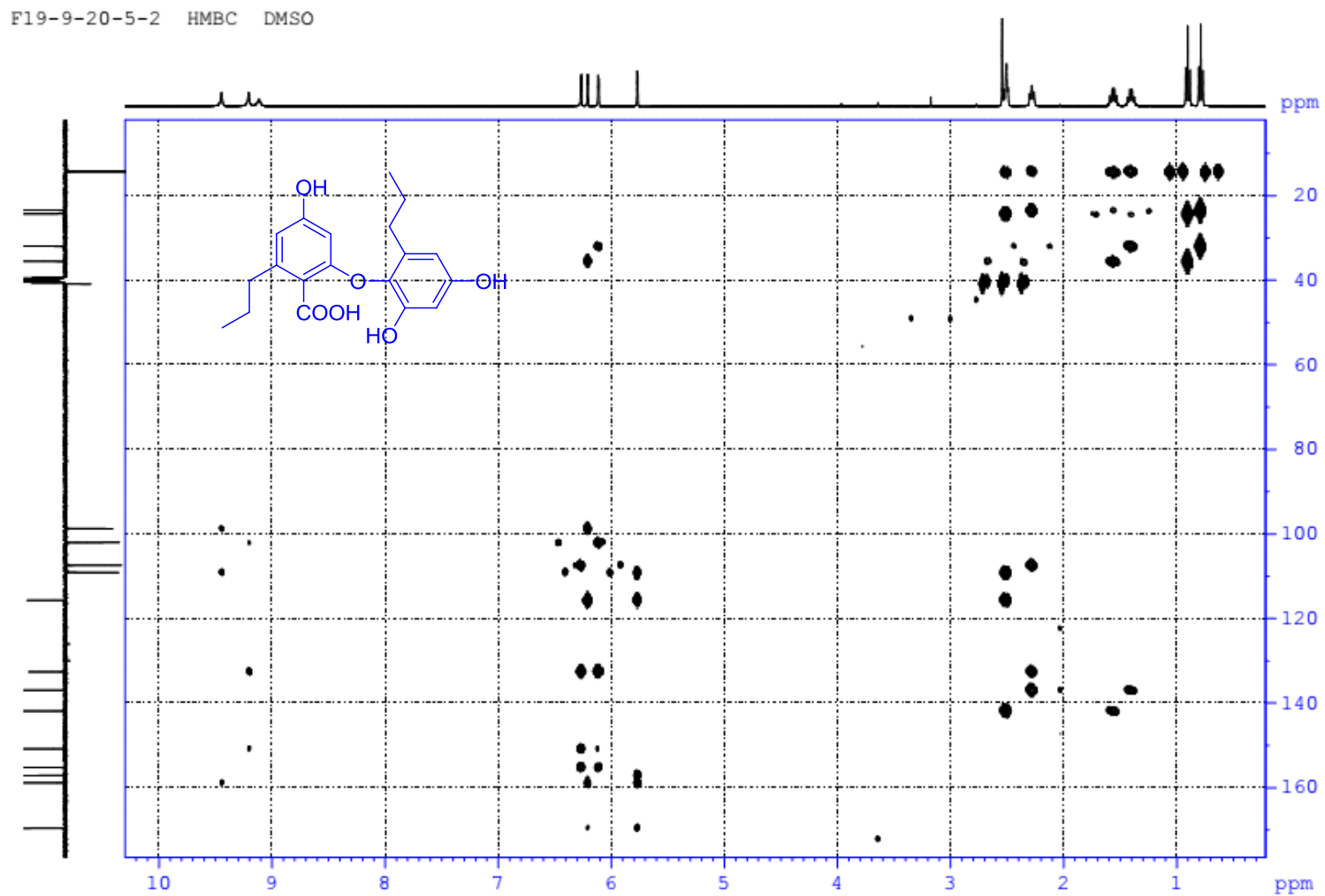


Figure S29. HMBC spectrum of compound 4 in DMSO-d₆.

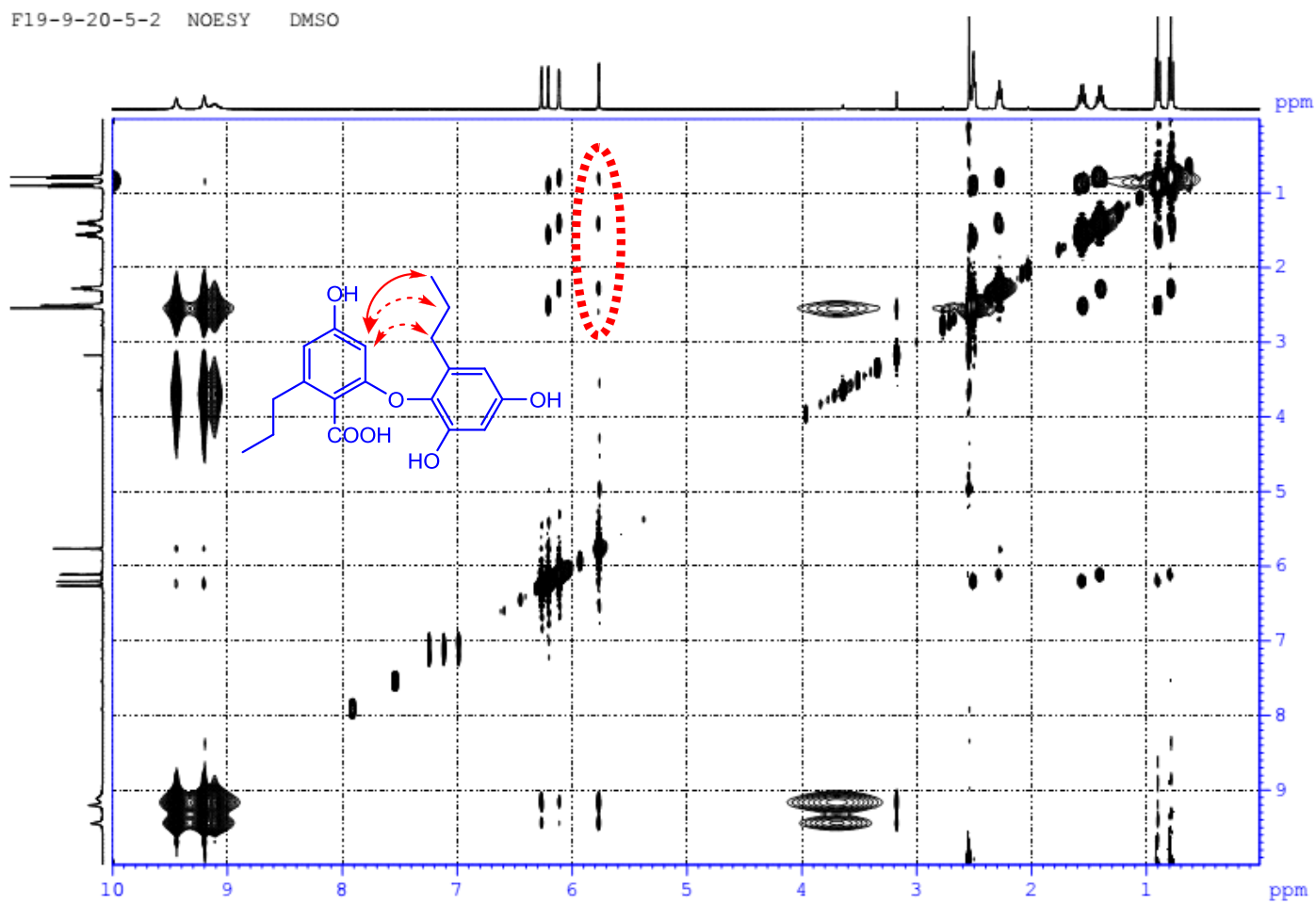


Figure S30. NOESY spectrum of compound 4 in DMSO-d6.

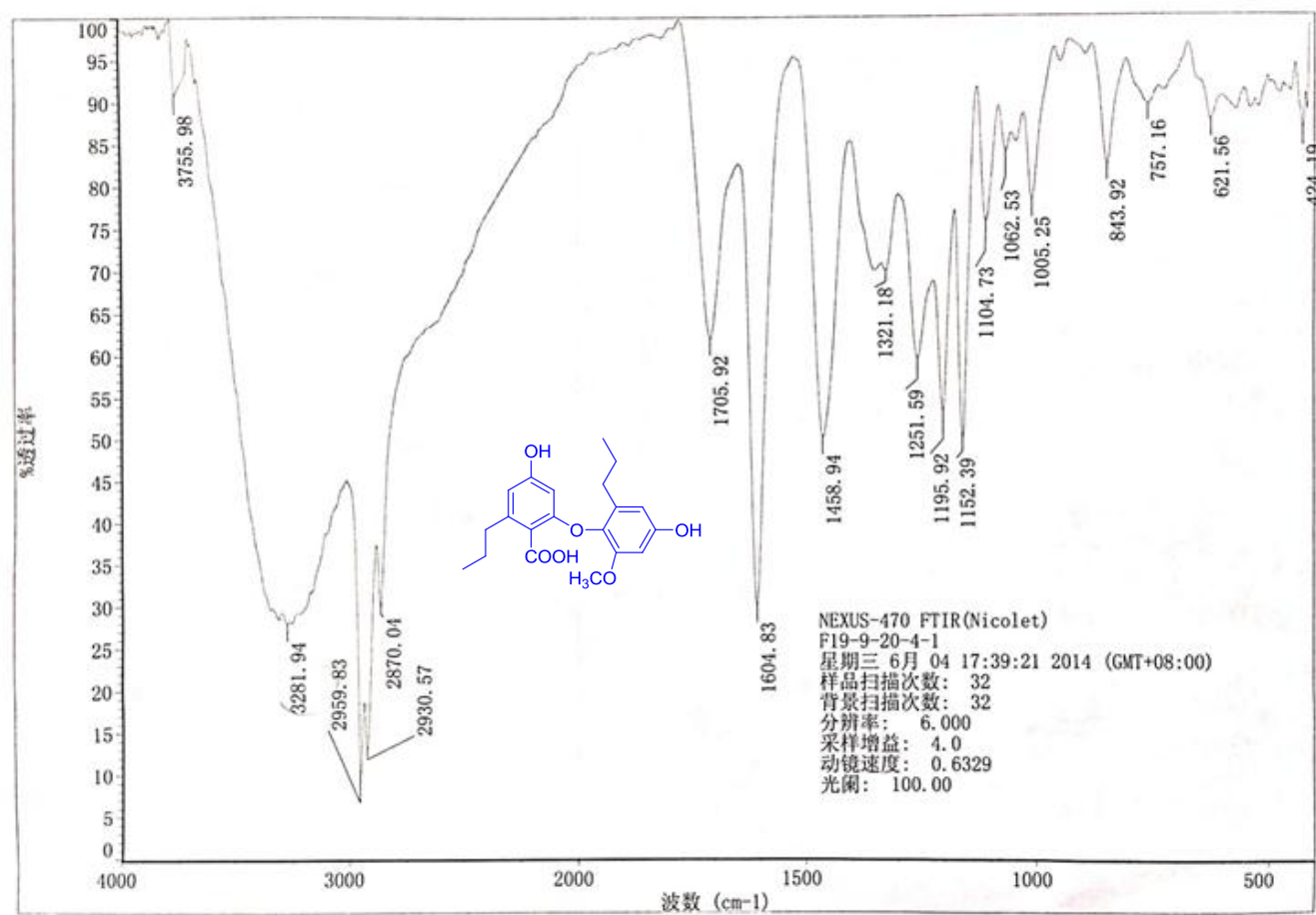


Figure S31. IR spectrum of compound 5.

Xevo G2 Q-TOF/YCA166#

07-Jul-2014

Waters

F19-9-20-4-1 11 (0.216) Cm(11:15-(36+2253))

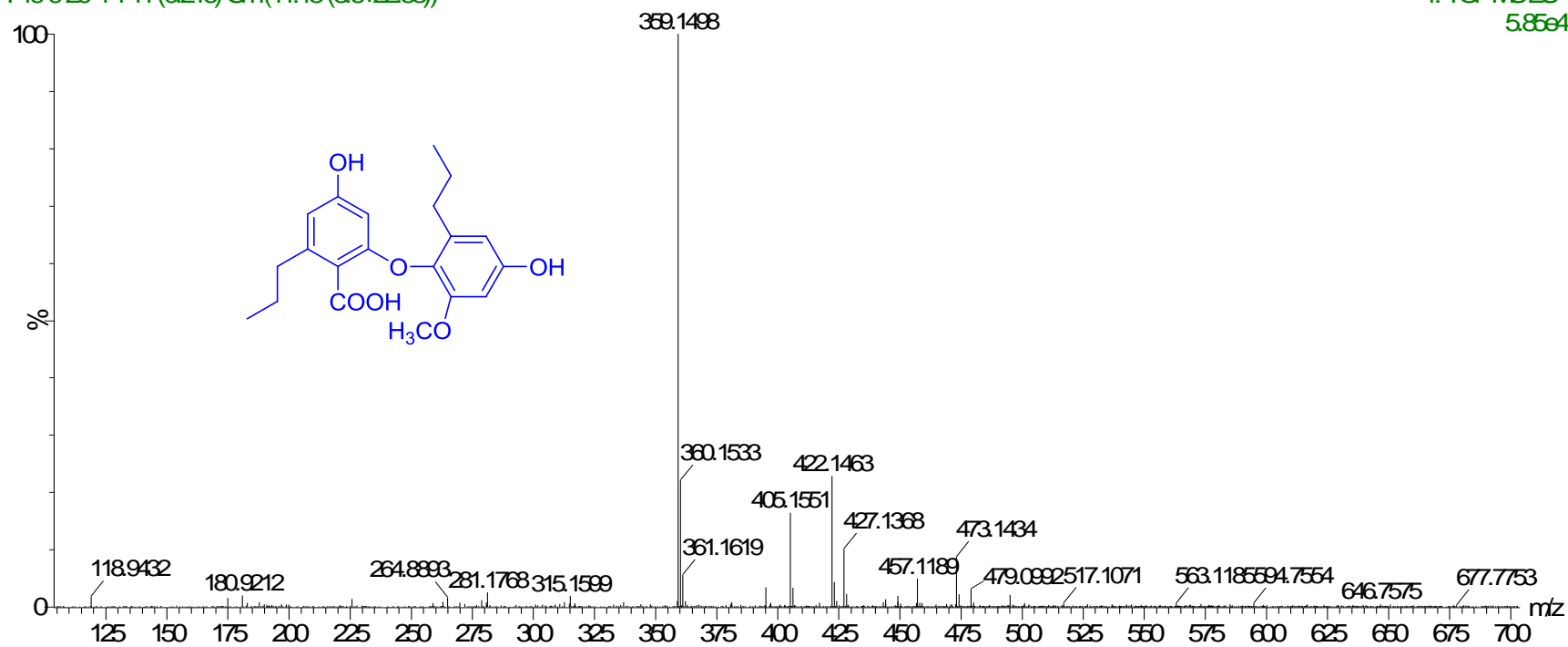
1: TOFMS ES-
5.85e4

Figure S32. Negative mode HRESIMS data of compound 5.

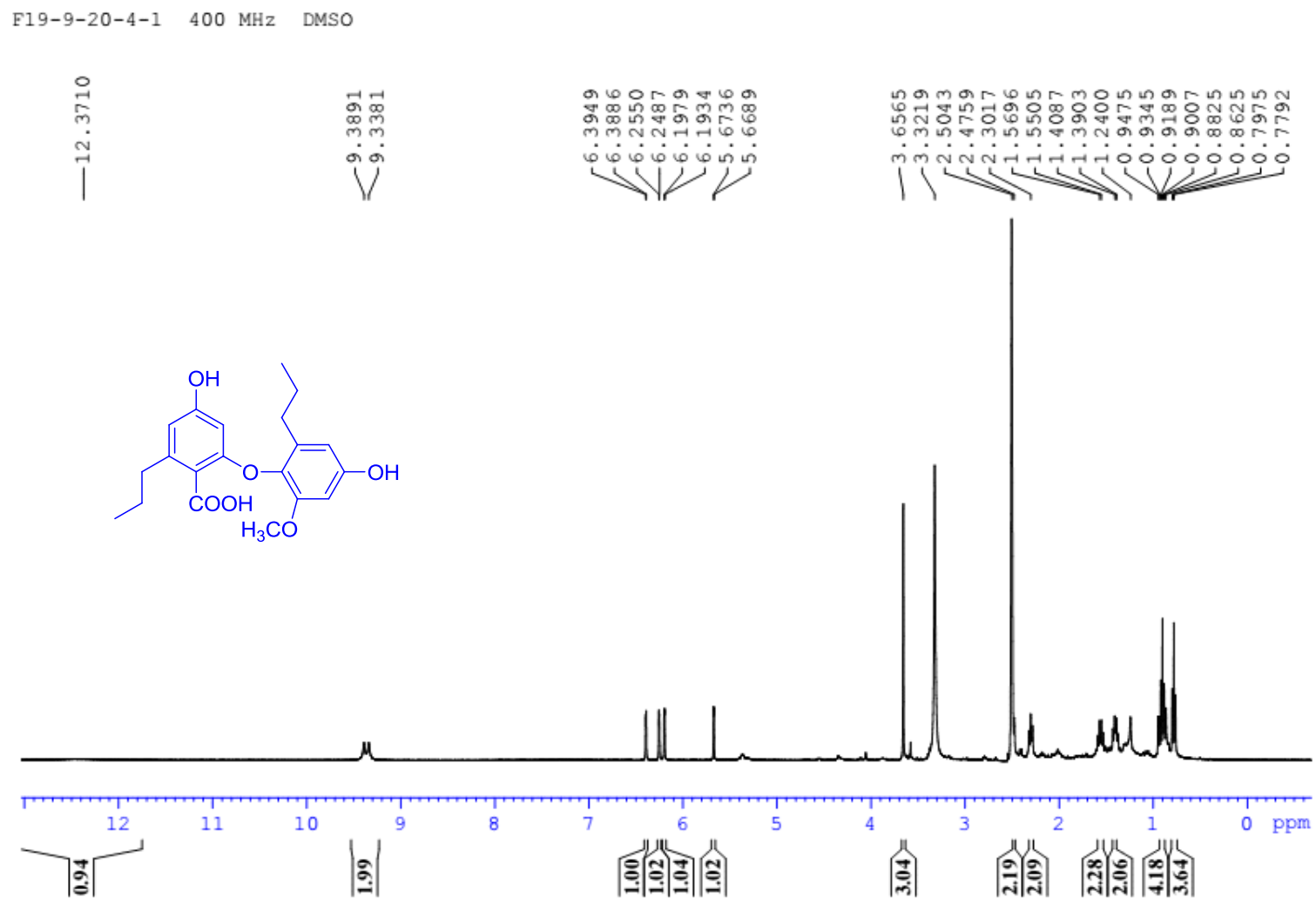


Figure S33. ¹H NMR spectrum of compound 5 in DMSO-d₆ (400 MHz).

F19-9-20-4-1 APT 100 MHz DMSO

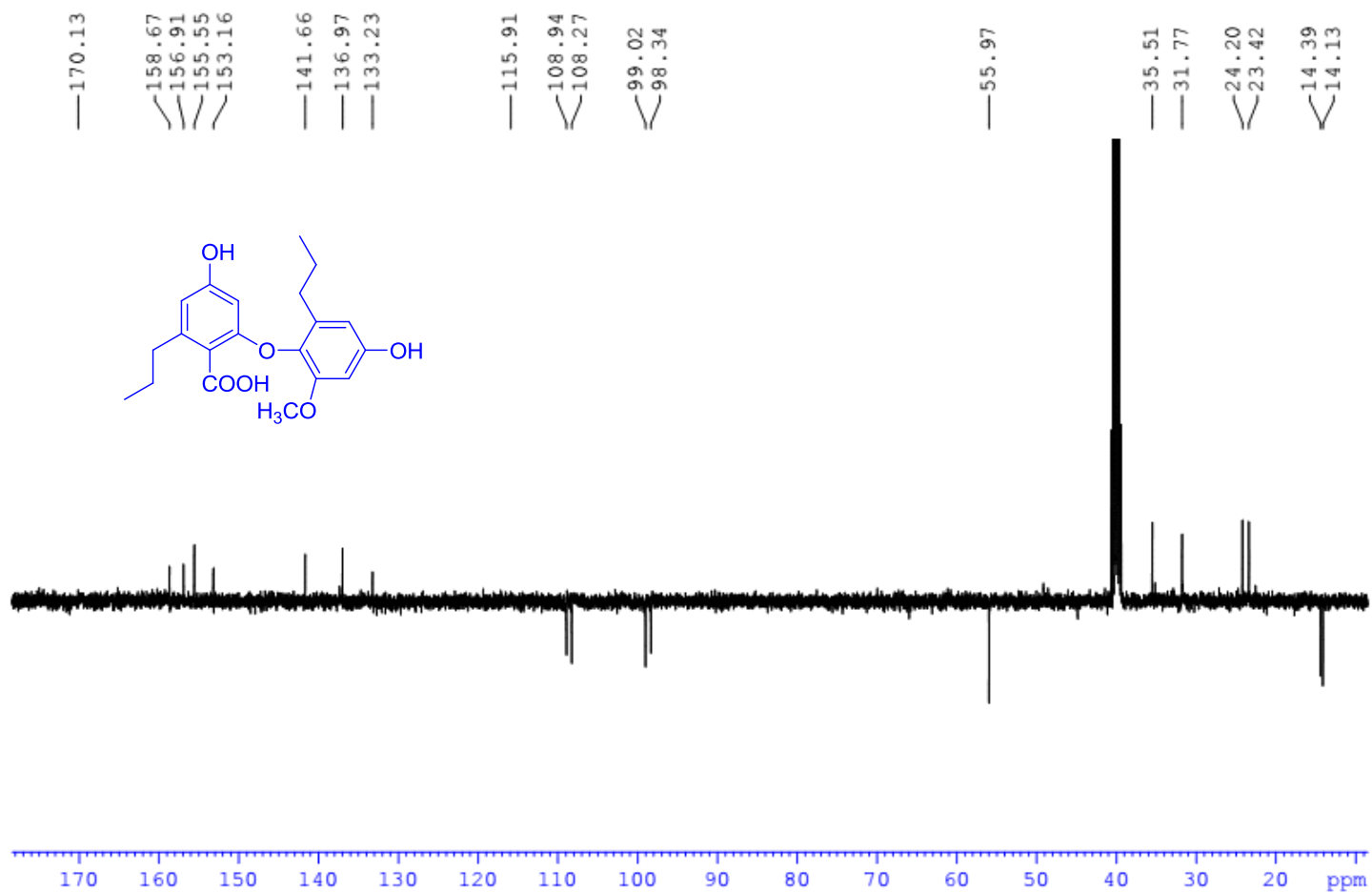


Figure S34. ¹³C NMR spectrum of compound 5 in DMSO-d₆ (100 MHz).

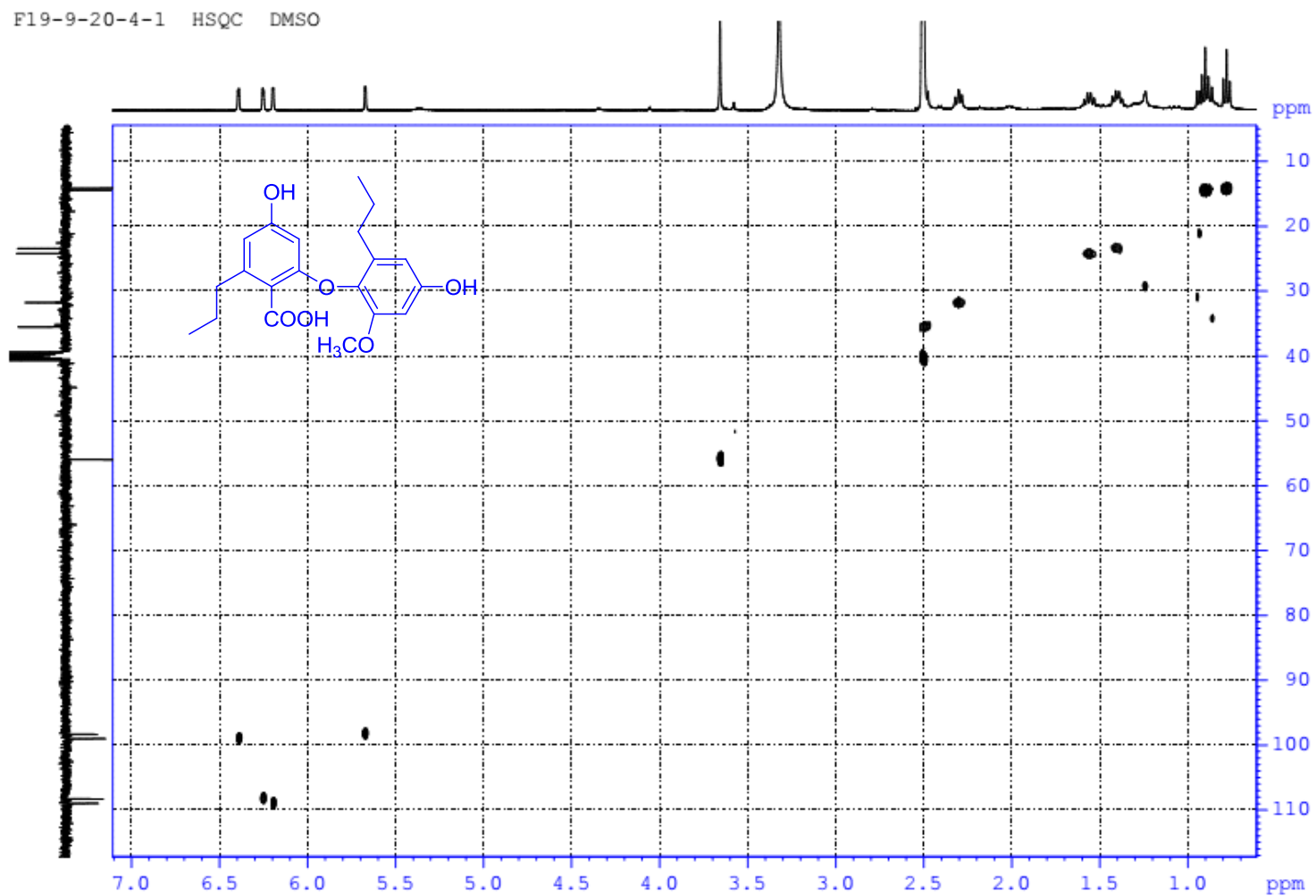


Figure S35. HSQC spectrum of compound 5 in DMSO-d6.

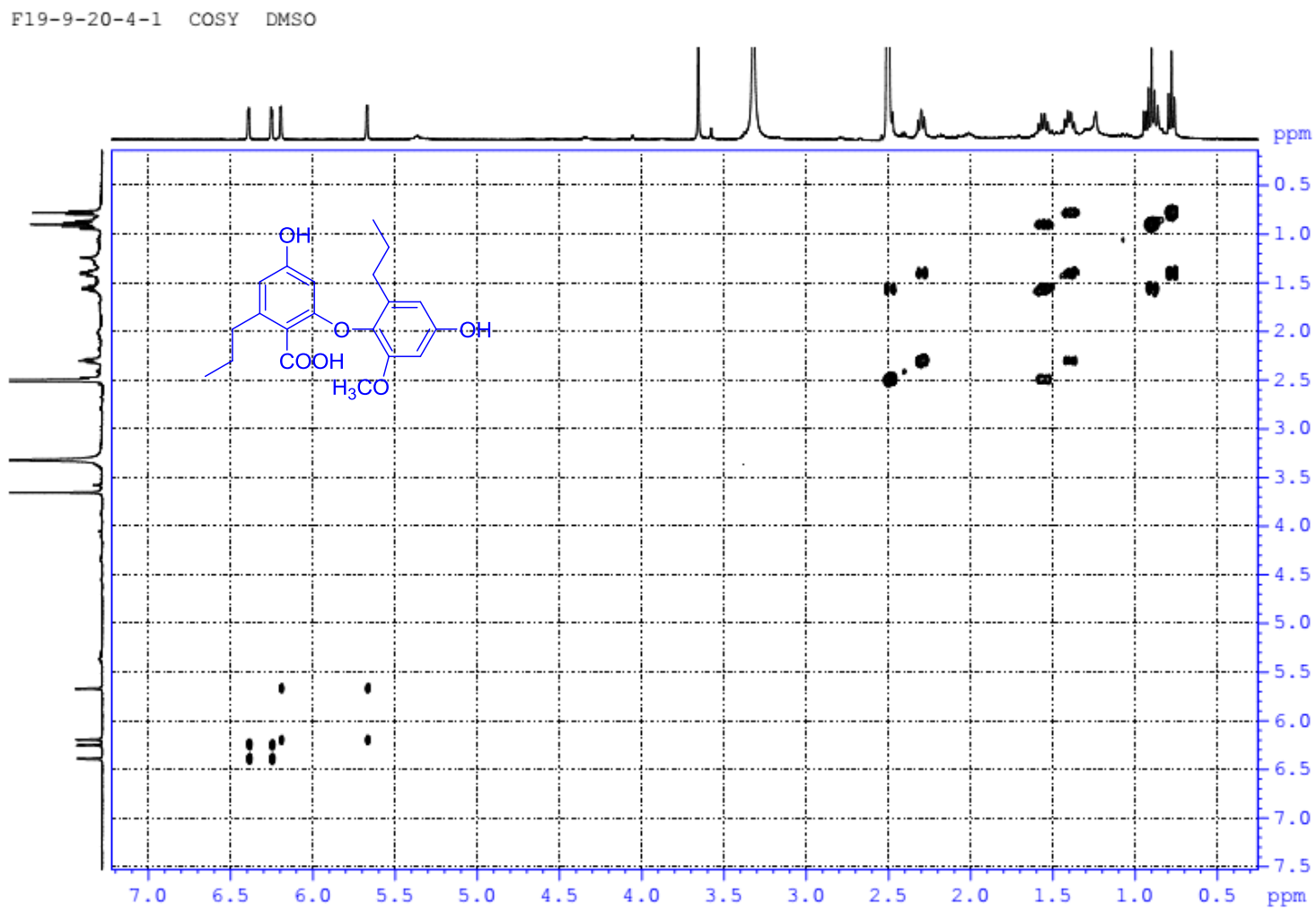


Figure S36. ¹H-¹H COSY spectrum of compound 5 in DMSO-d₆.

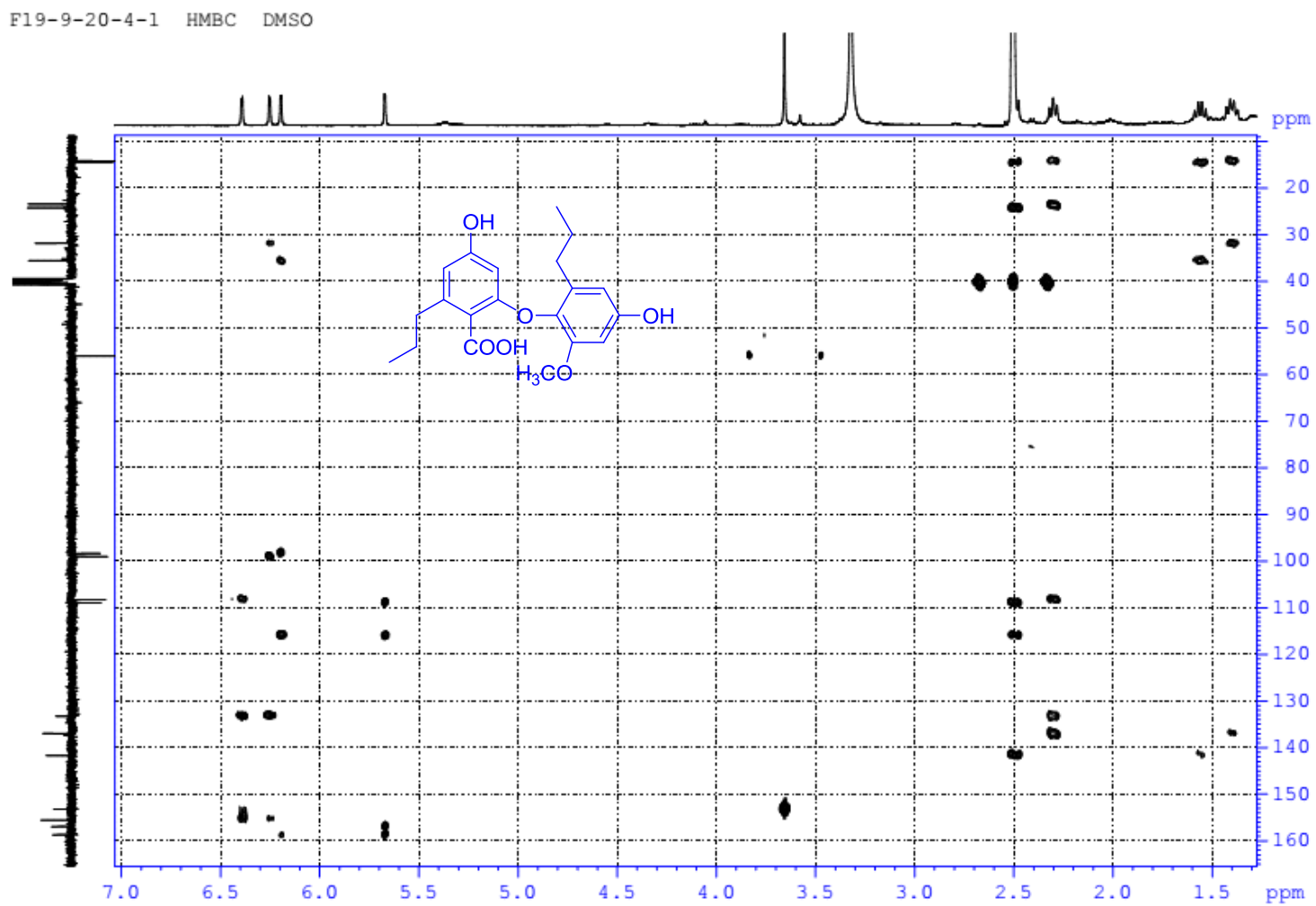


Figure S37. HMBC spectrum of compound 5 in DMSO-d₆.

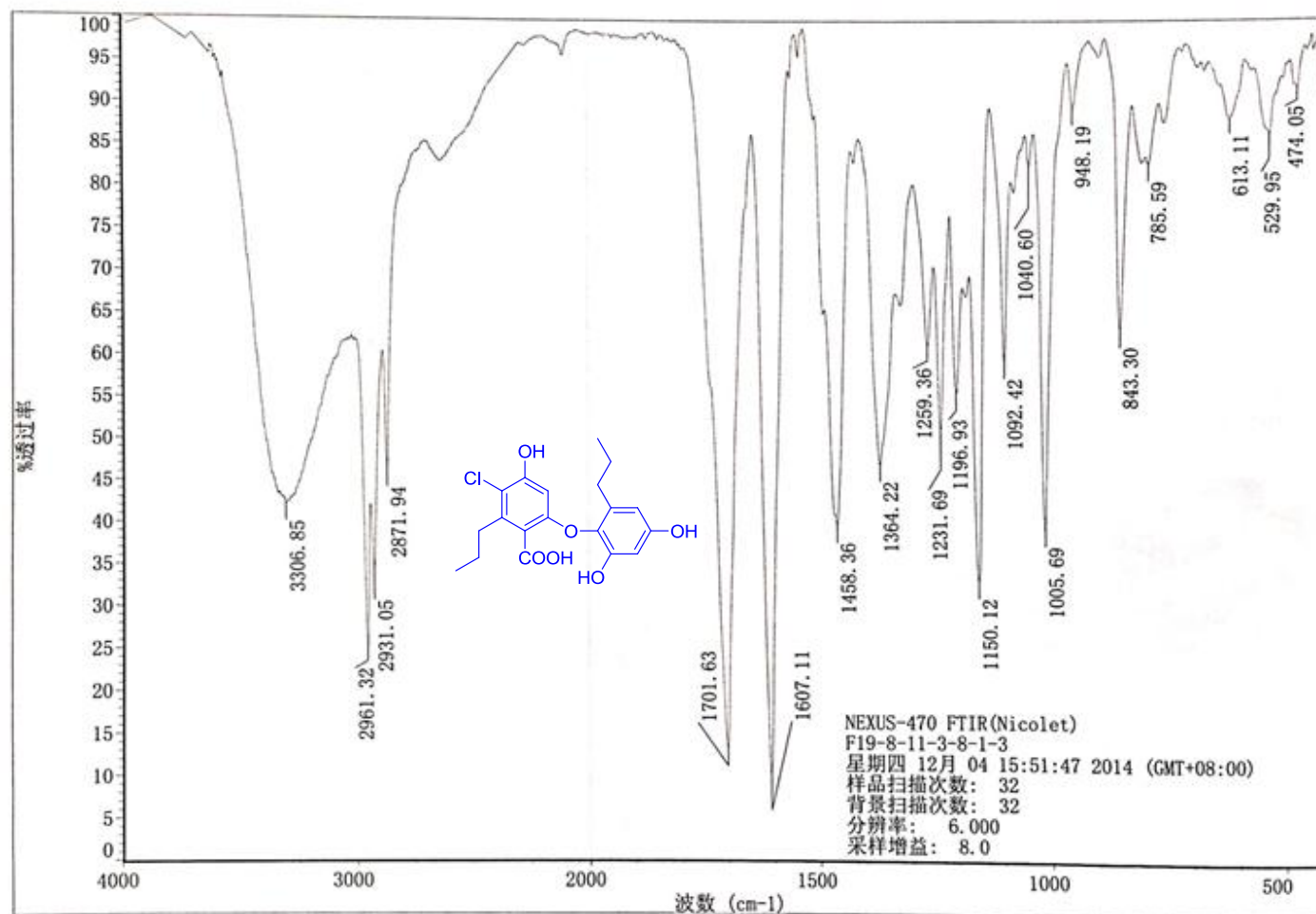


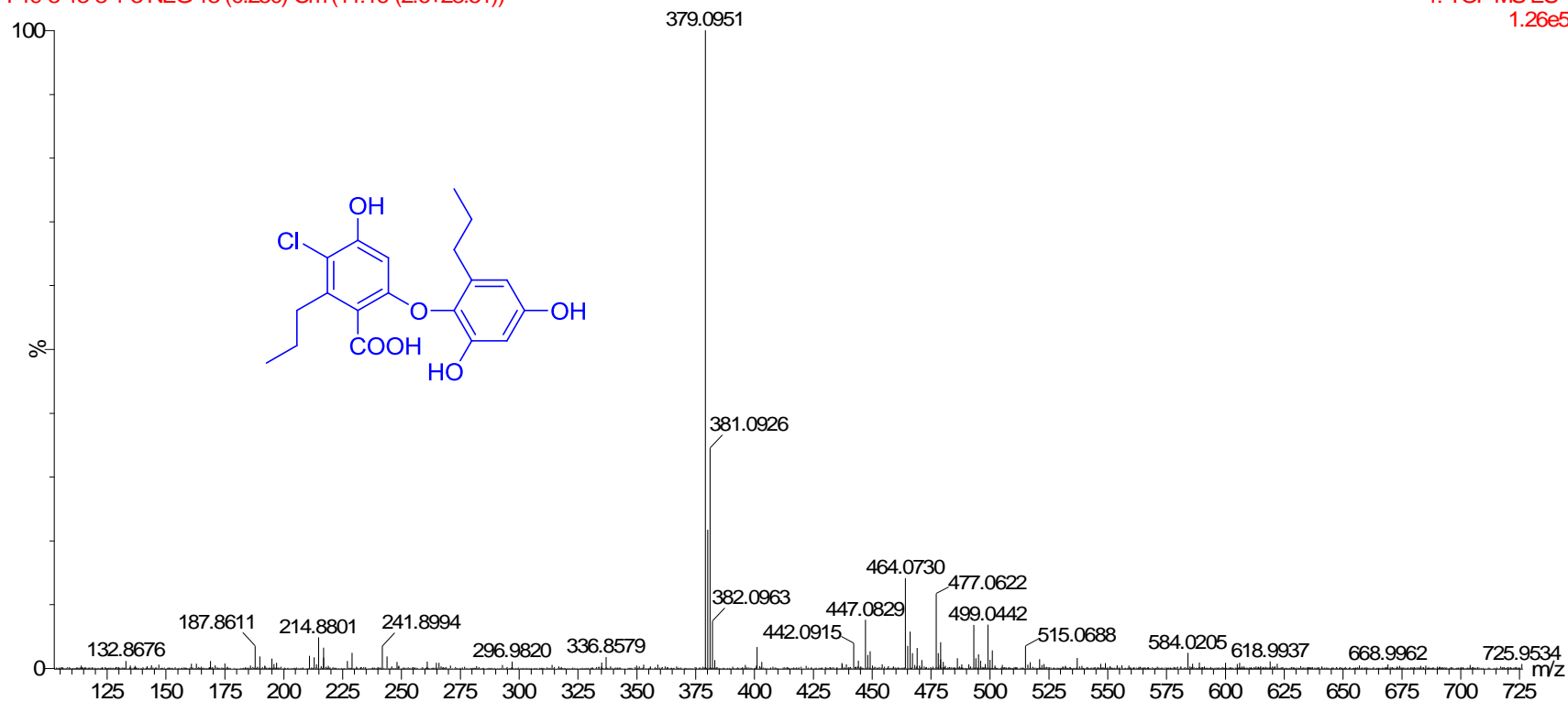
Figure S38. IR spectrum of compound 6.

Xevo G2 Q-TOF/YCA166#

02-Dec-2014

Waters

F19-8-13-8-1-3 NEG 13 (0.250) Cm (11:16-(2:6+28:51))

1: TOF MS ES-
1.26e5**Figure S39.** Negative mode HRESIMS data of compound 6.

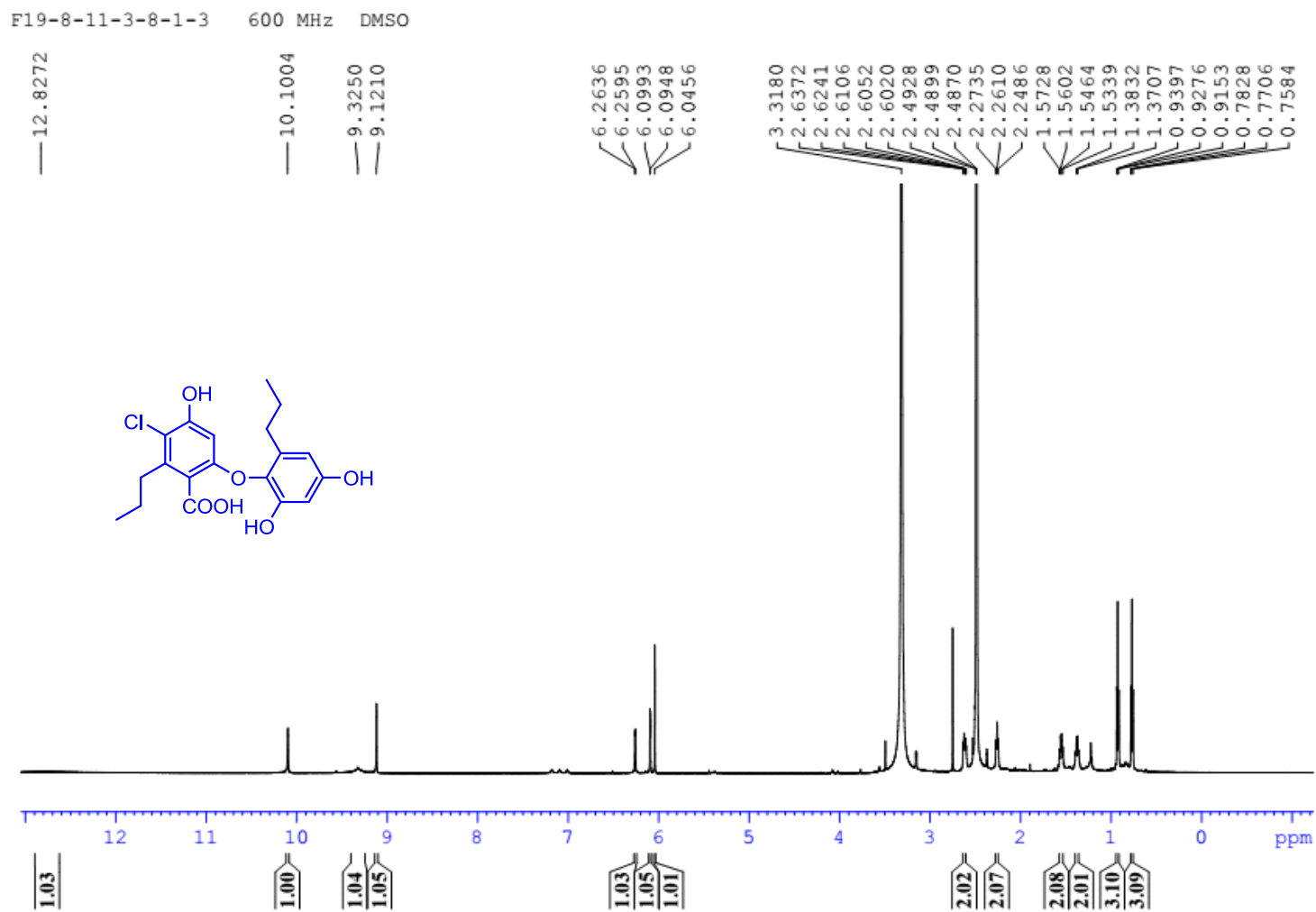


Figure S40. ^1H NMR spectrum of compound **6** in DMSO- d_6 (600 MHz).

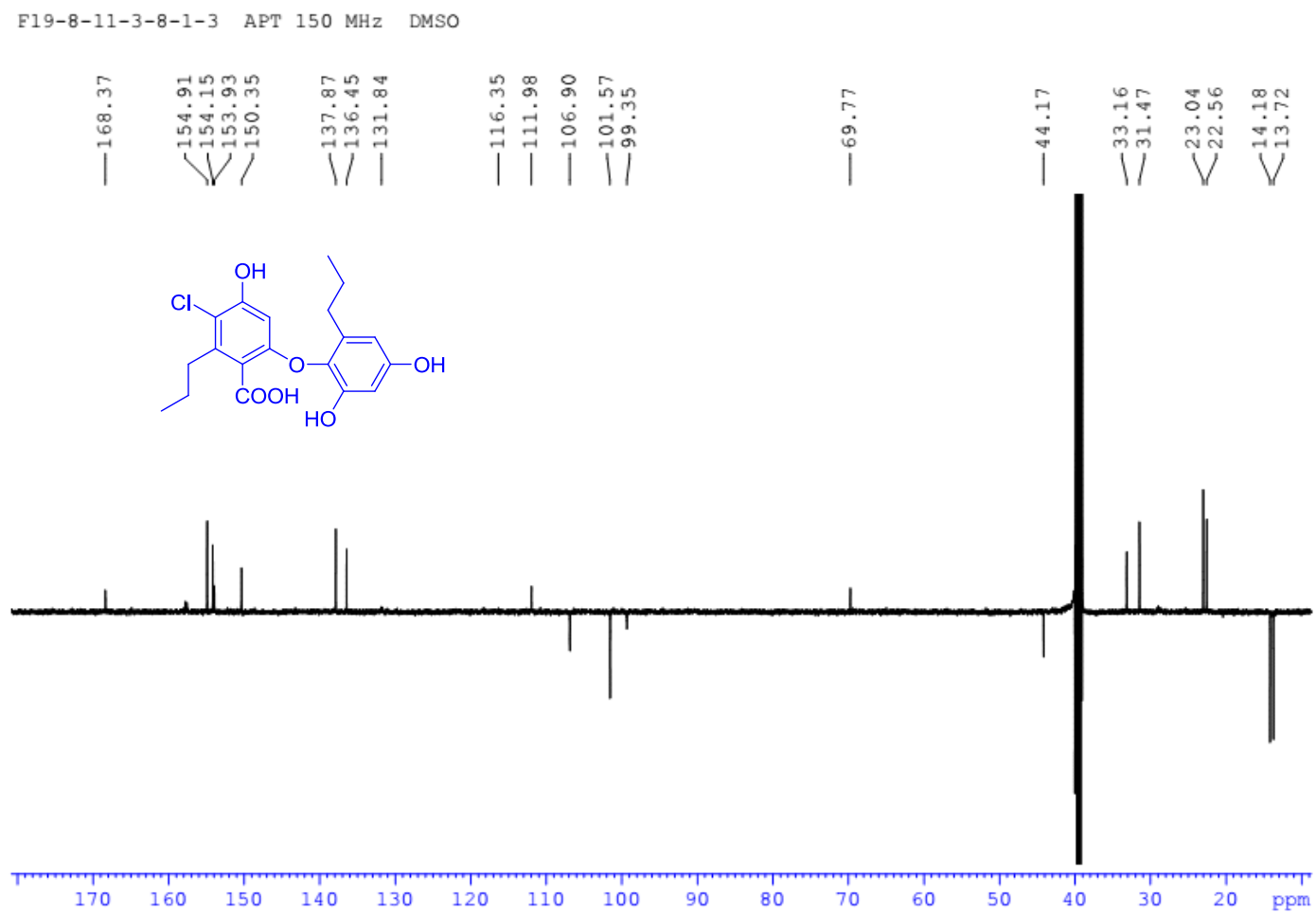


Figure S41. ^{13}C NMR spectrum of compound **6** in DMSO-d₆ (150 MHz).

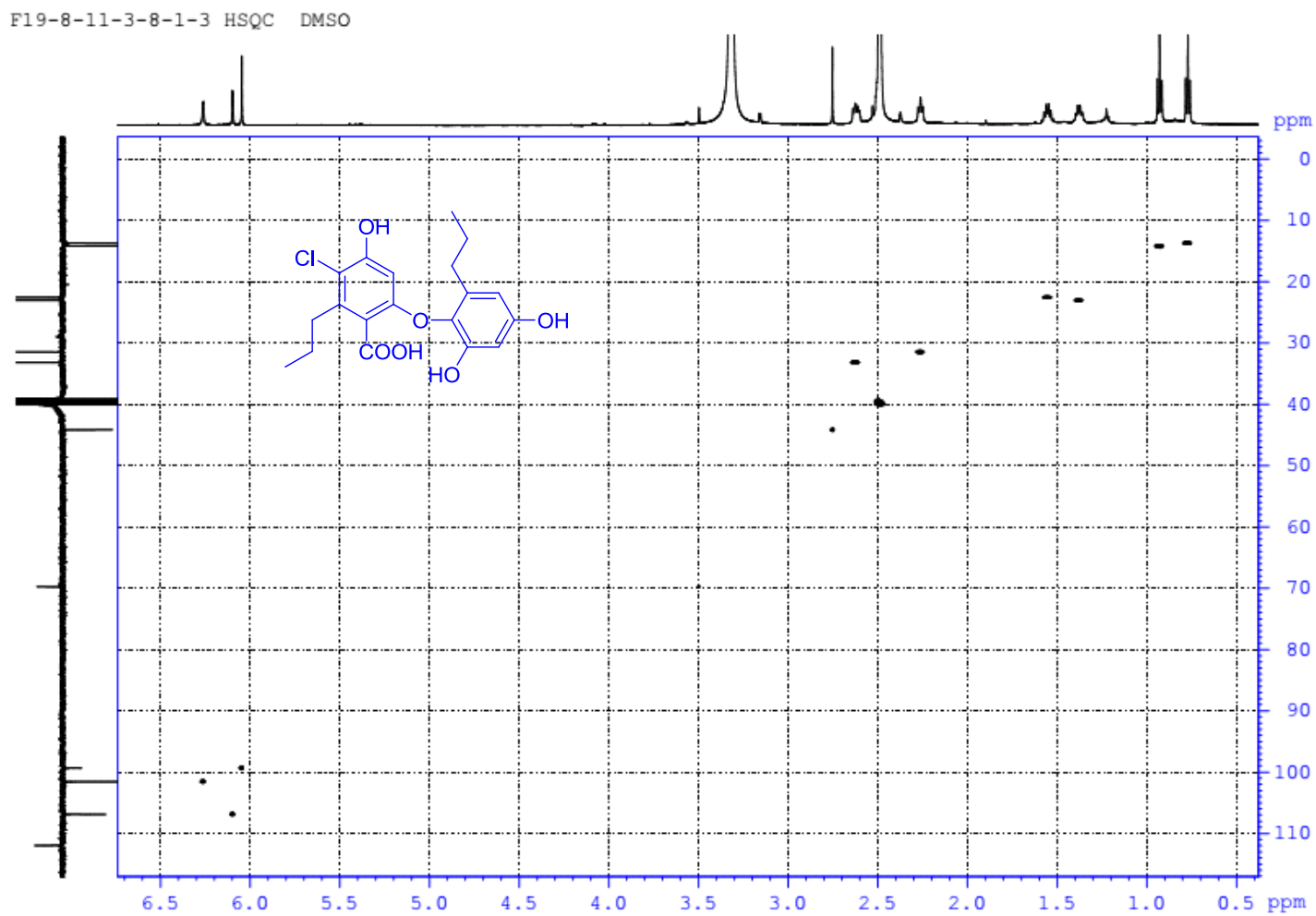


Figure S42. HSQC spectrum of compound 6 in DMSO-d6.

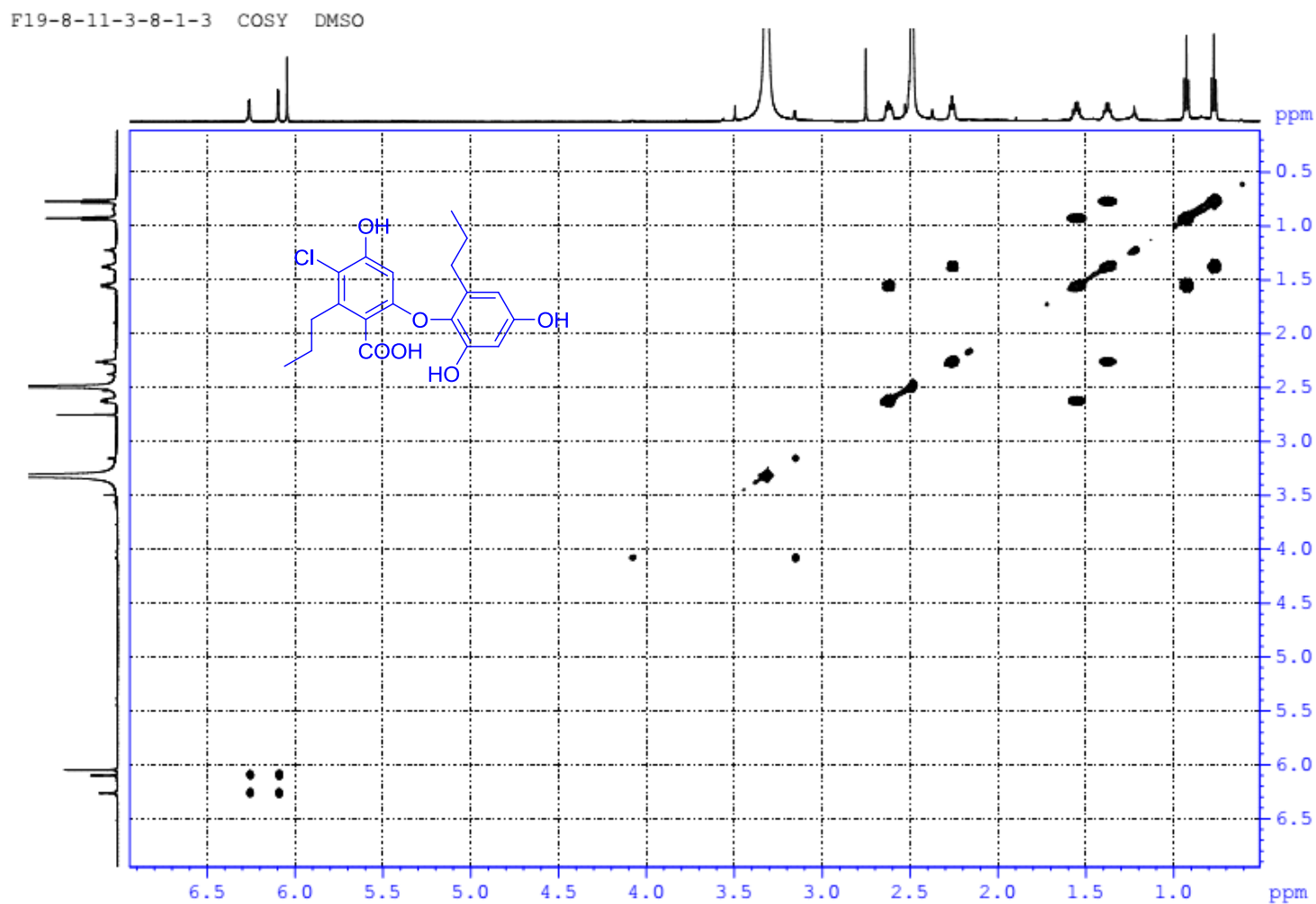


Figure S43. ^1H - ^1H COSY spectrum of compound **6** in DMSO- d_6 .

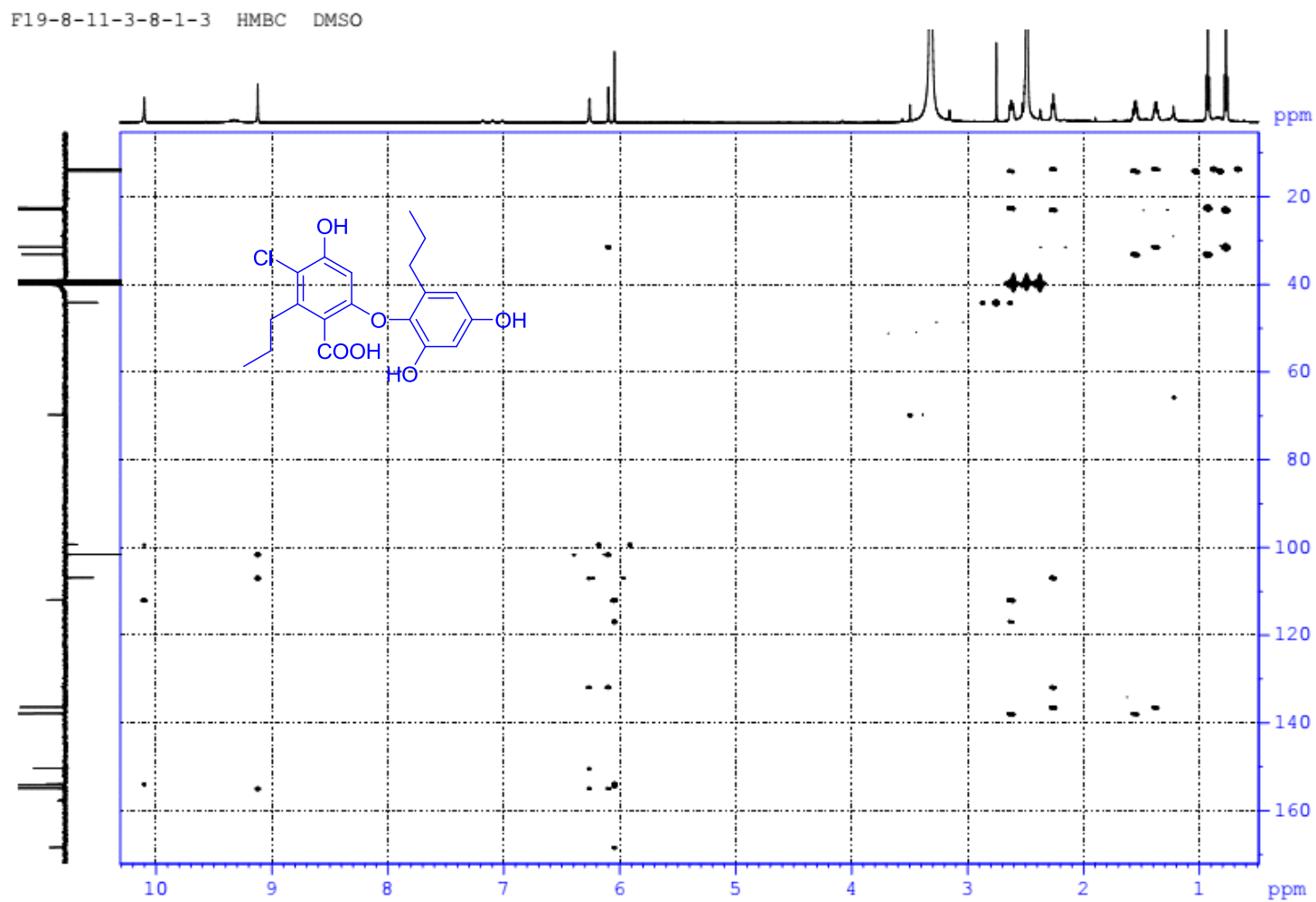


Figure S44. HMBC spectrum of compound 6 in DMSO-d6.

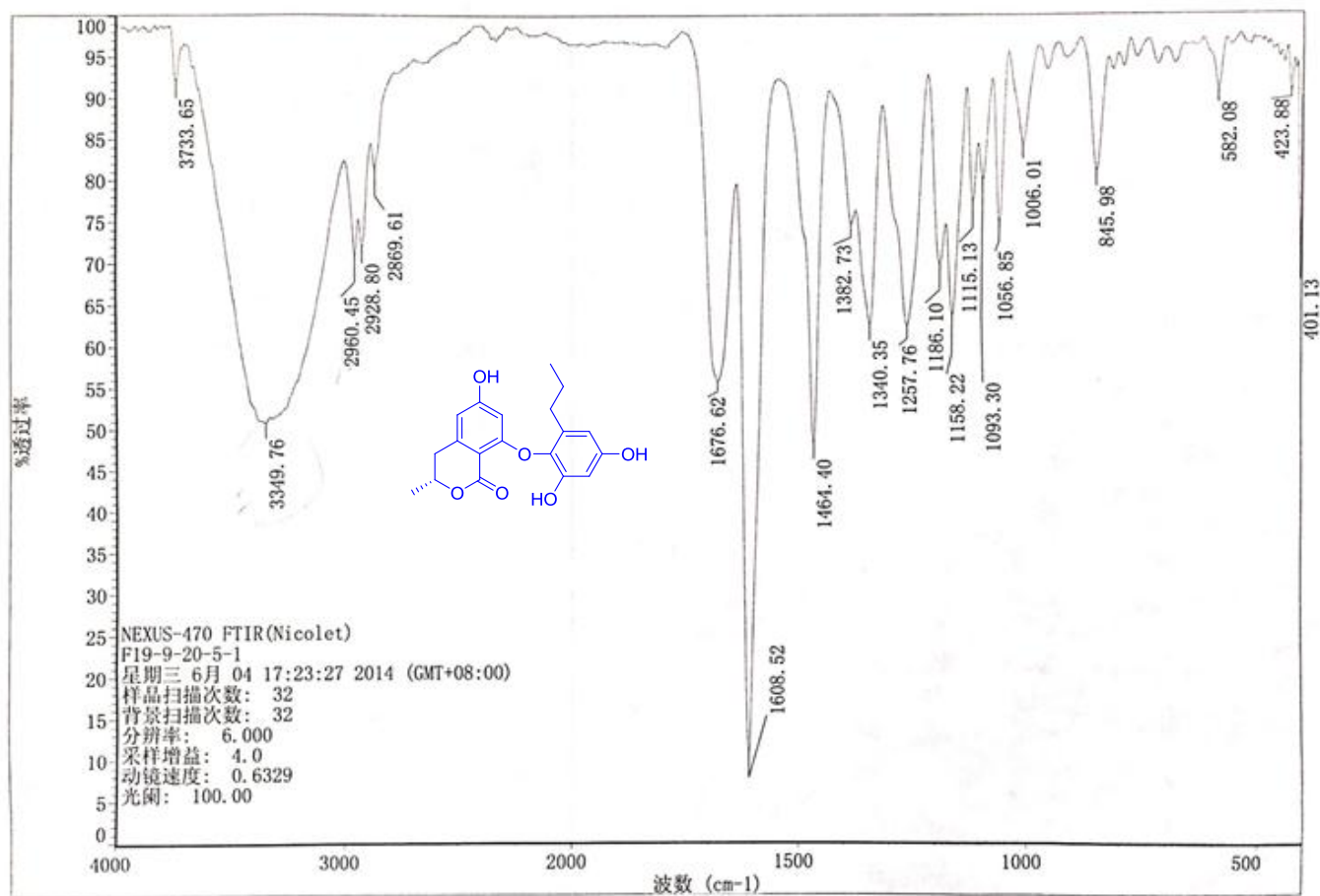


Figure S45. IR spectrum of compound 7.

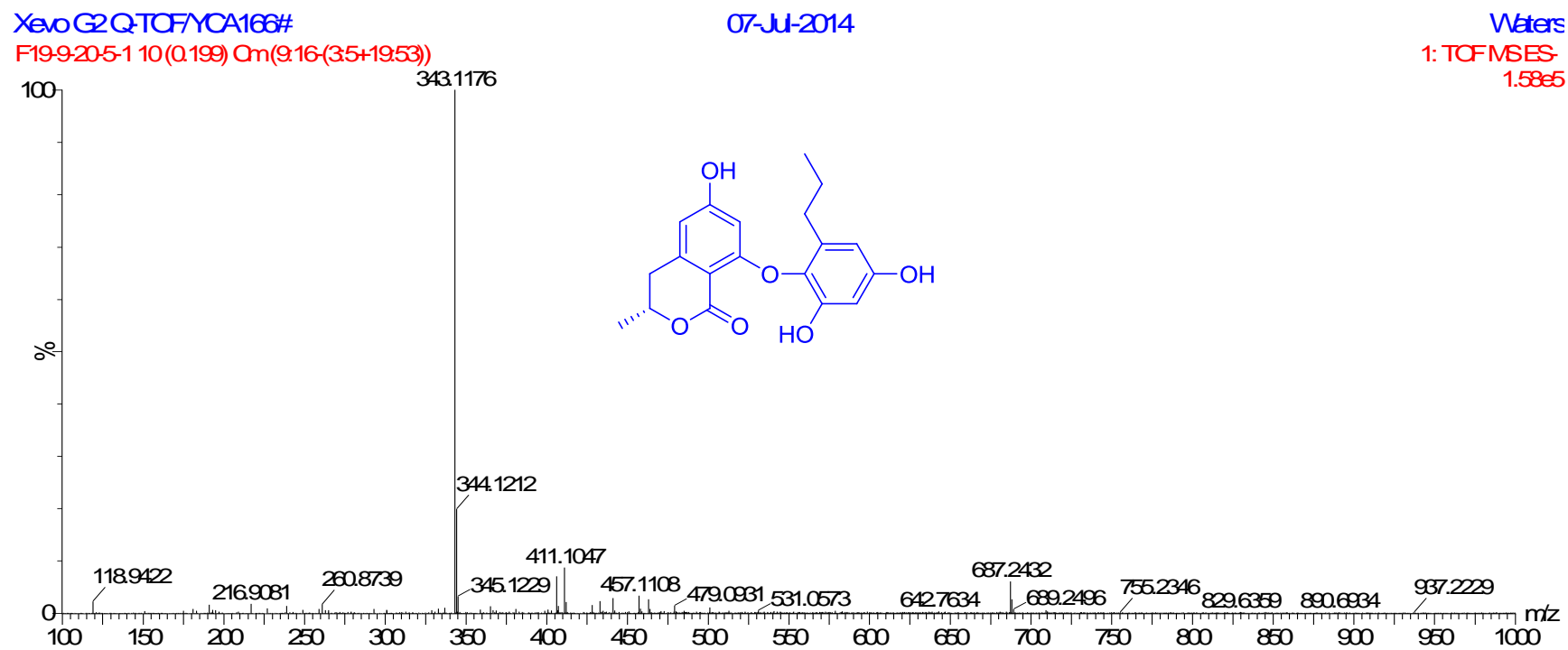


Figure S46. Negative mode HRESIMS data of compound 7.

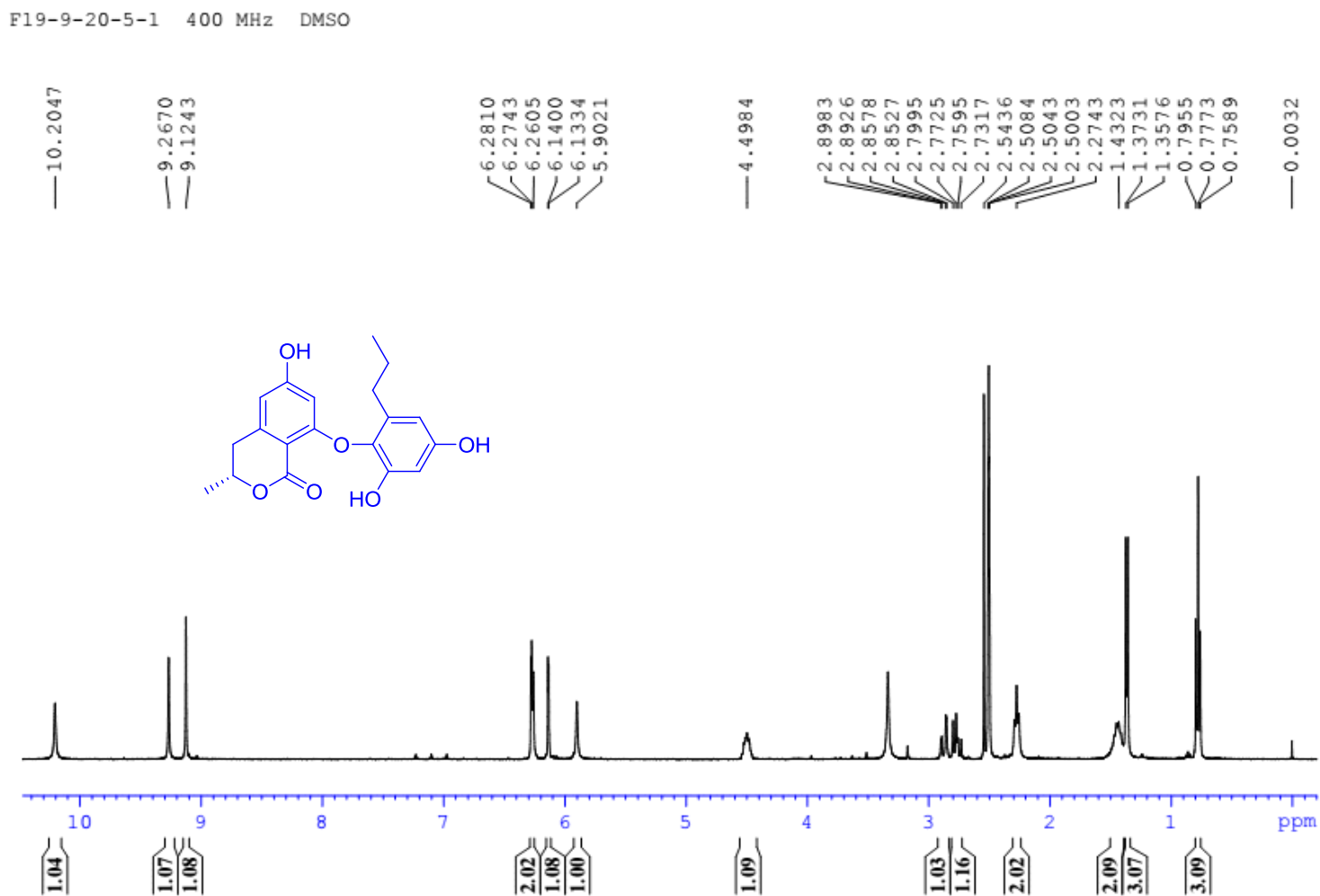


Figure S47. ^1H NMR spectrum of compound 7 in DMSO- d_6 (400 MHz).

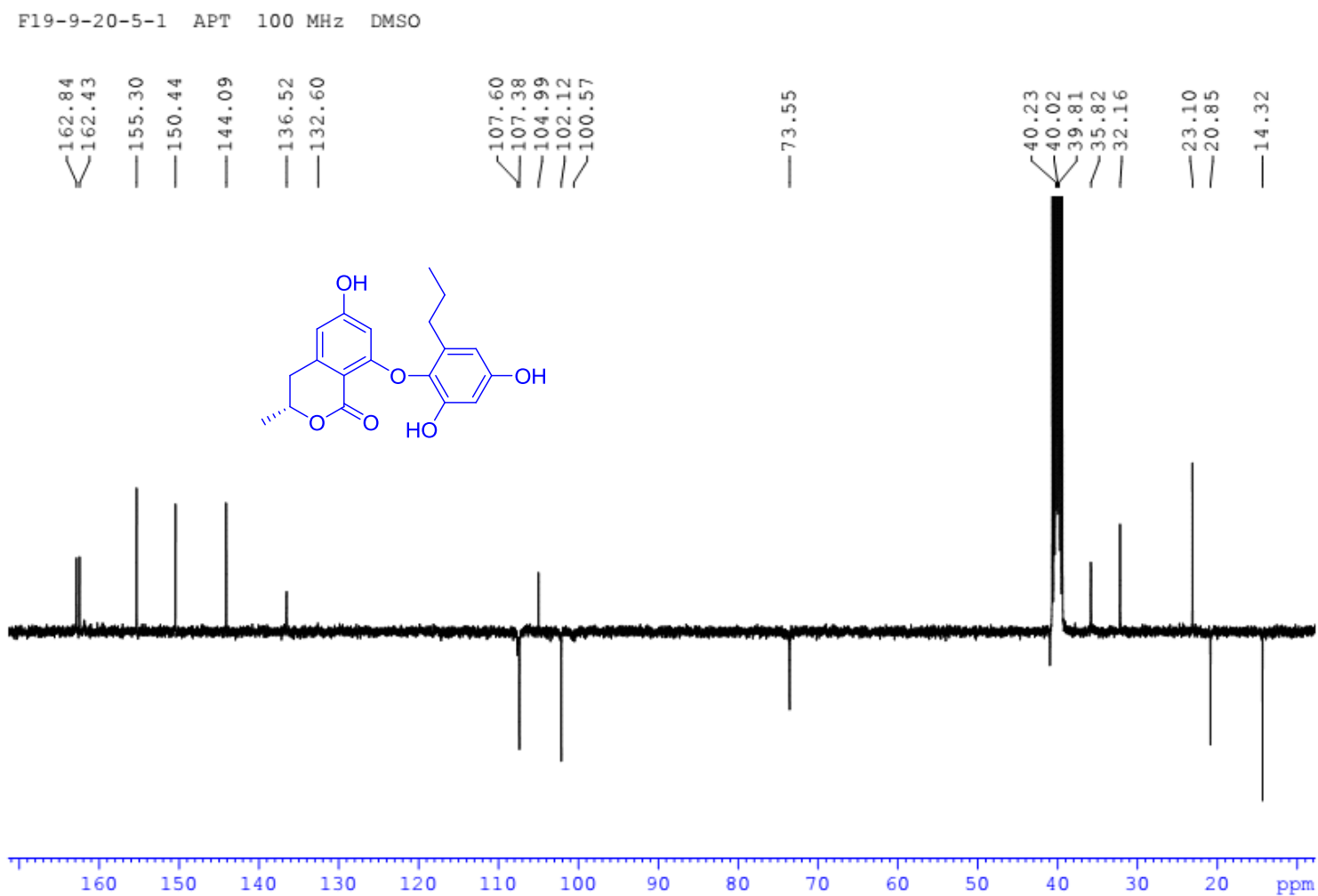


Figure S48. ^{13}C NMR spectrum of compound 7 in DMSO-d₆ (100 MHz).

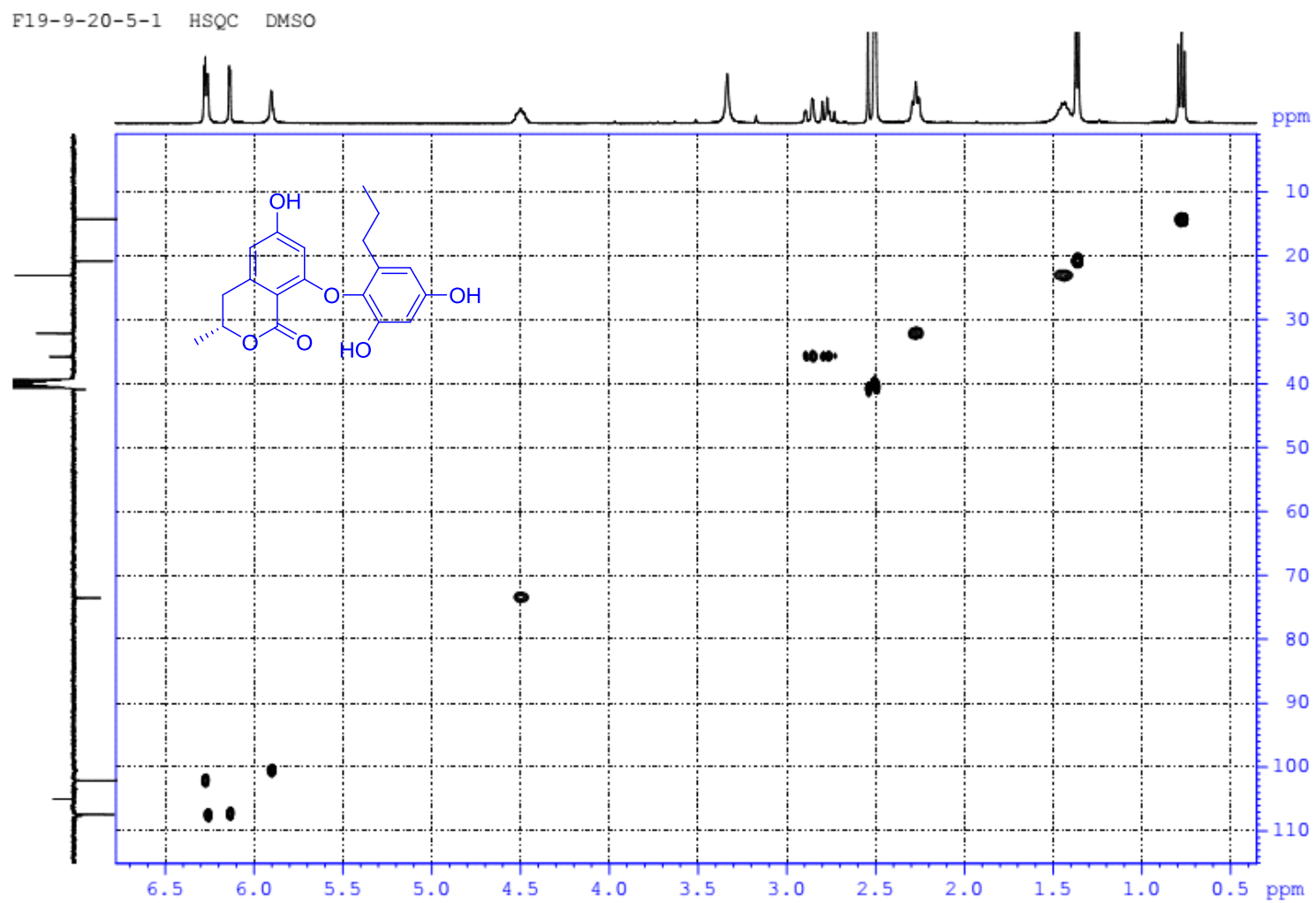


Figure S49. HSQC spectrum of compound 7 in DMSO-d₆.

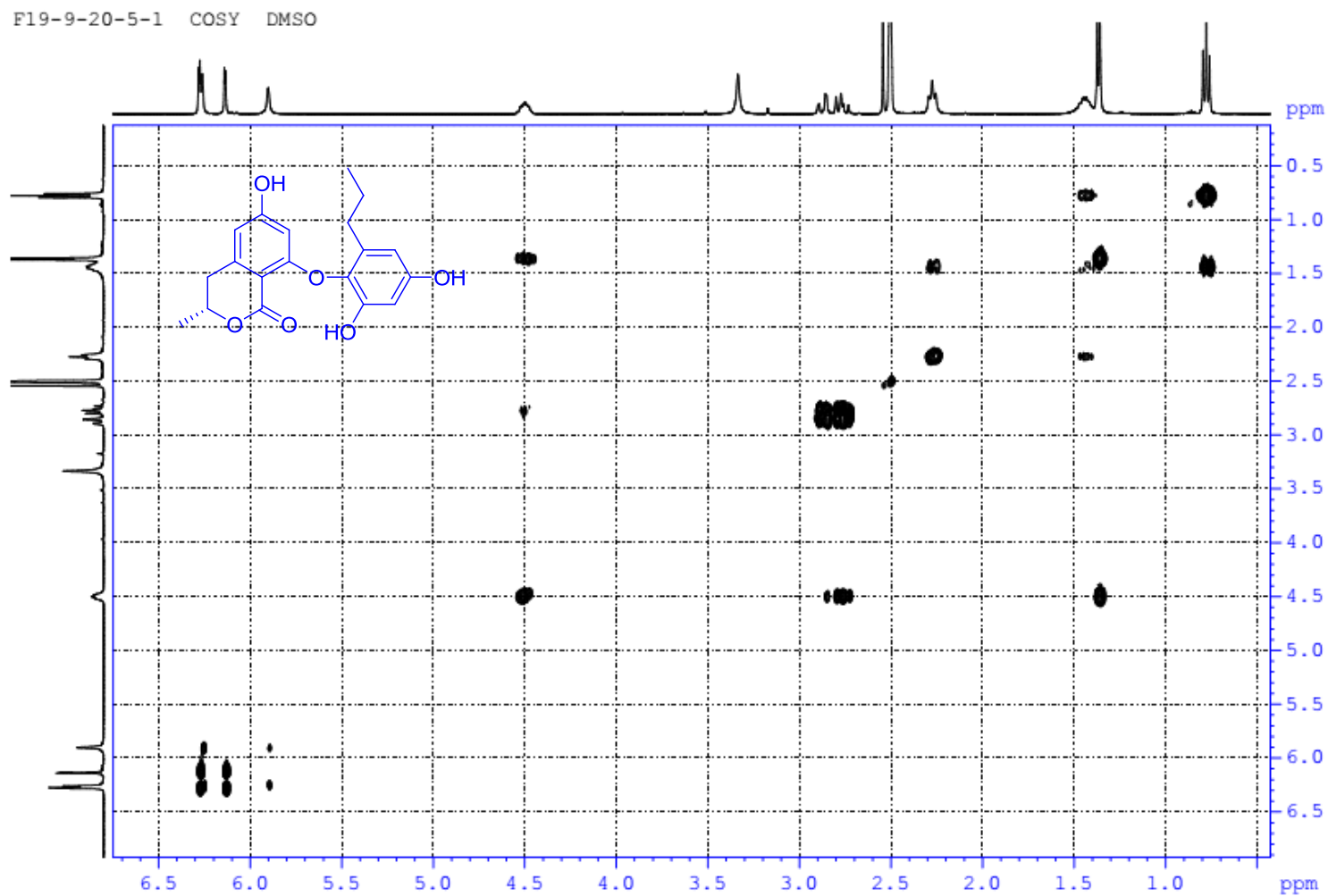


Figure S50. ¹H-¹H COSY spectrum of compound 7 in DMSO-d₆.

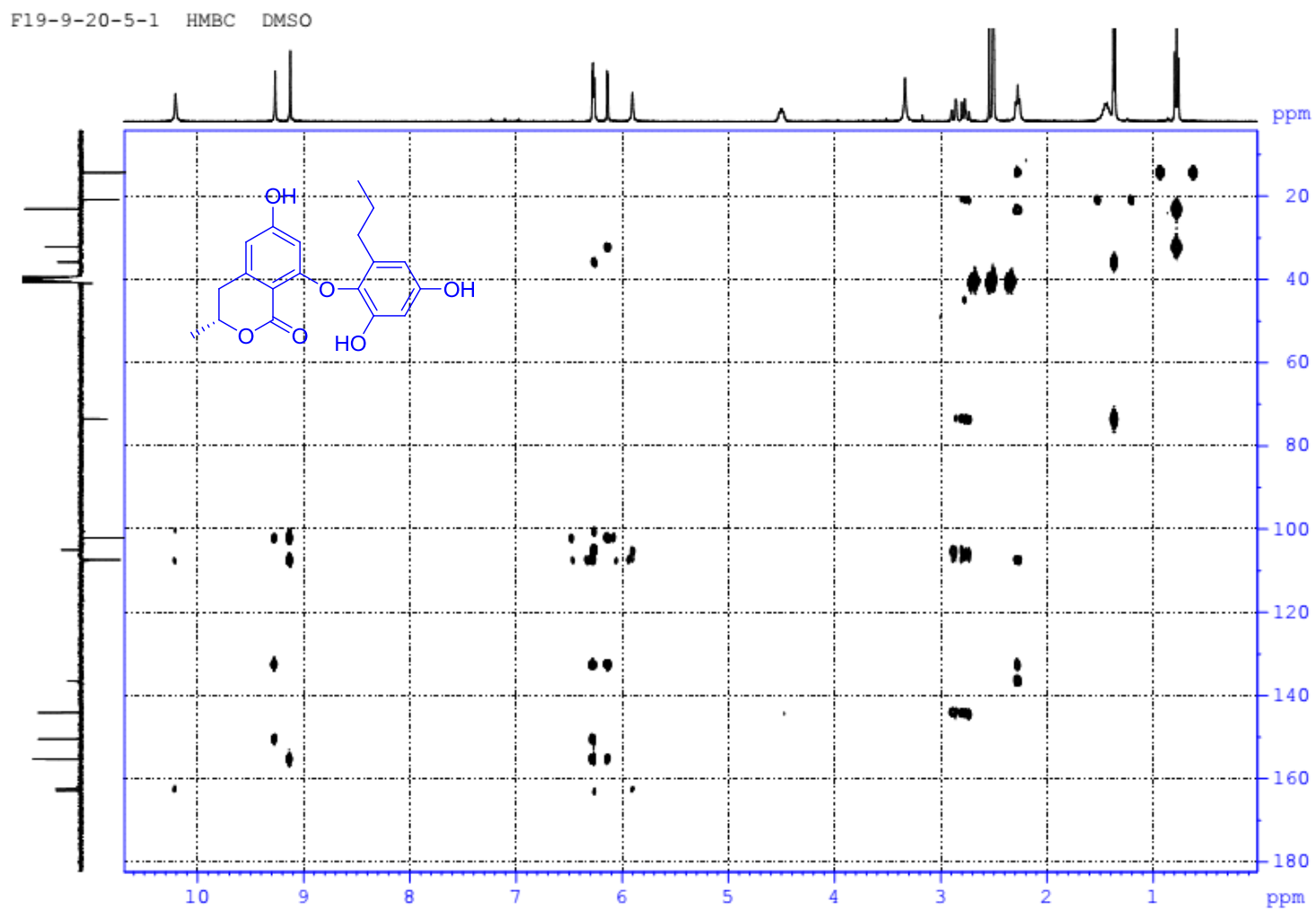


Figure S51. HMBC spectrum of compound 7 in DMSO-d₆.

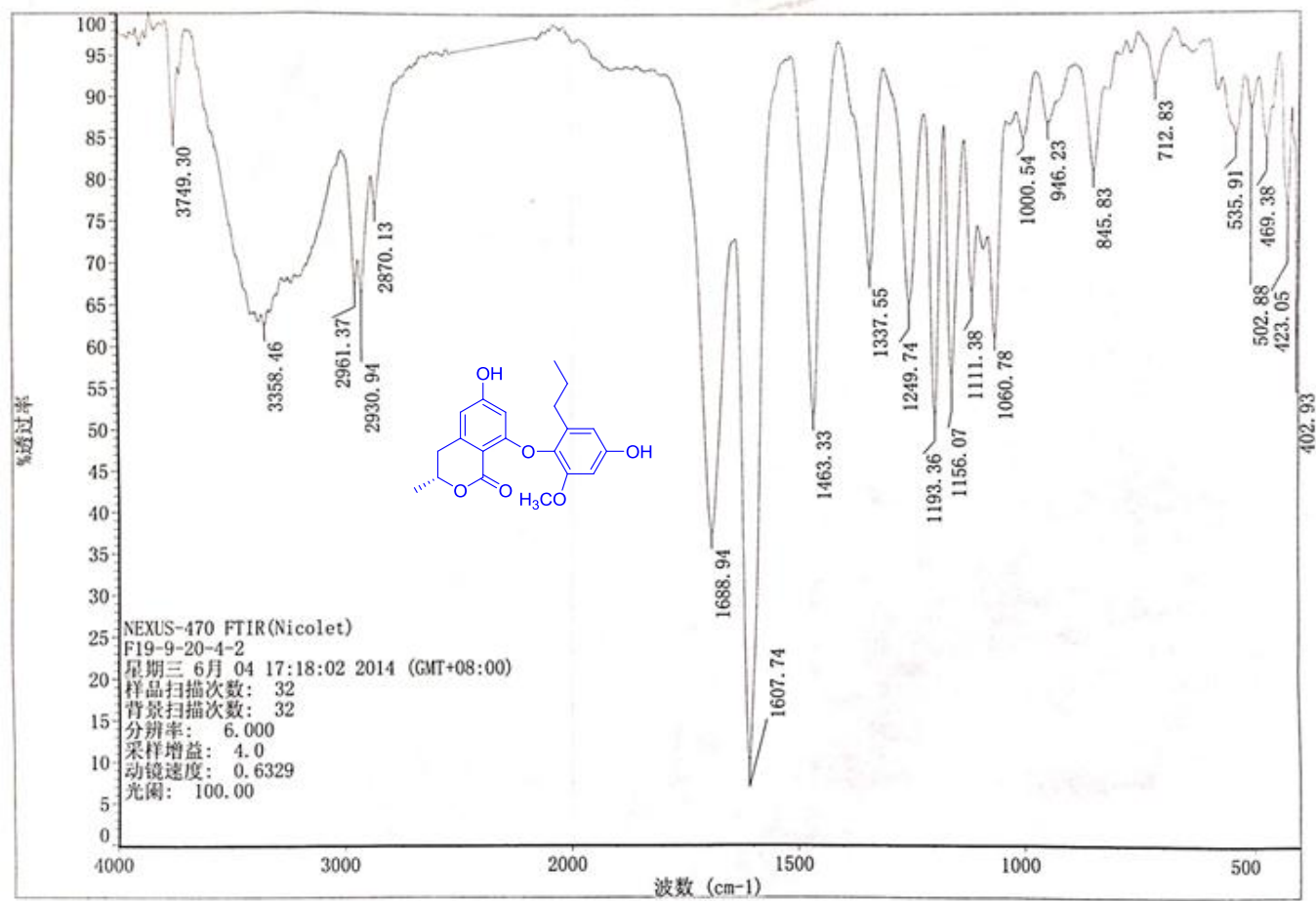


Figure S52. IR spectrum of compound 8.

Xevo G2 Q-TOF/YCA166#

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Waters

F19-9-20-4-2 10 (0.199) Cm (10:19-(36+21:53))

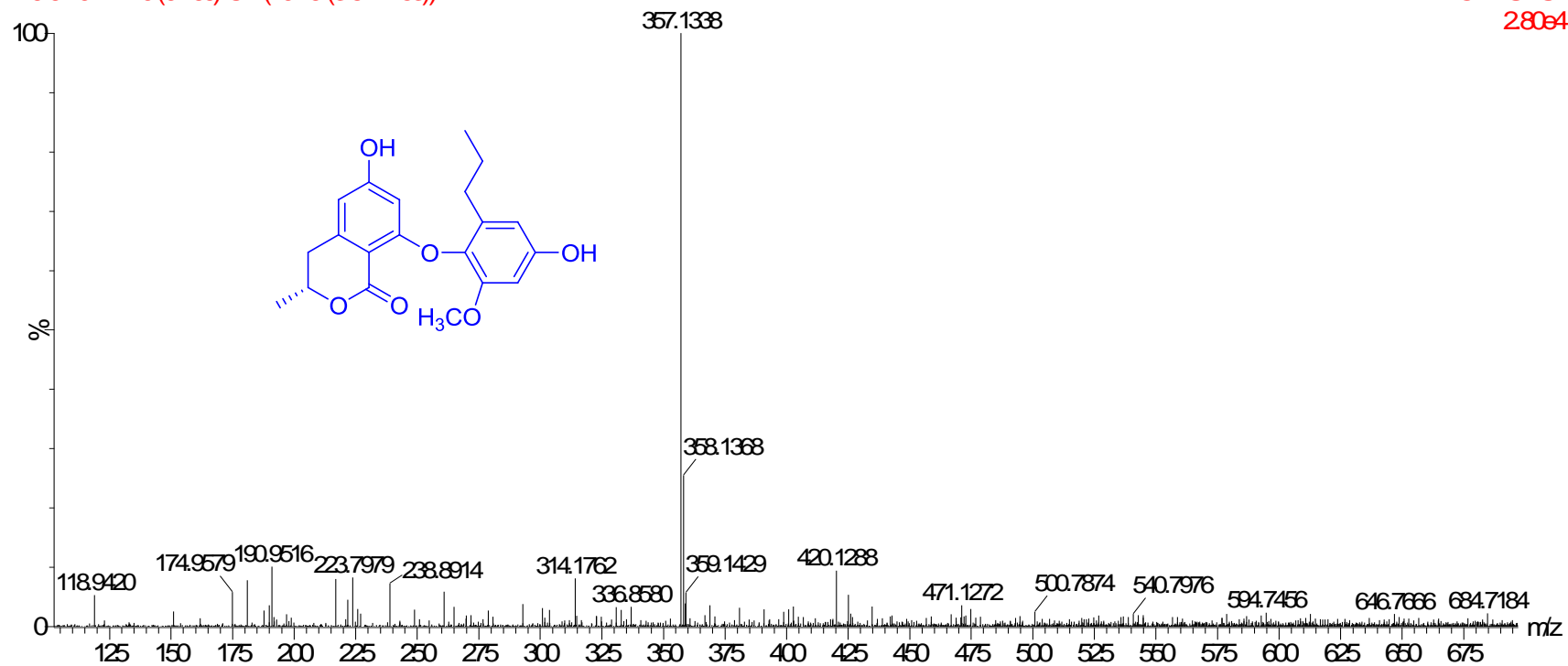
1: TOF MS ES-
280.4

Figure S53. Negative mode HRESIMS data of compound 8.

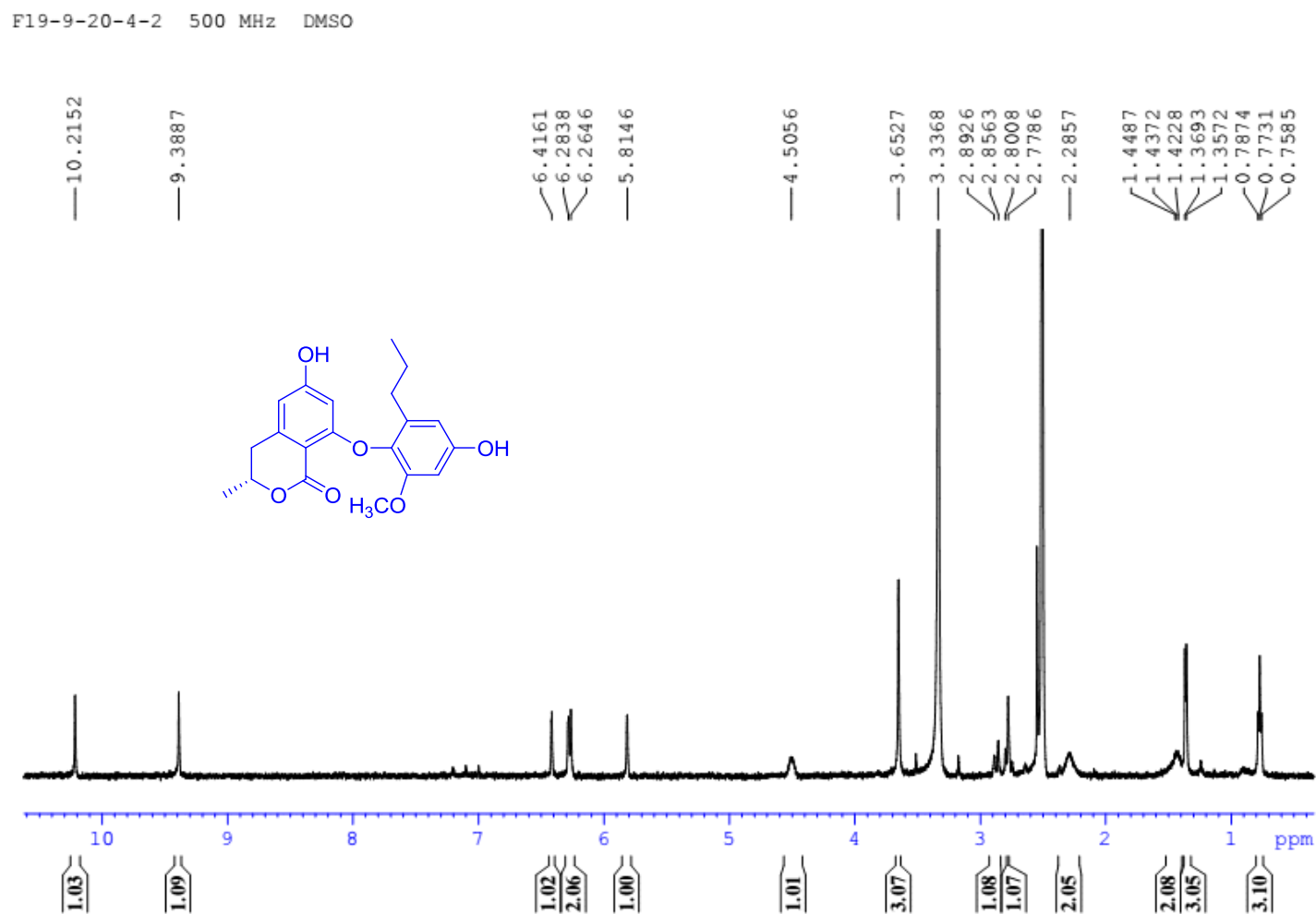


Figure S54. ^1H NMR spectrum of compound **8** in DMSO- d_6 (500 MHz).

F19-9-20-4-2 APT 125 MHz DMSO

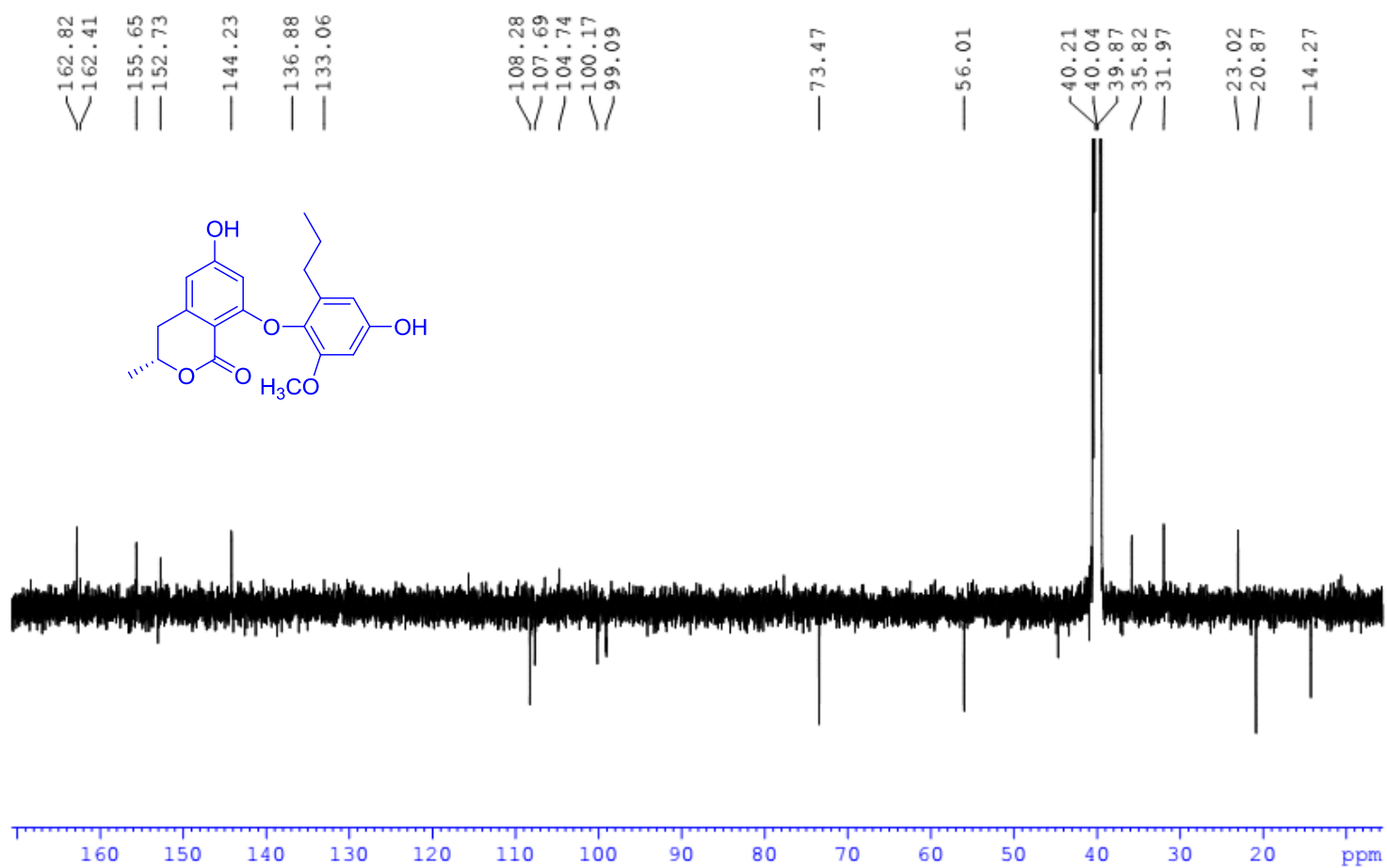


Figure S55. ¹³C NMR spectrum of compound 8 in DMSO-d₆ (125 MHz).

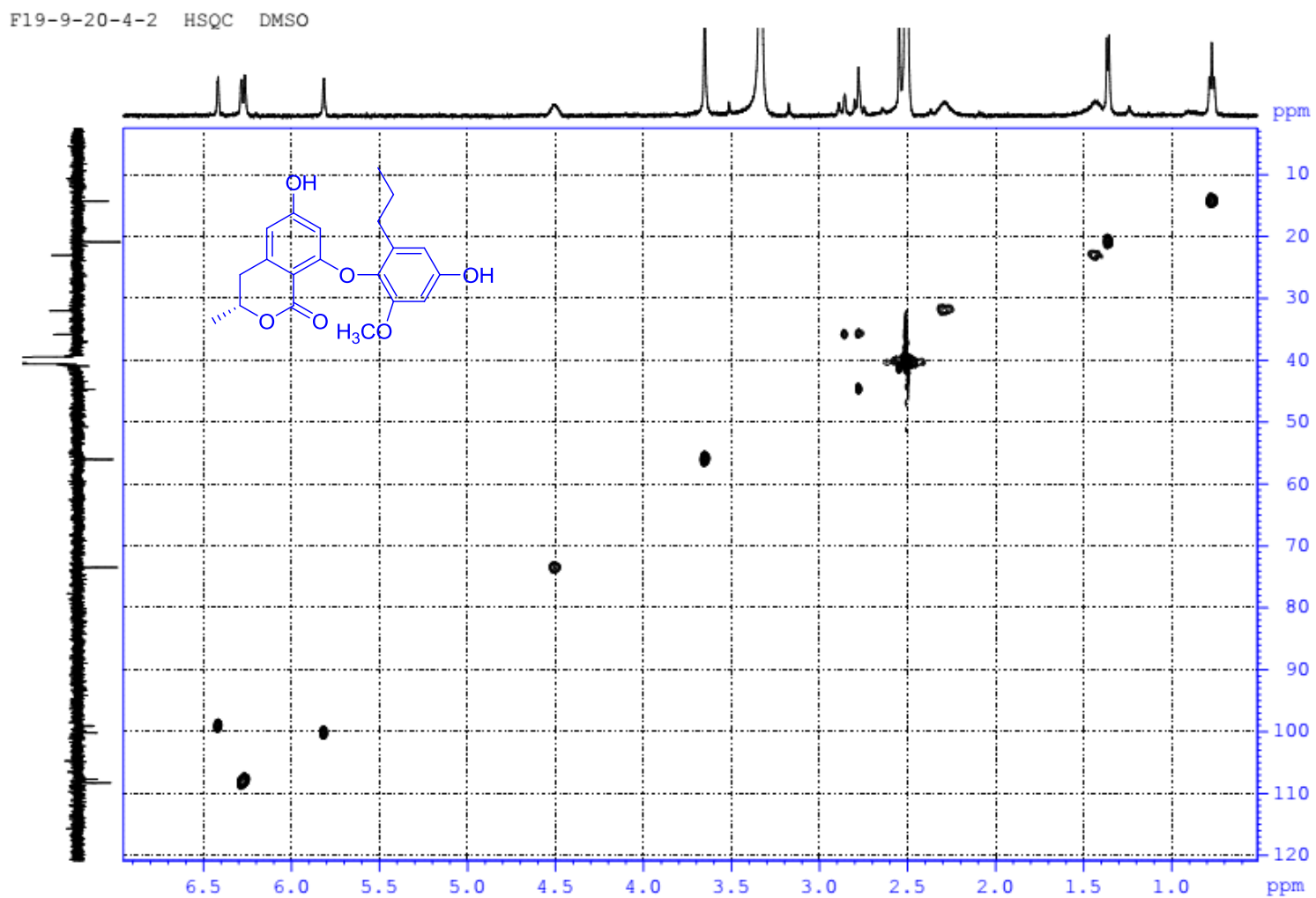


Figure S56. HSQC spectrum of compound **8** in DMSO-d₆.

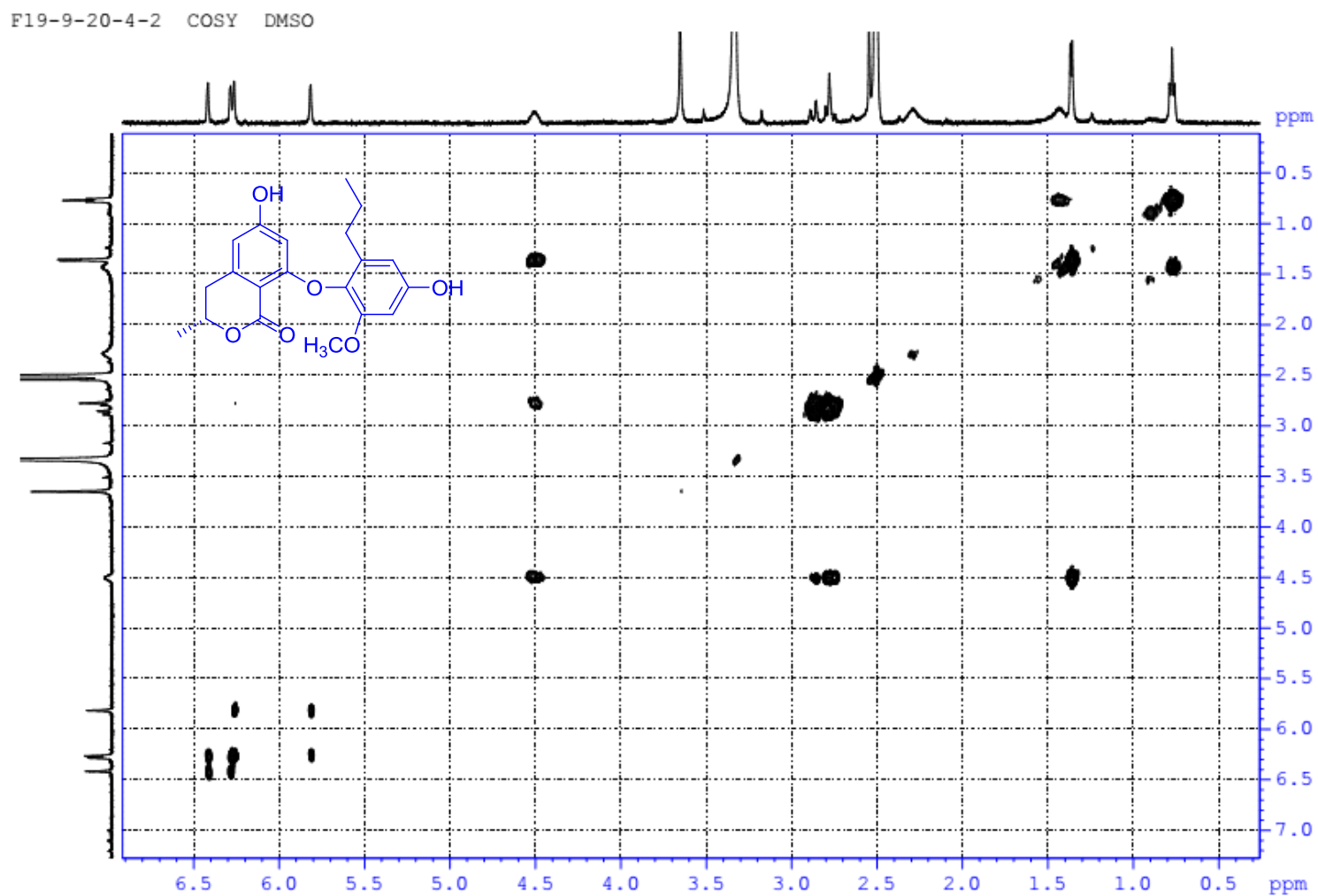


Figure S57. ^1H - ^1H COSY spectrum of compound 8 in DMSO- d_6 .

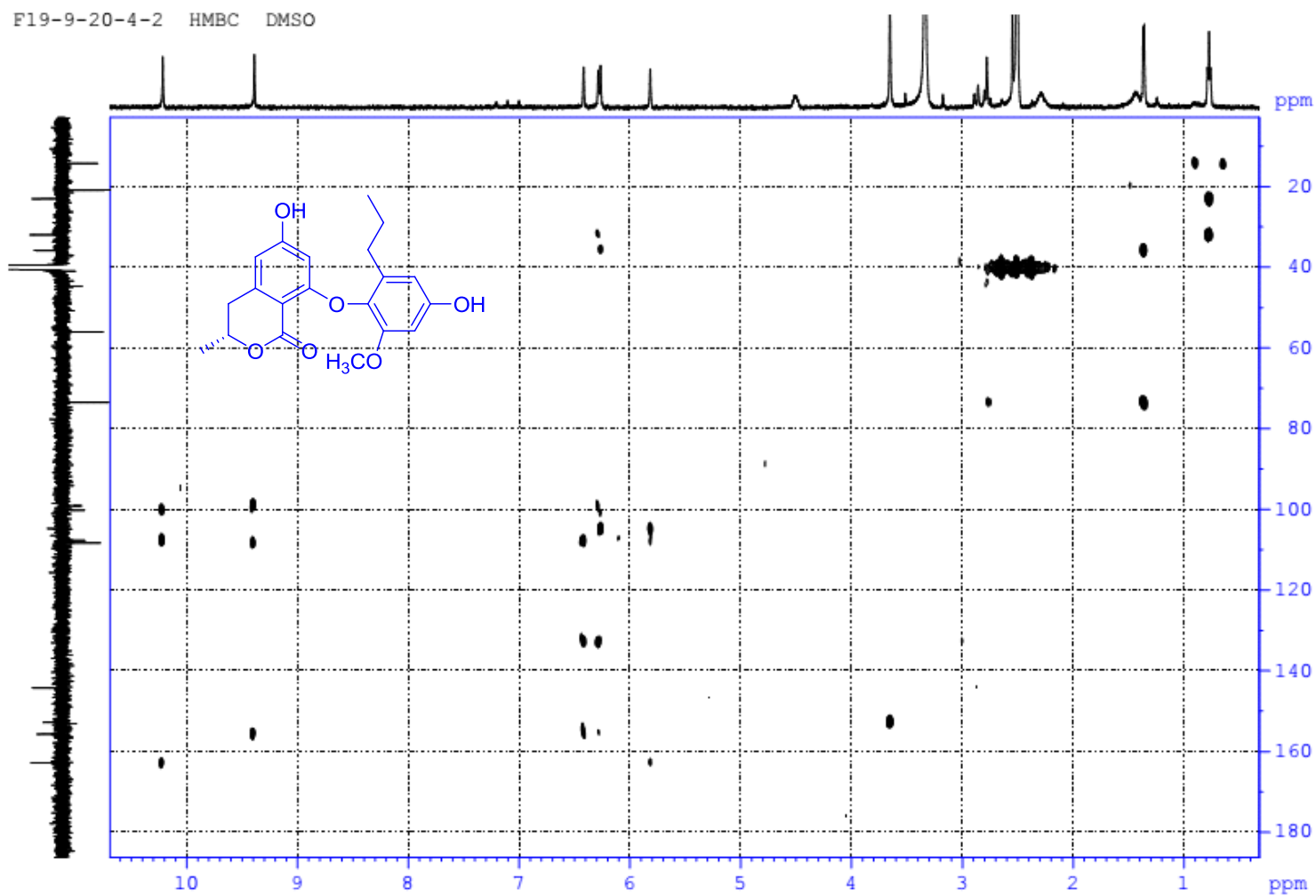


Figure S58. HMBC spectrum of compound 8 in DMSO-d₆.

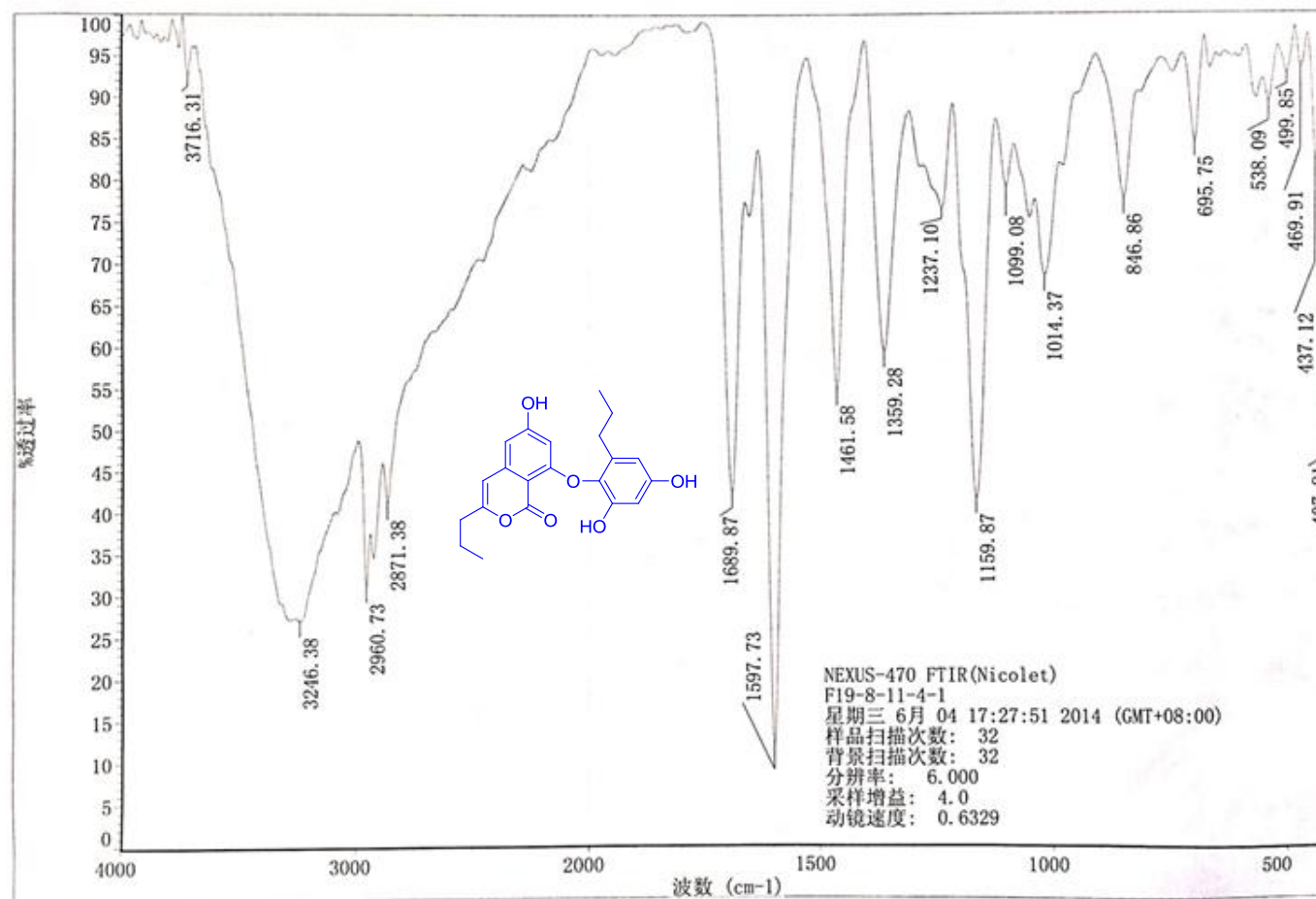


Figure S59. IR spectrum of compound 9.

Xevo G2 Q.TOF/YCA166#

07-Jul-2014

Waters

F198-11-4-1 10(0.199) Cm(10:16-(36+24:54))

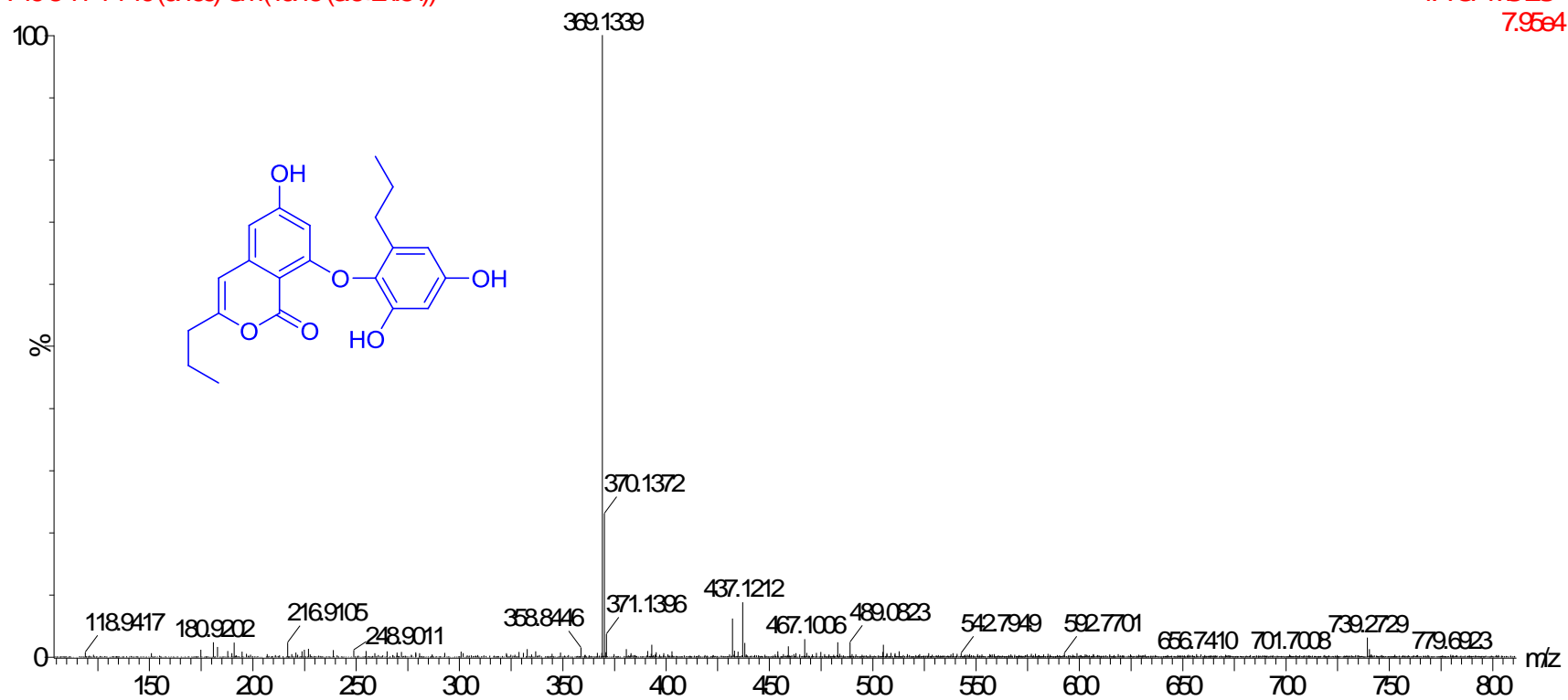
1: TCFMSES
7.95e4

Figure S60. Negative mode HRESIMS data of compound 9.

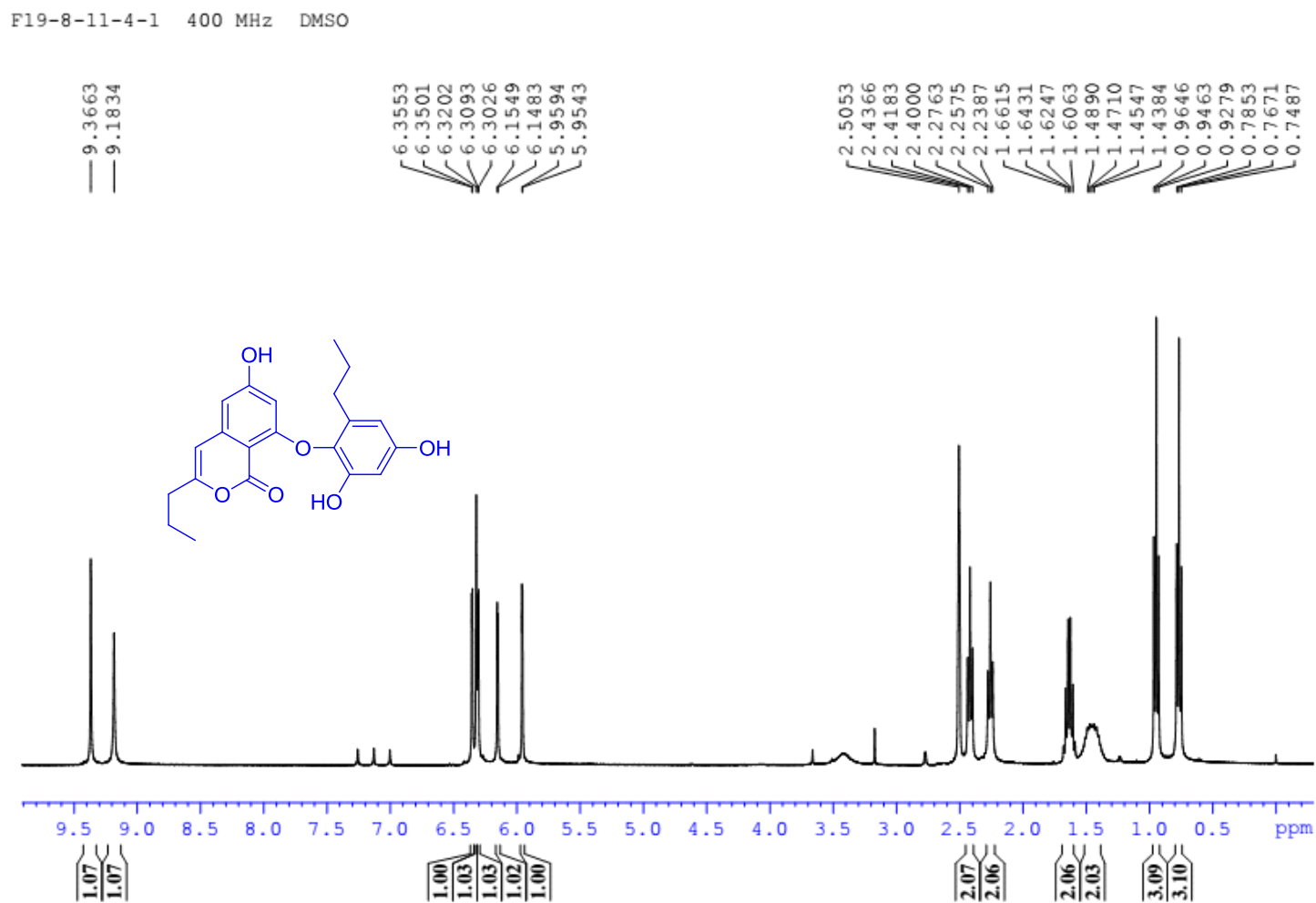


Figure S61. ^1H NMR spectrum of compound **9** in DMSO- d_6 (400 MHz).

F19-8-11-4-1 APT 100 MHz DMSO

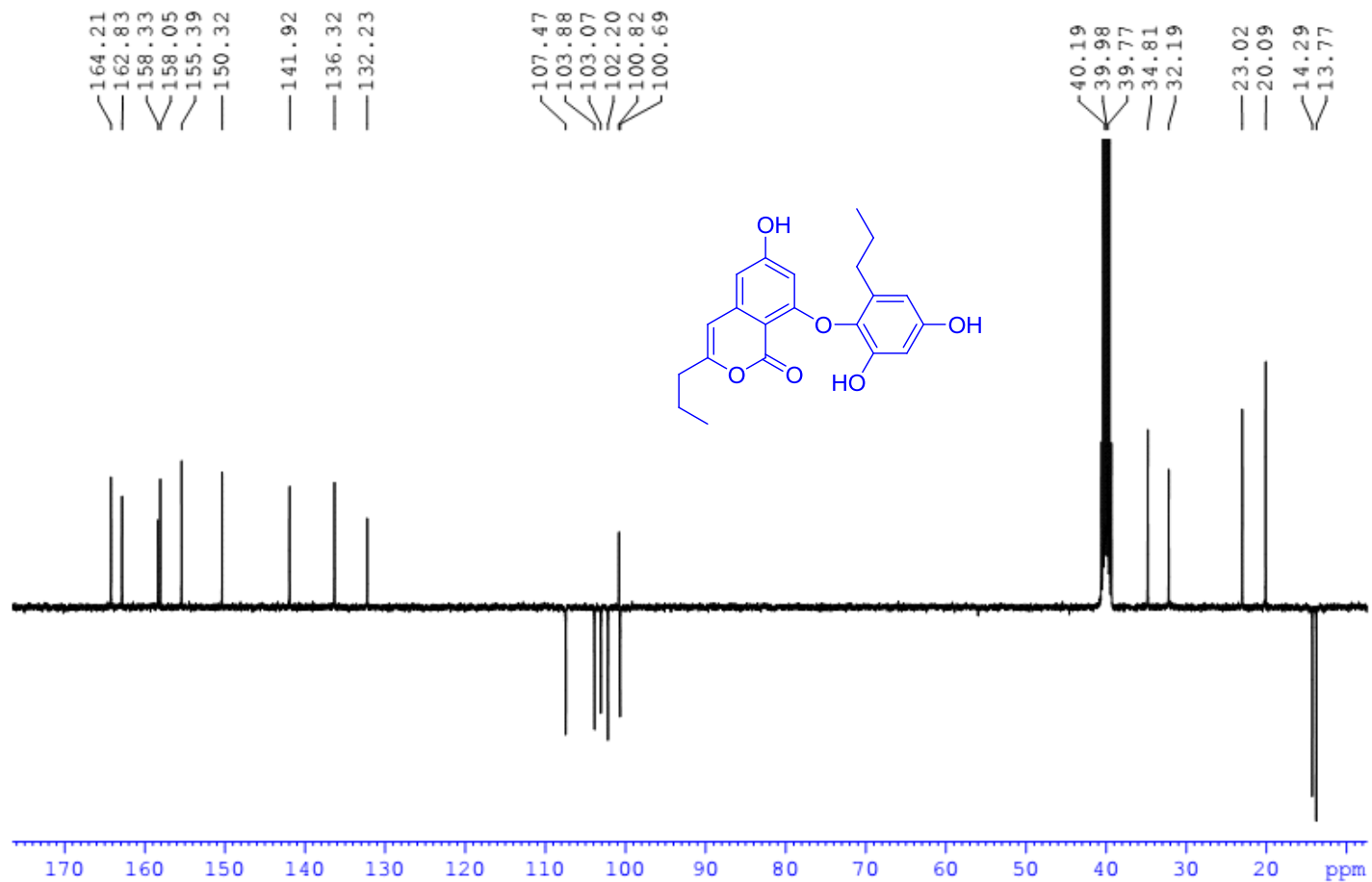


Figure S62. ¹³C NMR spectrum of compound 9 in DMSO-d₆ (100 MHz).

F19-8-11-4-1 HSQC DMSO

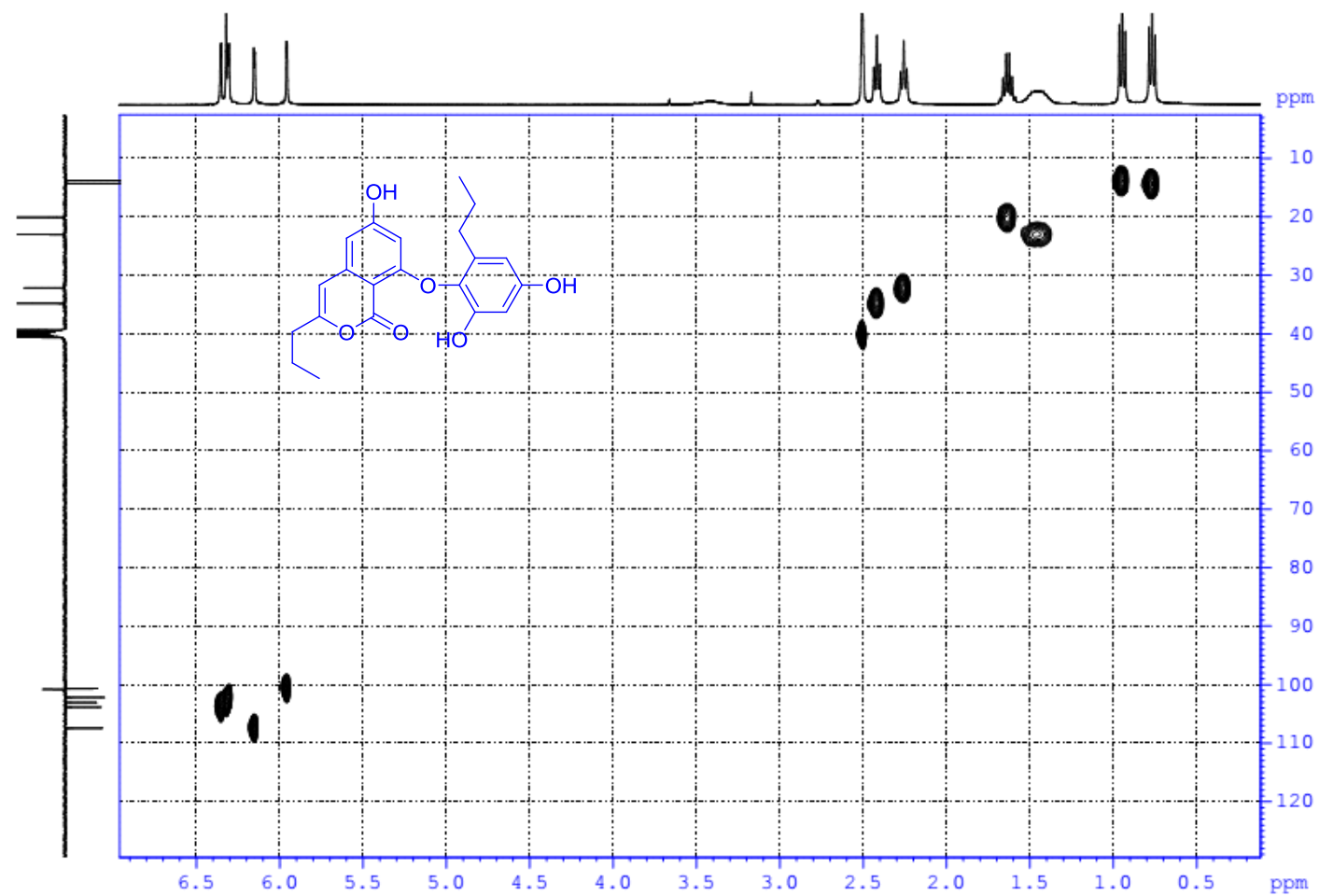


Figure S63. HSQC spectrum of compound **9** in DMSO-d₆.

F19-8-11-4-1 COSY DMSO

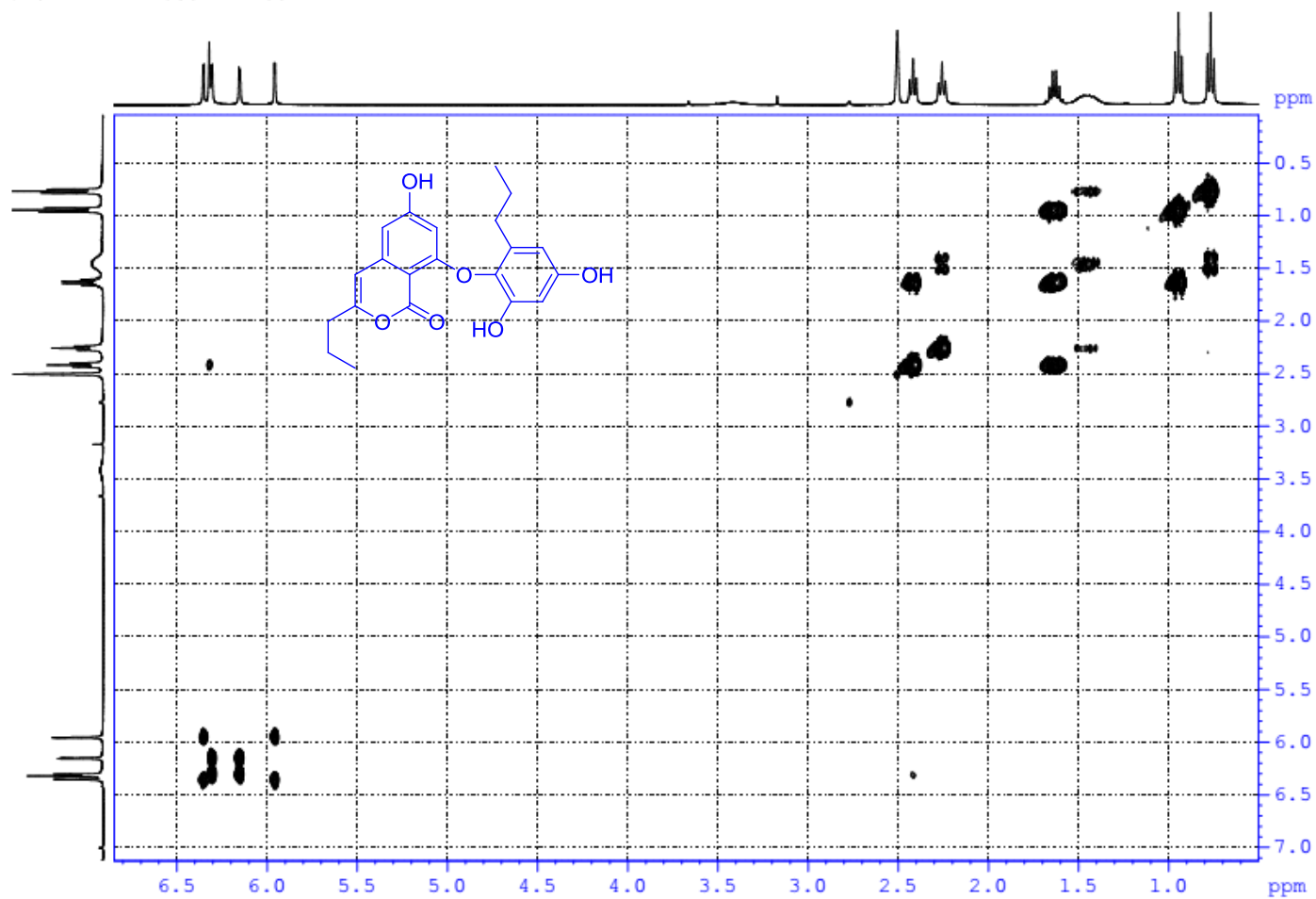


Figure S64. ^1H - ^1H COSY spectrum of compound **9** in DMSO- d_6 .

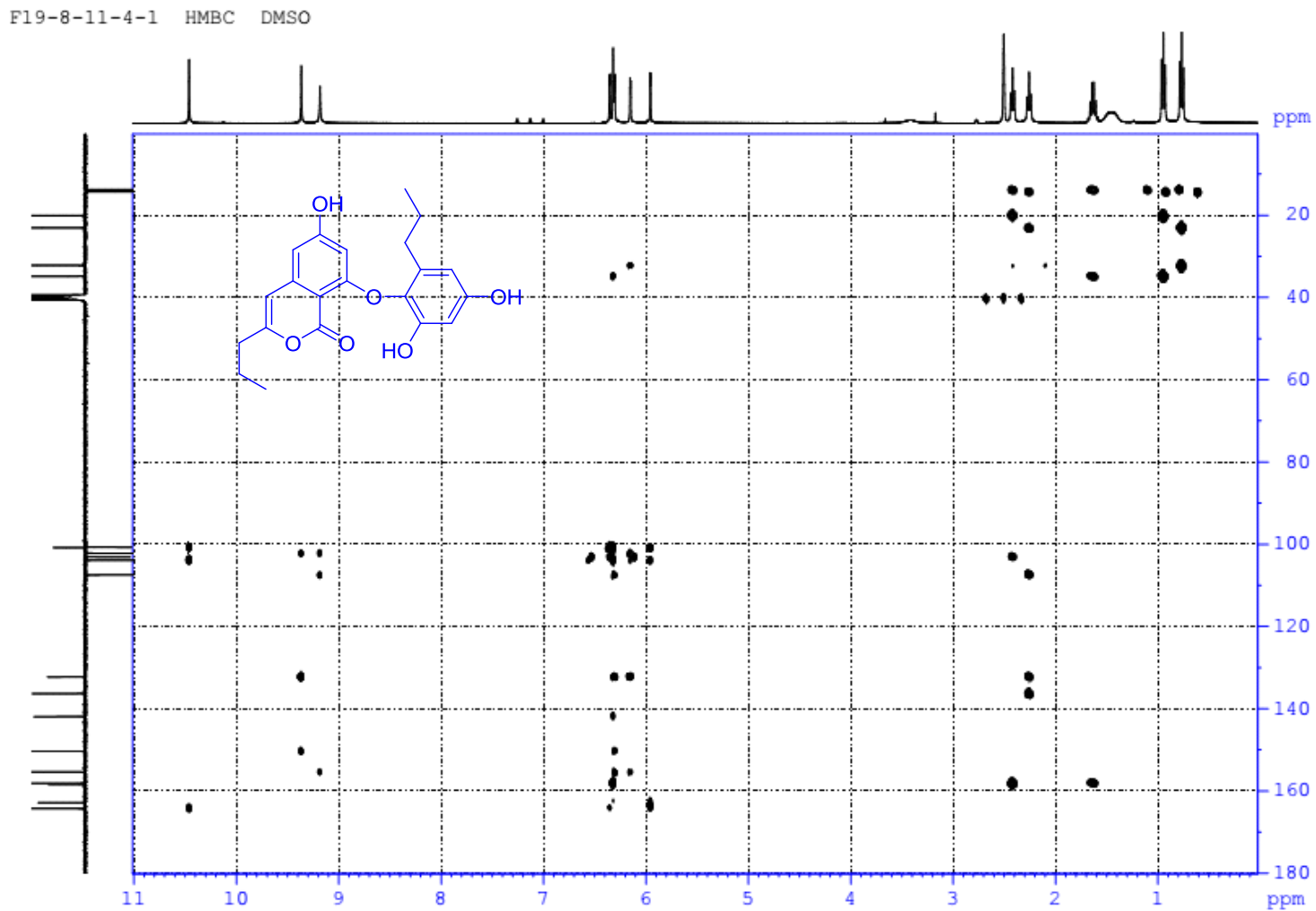


Figure S65. HMBC spectrum of compound 9 in DMSO-d₆.

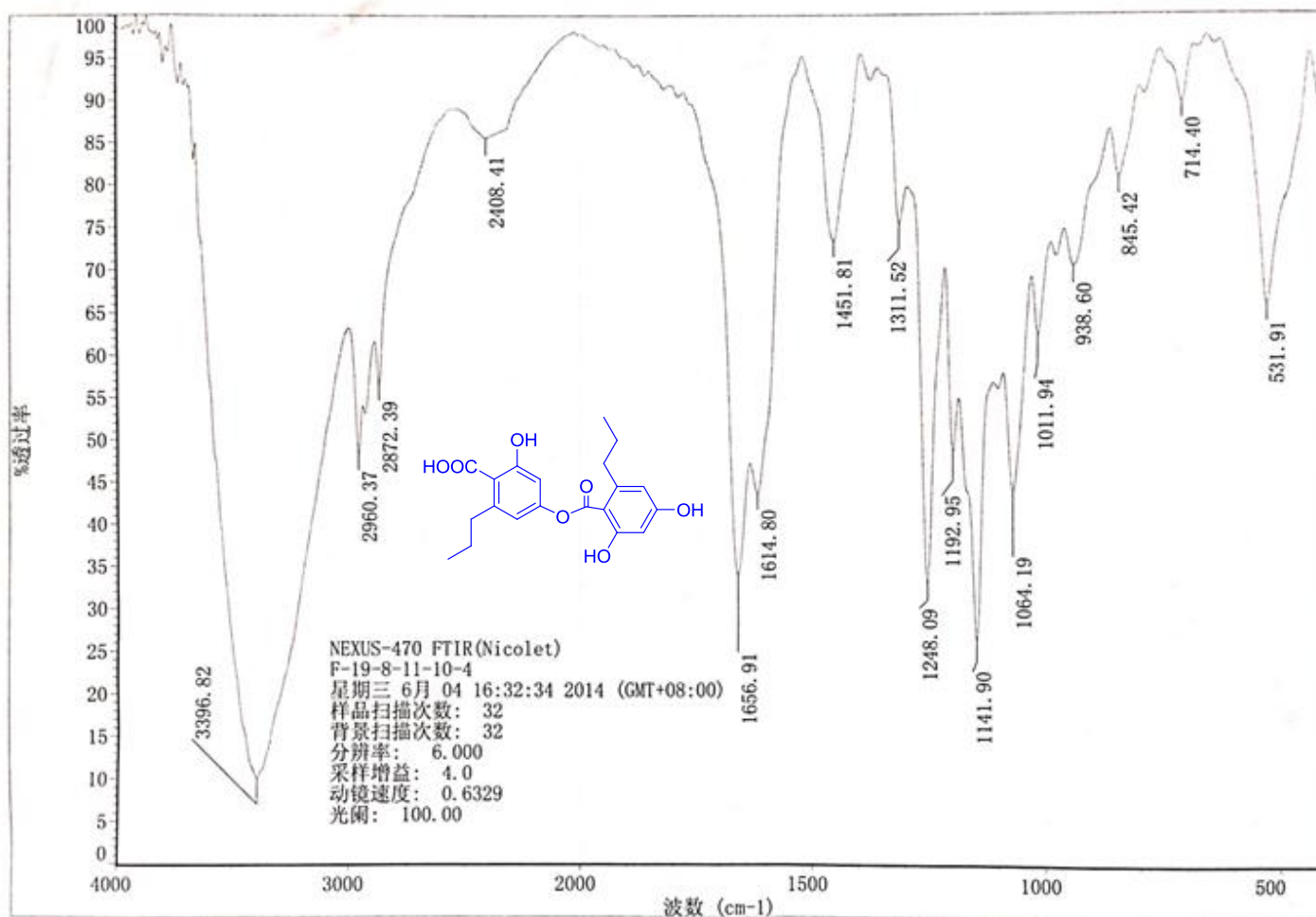


Figure S66. IR spectrum of compound 10.

Xevo G2 Q-TOF/CA166#

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Waters

F19-8-11-10-4 11 (0.216) Cm(11:16-(48+20.50))

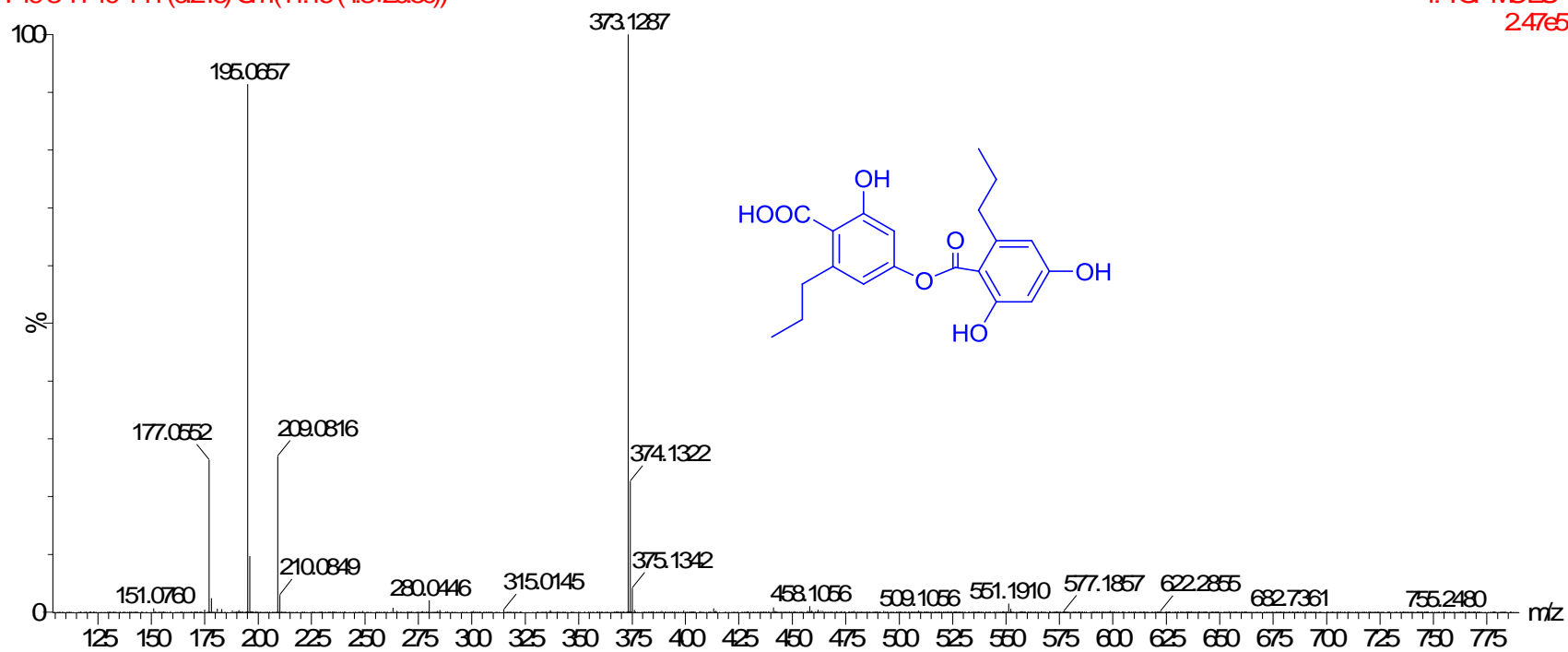
1: TOFMS ES-
247e5

Figure S67. Negative mode HRESIMS data of compound 10.

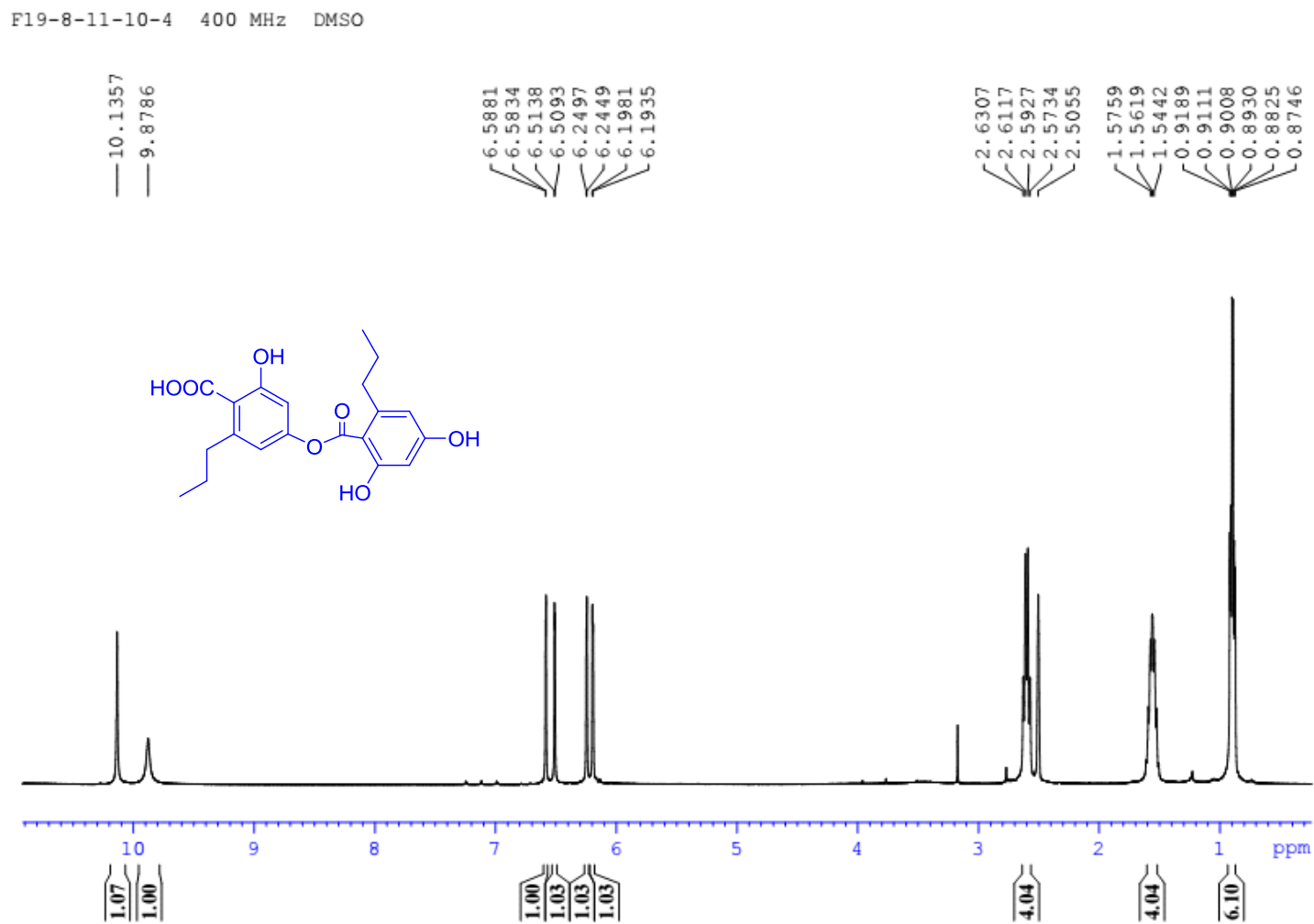


Figure S68. ^1H NMR spectrum of compound **10** in DMSO- d_6 (400 MHz).

F19-8-11-10-4 APT 100 MHz DMSO

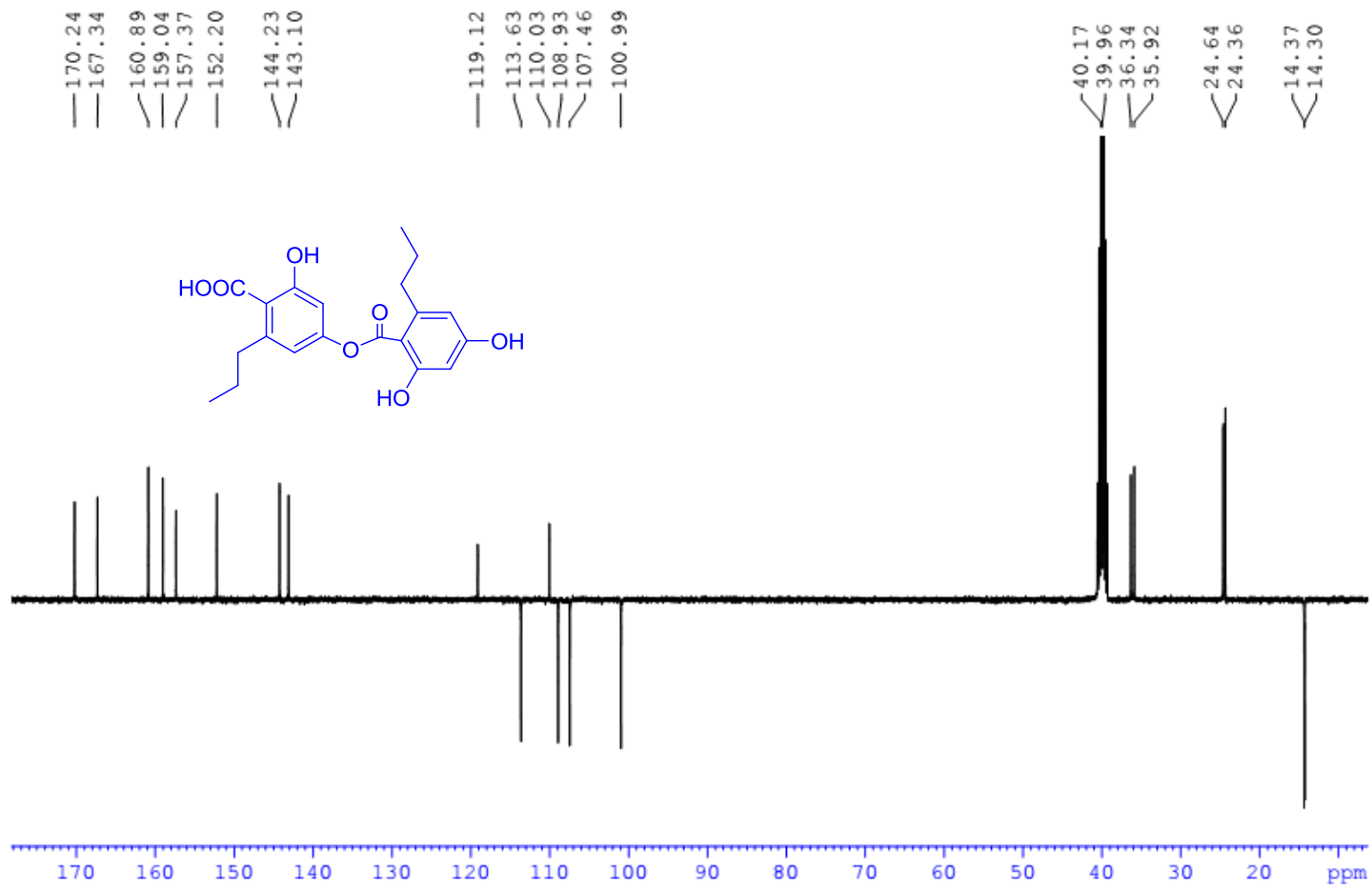


Figure S69. ¹³C NMR spectrum of compound 10 in DMSO-d₆ (100 MHz).

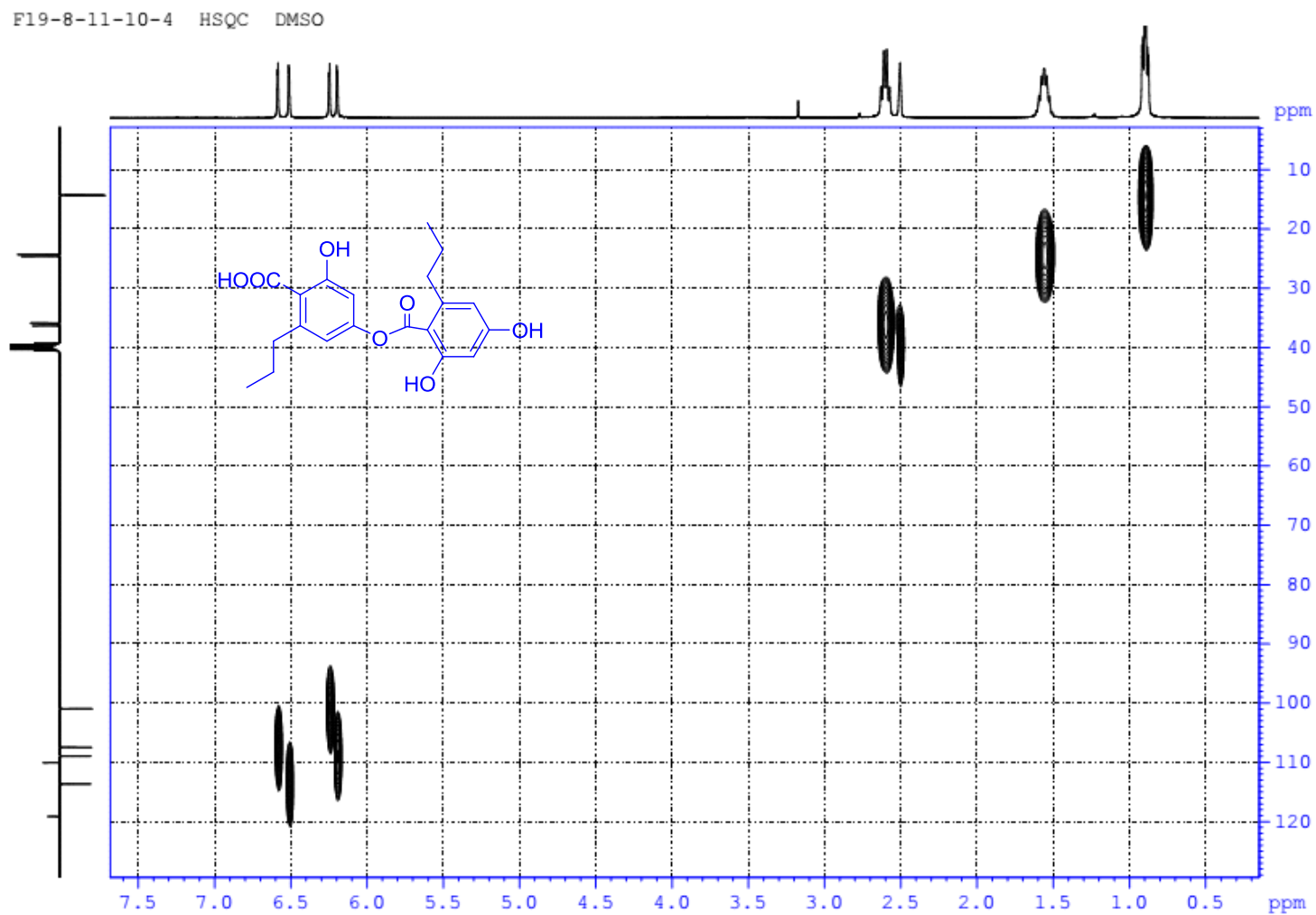


Figure S70. HSQC spectrum of compound 10 in DMSO-d6.

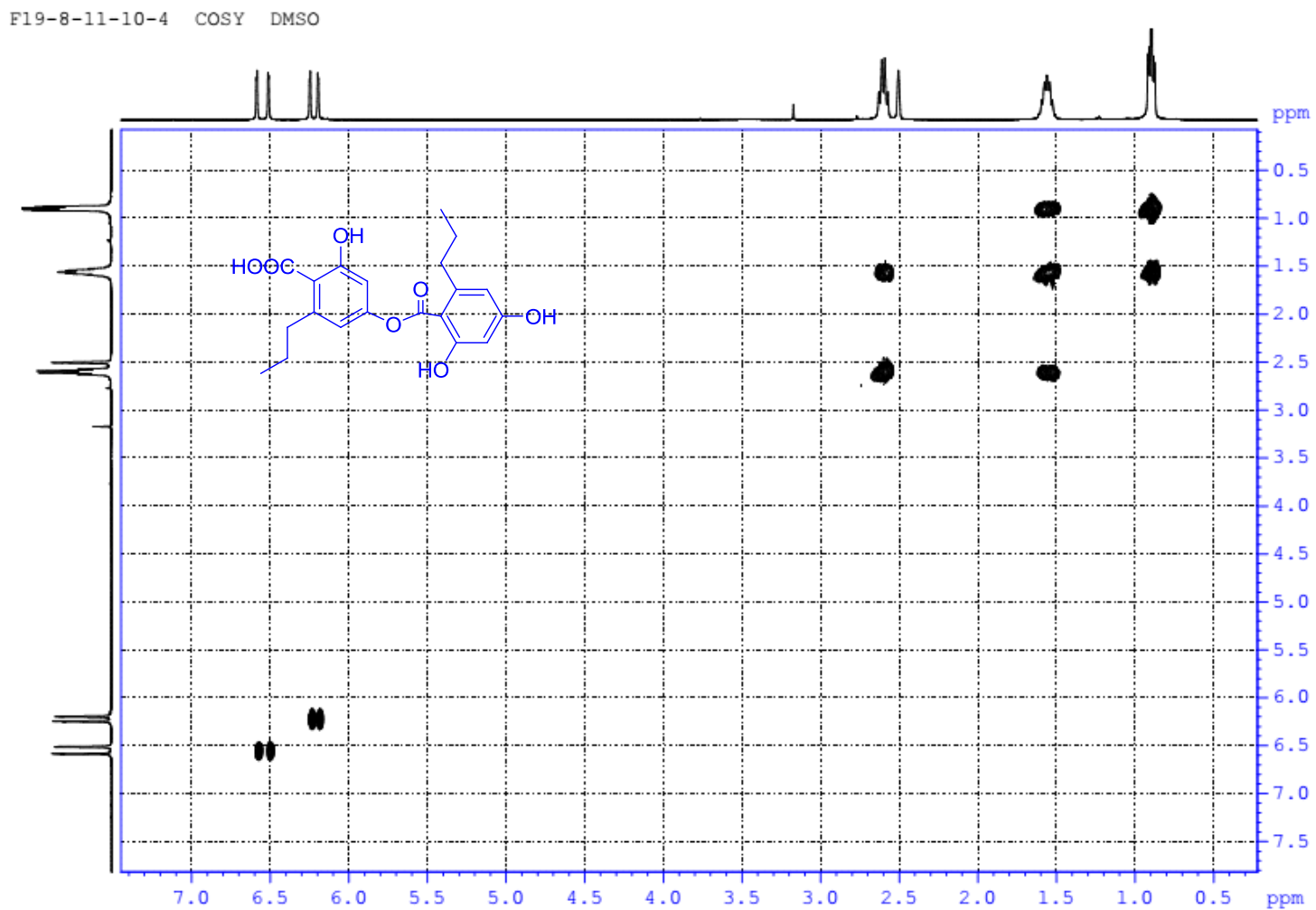


Figure S71. ¹H-¹H COSY spectrum of compound **10** in DMSO-d₆.

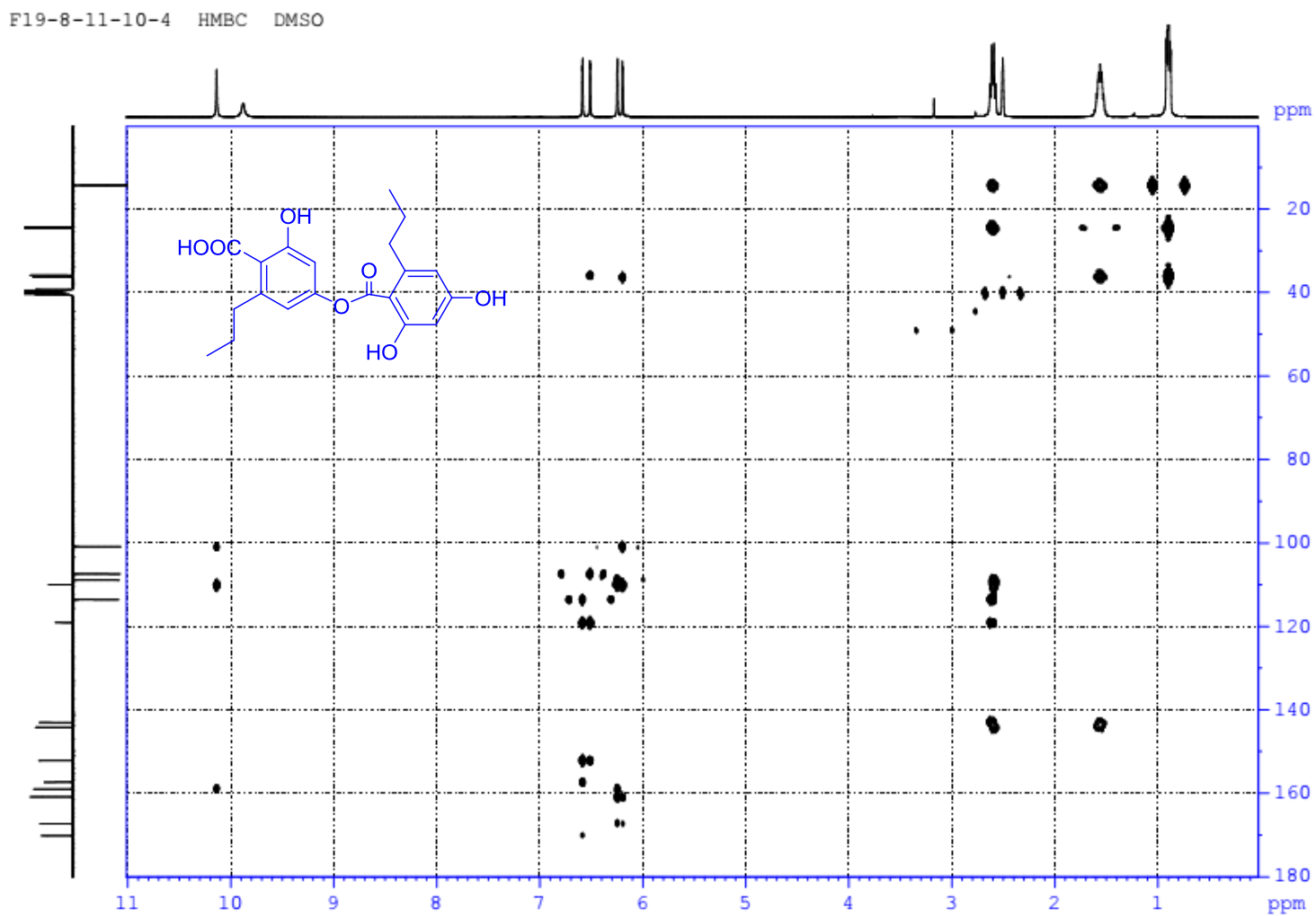


Figure S72. HMBC spectrum of compound 10 in DMSO-d6.

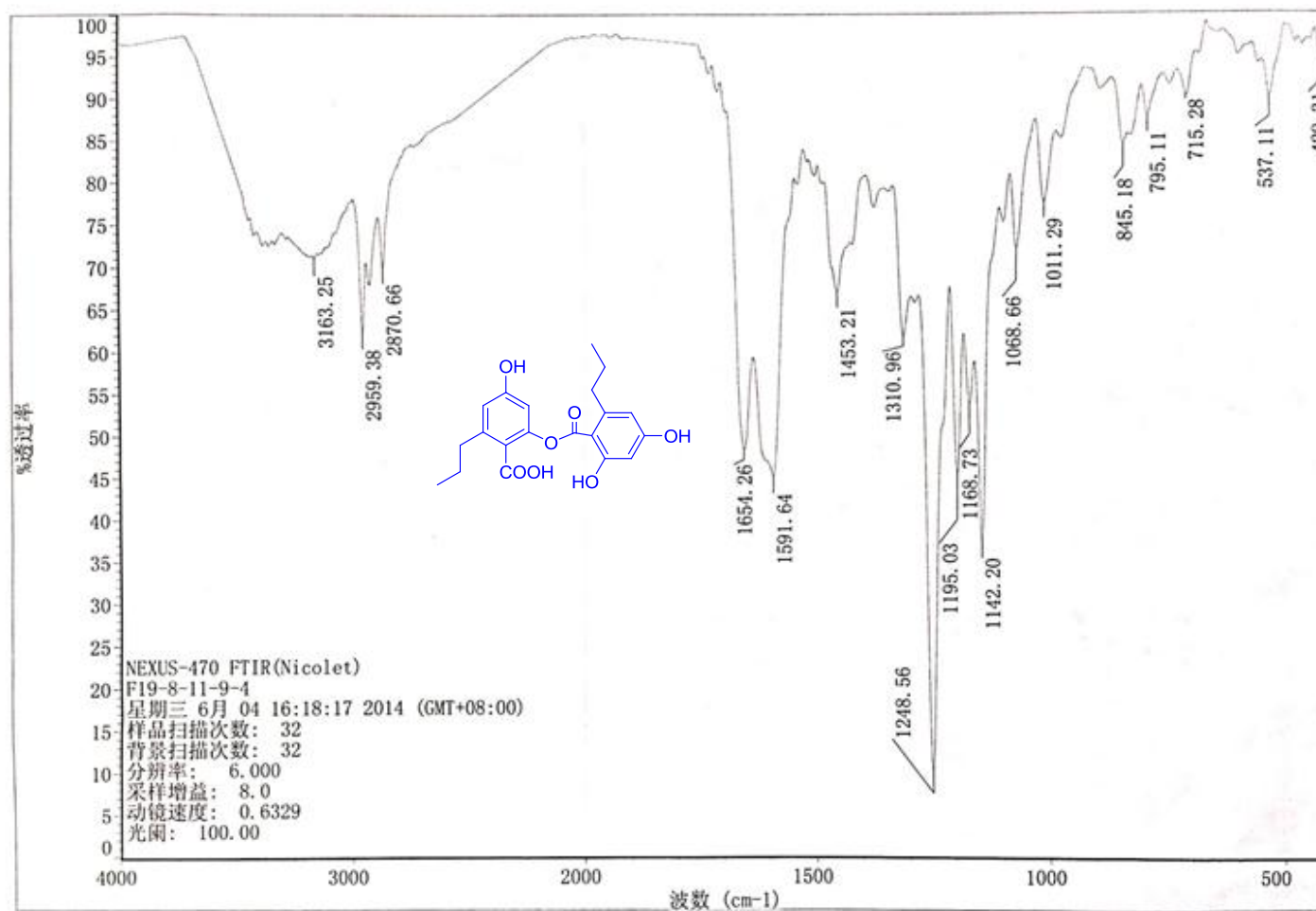


Figure S73. IR spectrum of compound 11.

Xevo G2 Q-TOF/YCA166#

F19-8-11-9-4 12 (0.233) Cm (10:16-(2:7+20:51))

07-Jul-2014

Waters

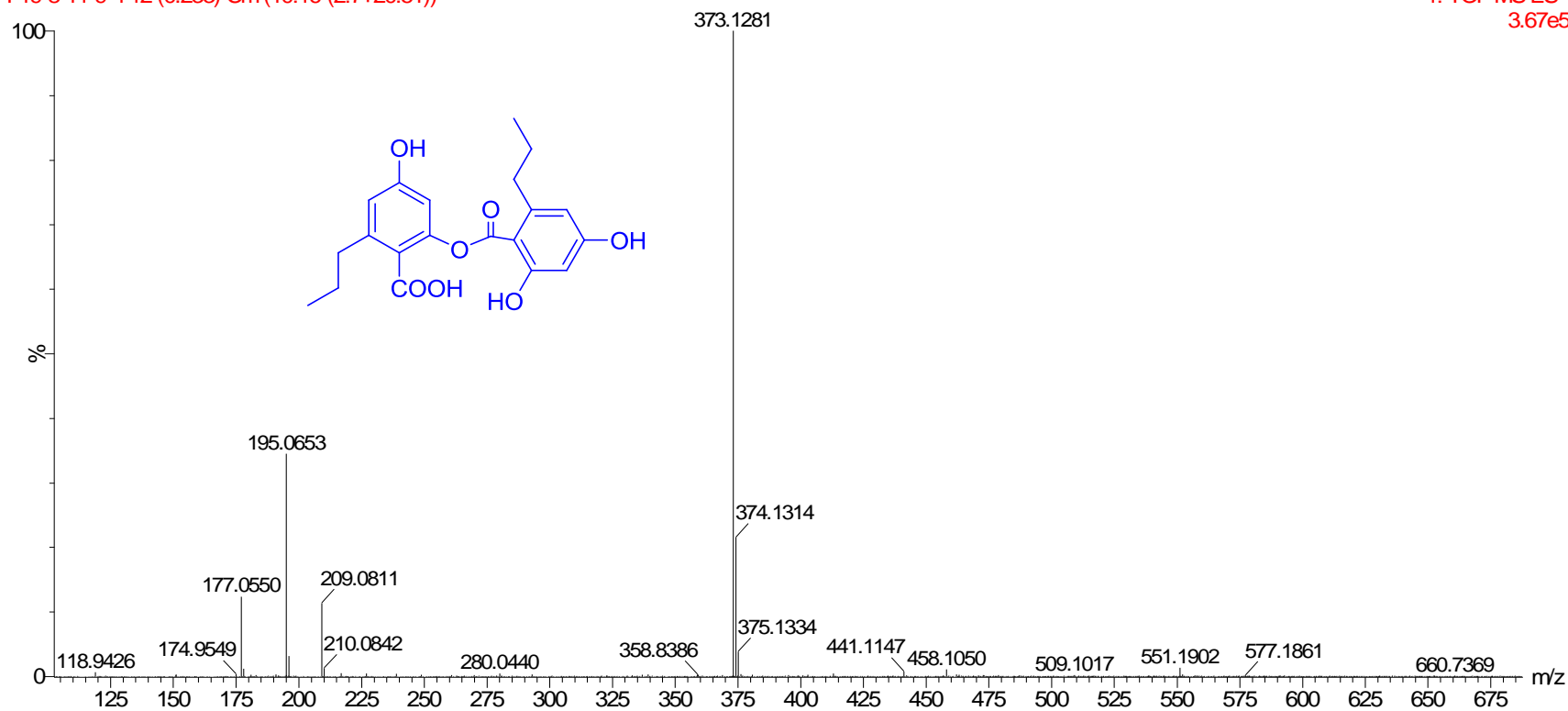
1: TOF MS ES-
3.67e5

Figure S74. Negative mode HRESIMS data of compound 11.

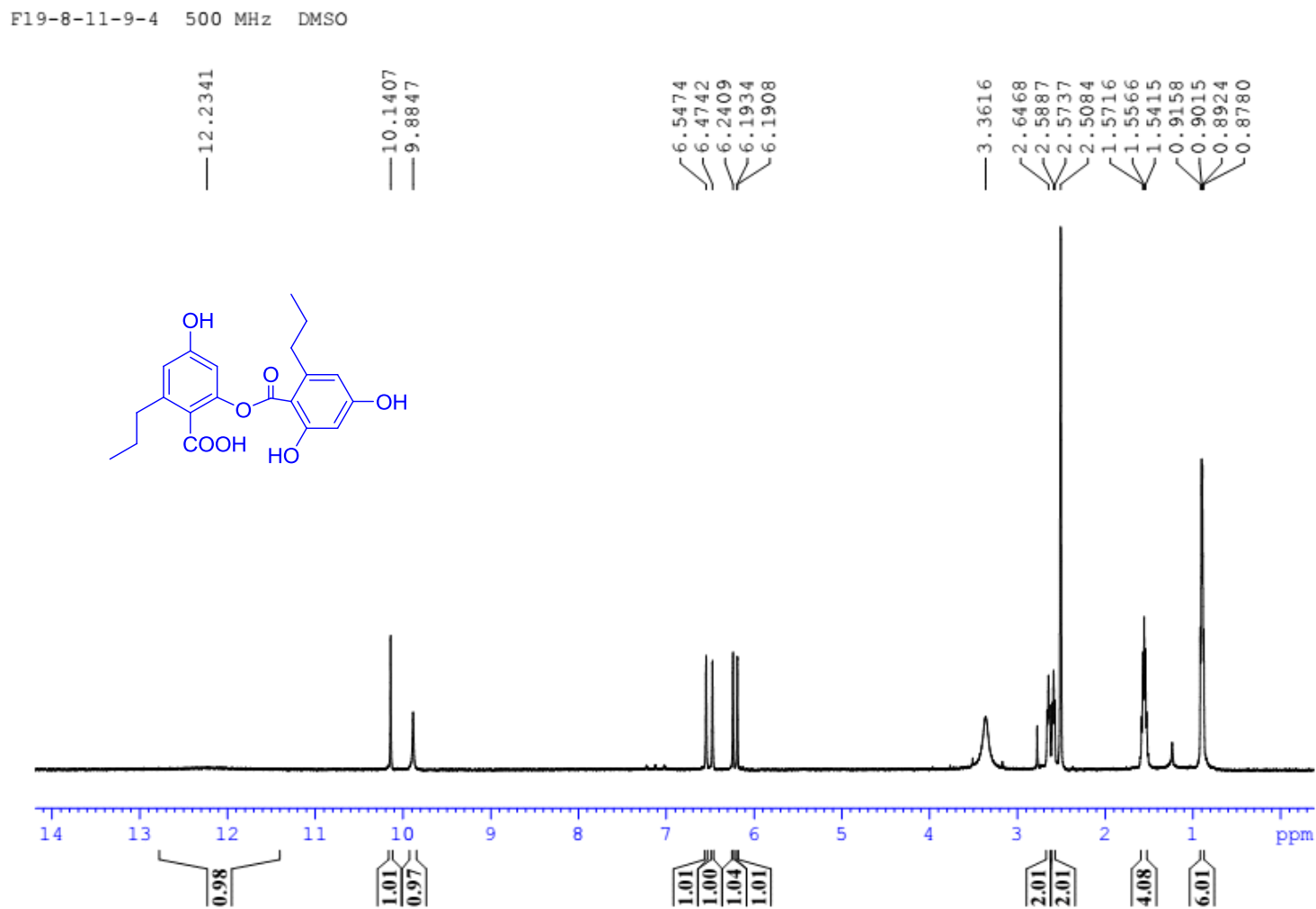


Figure S75. ^1H NMR spectrum of compound **11** in DMSO- d_6 (500 MHz).

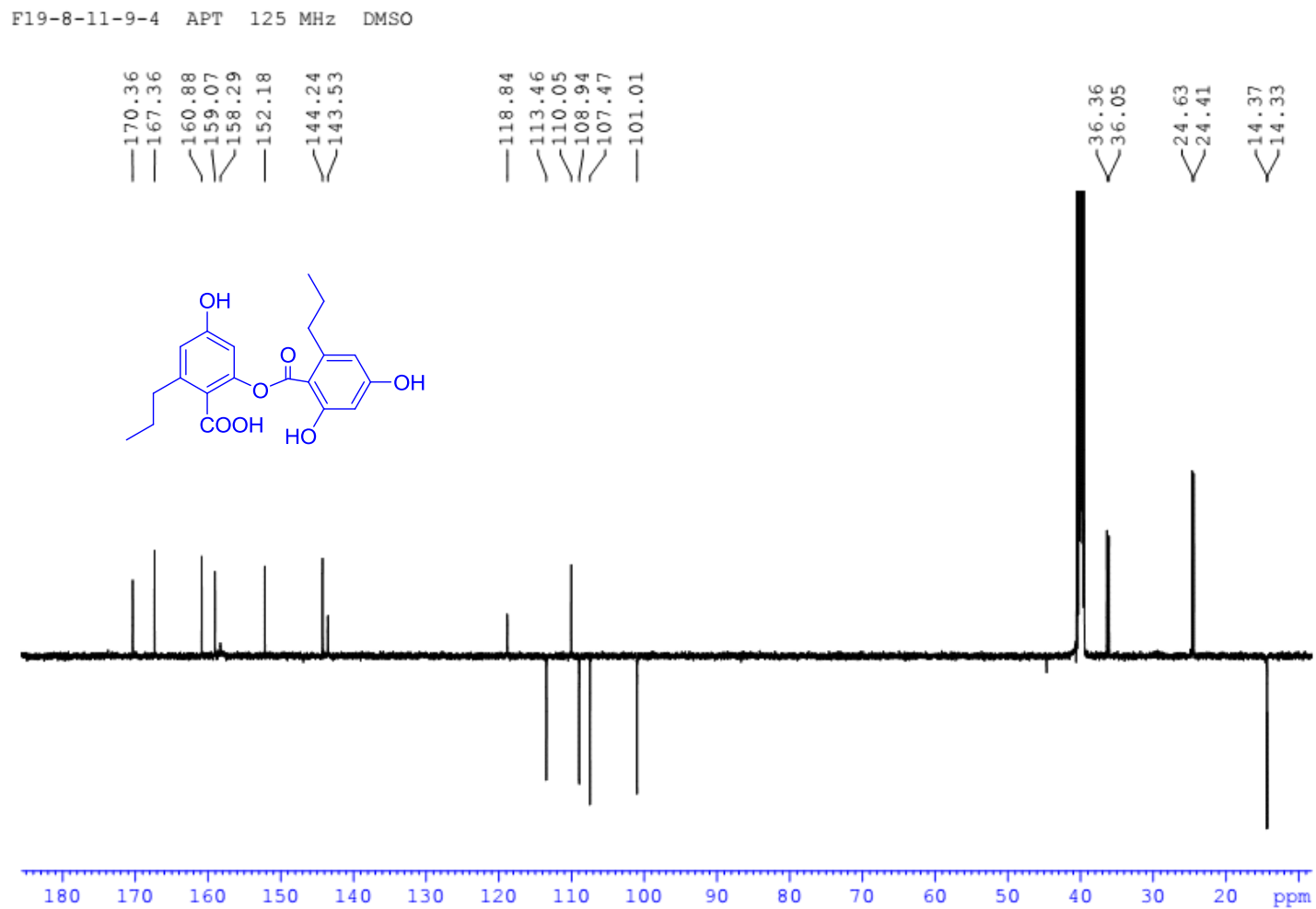


Figure S76. ^{13}C NMR spectrum of compound **11** in DMSO- d_6 (100MHz).

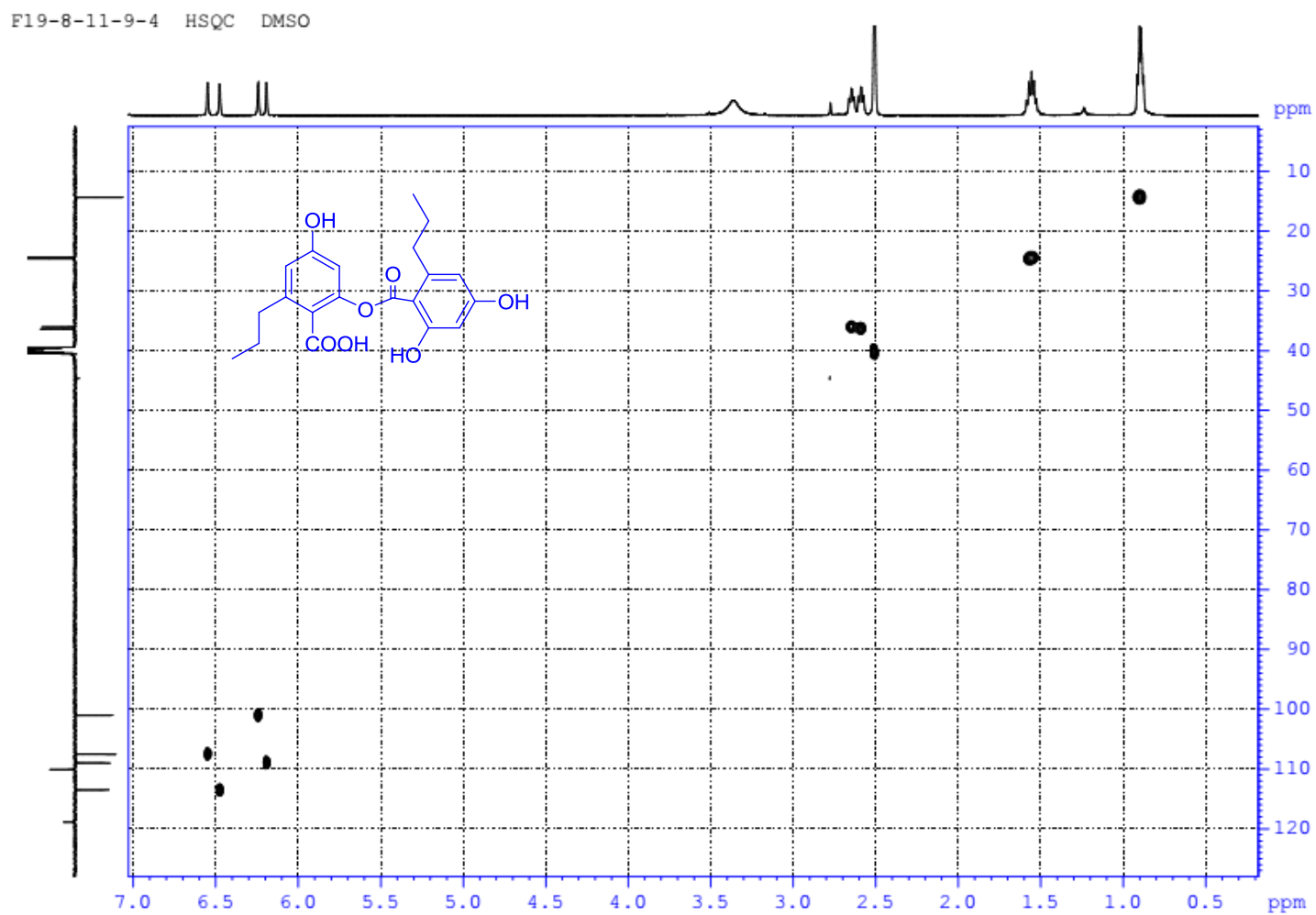


Figure S77. HSQC spectrum of compound 11 in DMSO-d₆.

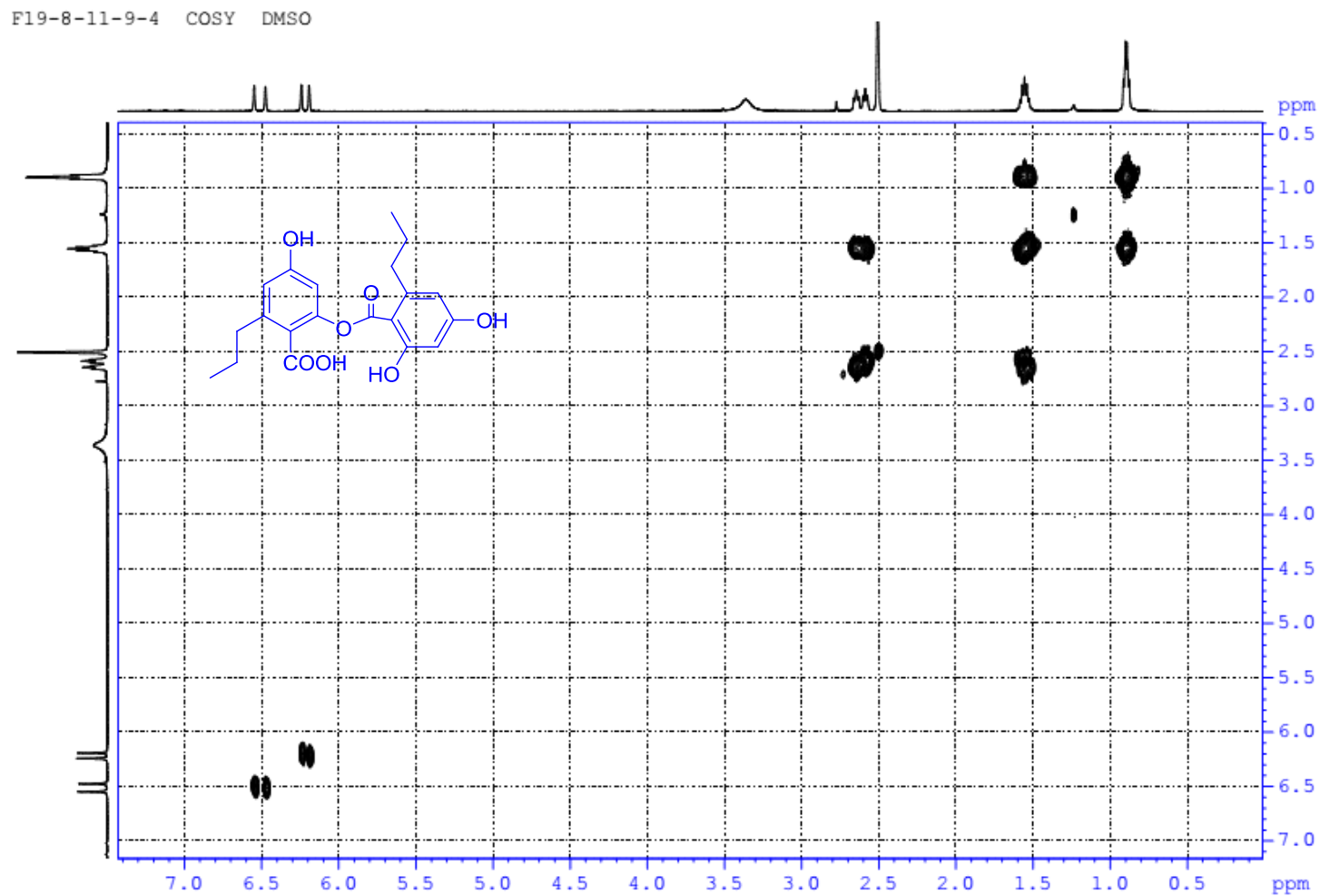


Figure S78. ^1H - ^1H COSY spectrum of compound **11** in DMSO- d_6 .

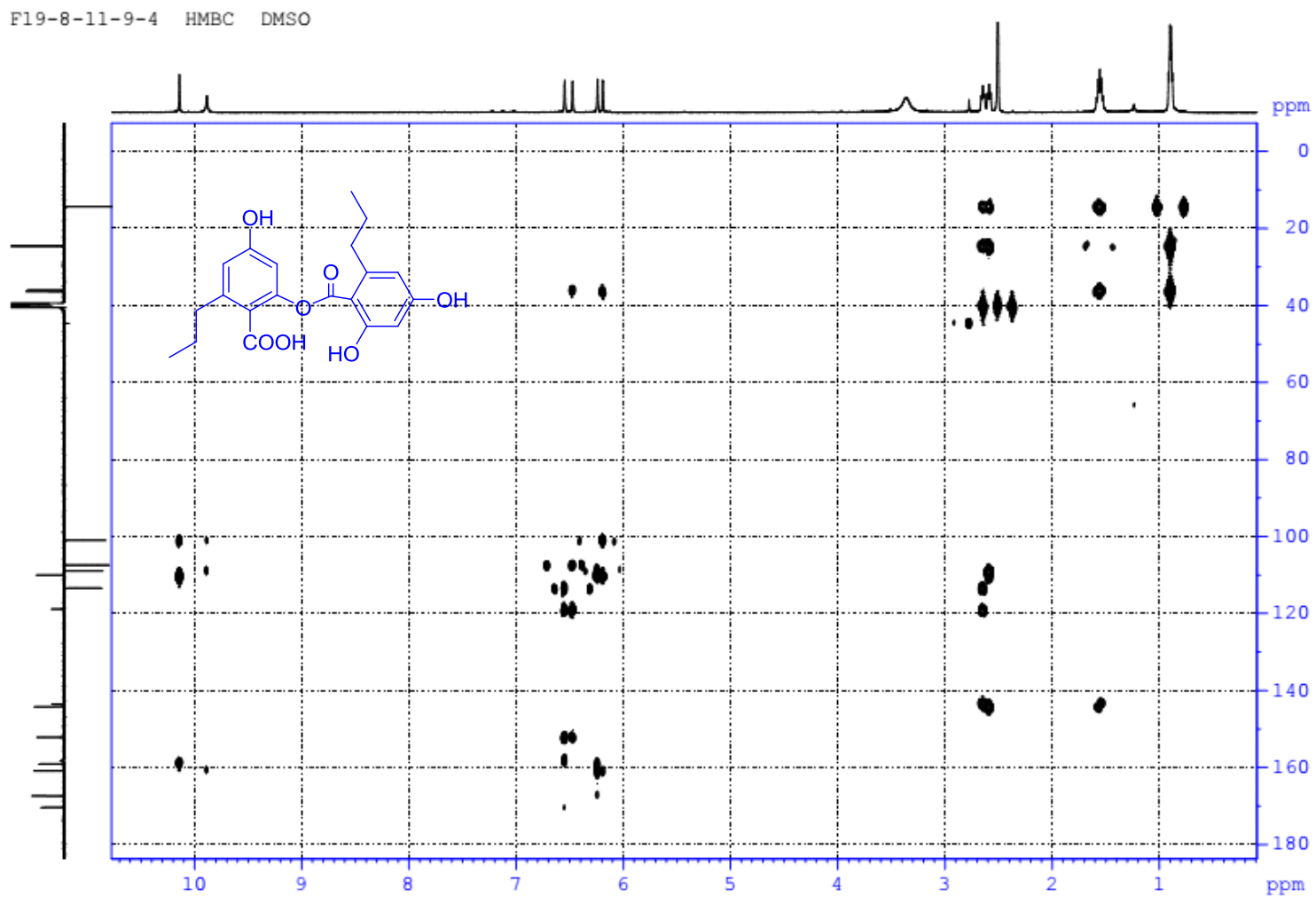


Figure S79. HMBC spectrum of compound 11 in DMSO-d6.

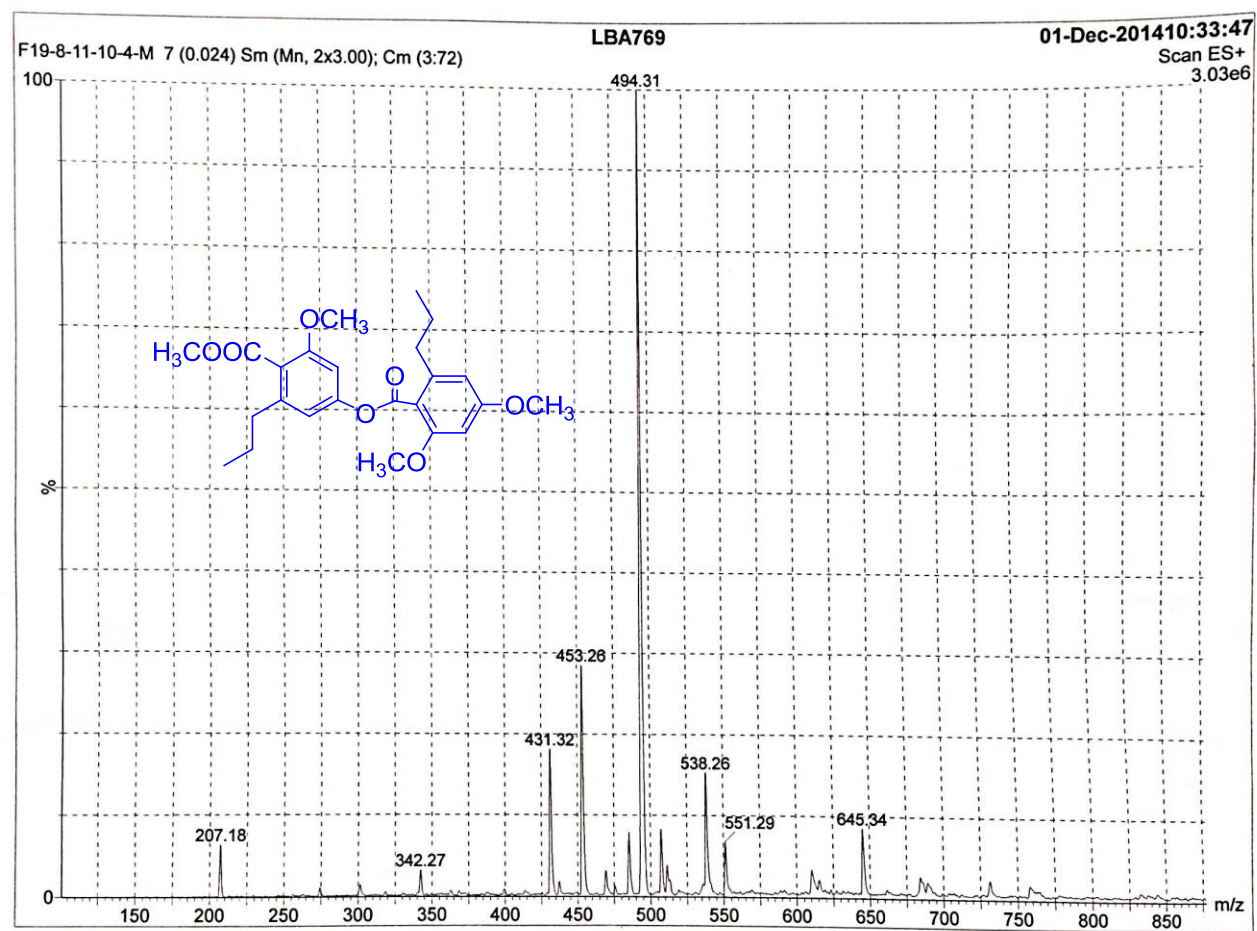


Figure S80. Negative mode ESIMS data of compound 10a.

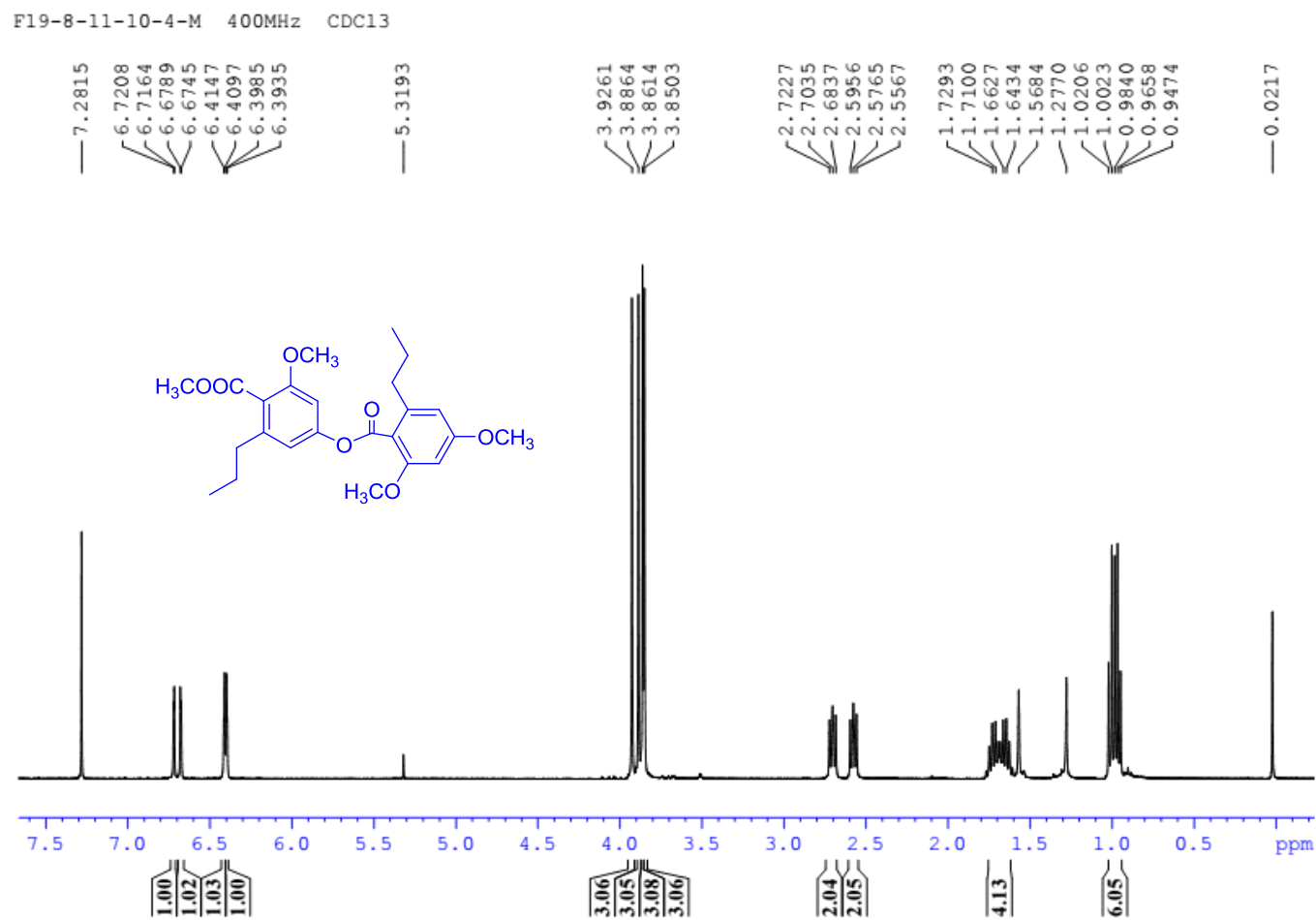


Figure S81. ¹H NMR spectrum of compound **10a** in CDCl₃ (400 MHz).

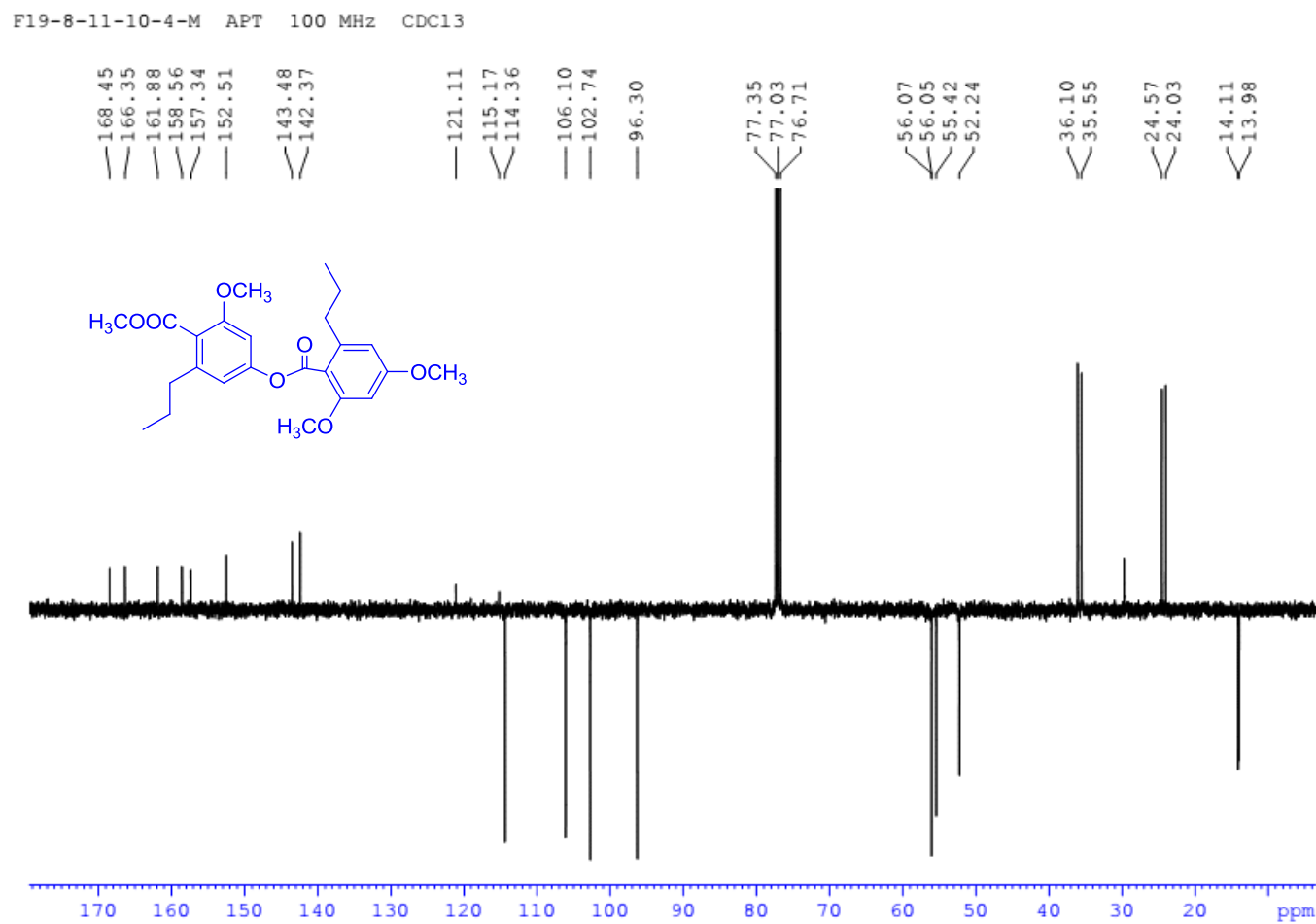


Figure S82. ¹³C NMR spectrum of compound **10a** in CDCl₃ (100 MHz).

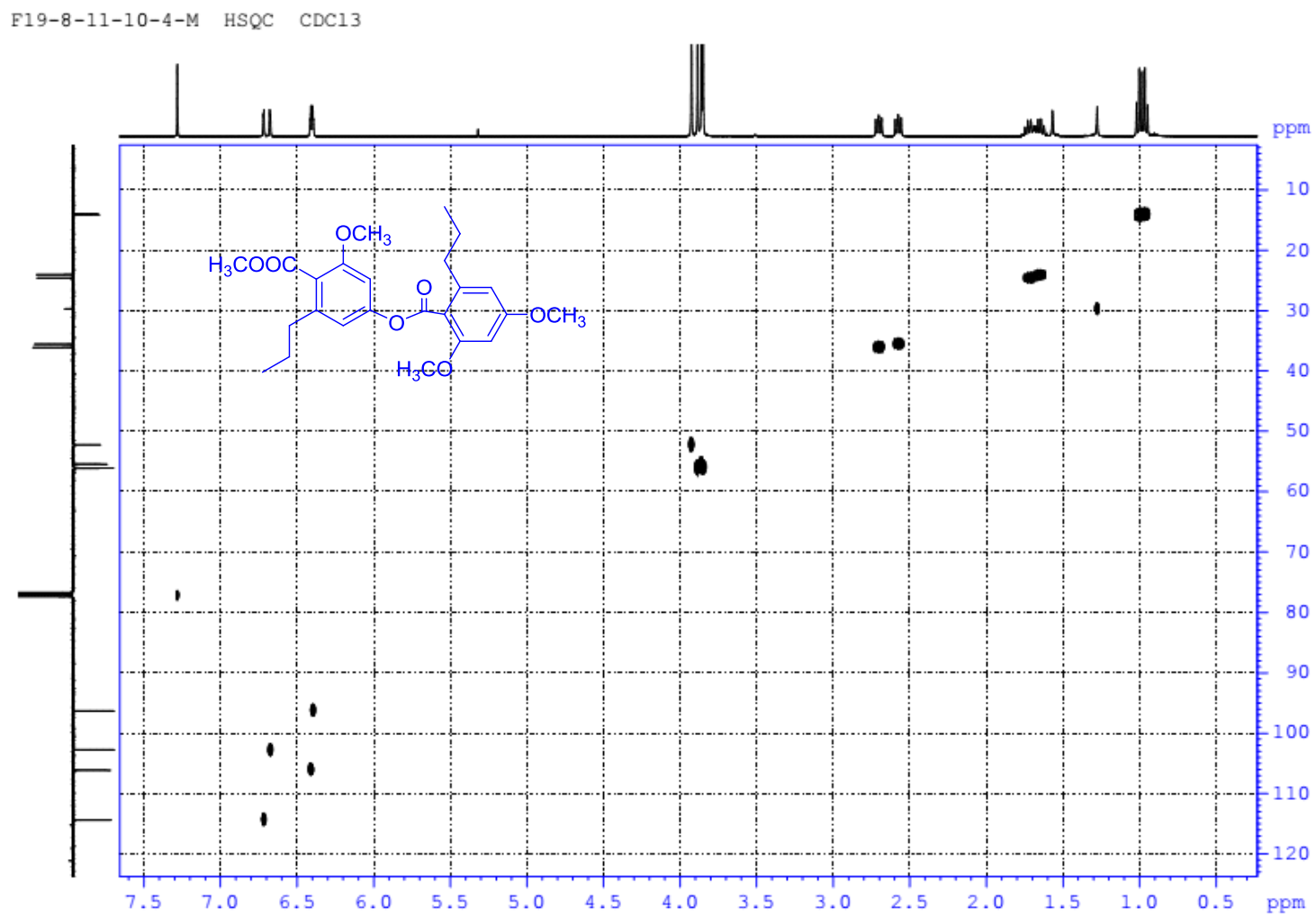


Figure S83. HSQC spectrum of compound **10a** in CDCl₃.

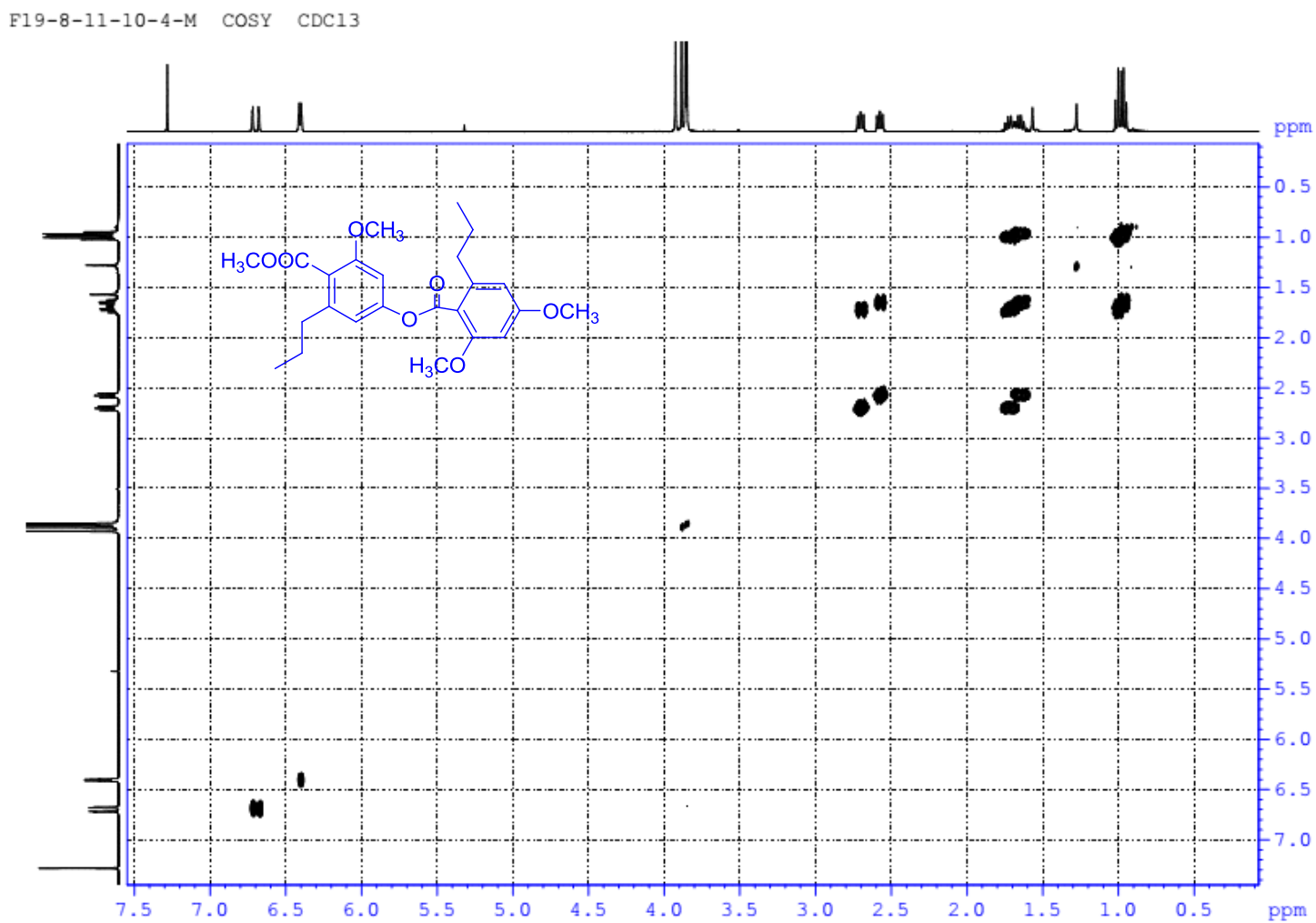


Figure S84. ^1H - ^1H COSY spectrum of compound **10a** in CDCl_3 .

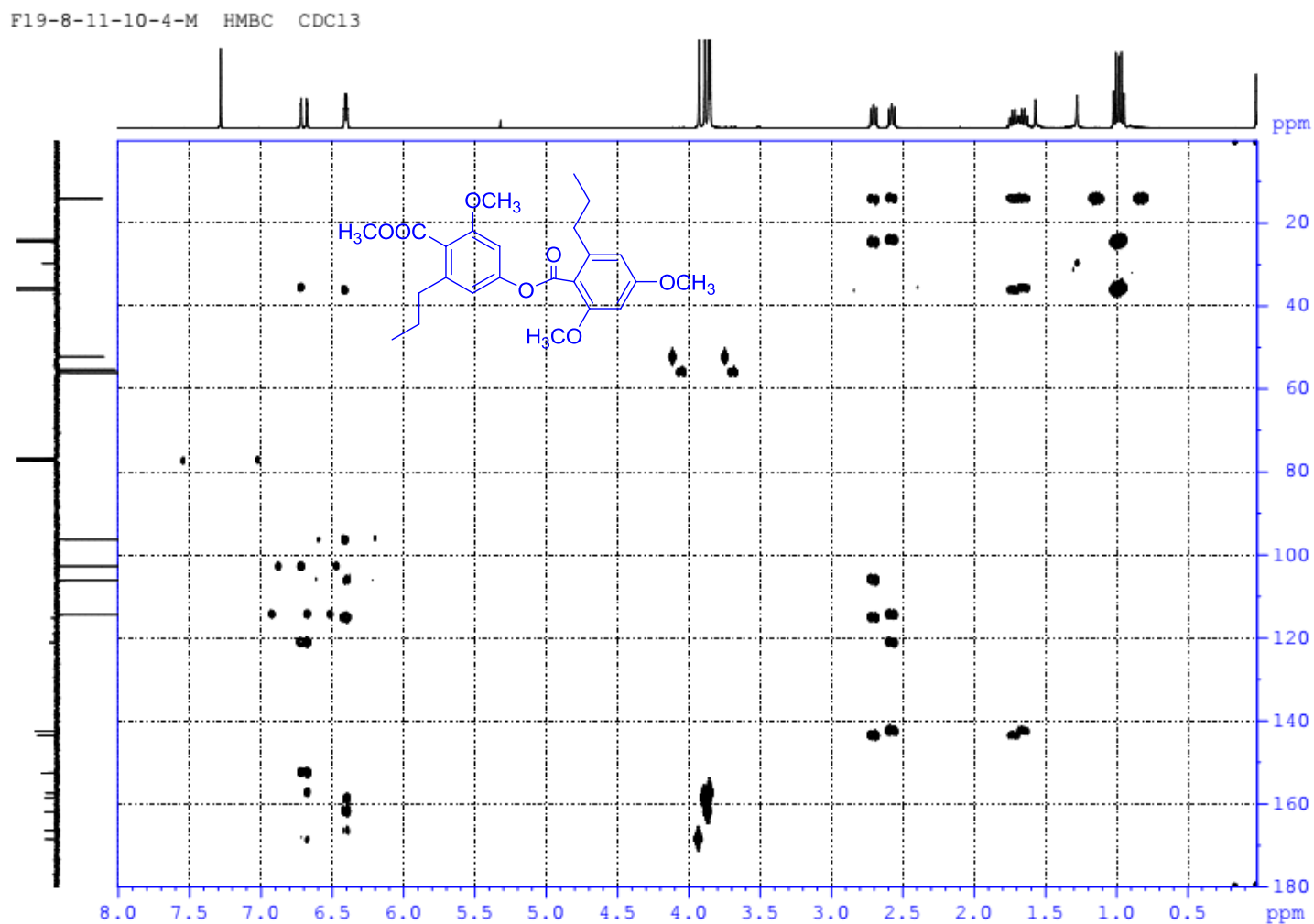


Figure S85. HMBC spectrum of compound **10a** in CDCl₃.