Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supplementary information

Curtachalasans, immunosuppressive agents from endophytic fungus *Xylaria* cf. *curta*

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Content

Table S1. ^{1}H NMR data of **1**–**11** ($CDCl_3$, 600 MHz, *J* in Hz).

No	**1**	**2**	**3**	**4**	**5**
3	3.66 (dd, 7.5, 7.5)	3.38 m	3.32 (br dd, 8.2, 6.9)	4.97 m	3.33 overlapped
4	2.29 overlapped	2.10 br s	2.44 br s	2.28 overlapped	2.34 br s
5		2.50 m			
7	4.00 (d, 10.1)	4.46 br s	3.92 br s	4.20 (d, 3.0)	4.24 (d, 9.6)
8	2.46 (dd, 10.1, 10.1)				1.88 (dd, 9.6, 9.6)
10	2.93 m	2.62 (dd, 13.8, 9.0); 2.91 (dd, 13.8, 3.8)	3.00 (dd, 13.2, 8.2); 3.06 (dd, 13.2, 6.9)	3.08 (dd, 12.9, 4.7); 2.49 (dd, 12.9, 10.5)	2.94 (dd, 13.6, 6.7); 2.86 (dd, 13.6, 7.9)
11	1.09 s	1.04 (d, 6.3)	1.26 s	0.80 s	1.20 s
12	1.34 s	5.07 br s; 5.48 br s	1.64 s	1.47 s	1.61 s
13	4.76 (dd, 10.1, 10.1)	5.96 br s	5.86 br s	2.09 (dd, 15.4, 3.6); 1.59 (dd, 15.4, 12.6)	4.70 (dd, 9.6, 9.6)
14	1.58 (dddd, 12.3, 10.1, 10.1, 3.4)	2.07 overlapped		1.81 (ddddd, 12.0, 12.0, 12.0, 3.9, 3.9)	1.61 overlapped
15	1.92 m; 1.29 (ddd, 12.3, 12.3, 12.3)	1.59 (ddd, 12.9, 4.0, 4.0); 1.35 (ddd, 12.9, 12.9, 12.9)	2.0 (br dd, 13.4, 4.0); 2.29 br dd, 13.4, 13.4	1.30 m; 1.49 overlapped	1.93 (br dd, 11.0, 4.0); 1.27 (ddd, 11.0, 11.0, 11.0)
16	1.84 m	1.93 m	1.89 m	1.87 m	1.85 m
19	3.40 (d, 10.1)	3.46 (d, 10.0)	3.64 (dd, 9.6, 8.6)	3.47 (dd, 10.4, 10.4)	3.41 (dd, 10.5, 8.1)
20	2.31 (ddd, 10.1, 10.1, 2.0)	2.74 (dd, 10.0, 10.0)	2.84 (dd, 9.6, 3.8)	2.29 overlapped	2.36 overlapped
21	5.35 (d, 2.0)	5.30 br s	5.69 (d, 3.8)	5.56 (d, 1.8)	5.50 br s
22	2.25 s	2.26 s	2.25 s	2.27 s	2.24 s
23	0.74 (d, 6.7)	0.75 (d, 6.6)	0.71 (d, 6.6)	0.74 (d, 6.6)	0.72 (d, 6.5)
25/29	7.15 (d, 7.6)	7.13 (d, 7.5)	7.20 (d, 7.5)	7.17 (d, 7.4)	7.13 (d, 7.0)
26/28	7.30 (dd, 7.6, 7.6)	7.27 (dd, 7.5, 7.5)	7.29 (dd, 7.5, 7.5)	7.31 (dd, 7.4, 7.4)	7.26 (dd, 7.0, 7.0)
27	7.23 (t, 7.6)	7.20 (t, 7.5)	7.22 overlapped	7.22 (dd, 7.4)	7.18 (t, 7.0)
OAc	2.30 s	2.11 s	2.20 s	2.19 s	2.24 s

Table S1. Continued.

No	**6**	**7**	**8**	**9**	**10**	**11**
3	3.40 (dd, 7.2, 7.2)	3.34 m	3.49 m	3.55 (dd, 7.3, 7.3)	3.64 overlapped	3.33 m
4	2.31 br s	2.78 br s	2.94 br s	3.68 br s	2.87 br s	3.00 br s
7	4.36 br s	5.82 br s	5.97 br s			3.78 overlapped
8	2.11 overlapped	2.59 overlapped				1.74 (ddd, 13.5, 9.8, 4.4)
10	2.97 (dd, 13.6, 6.7); 2.82 (dd, 13.6, 7.6)	2.95 (dd, 13.3, 7.0); 2.82 (dd, 13.3, 8.3)	2.92, overlapped; 2.84 overlapped	3.04 (dd, 13.3, 6.4); 2.91 (dd, 13.3, 8.4)	3.16 (dd, 13.2, 5.9); 2.89 (dd, 13.2, 9.3)	2.80 m
11	1.17 s	4.82 m; 4.26 m	4.83 br s; 4.22 br s	1.44 s	1.43 s	1.38 s
12	1.72 s	1.82 s	1.75 s	1.68 s	1.73 s	1.62 s
13	4.99 (dd, 11.0, 11.0)	4.81 (dd, 11.0, 11.0)	5.60 s	6.75 s	6.84 (d, 2.0)	3.05 (dd, 13.5, 13.5); 2.33 (dd, 13.5, 4.4)
14	1.81 (dddd, 11.0, 11.0, 11.0, 3.3)	1.80 (dddd, 11.0, 11.0, 11.0, 3.0)	2.06 m	2.38 m	2.23 overlapped	
15	2.10 overlapped; 1.40 (ddd, 11.0, 11.0, 11.0)	2.09 (ddd, 11.0, 3.0, 3.0); 1.39 (ddd, 11.0, 11.0, 11.0)	1.47 (ddd, 12.0, 12.0, 12.0); 1.53 m	1.66 m; 1.44 m	1.68 (ddd, 12.9, 3.7, 3.7); 1.52 (ddd, 12.9, 12.9, 12.9)	5.20 br s
16	1.87 m	1.87 m	1.85 m	1.95 m	1.95 m	3.89 m
19	3.43 (dd, 11.0, 8.0)	3.46 (dd, 10.4, 8.0)	3.40 (dd, 10.7)	3.92 (d, 10.0)	3.48 (dd, 10.5, 6.7)	5.93 (d, 11.6)
20	2.69 (ddd, 11.0, 11.0, 2.0)	2.62 overlapped	2.79 (br dd, 10.7, 10.7)	2.40 m	2.75 (br dd, 12.9, 10.5)	3.44 (br d, 11.6)
21	5.46 (d, 2.0)	5.52 (d, 1.9)	5.36 br s	4.29 br s	5.59 br s	3.82 (br d, 6.9)
22	2.27 s	2.26 s	2.20 s	2.29 s	2.28 s	1.28 s
23	0.79 (d, 6.7)	0.78 (d, 6.6)	0.71 (d, 6.6)	0.69 (d, 6.5)	0.76 (d, 6.6)	1.22 (d, 6.7)
25/29	7.17 (d, 7.3)	7.16 (d, 7.2)	7.10 (d, 7.2)	7.28 (d, 7.2)	7.23 (d, 7.3)	7.14 (d, 7.5)
26/28	7.28 (dd, 7.3, 7.3)	7.31 (dd, 7.2)	7.24 (dd, 7.2)	7.33 (dd, 7.2, 7.2)	7.34 (dd, 7.3, 7.3)	7.33 (dd, 7.5, 7.5)
27	7.20 (t, 6.8)	7.23 (t, 7.2)	7.16 (t, 7.2)	7.22(t, 7.2)	7.25 (t, 7.3)	7.26 (t, 7.5)
OAc	2.22 s	2.24 s	2.10 s		2.23 s	2.26, s

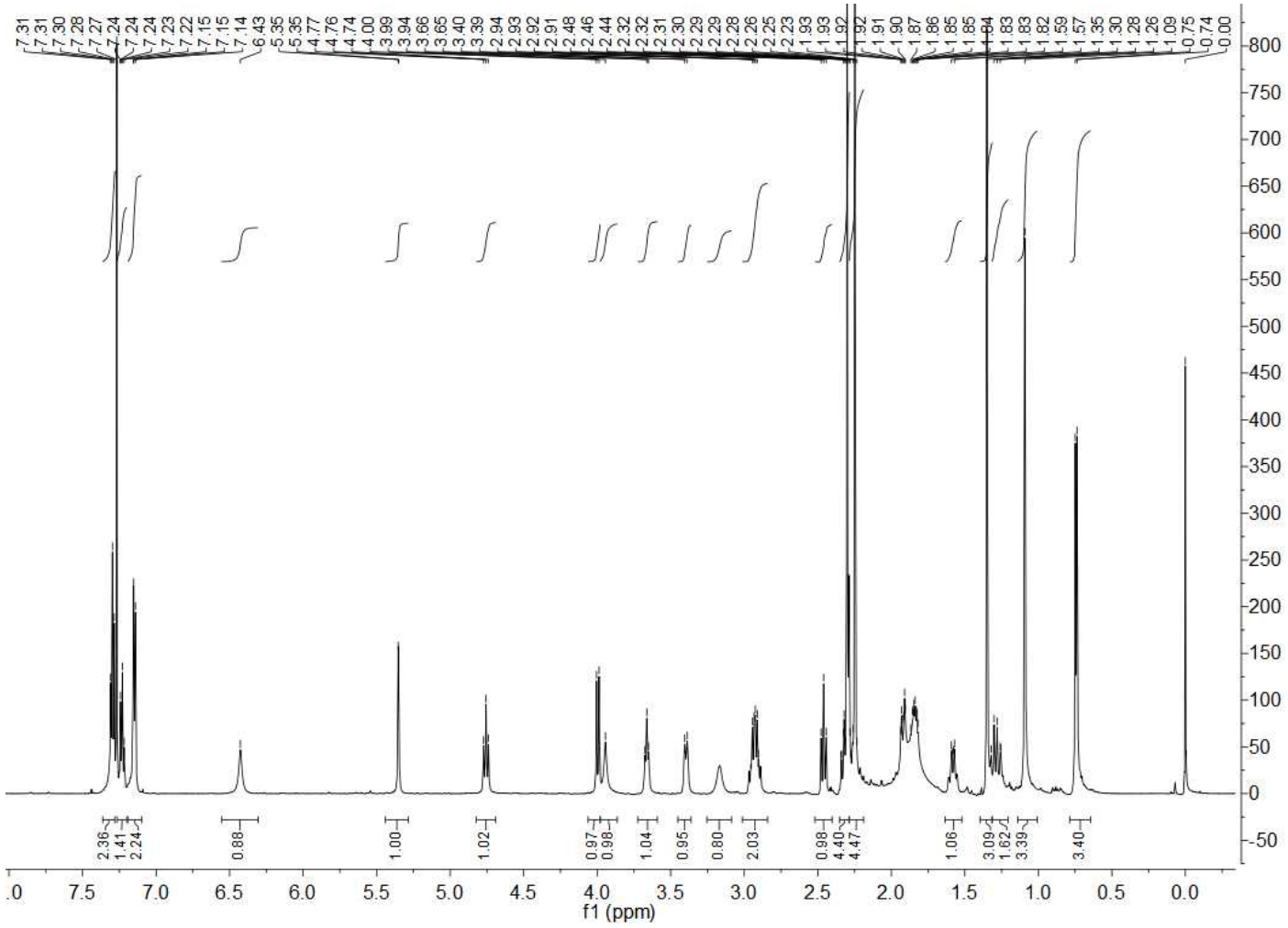

Fig. S1. ^{1}H NMR of **1** ($CDCl_3$, 600 MHz).

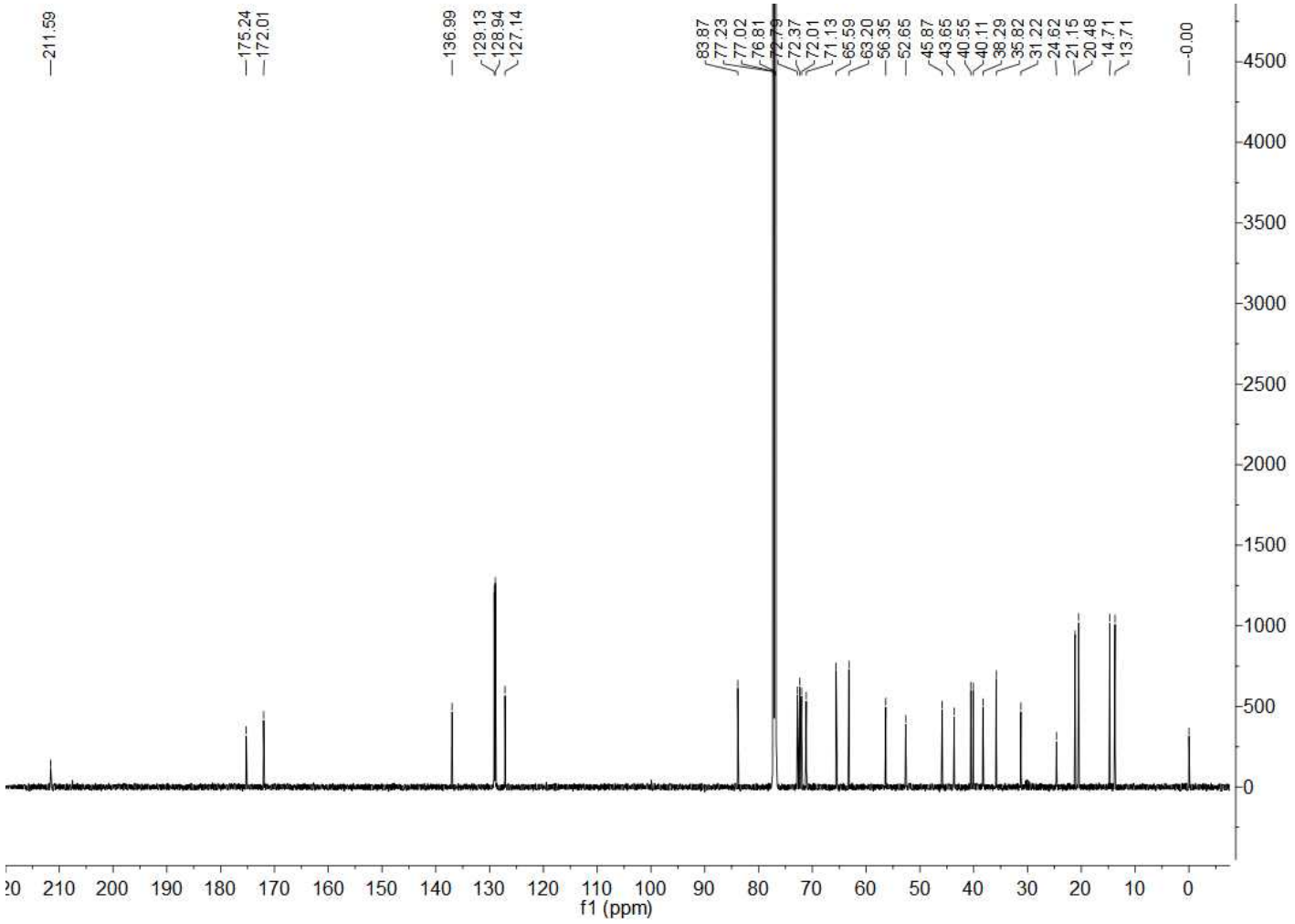

Fig. S2. ^{13}C NMR of **1** ($CDCl_3$, 150 MHz).

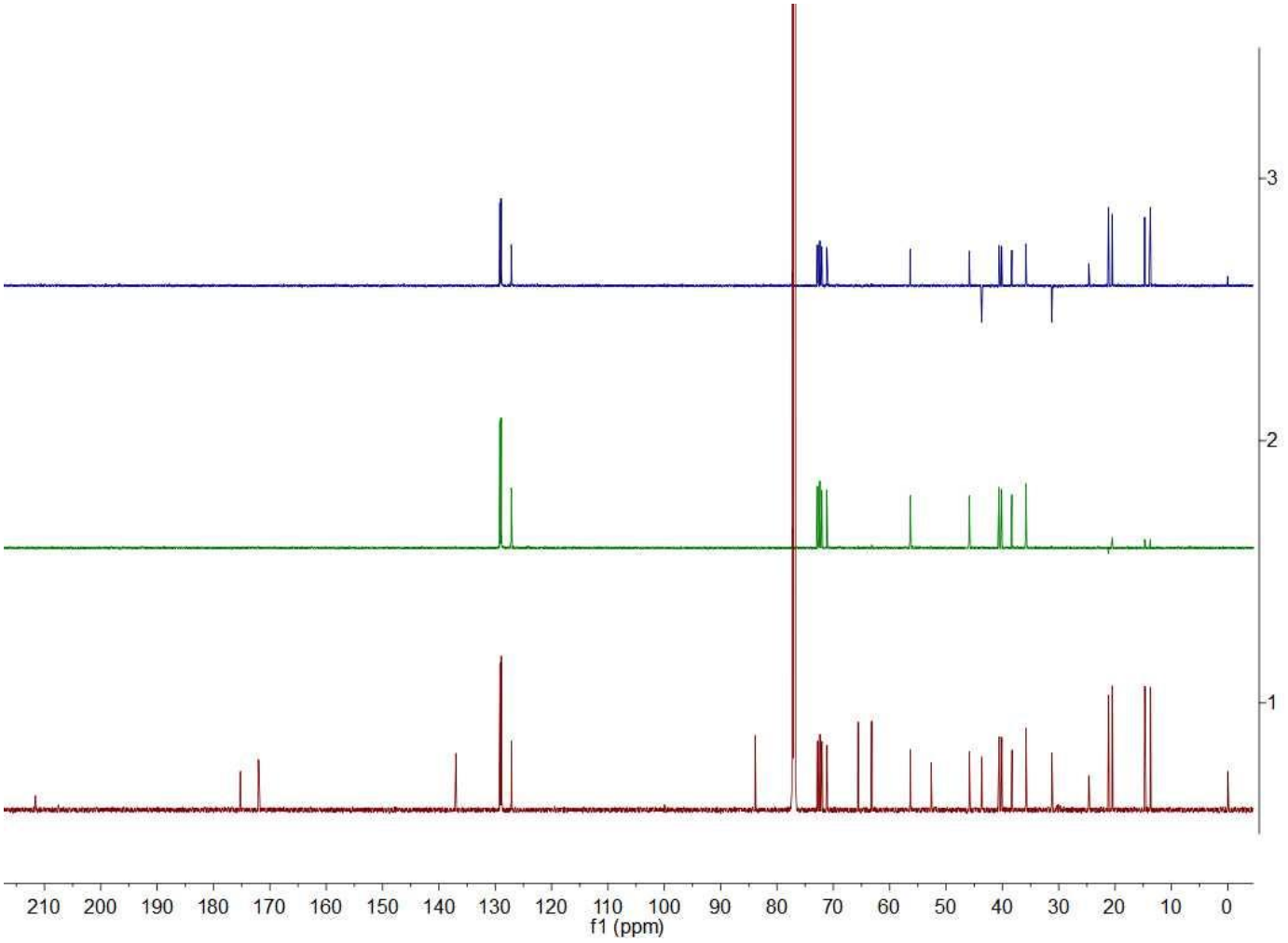

Fig. S3. DEPT of **1**.

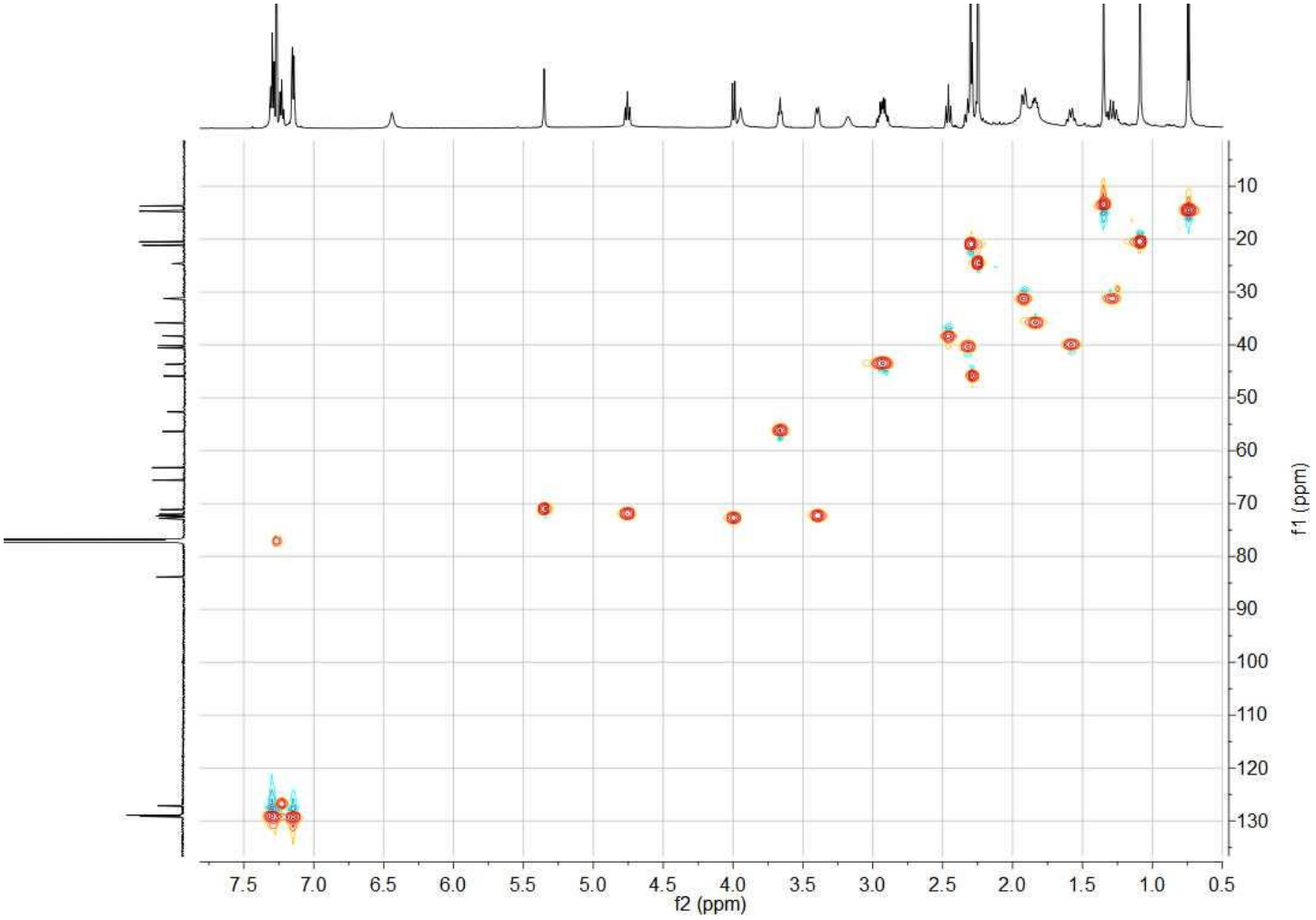

Fig. S4. HSQC of **1**.

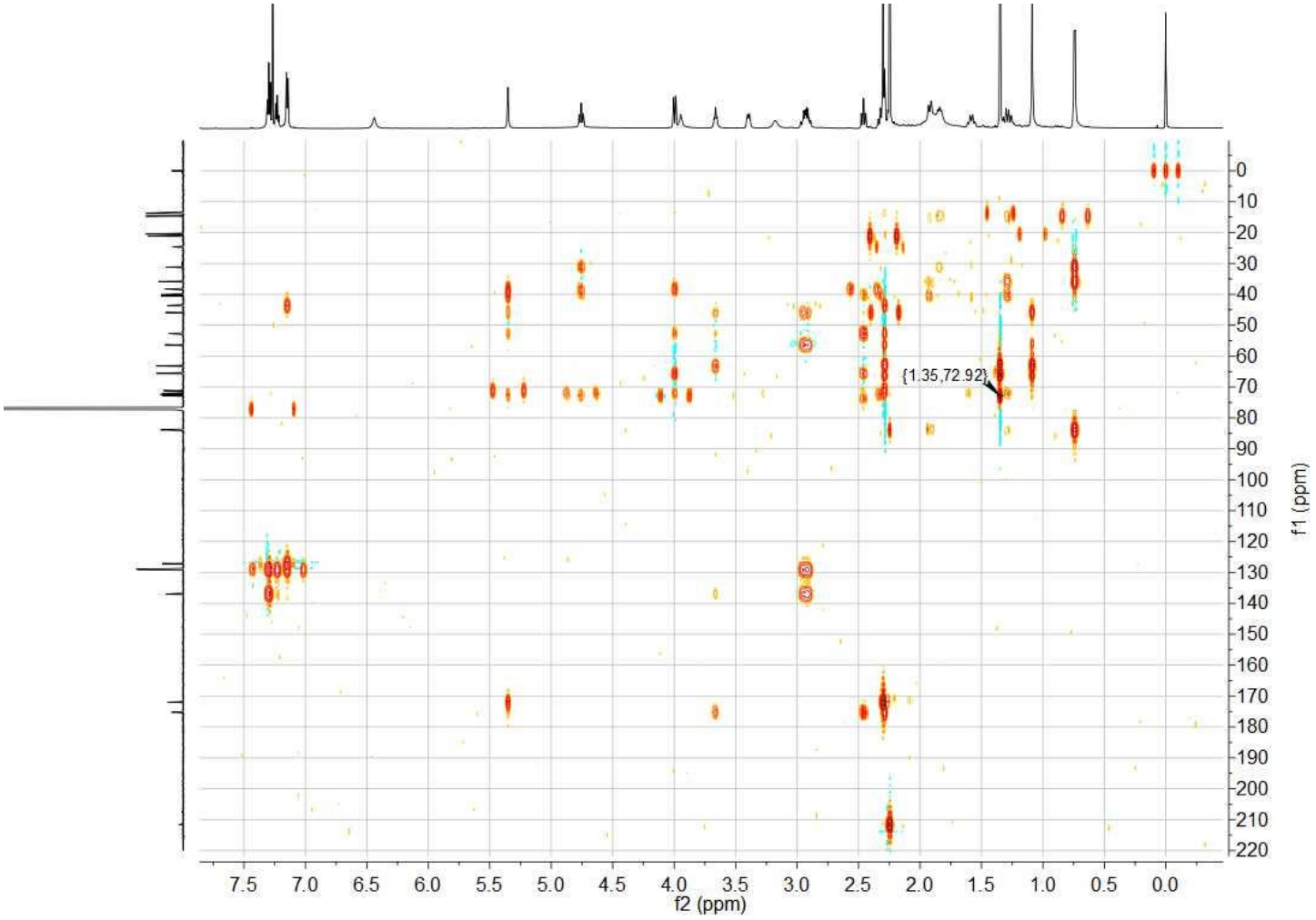

Fig. S5. HMBC of **1**.

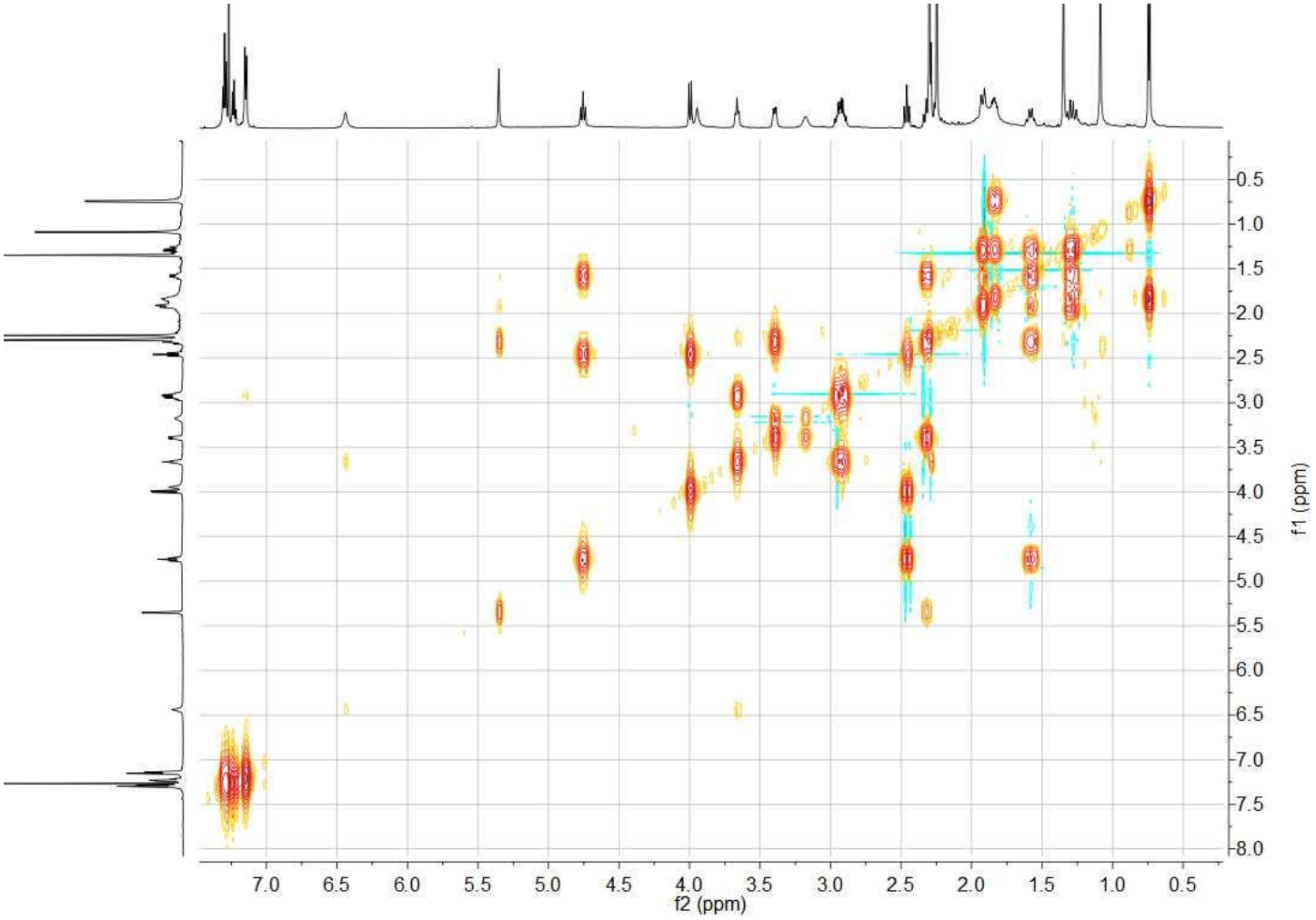

Fig. S6. ^{1}H-^{1}H COSY of **1**.

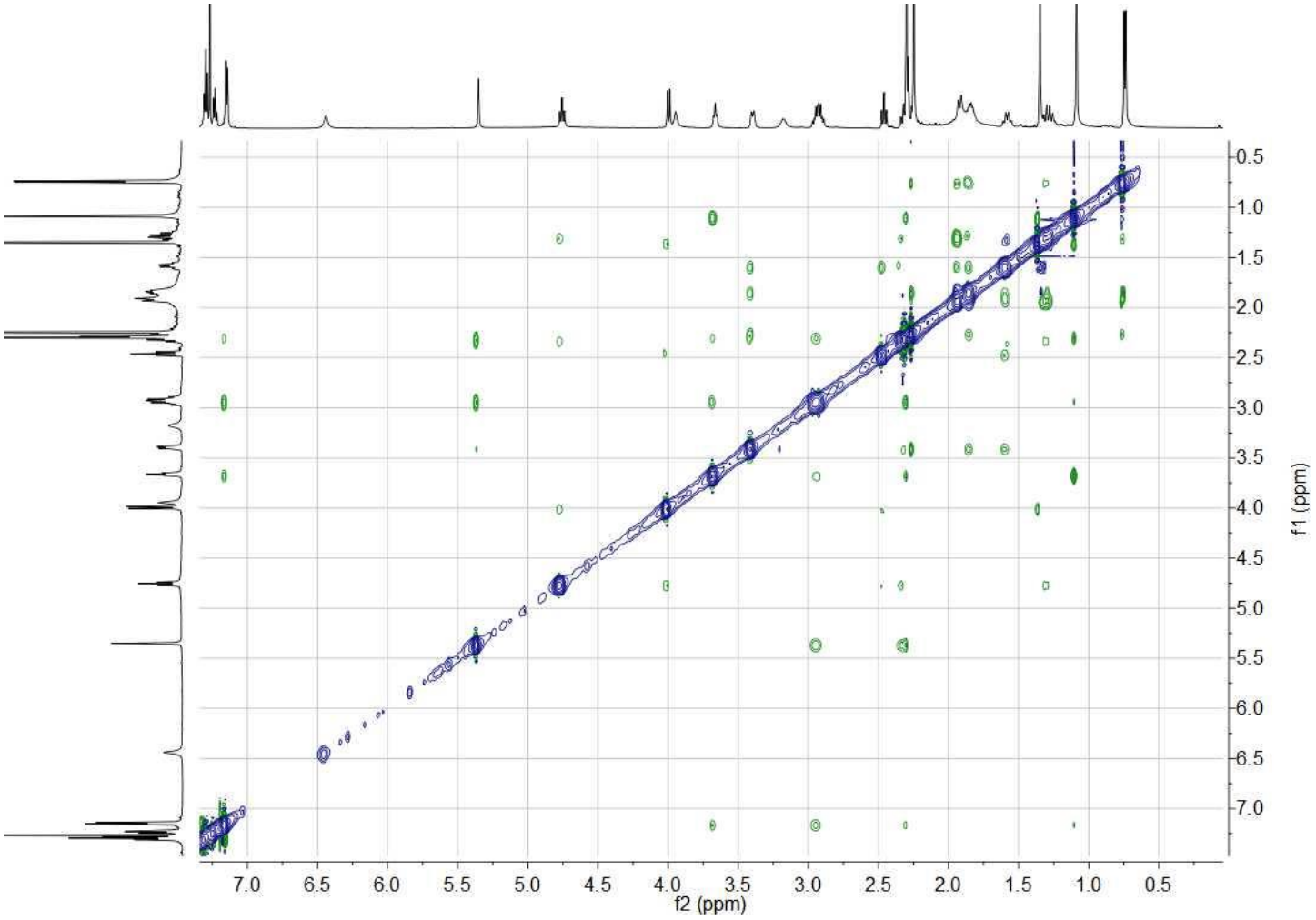

Fig. S7. ROESY of **1**.

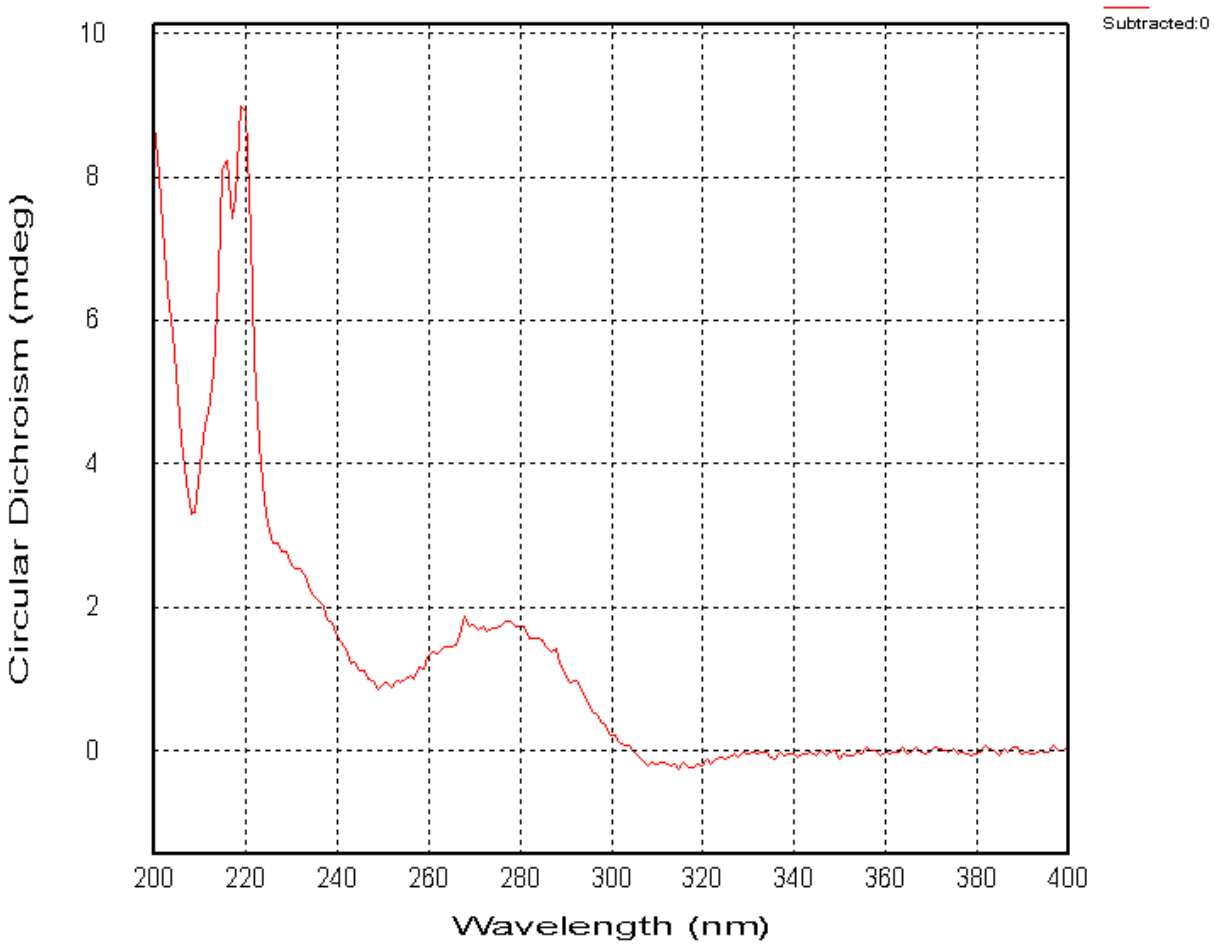

Fig. S8. Experimental ECD of **1**.

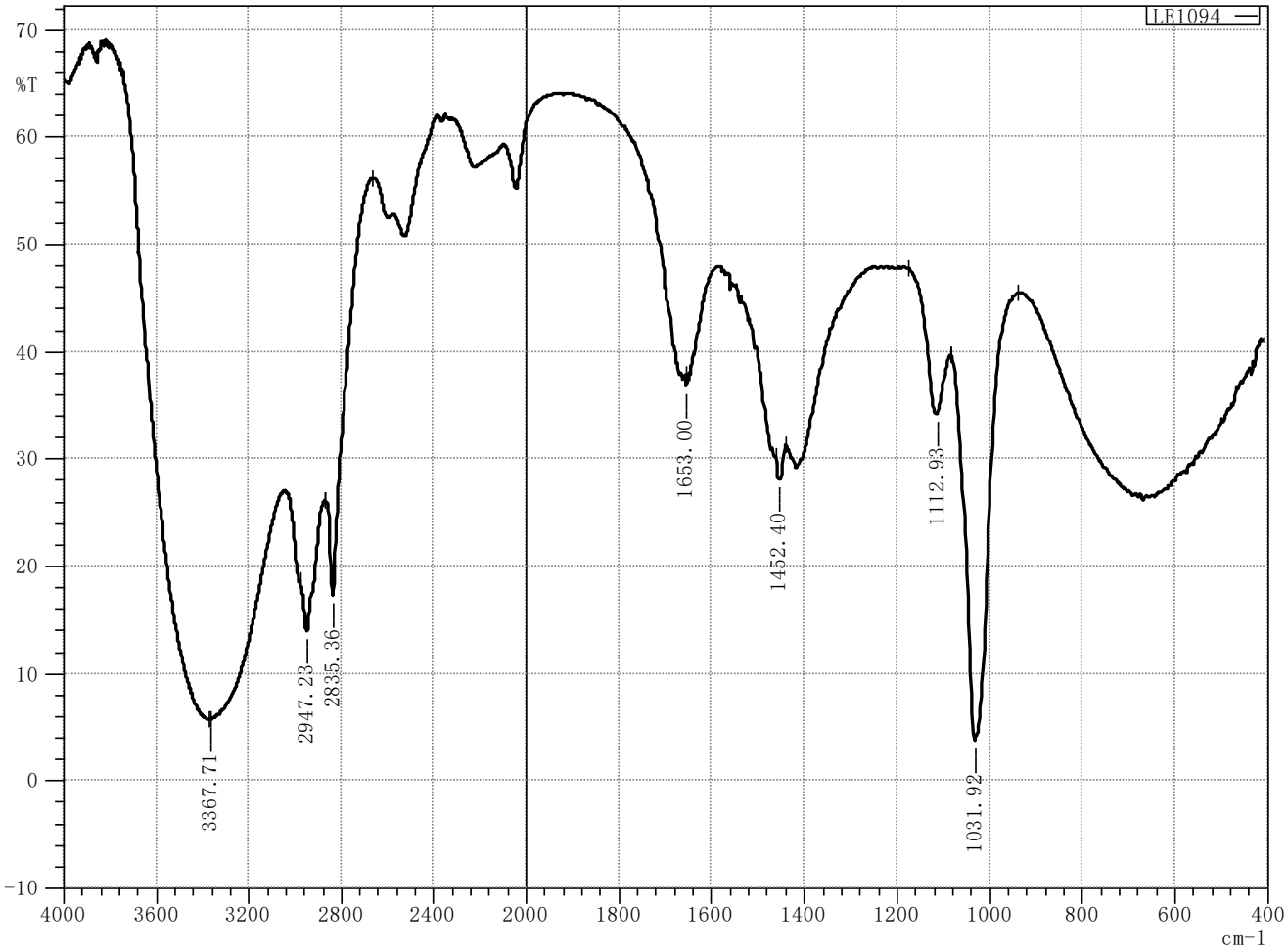

Fig. S9. IR spectrum of **1**.

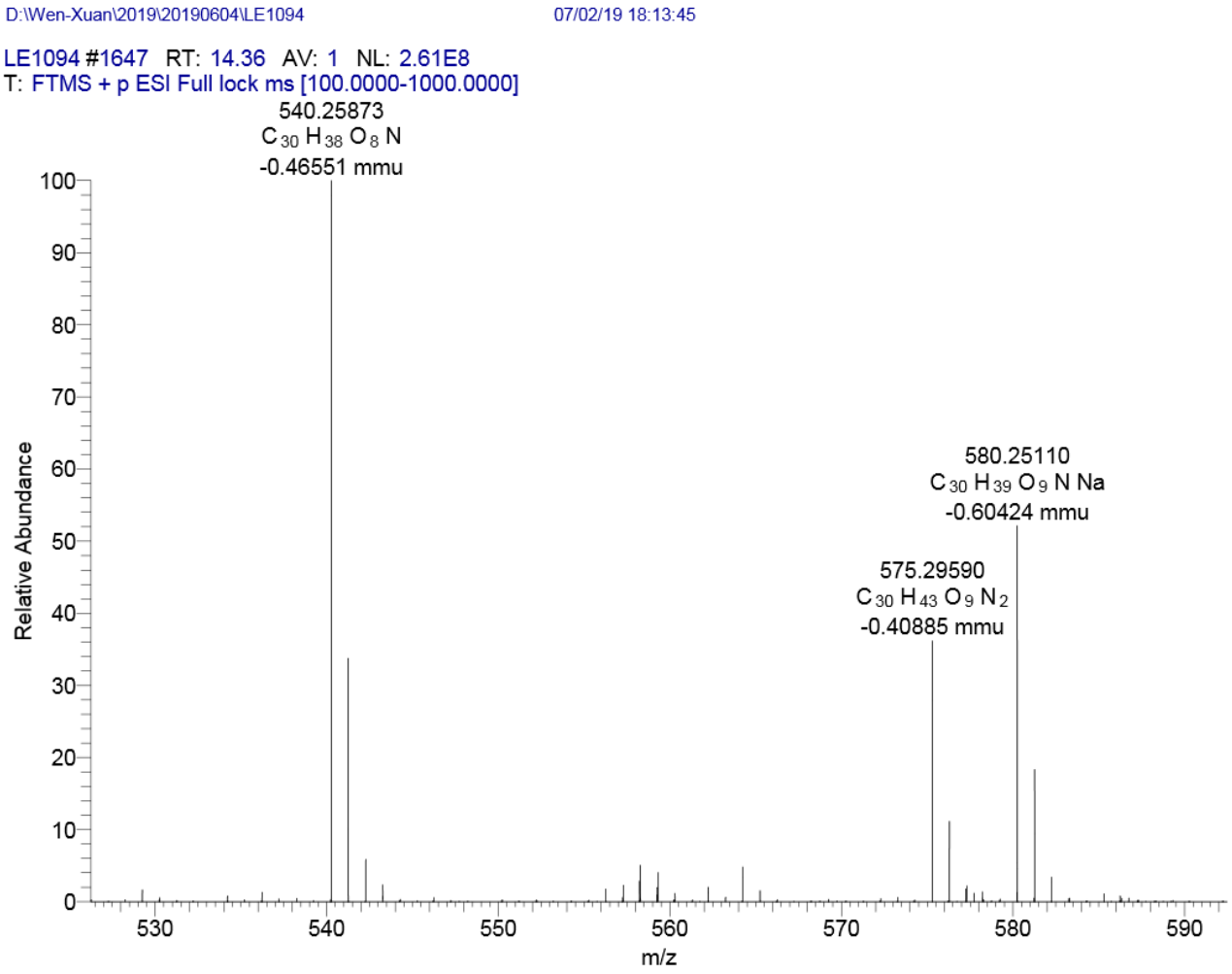

Fig. S10. HRESIMS of **1**.

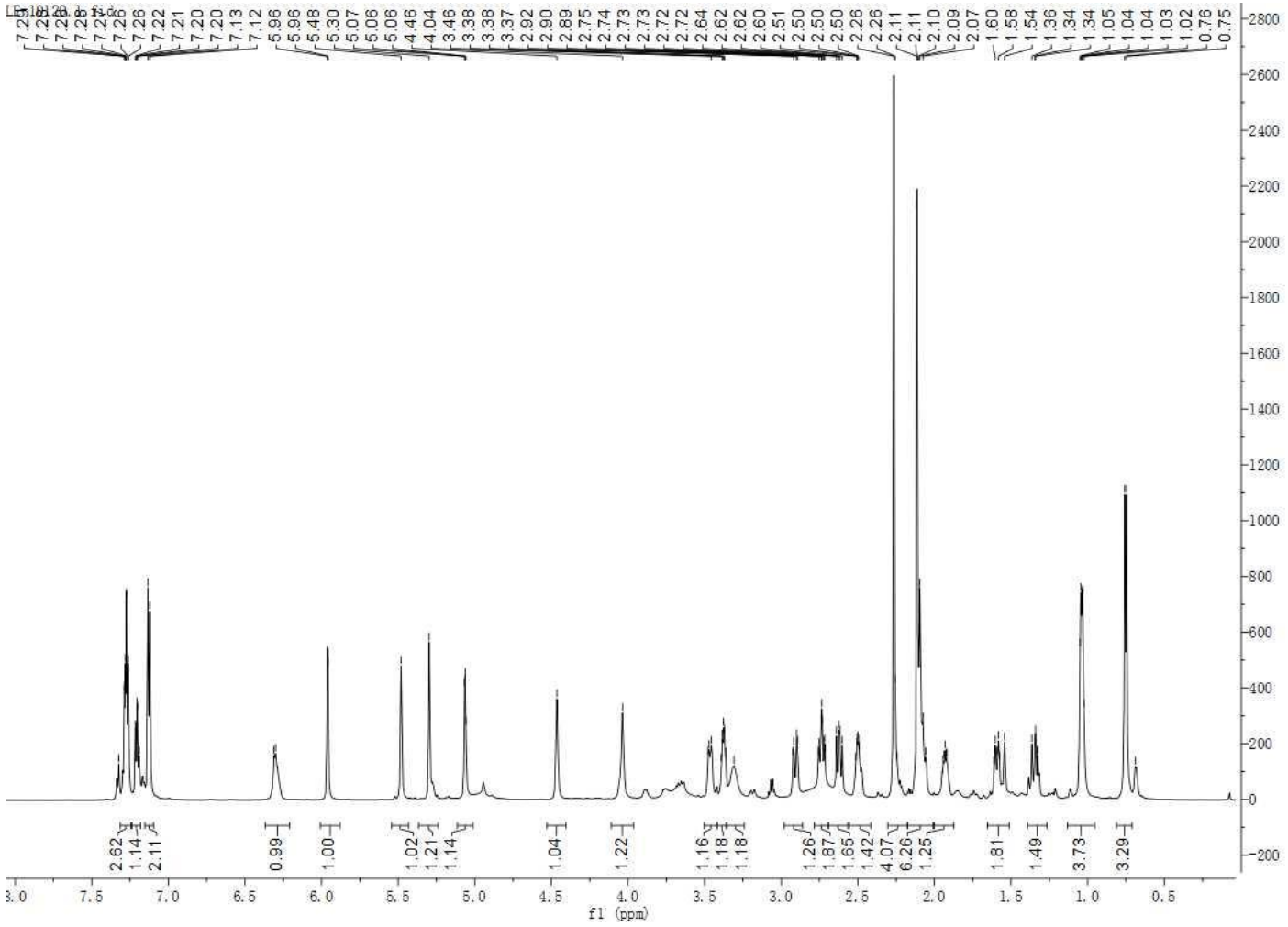

Fig. S11. ^{1}H NMR of **2** ($CDCl_3$, 600 MHz).

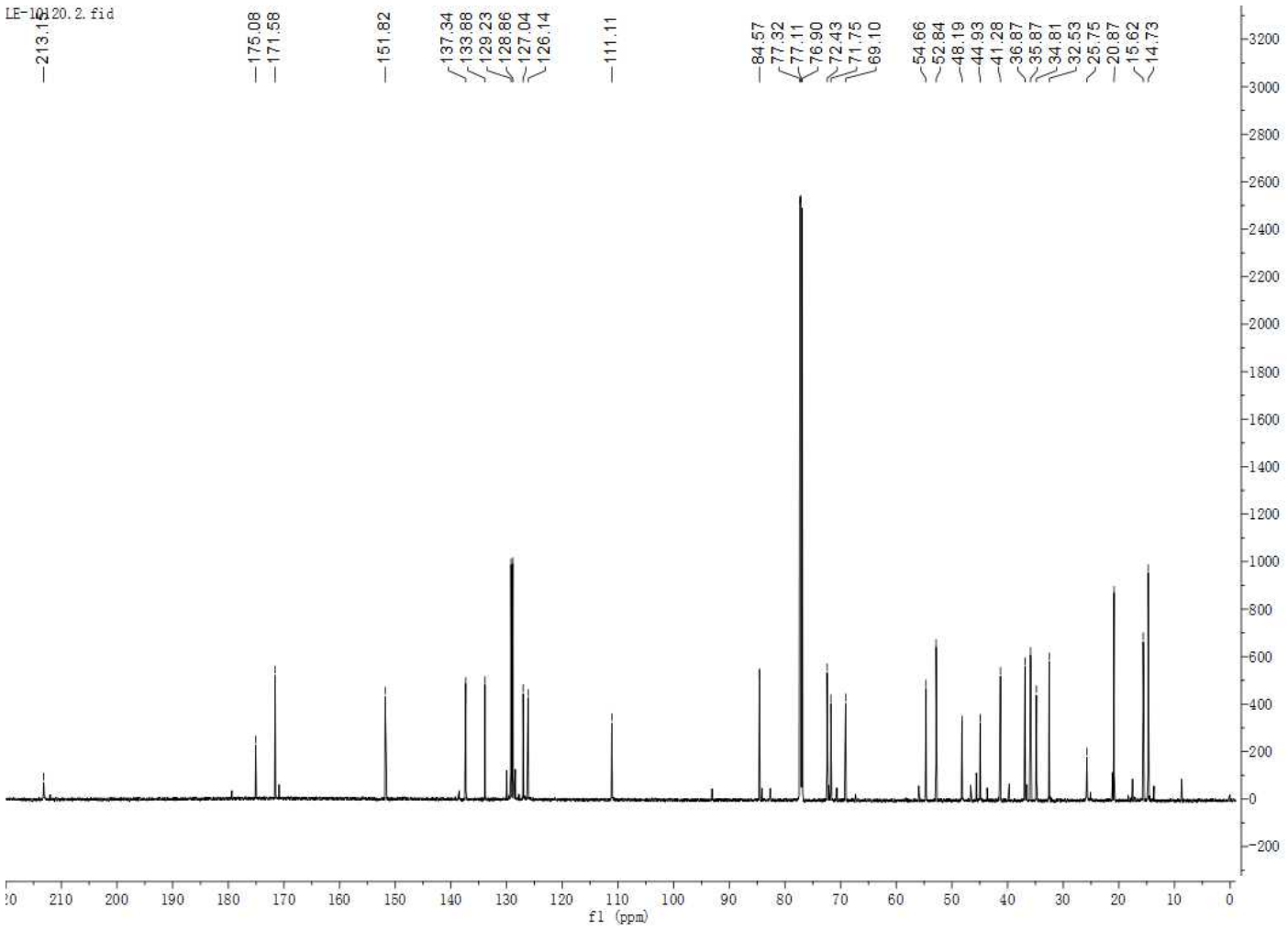

Fig. S12. ^{13}C NMR of **2** (CDCl3, 150 MHz).

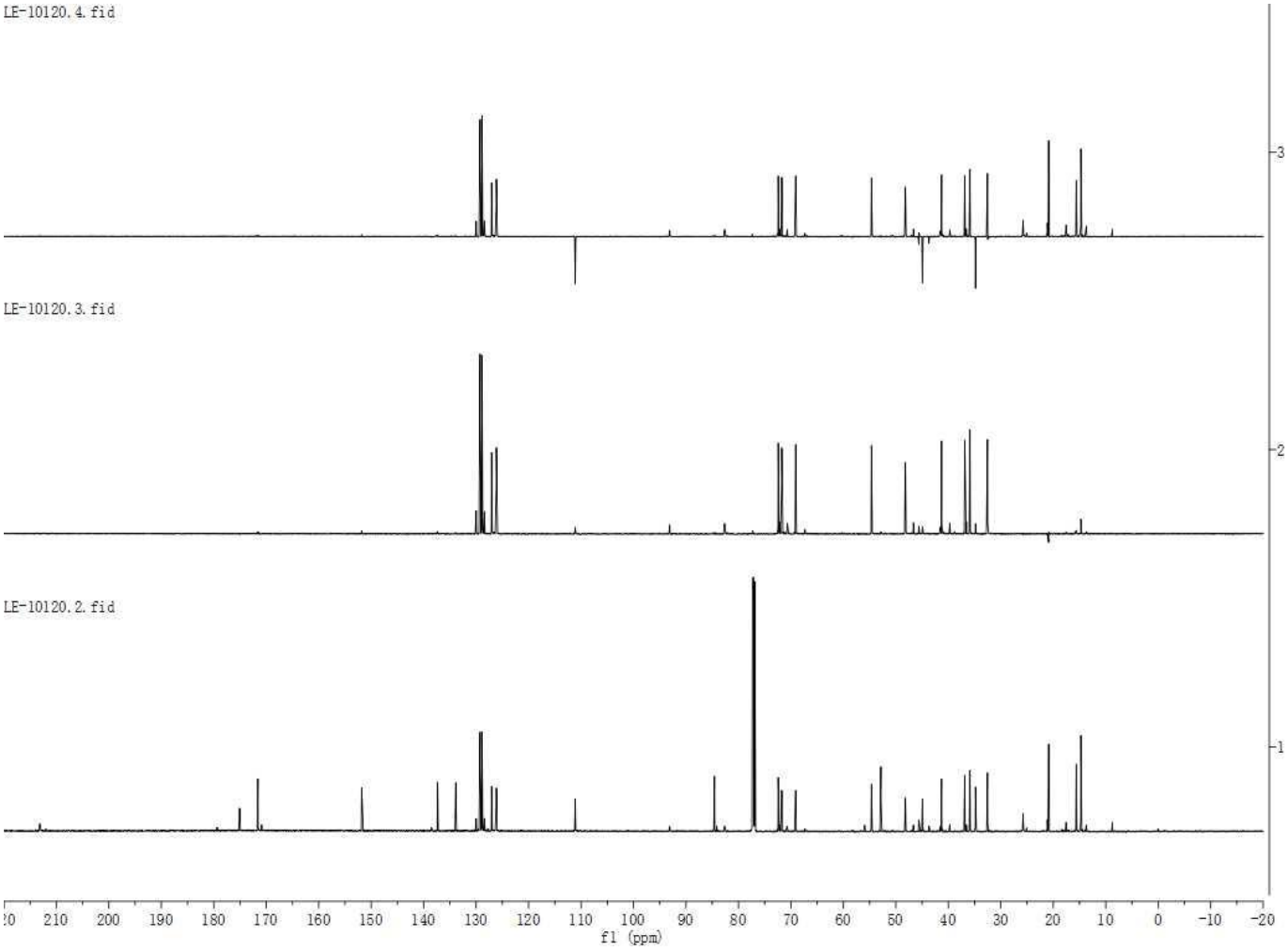

Fig. S13. DEPT of **2**.

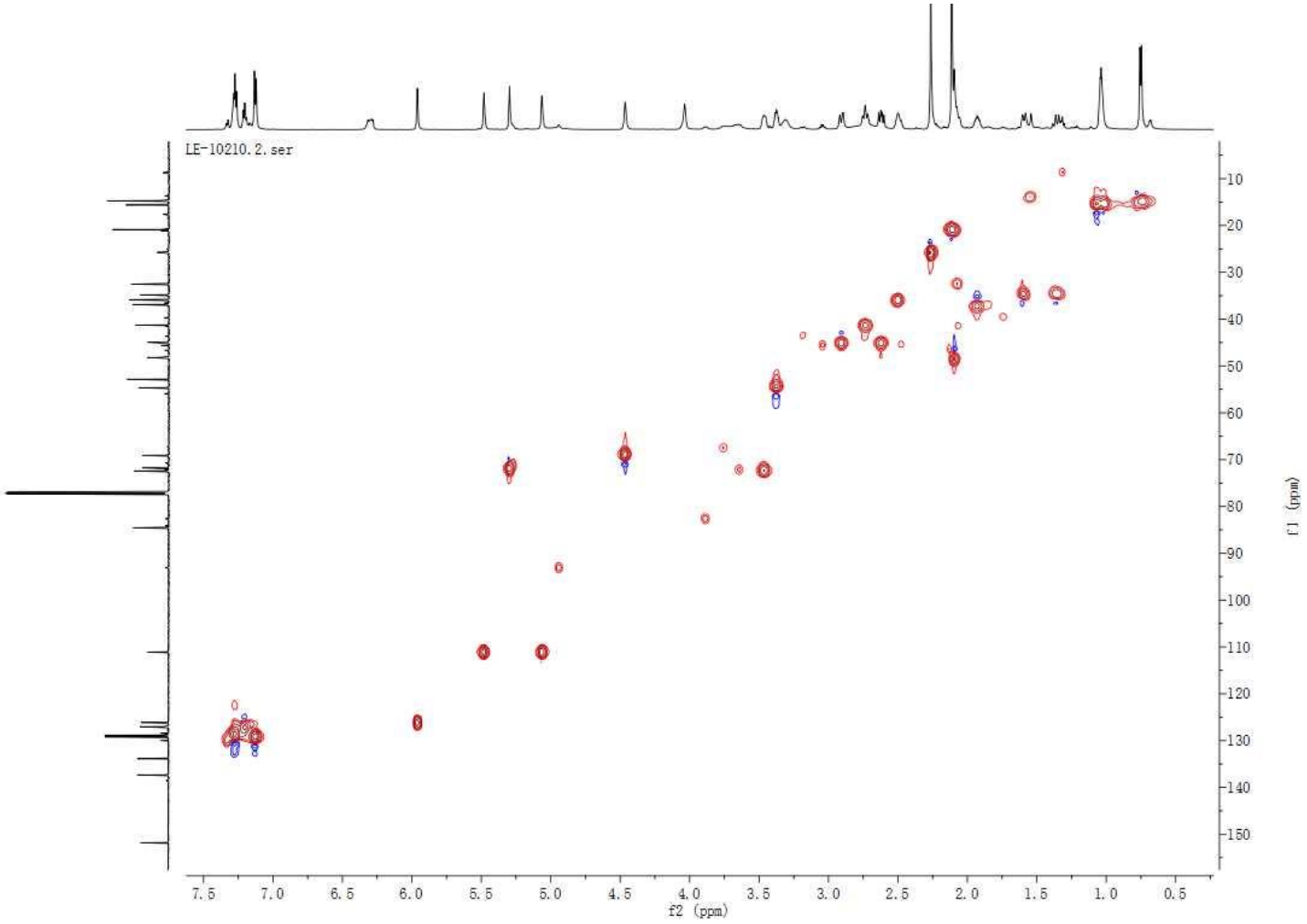

Fig. S14. HSQC of **2**.

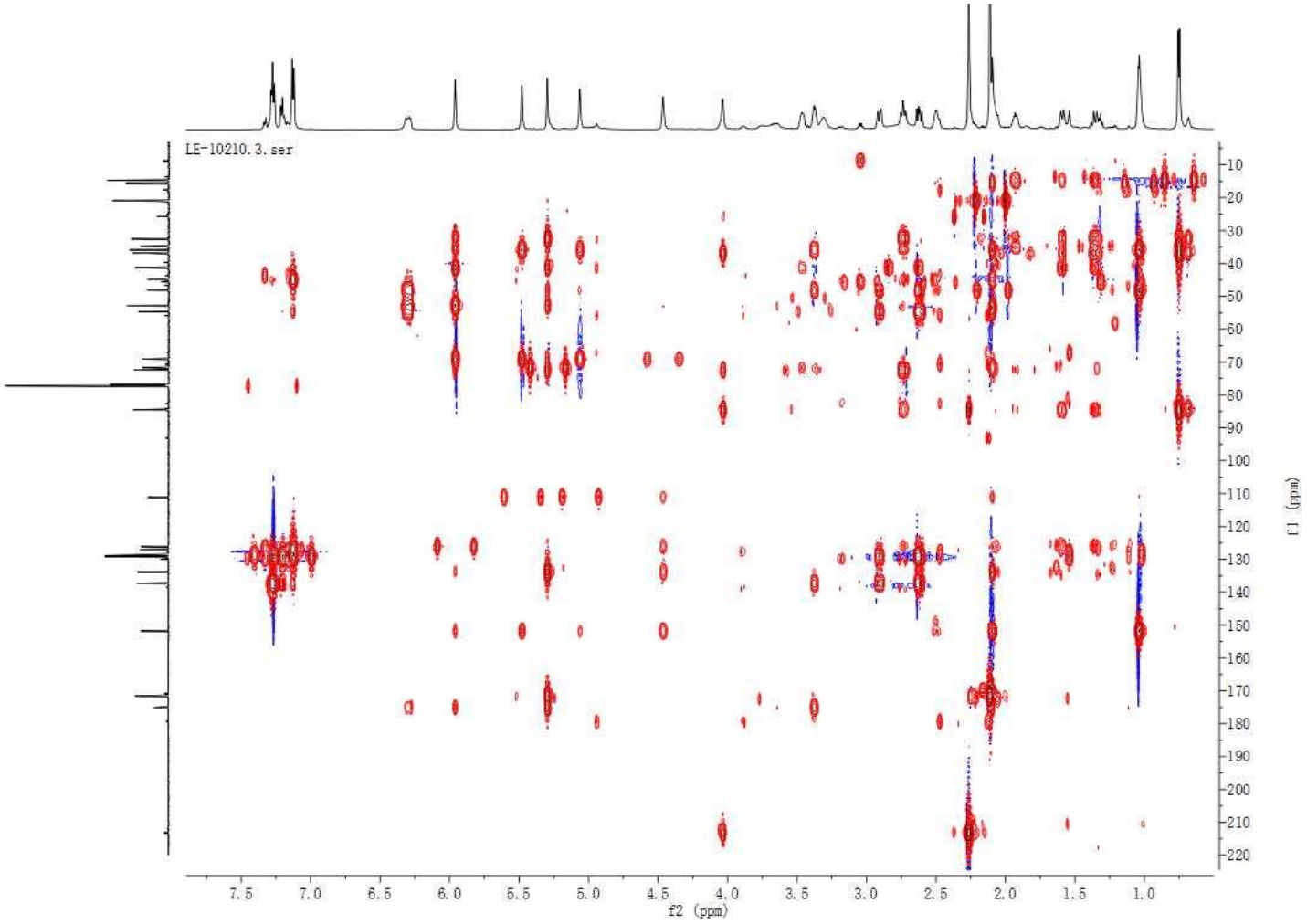

Fig. S15. HMBC of **2**.

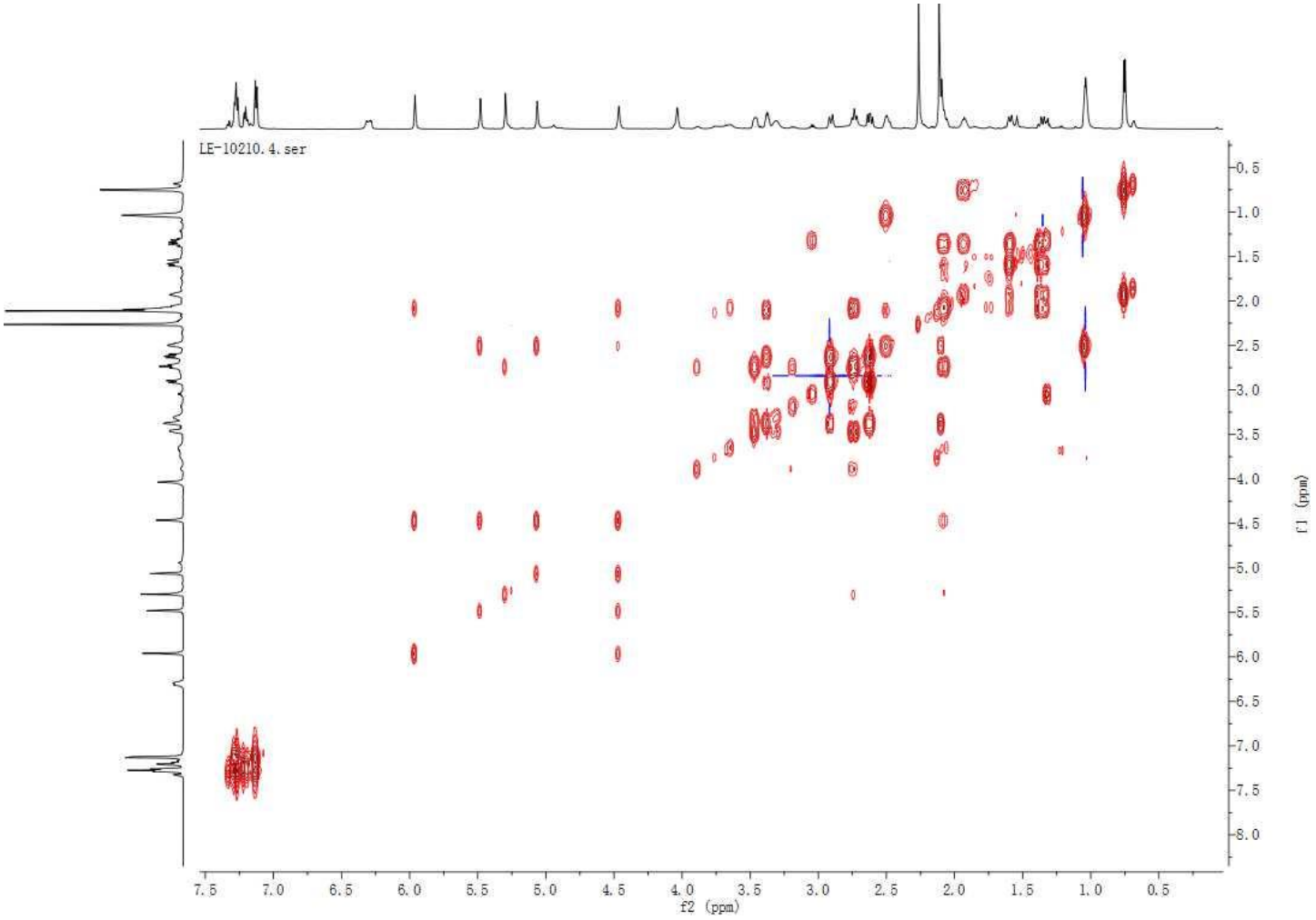

Fig. S16. ^{1}H-^{1}H COSY of **2**.

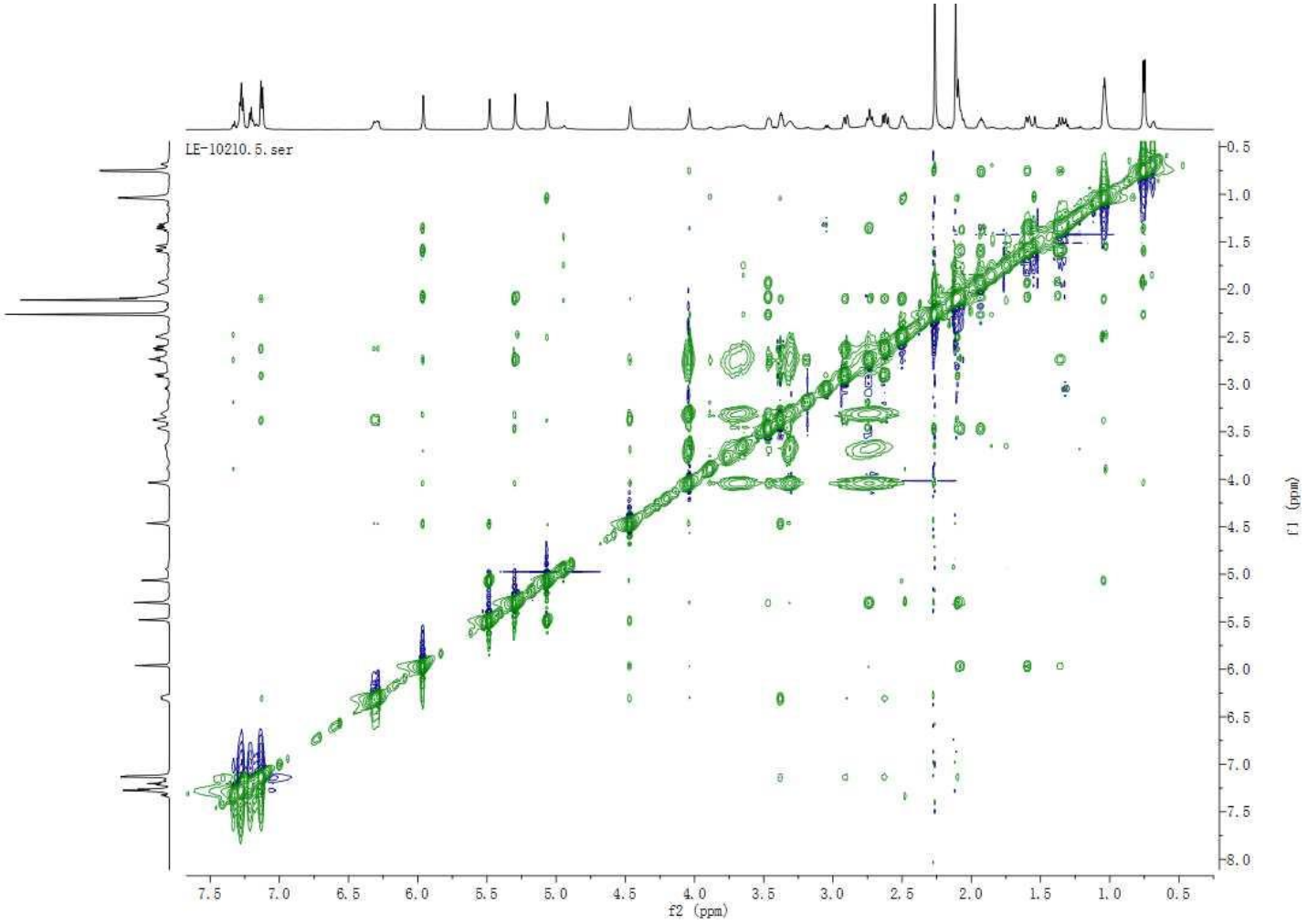

Fig. S17. ROESY of **2**.

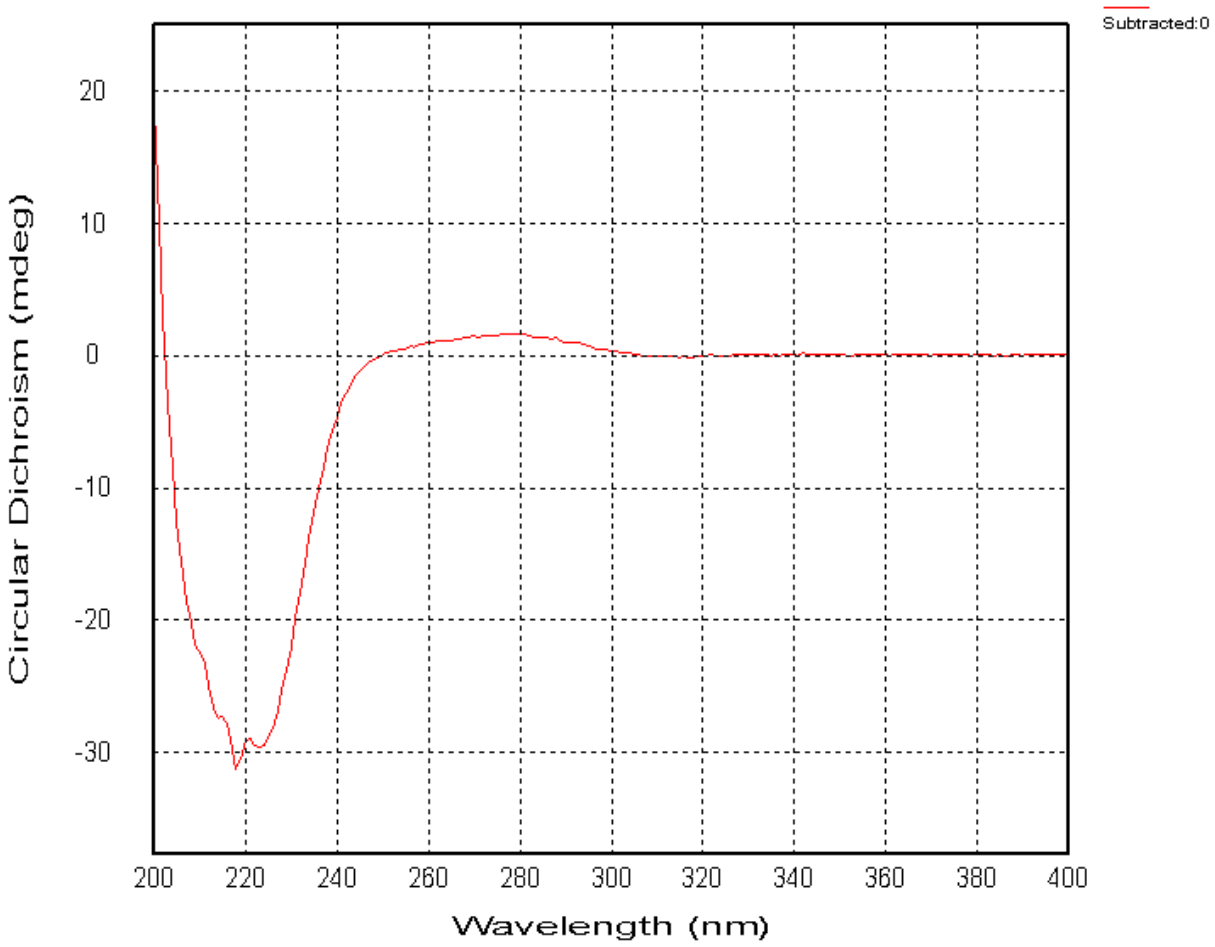

Fig. S18. Experimental ECD of **2**.

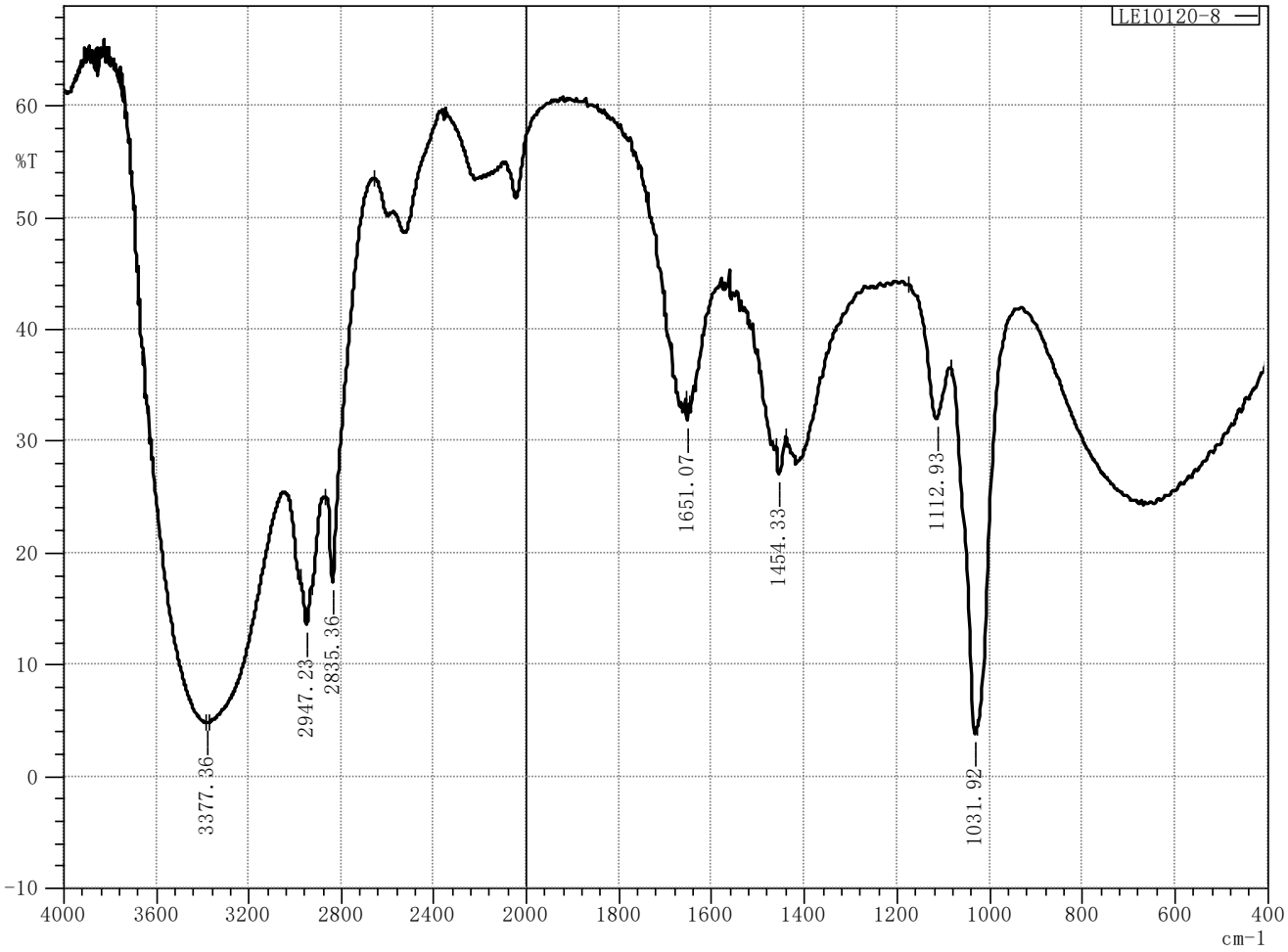

Fig. S19. IR of **2**.

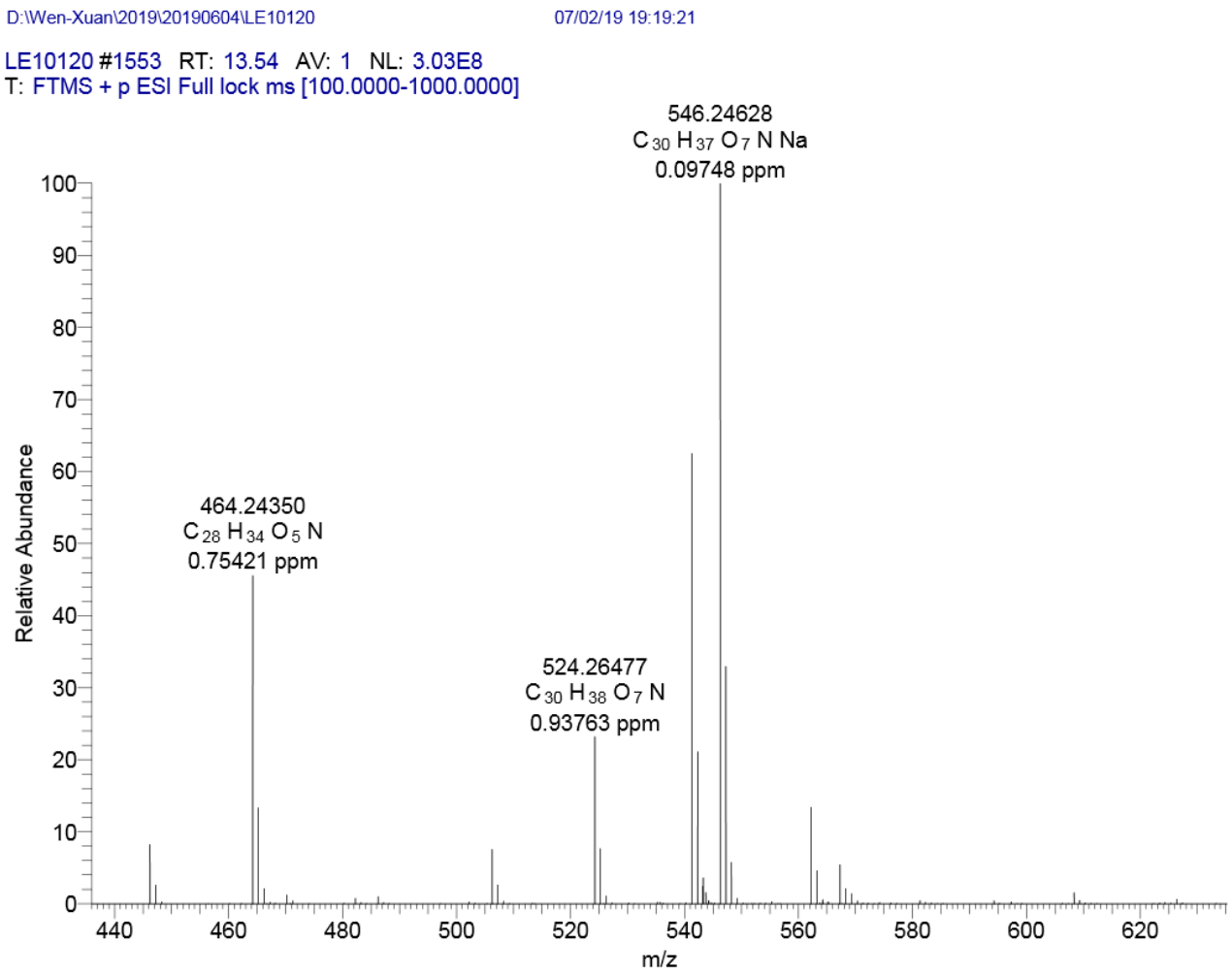

Fig. S20. HRESIMS of **2**.

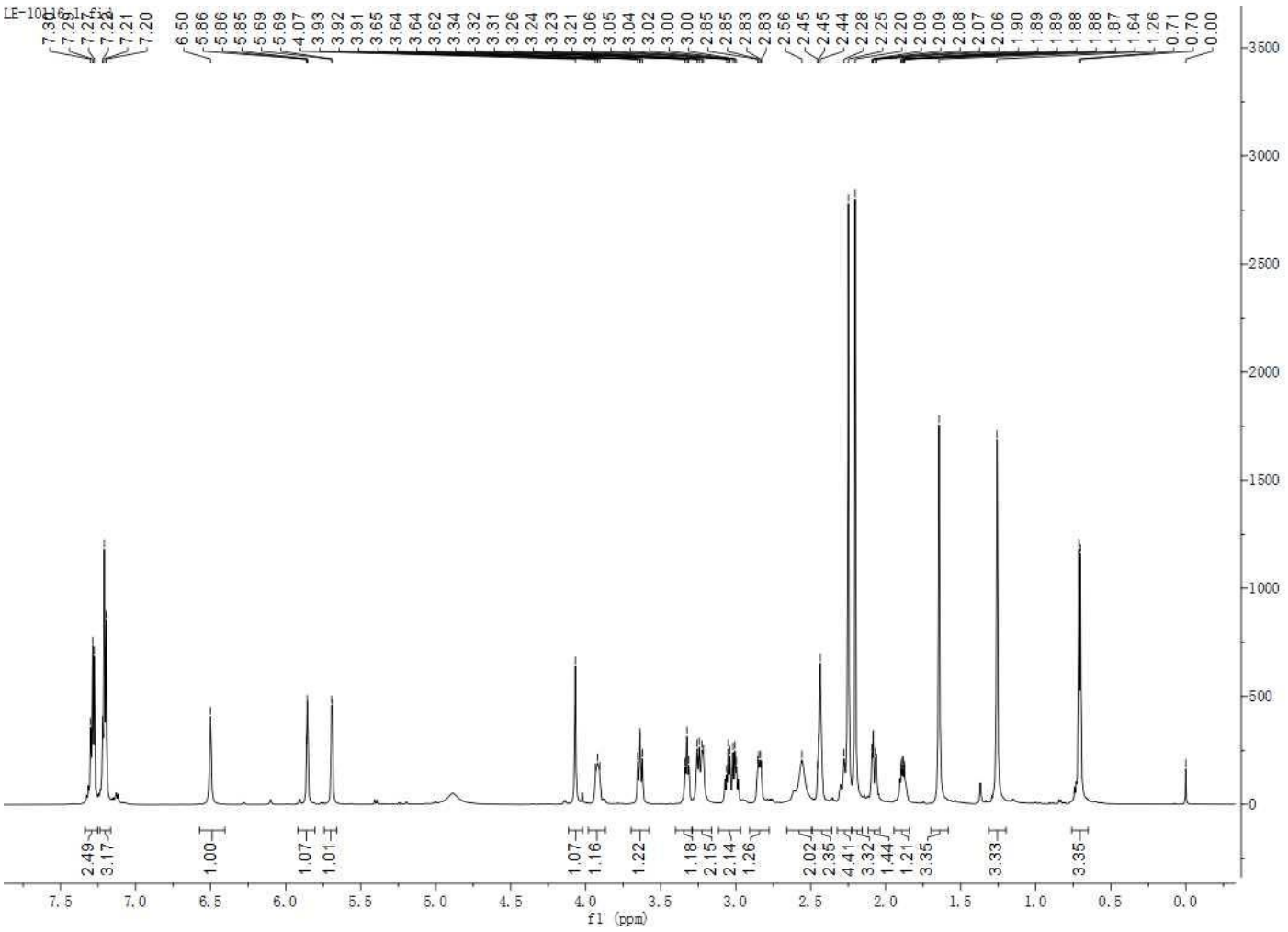

Fig. S21. ^{1}H NMR of **3** ($CDCl_3$, 600 MHz).

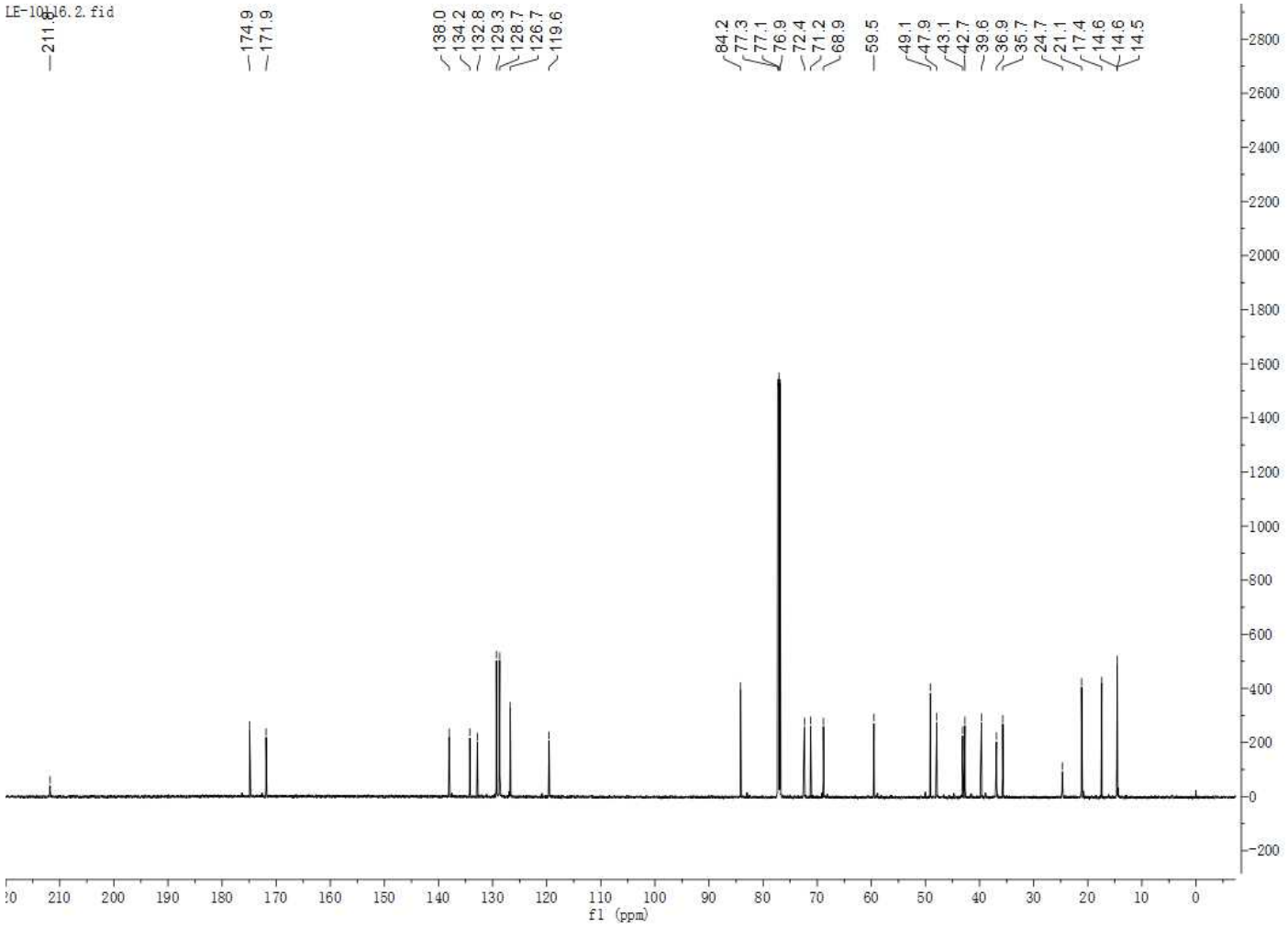

Fig. S22. ^{13}C NMR of **3** ($CDCl_3$, 150 MHz).

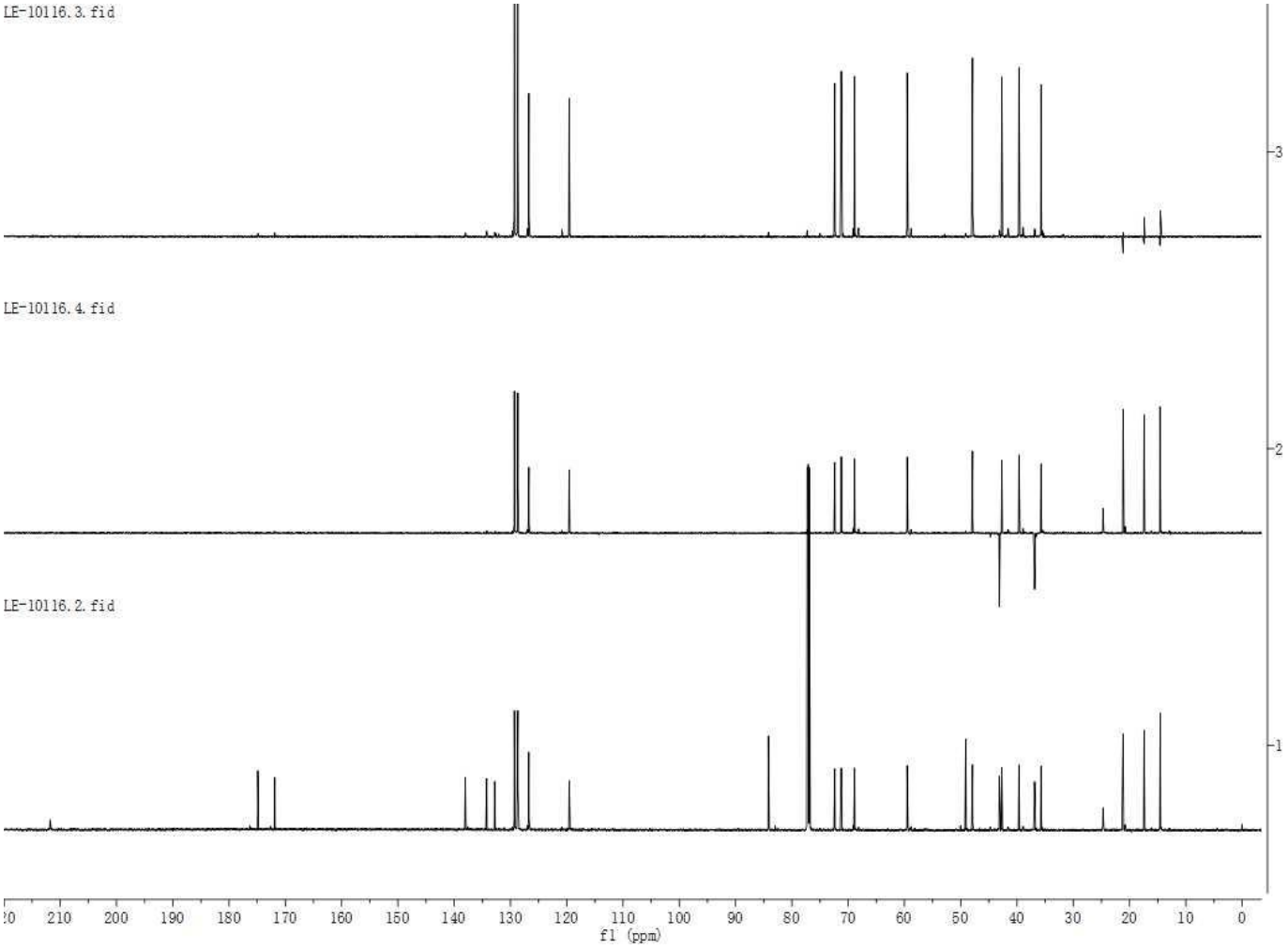

Fig. S23. DEPT of **3**.

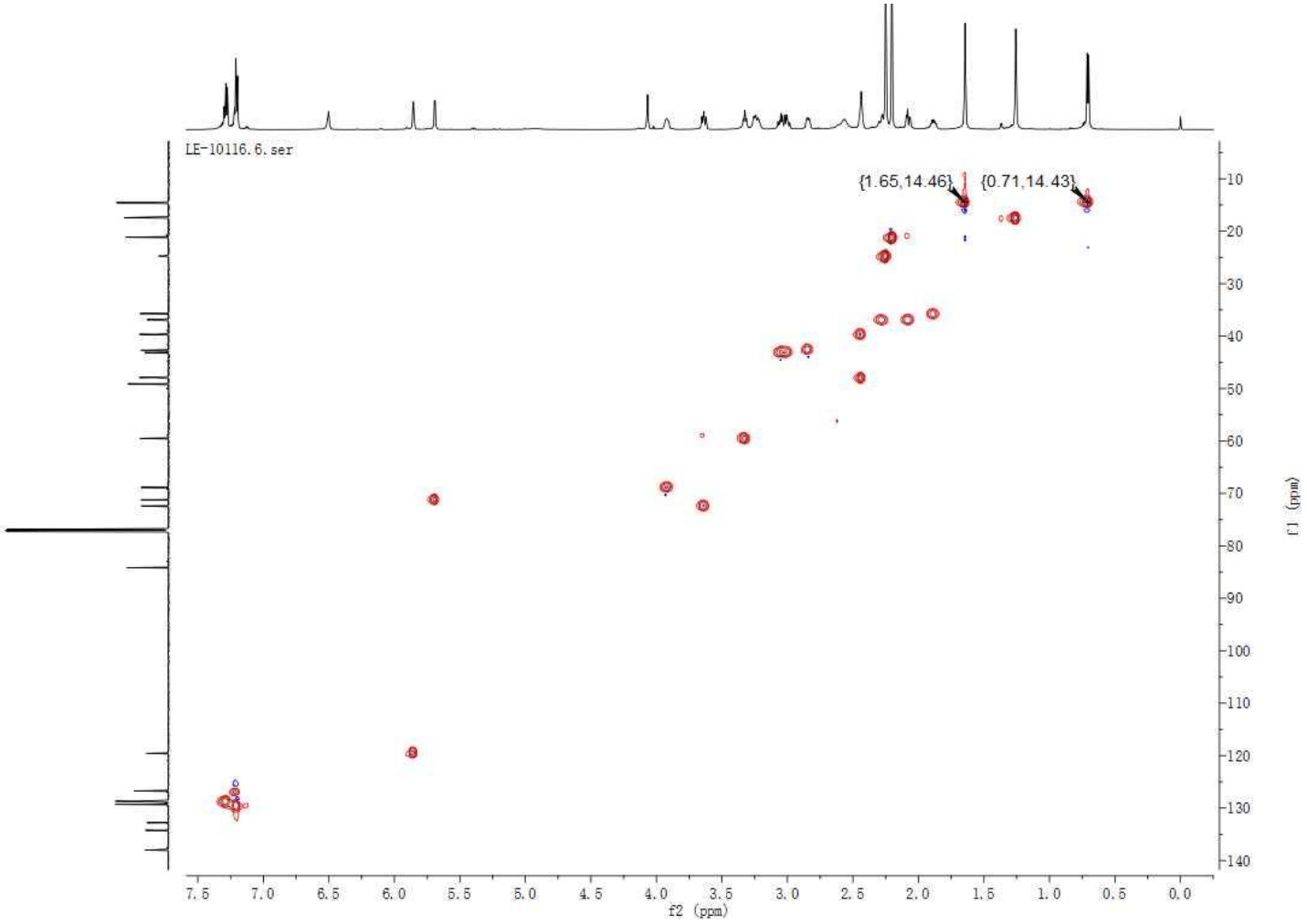

Fig. S24. HSQC of **3**.

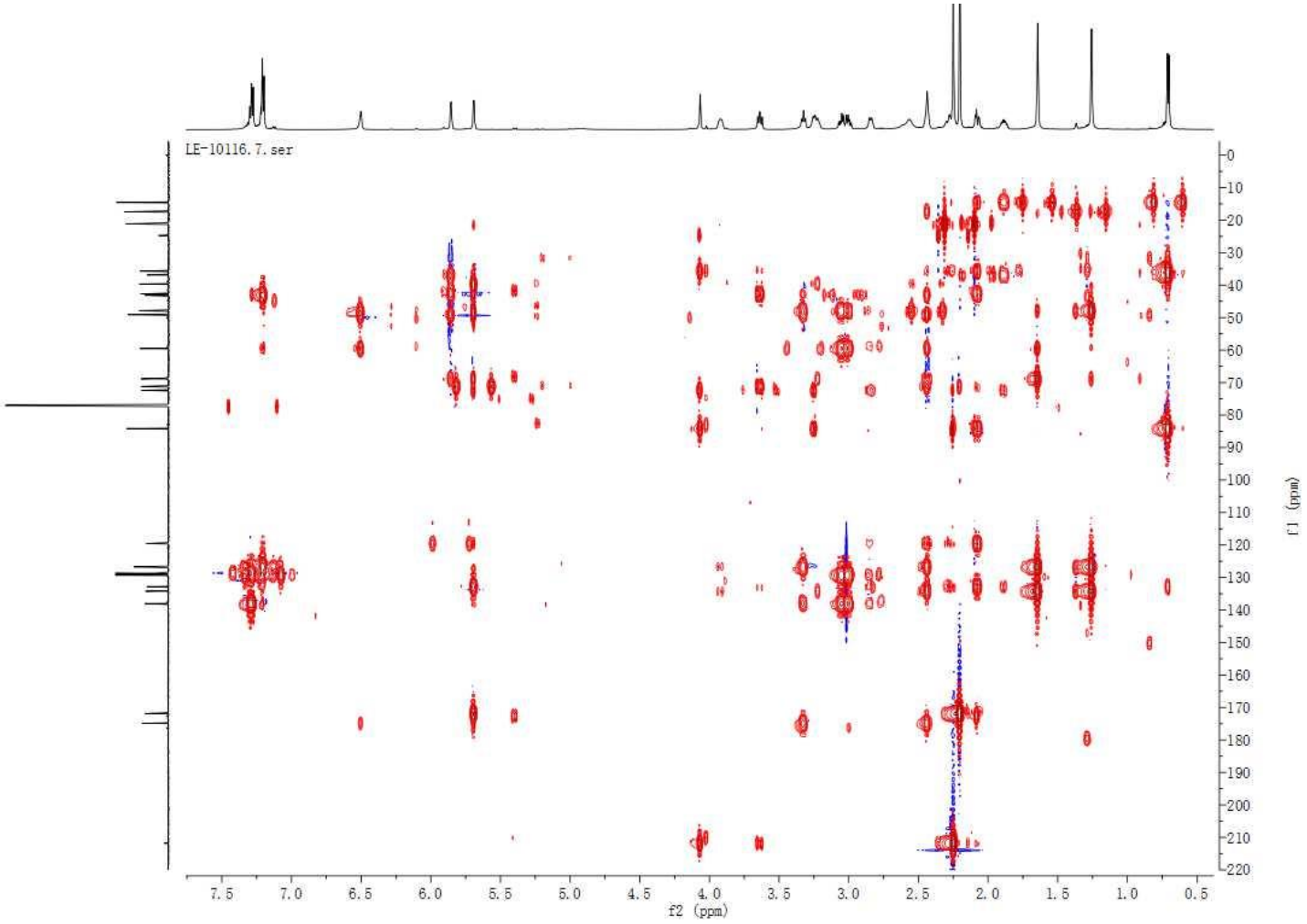

Fig. S25. HMBC of **3**.

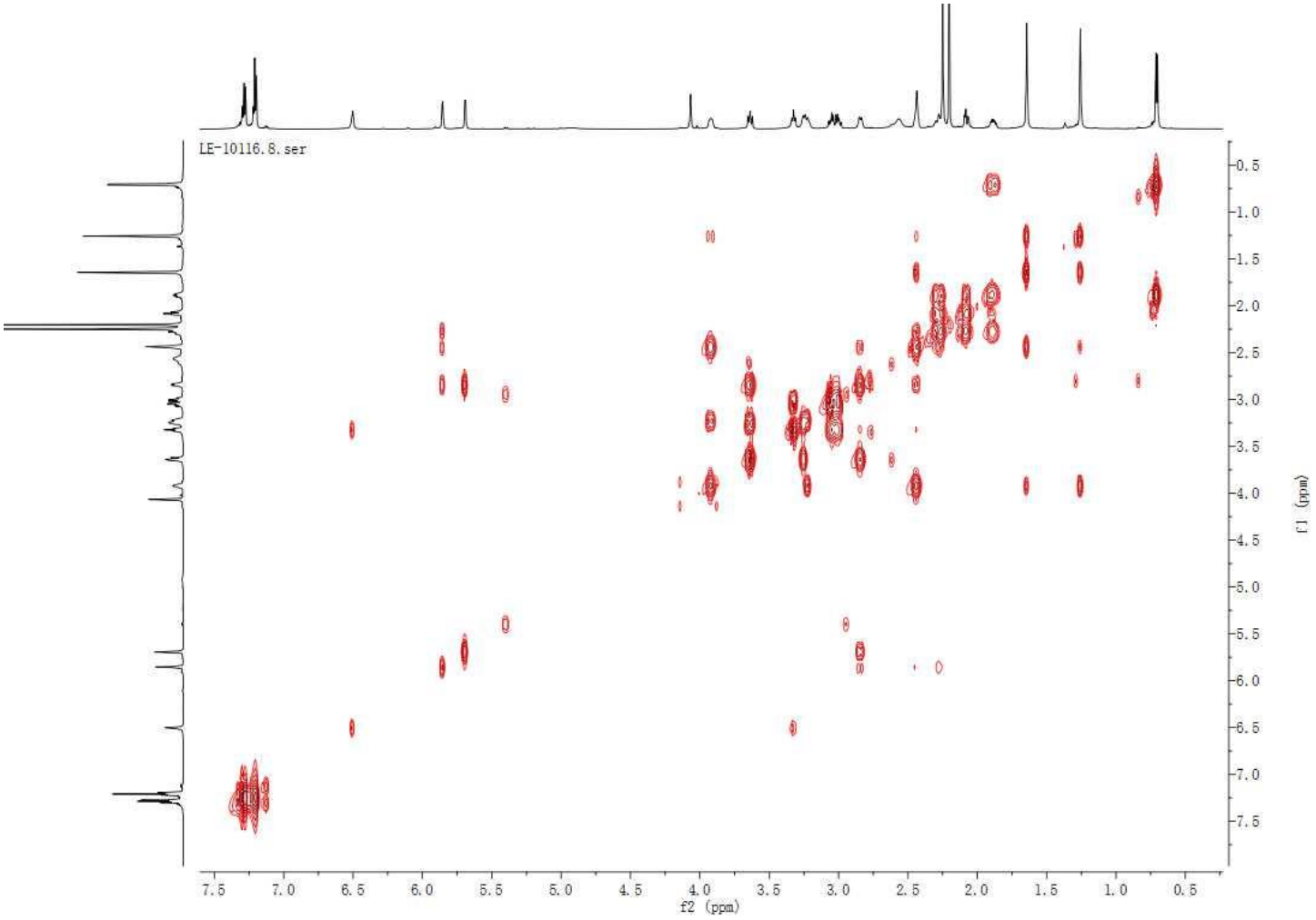

Fig. S26. ^{1}H-^{1}H COSY of **3**.

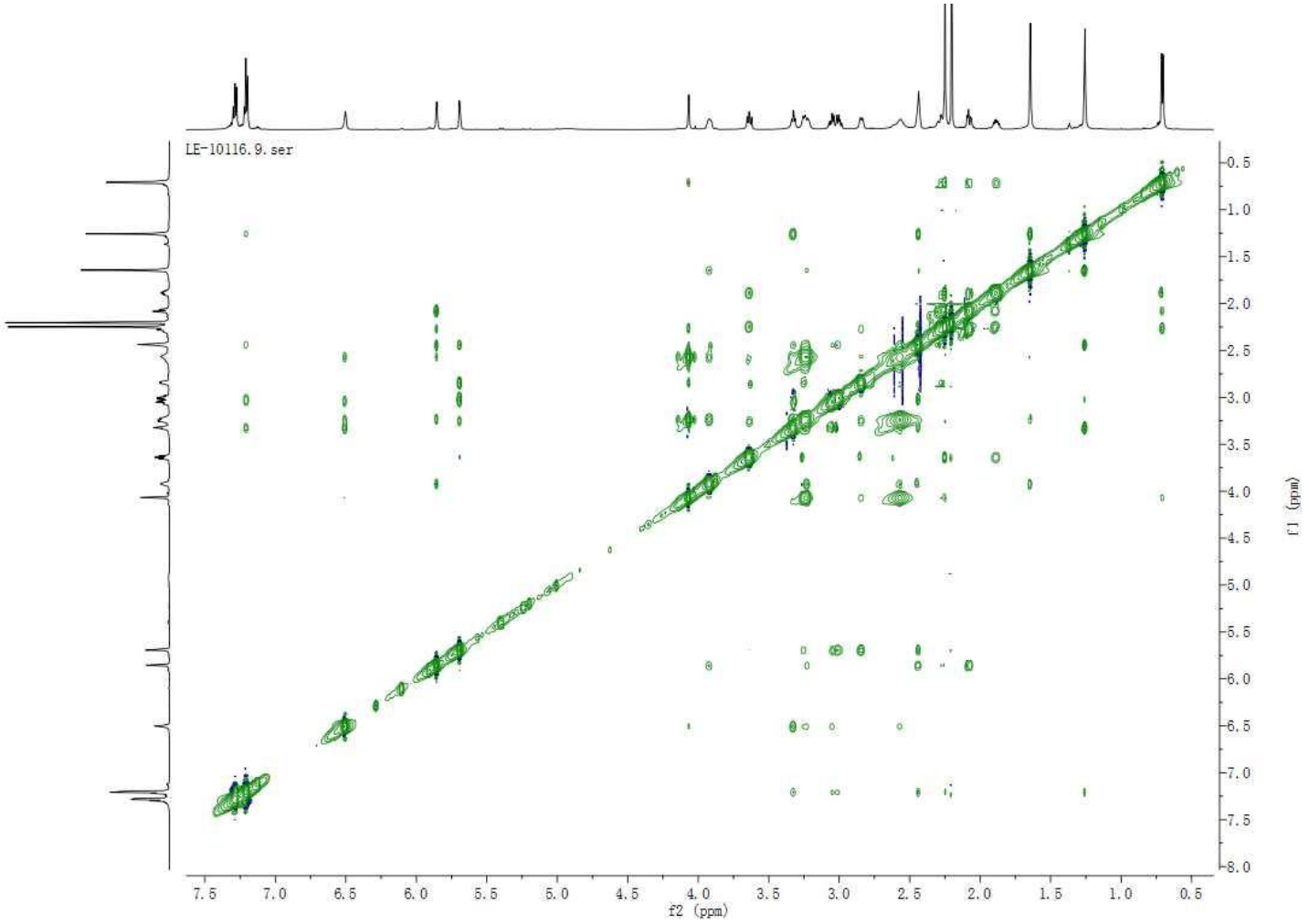

Fig. S27. ROESY of **3**.

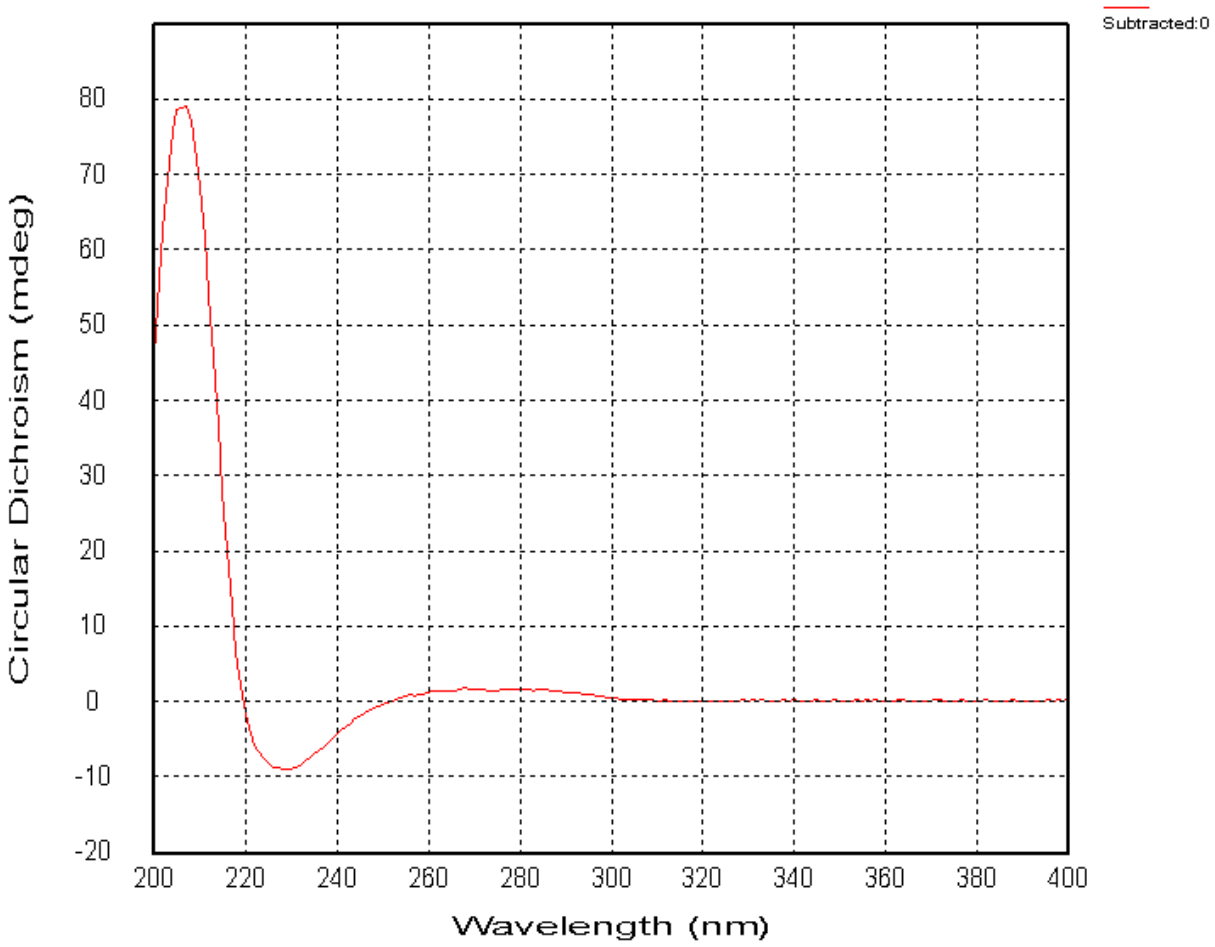

Fig. S28. Experimental ECD of **3**.

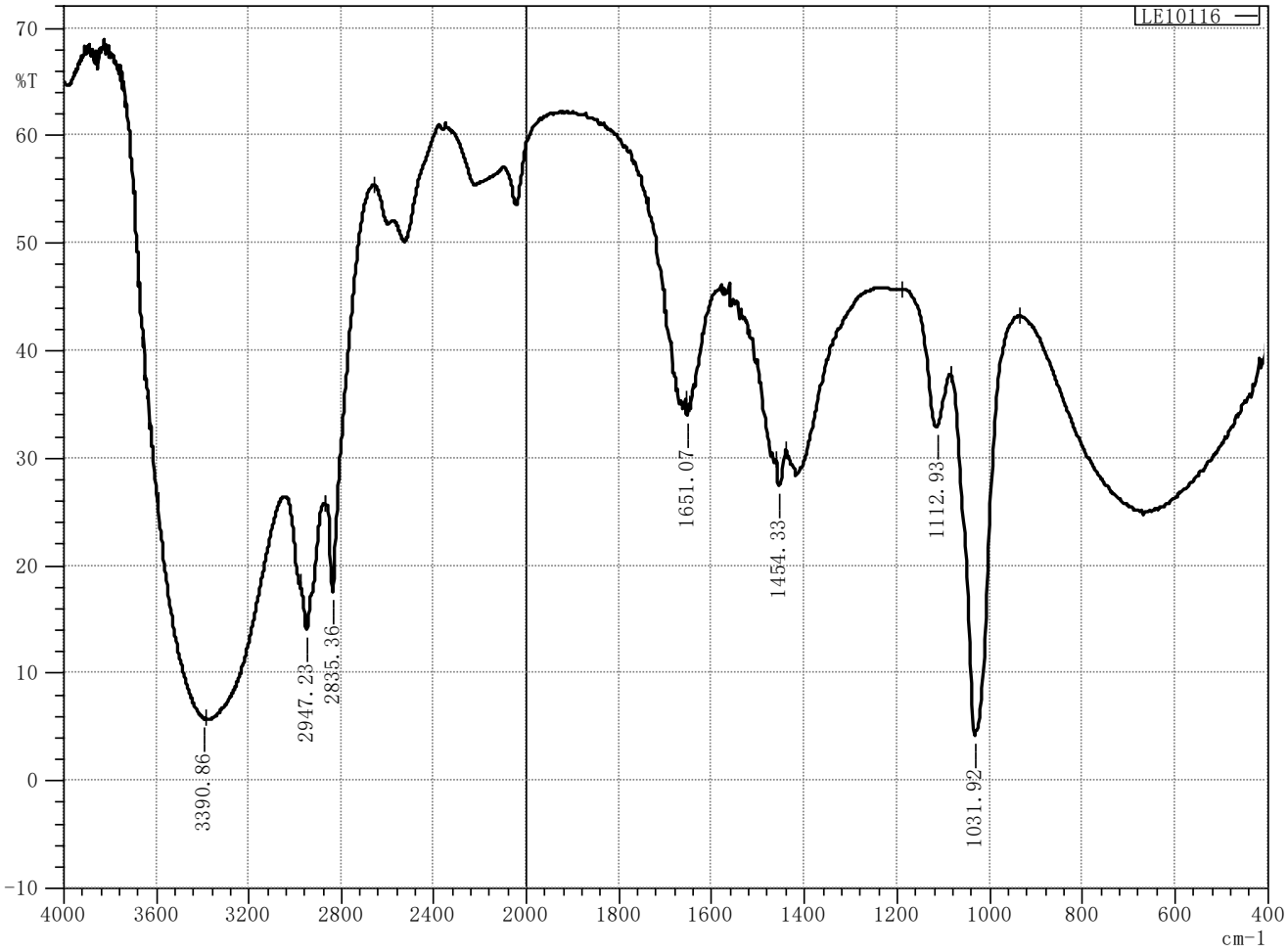

Fig. S29. IR of **3**.

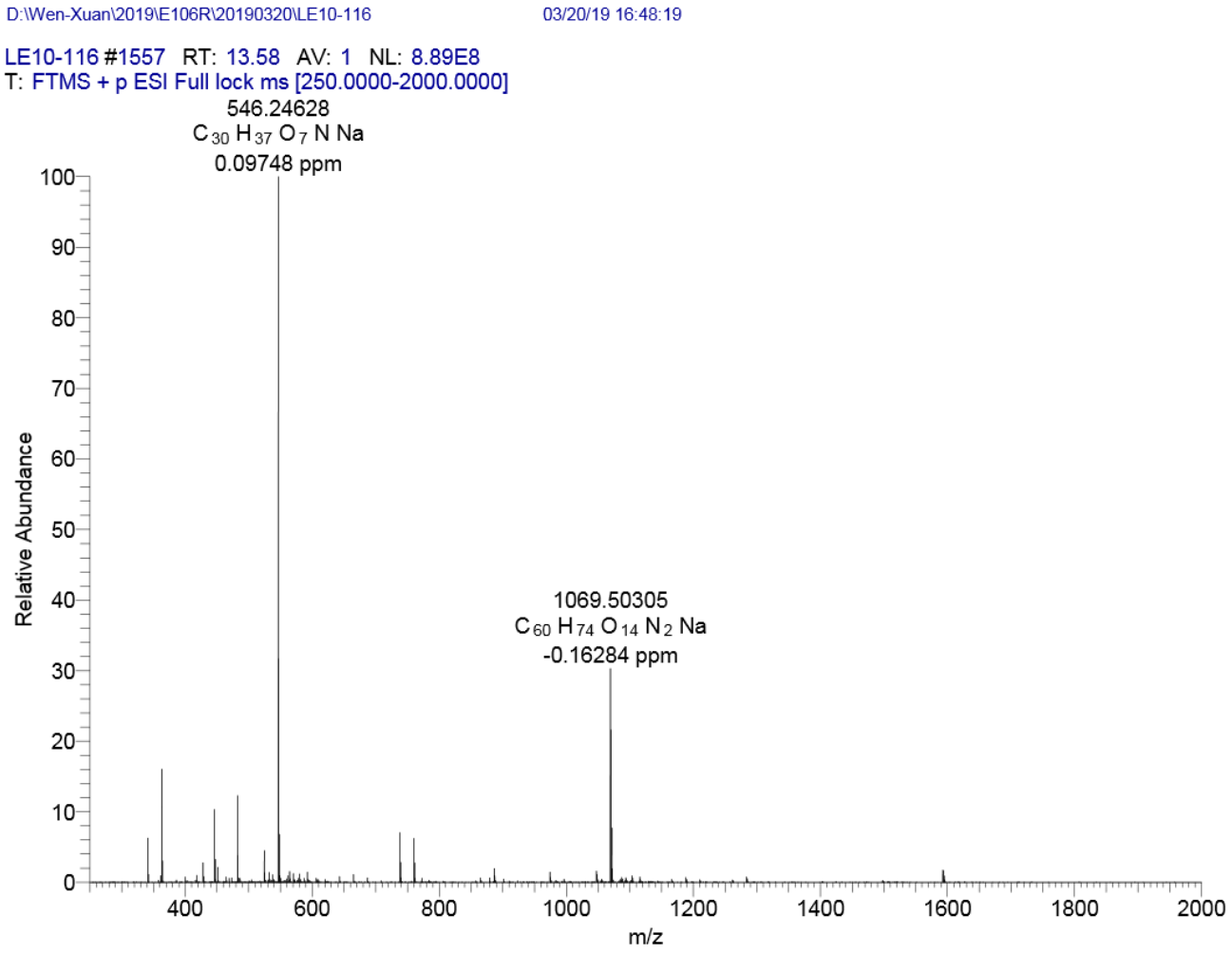

Fig. S30. HRESIMS of **3**.

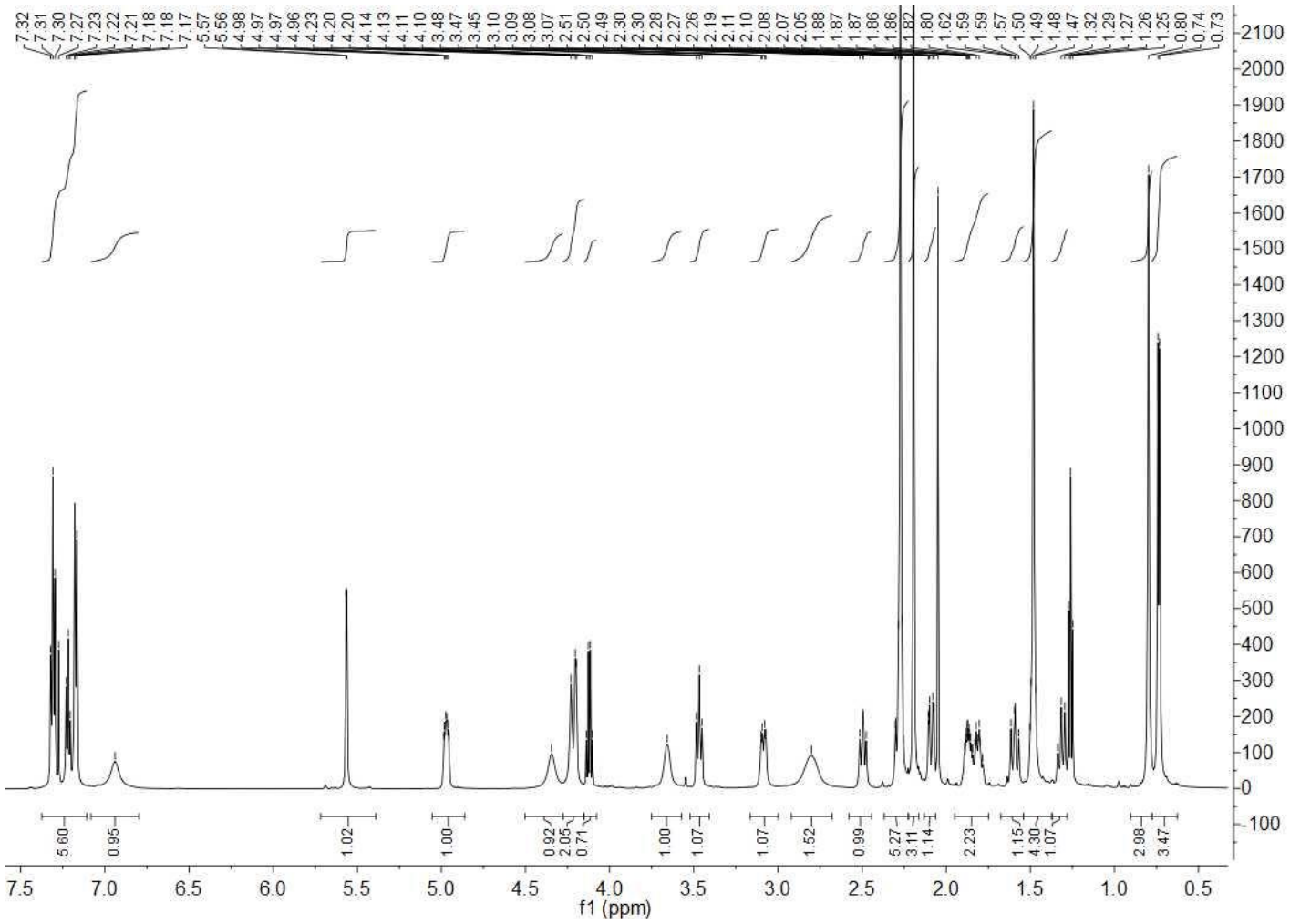

Fig. S31. ^{1}H NMR of **4** ($CDCl_3$, 600 MHz).

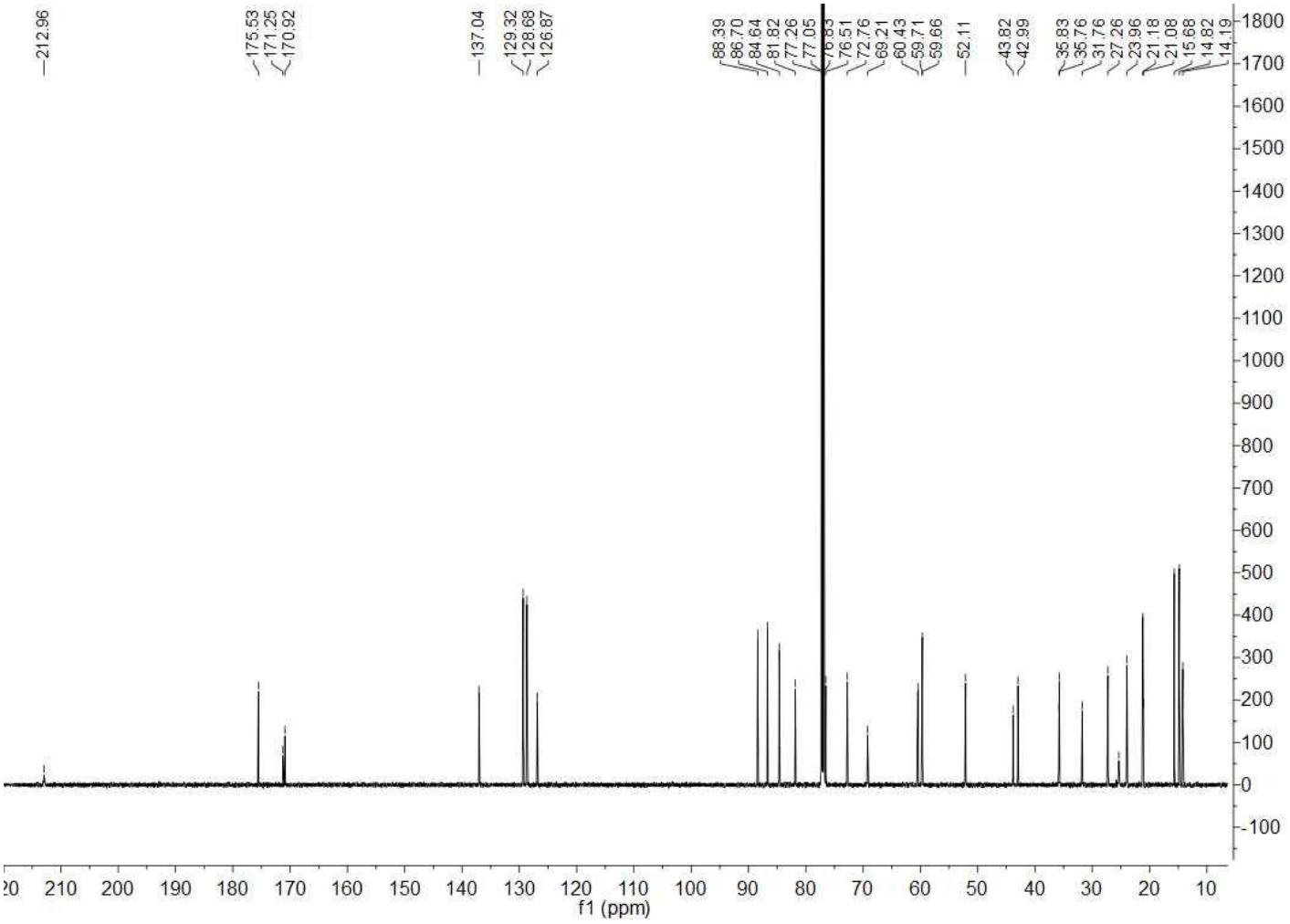

Fig. S32. ^{13}C NMR of **4** ($CDCl_3$, 150 MHz).

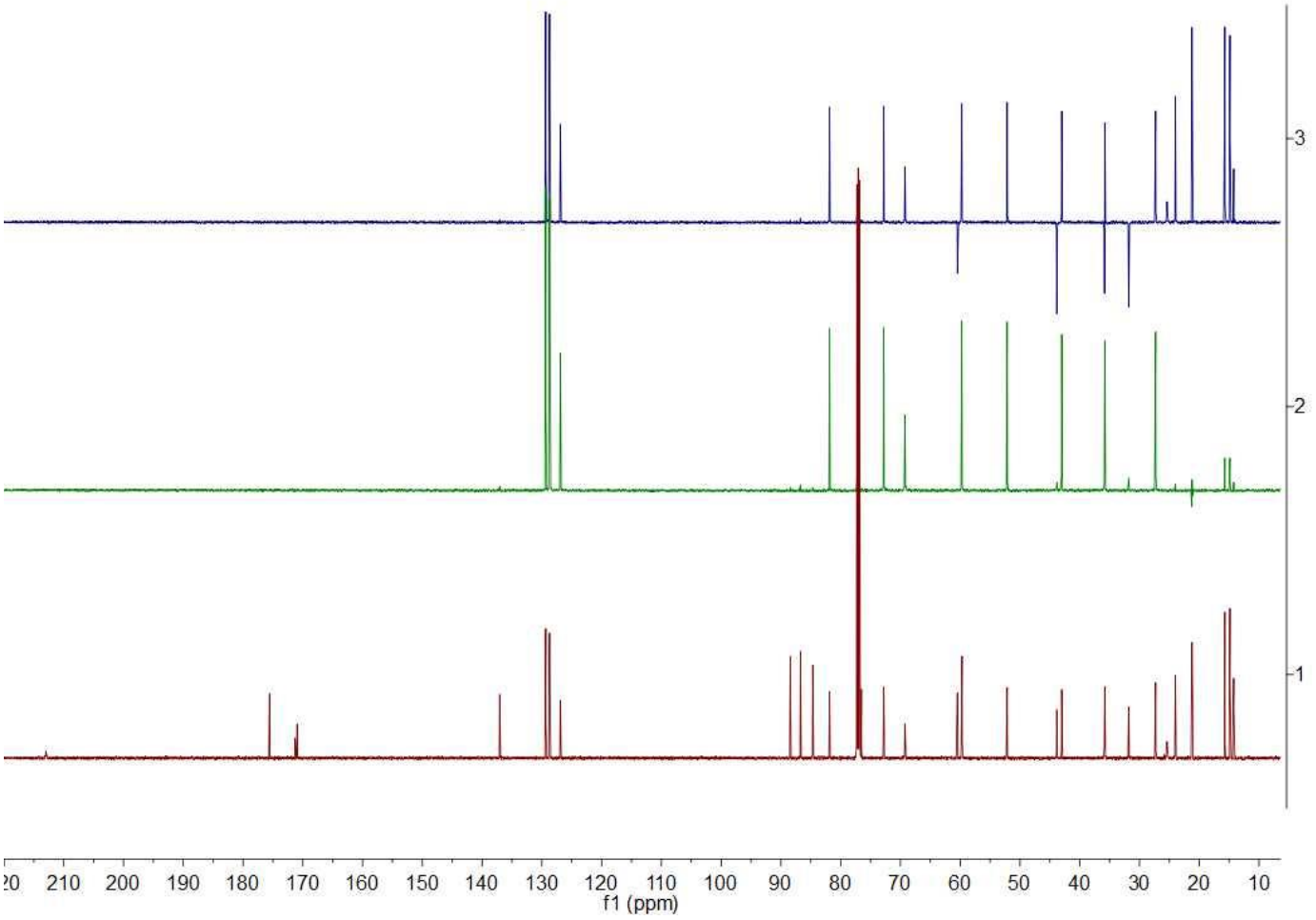

Fig. S33. DEPT of **4**.

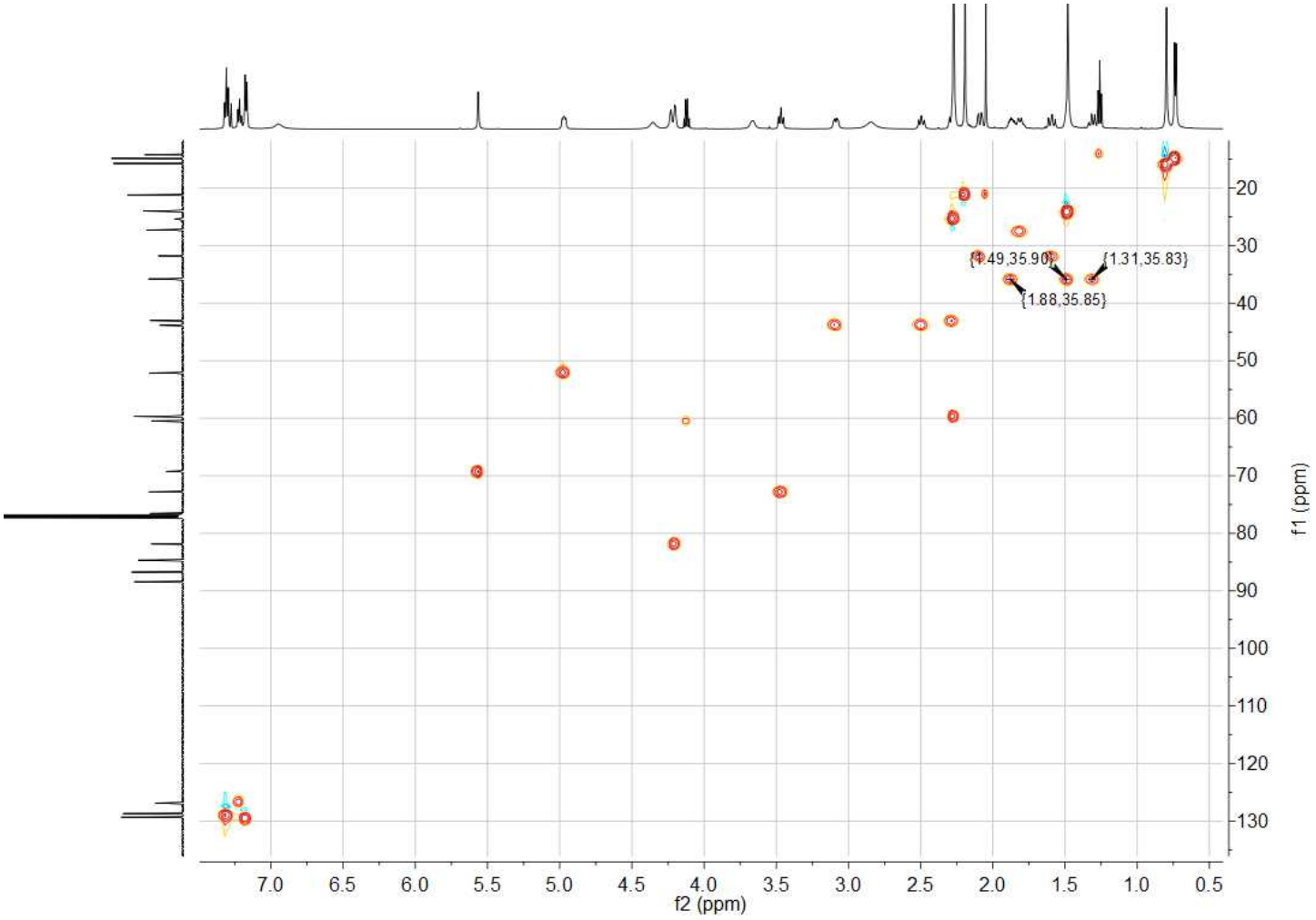

Fig. S34. HSQC of **4**.

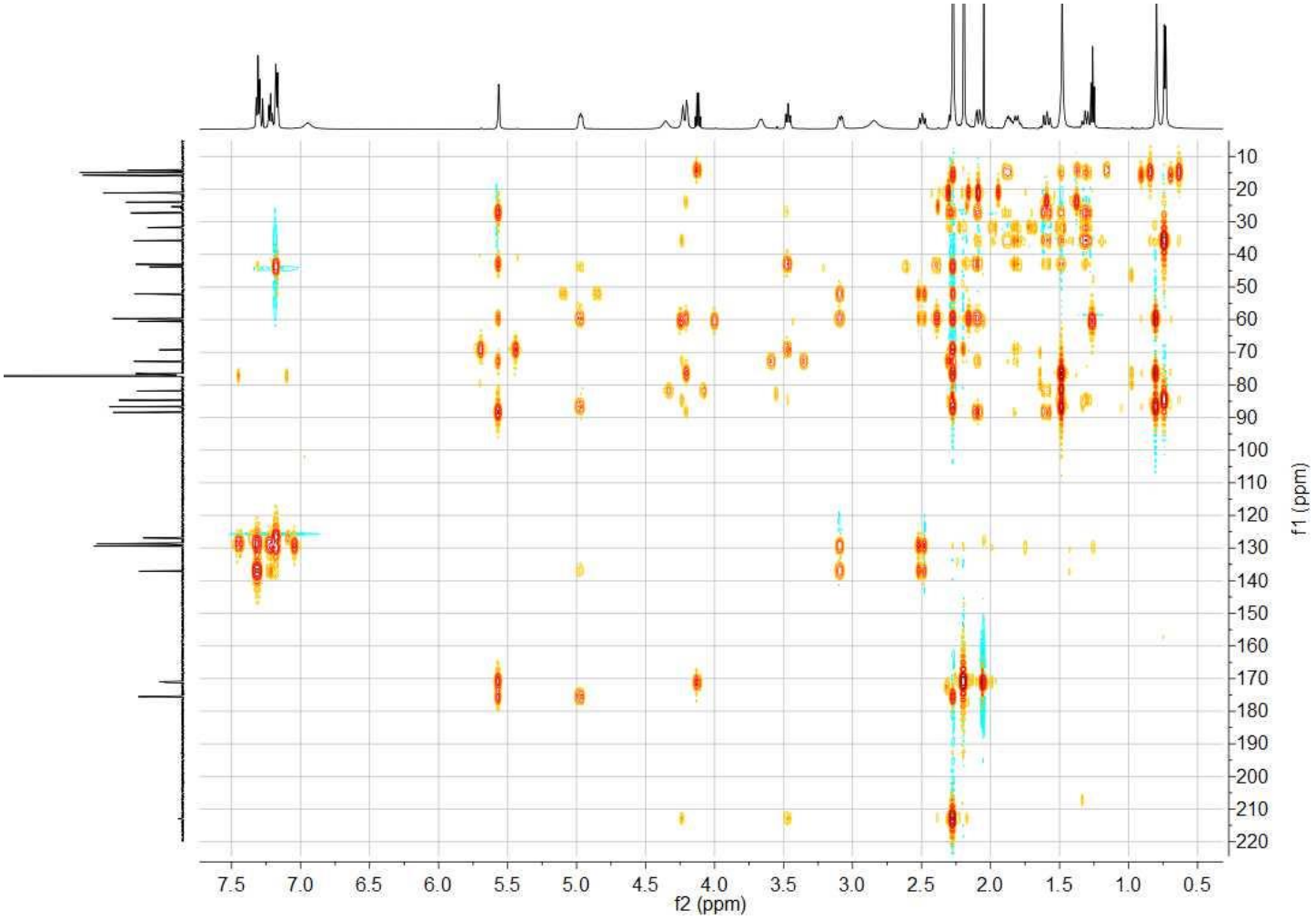

Fig. S35. HMBC of **4**.

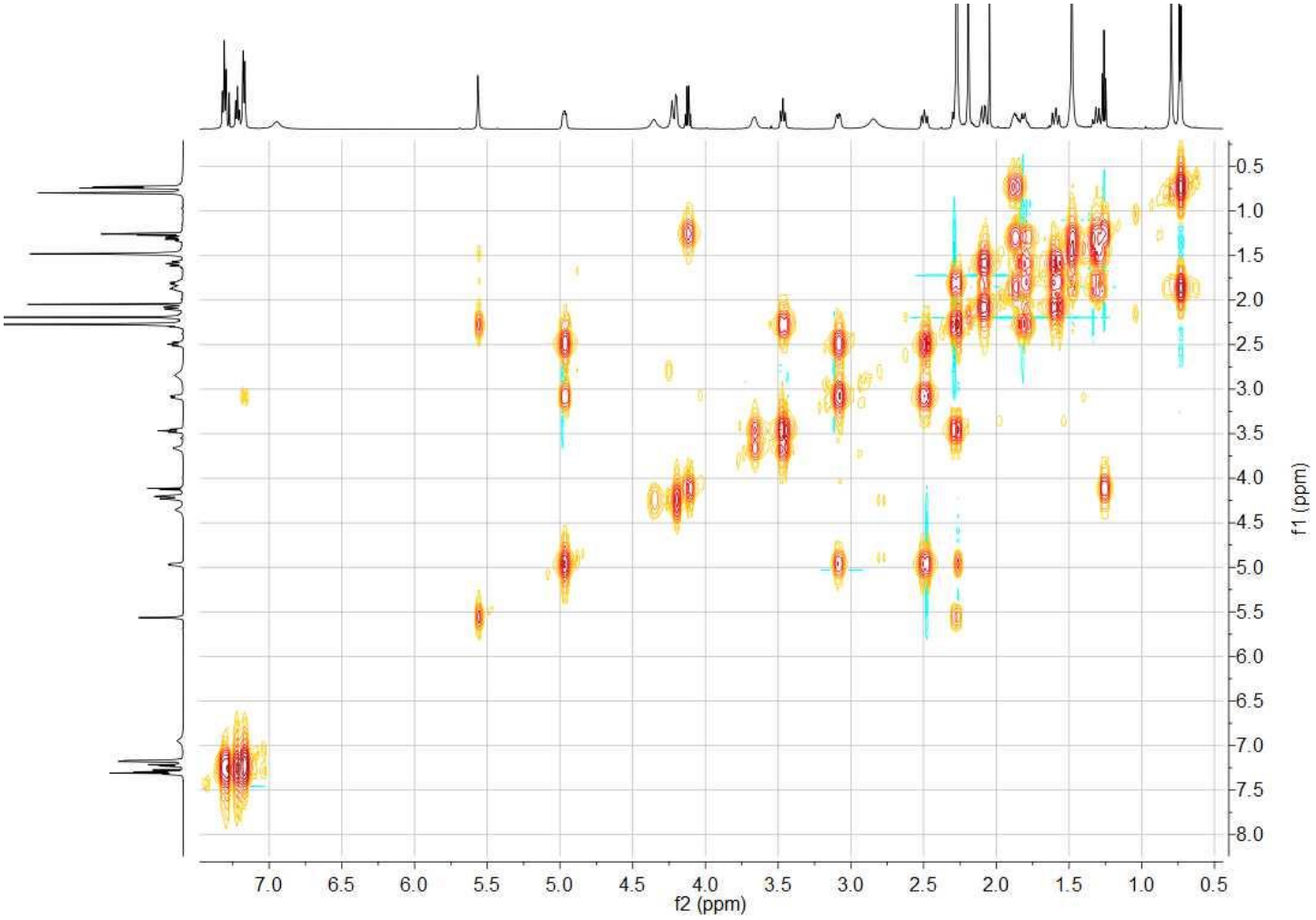

Fig. S36. ^{1}H-^{1}H COSY of **4**.

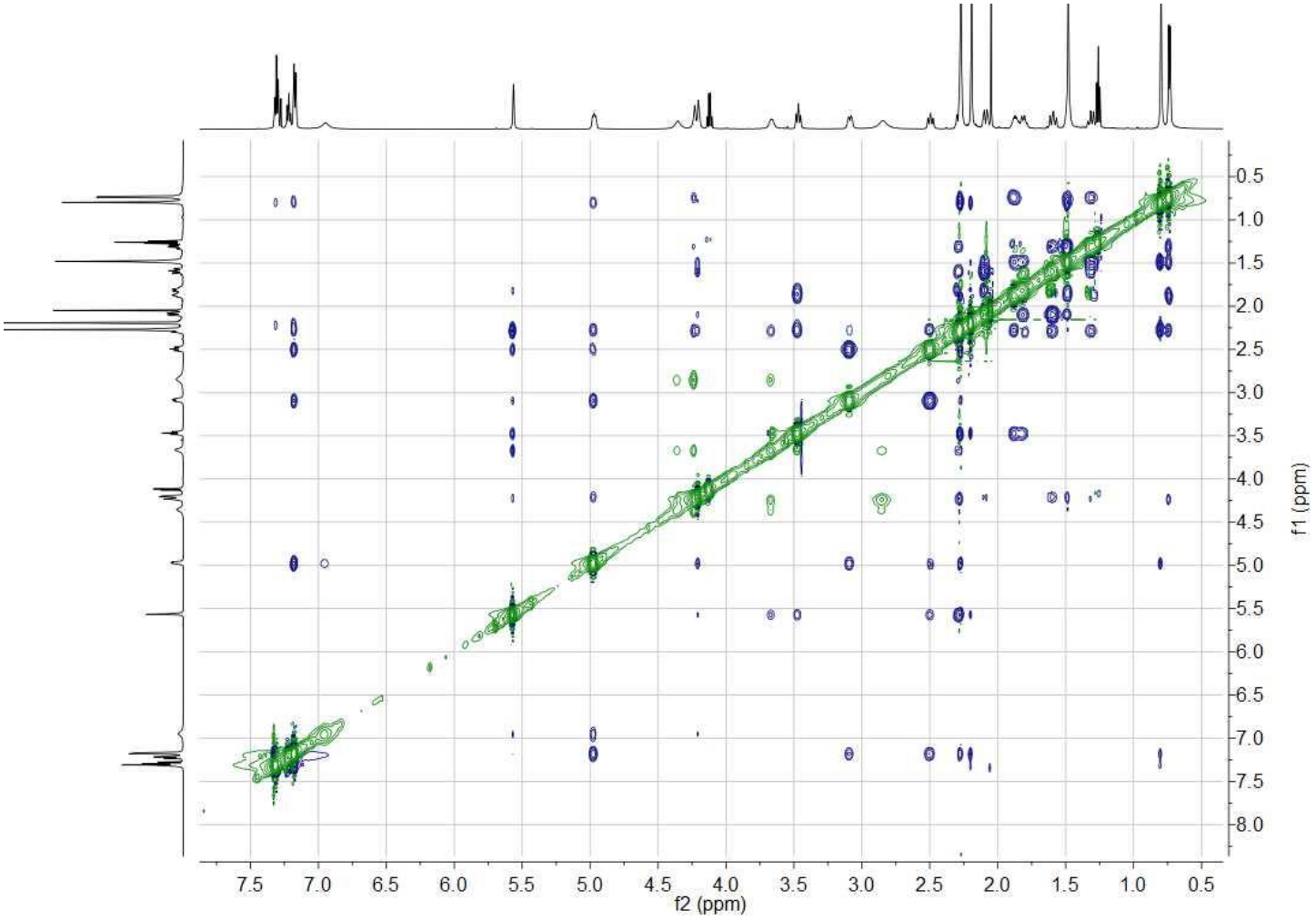

Fig. S37. ROESY of **4**.

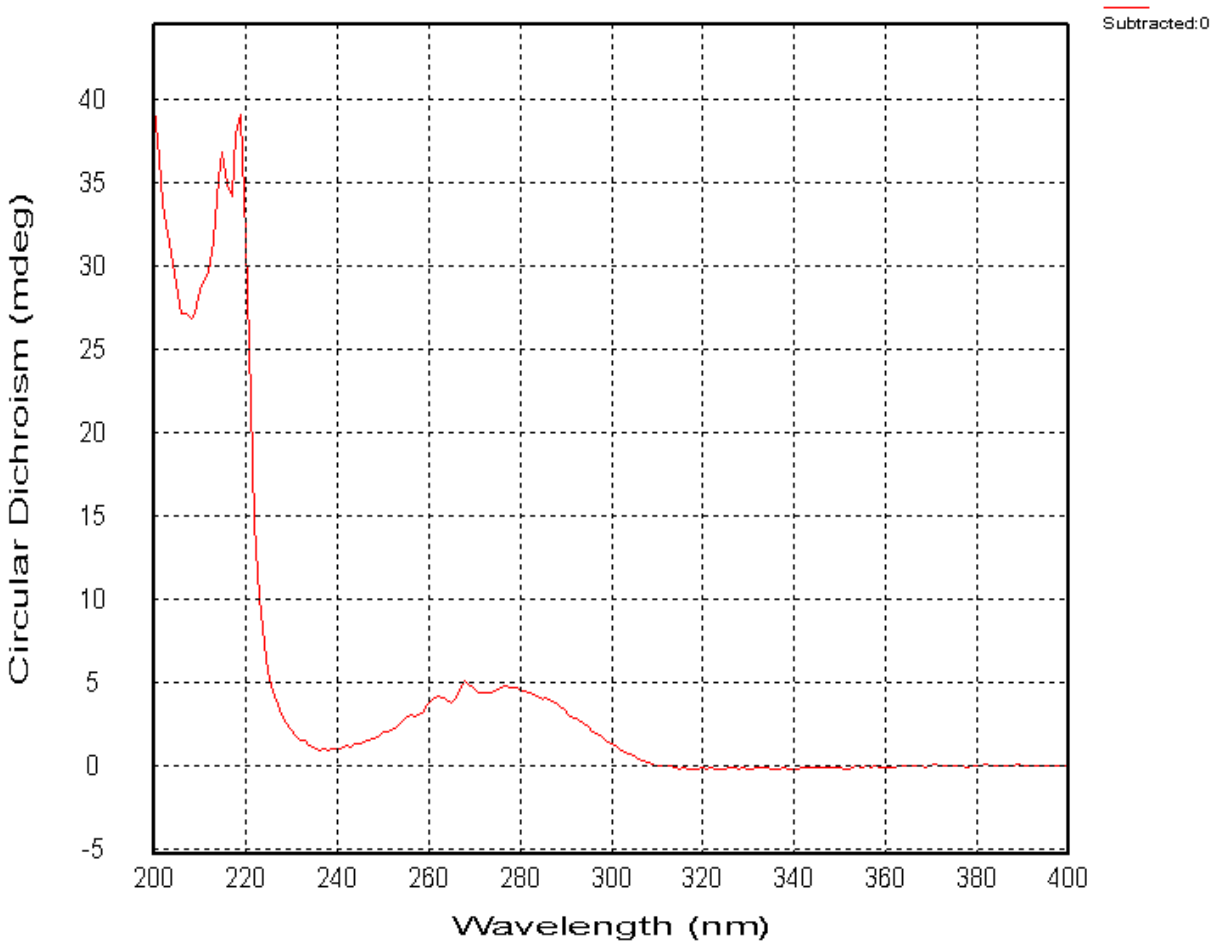

Fig. S38. Experimental ECD of **4**.

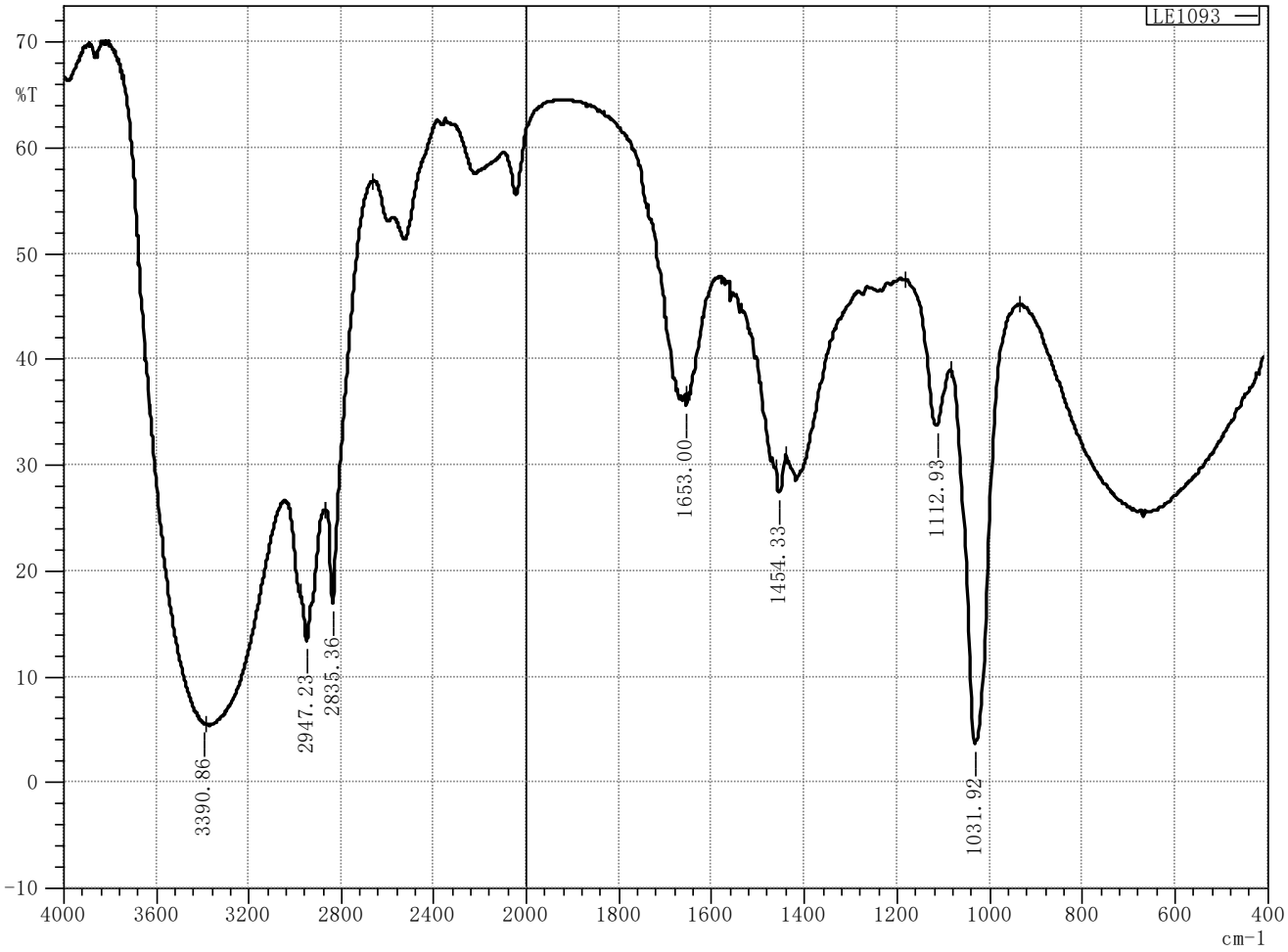

Fig. S39. IR of **4**.

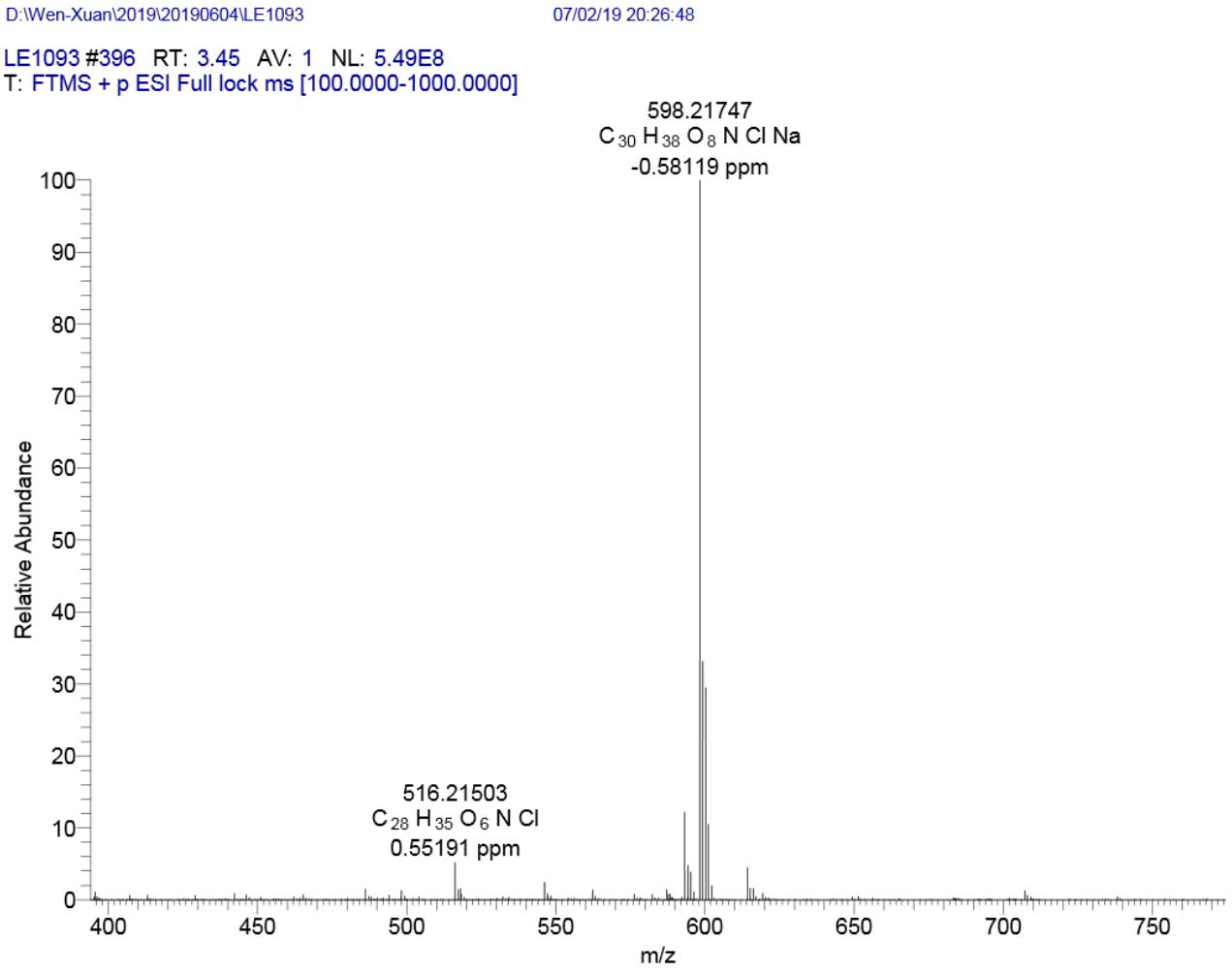

Fig. S40. HRESIMS of **4**.

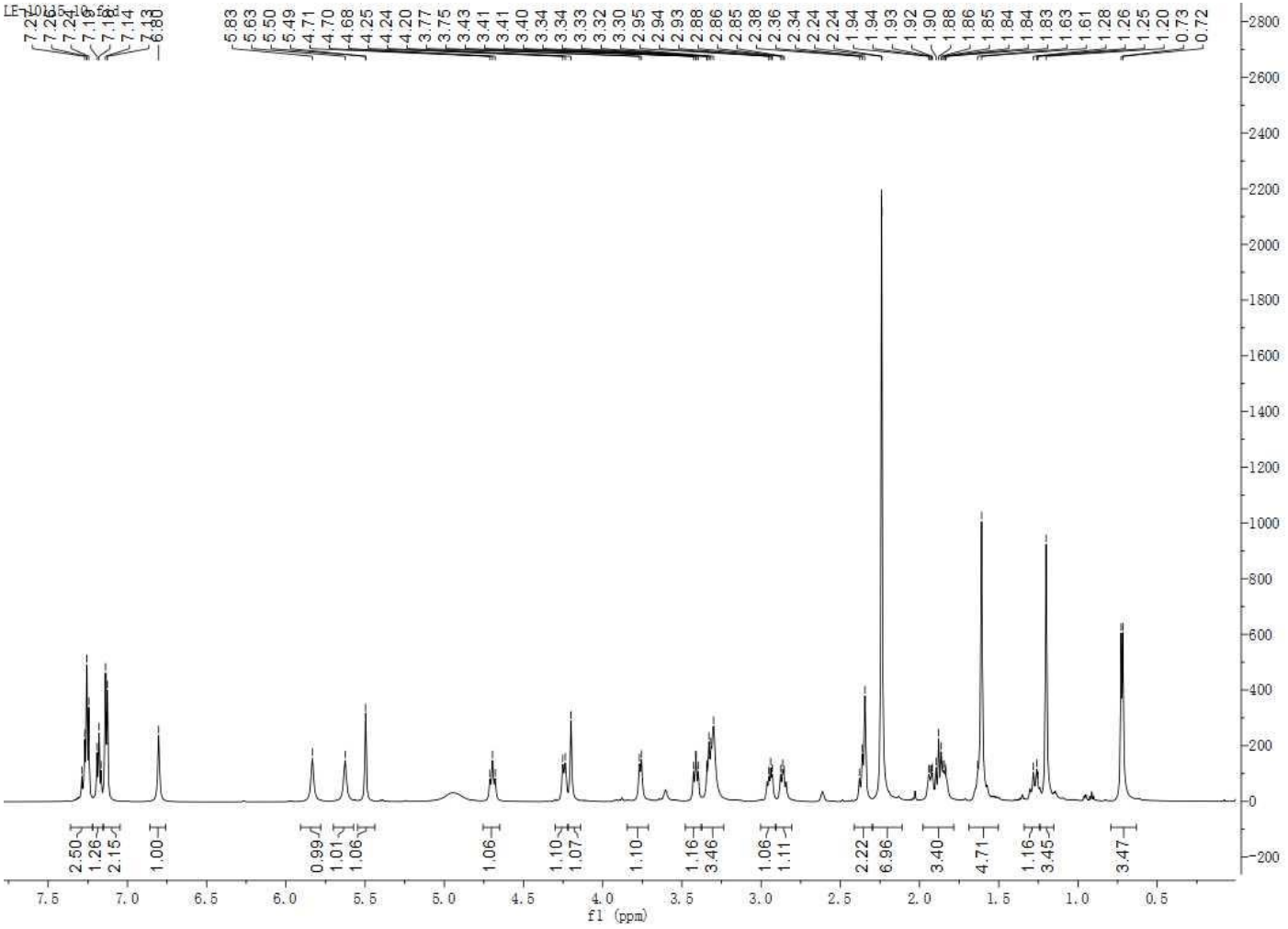

Fig. S41. ^{1}H NMR of **5** ($CDCl_3$, 600 MHz).

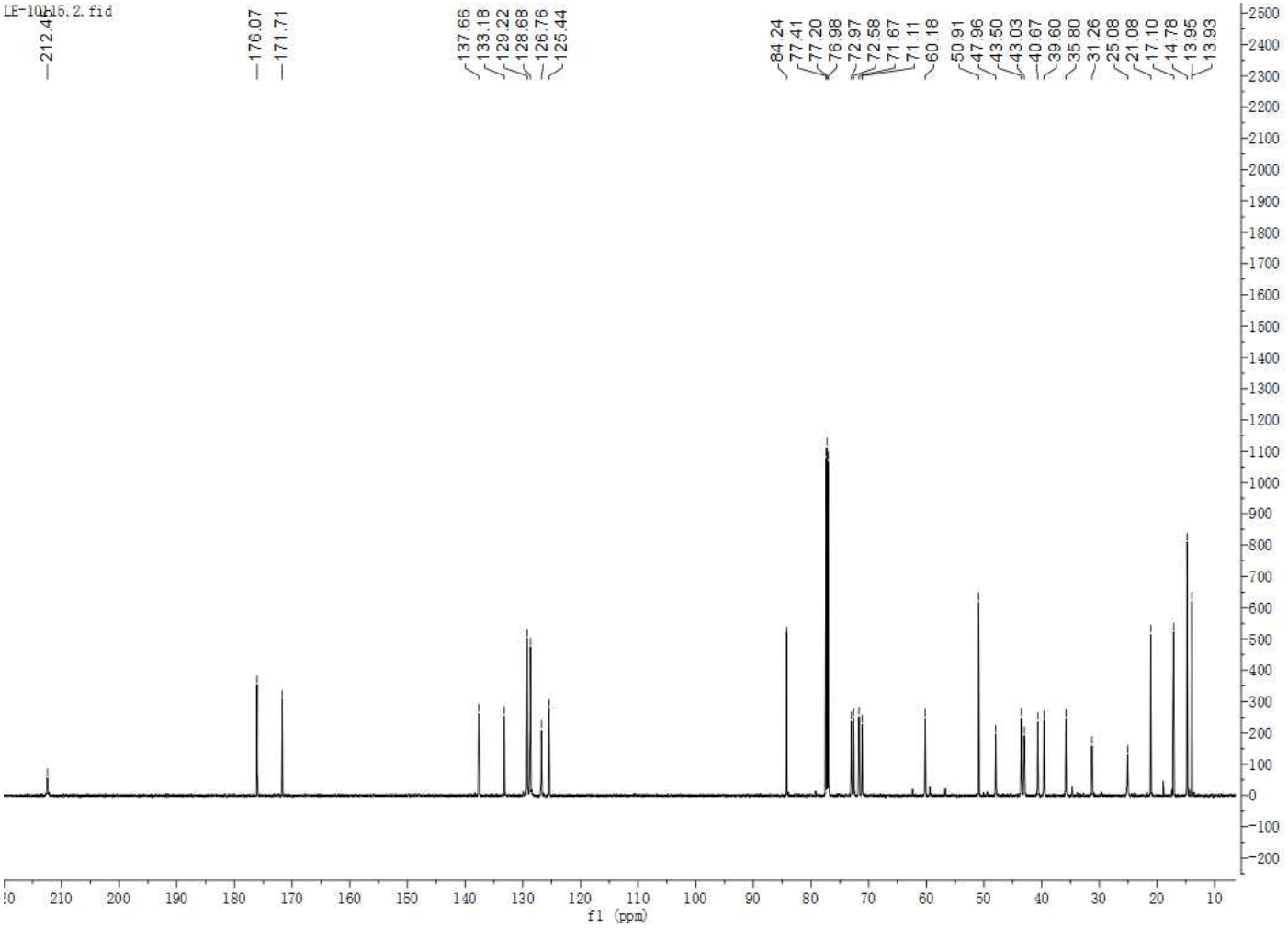

Fig. S42. ^{13}C NMR of **5** ($CDCl_3$, 150 MHz).

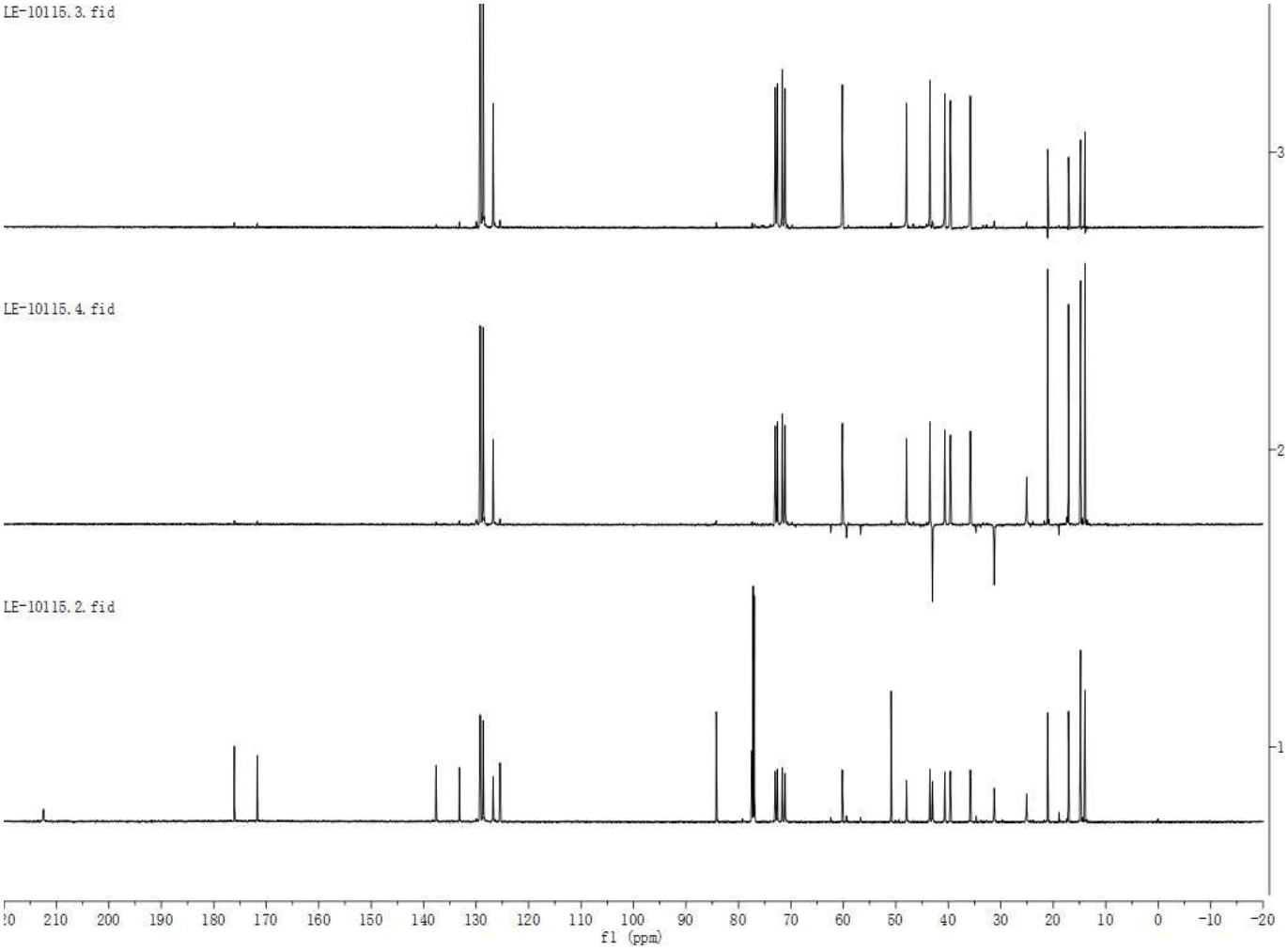

Fig. S43. DEPT of **5**.

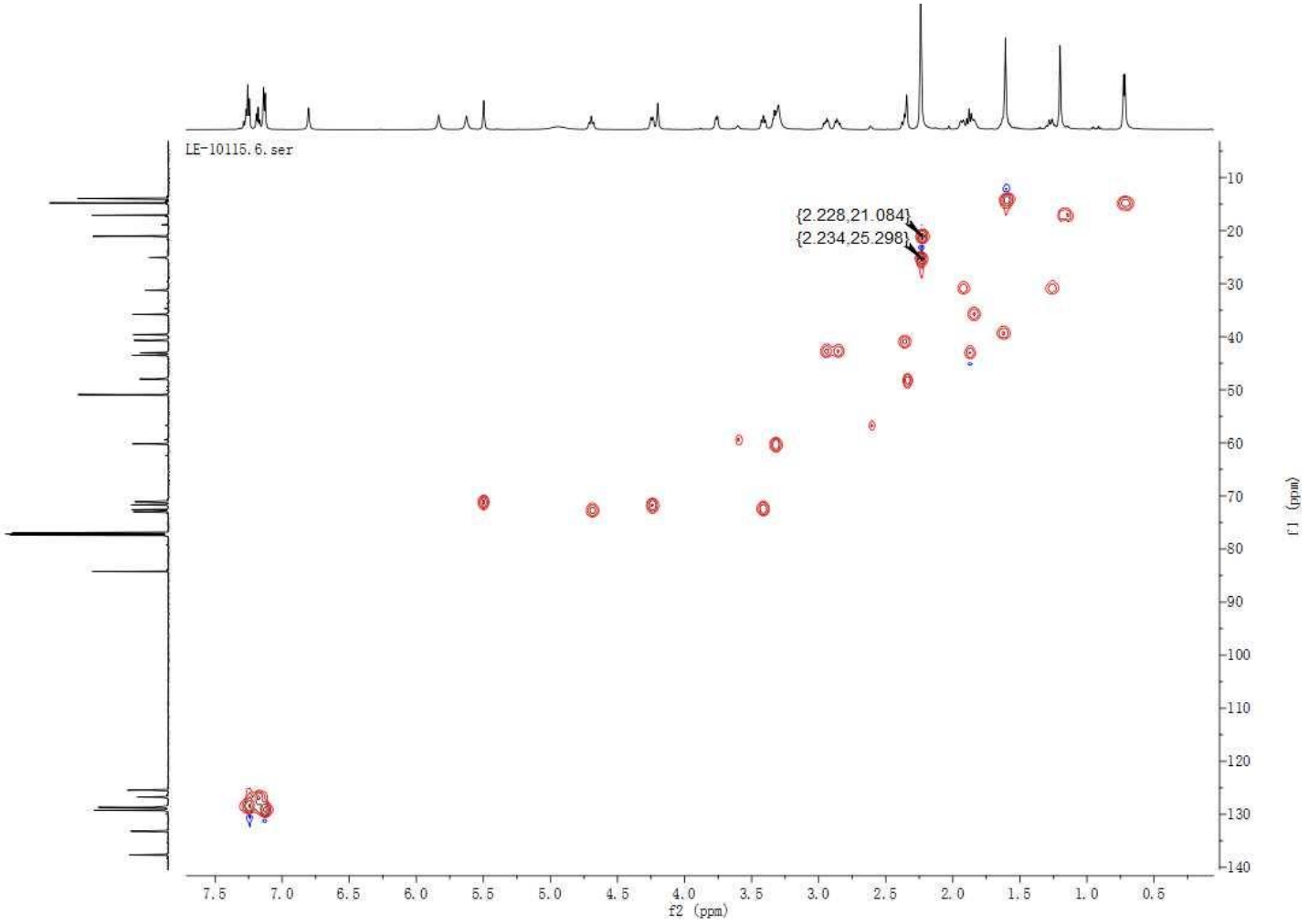

Fig. S44. HSQC of **5**.

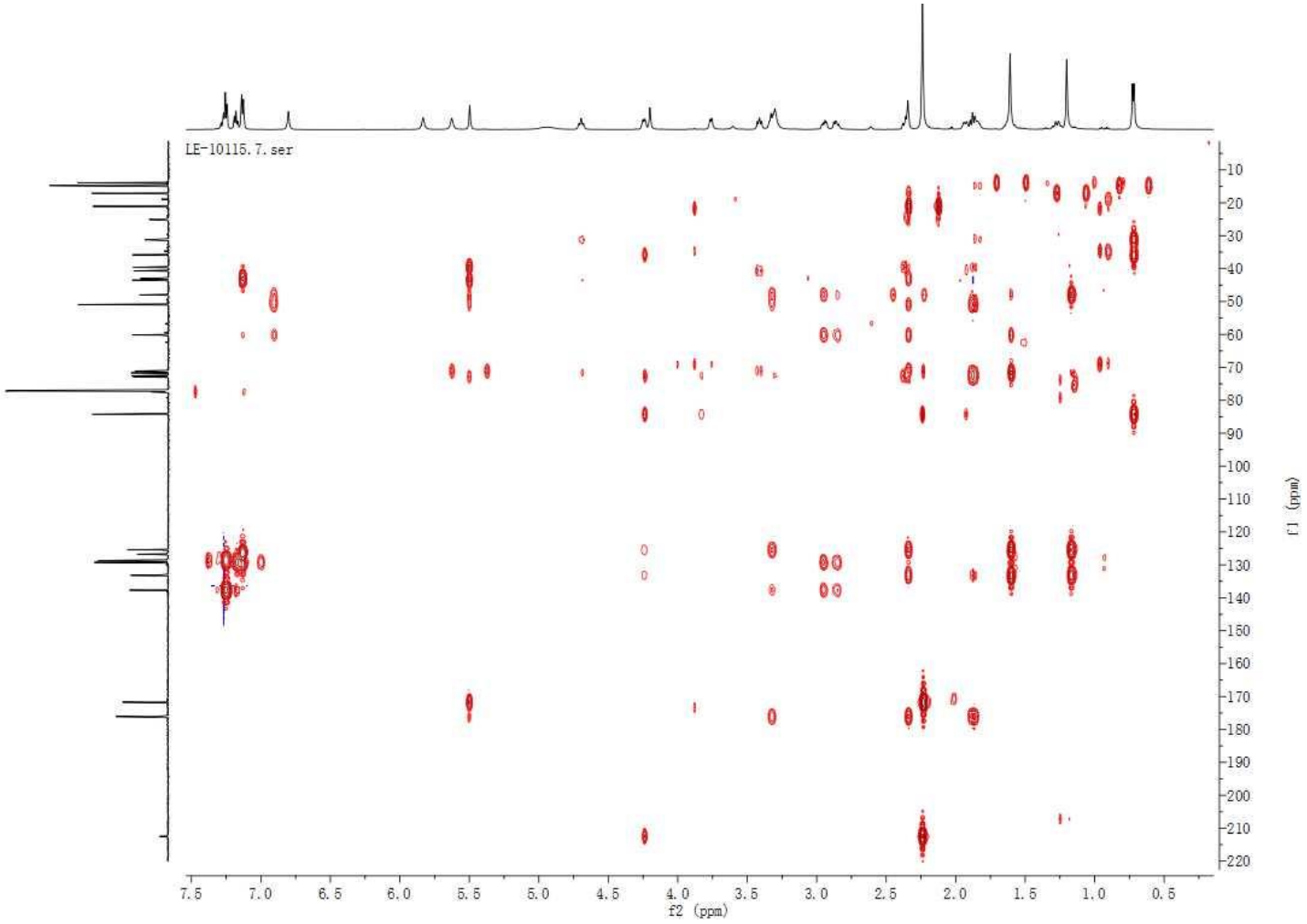

Fig. S45. HMBC of **5**.

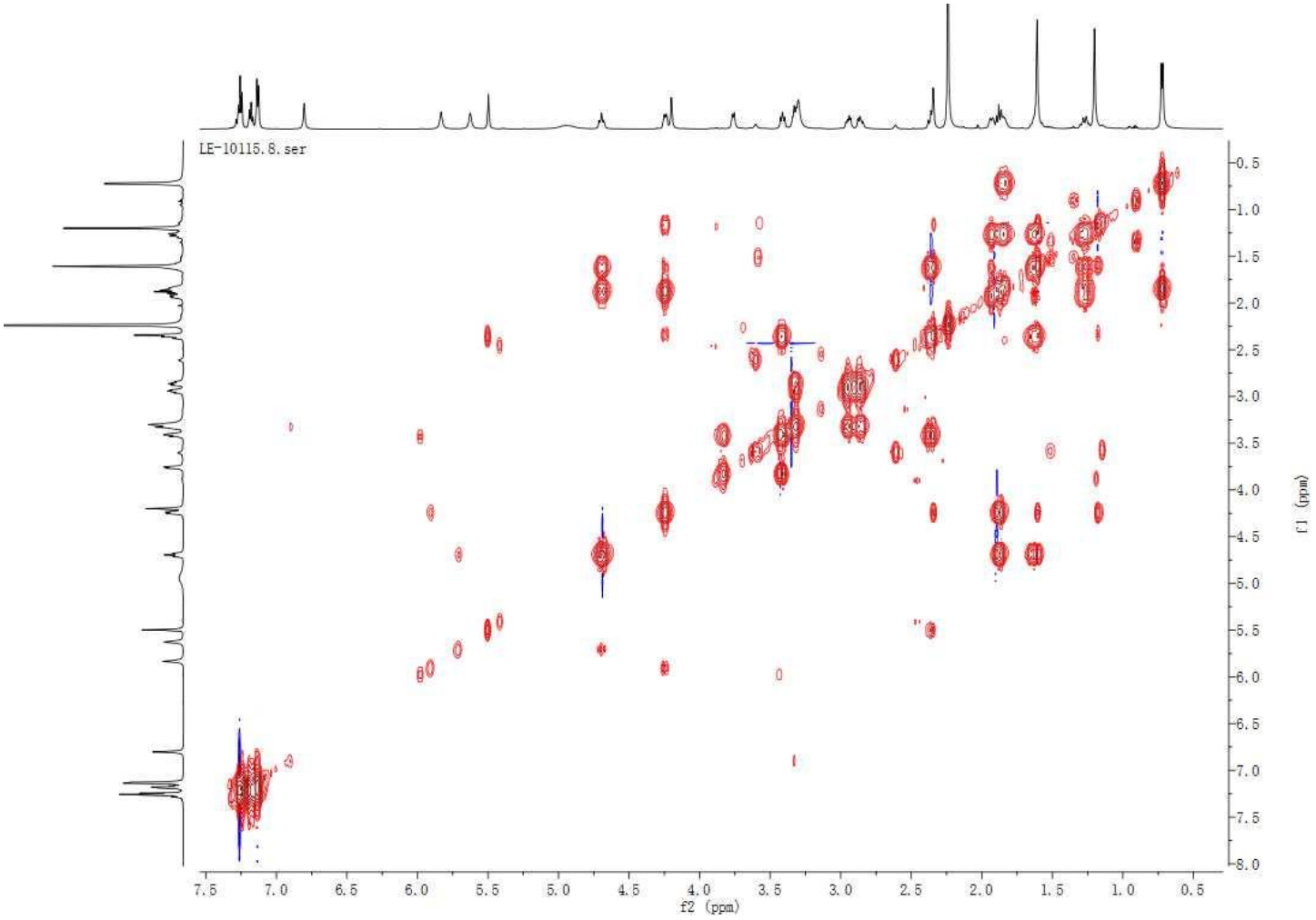

Fig. S46. ^{1}H-^{1}H COSY of **5**.

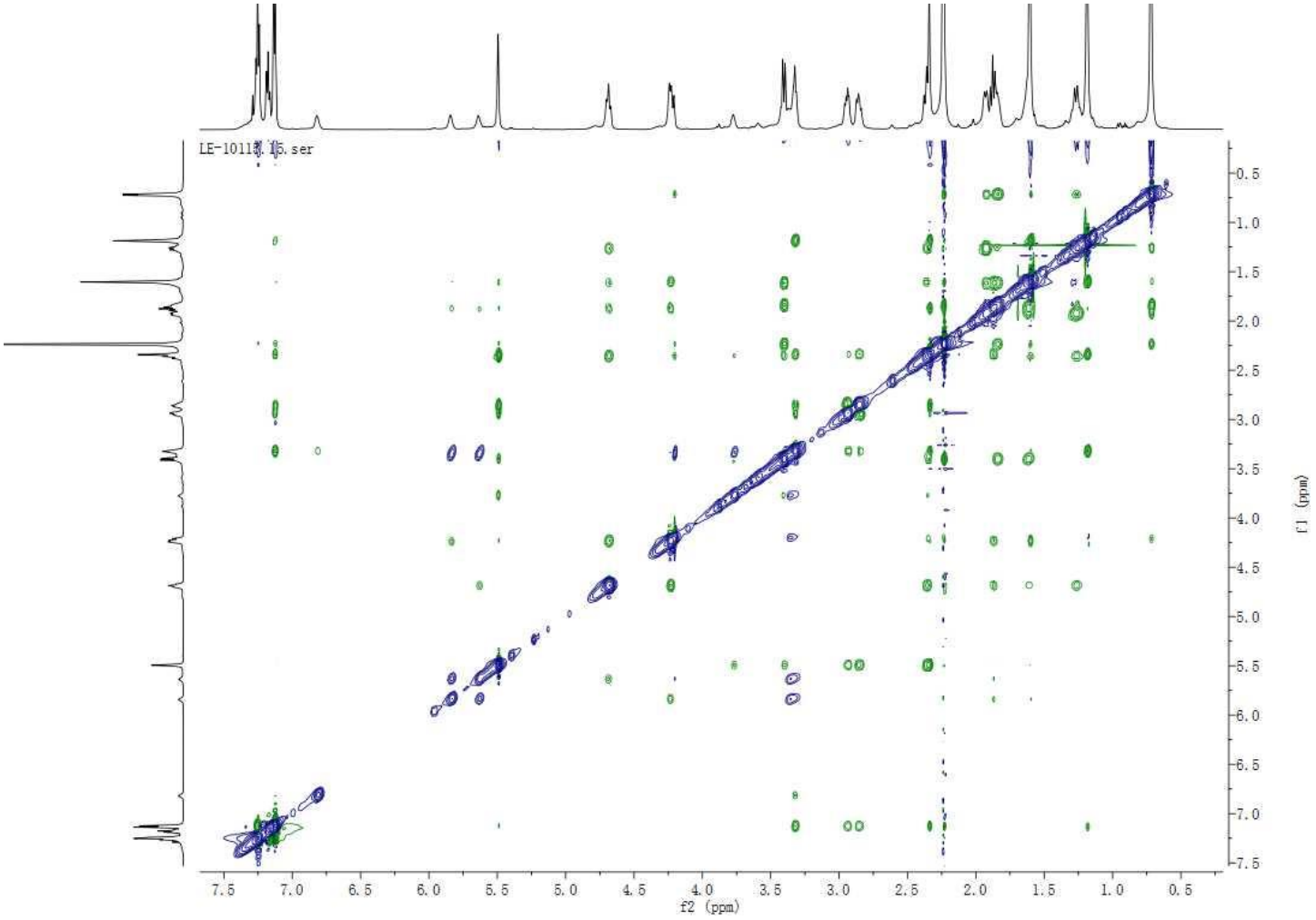

Fig. S47. ROESY of **5**.

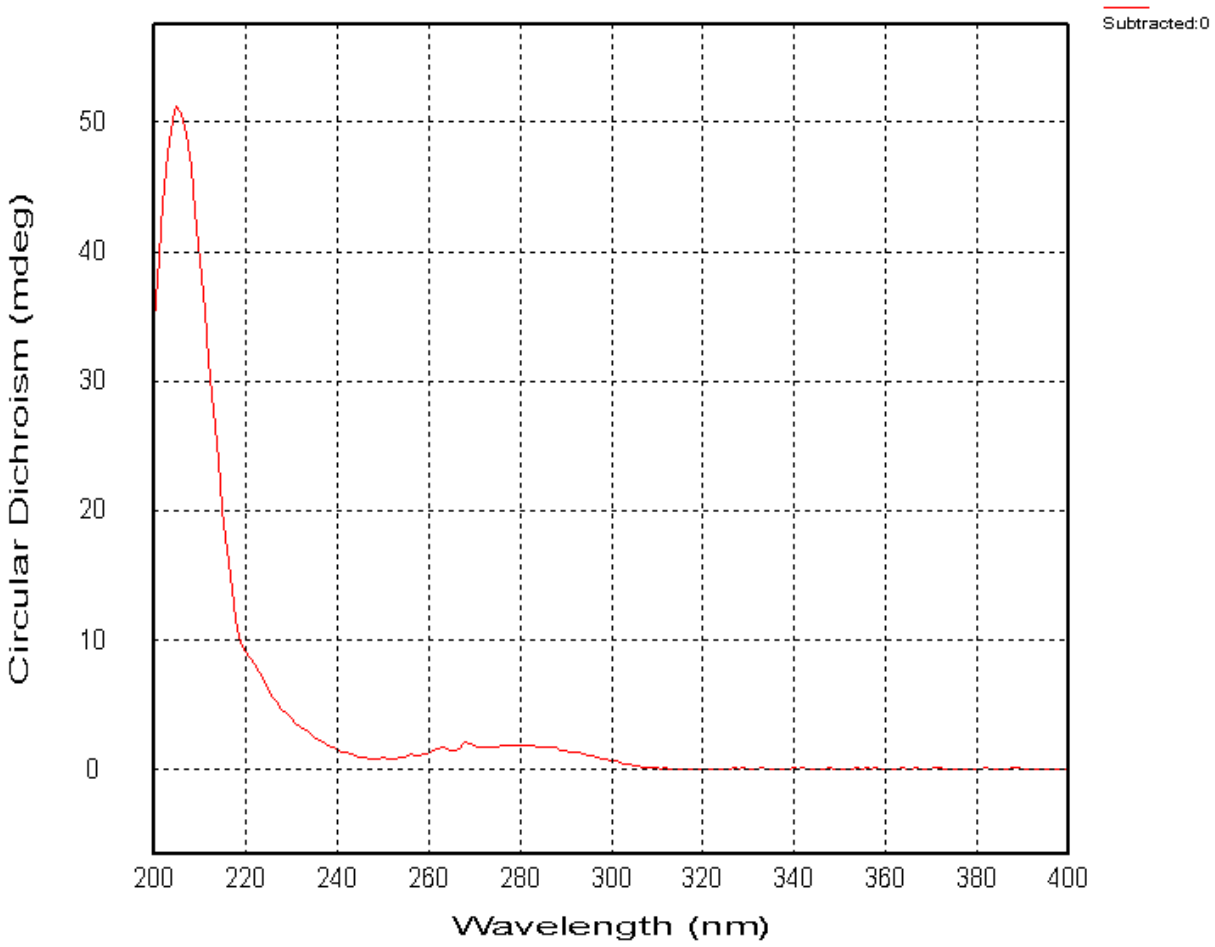

Fig. S48. Experimental ECD of **5**.

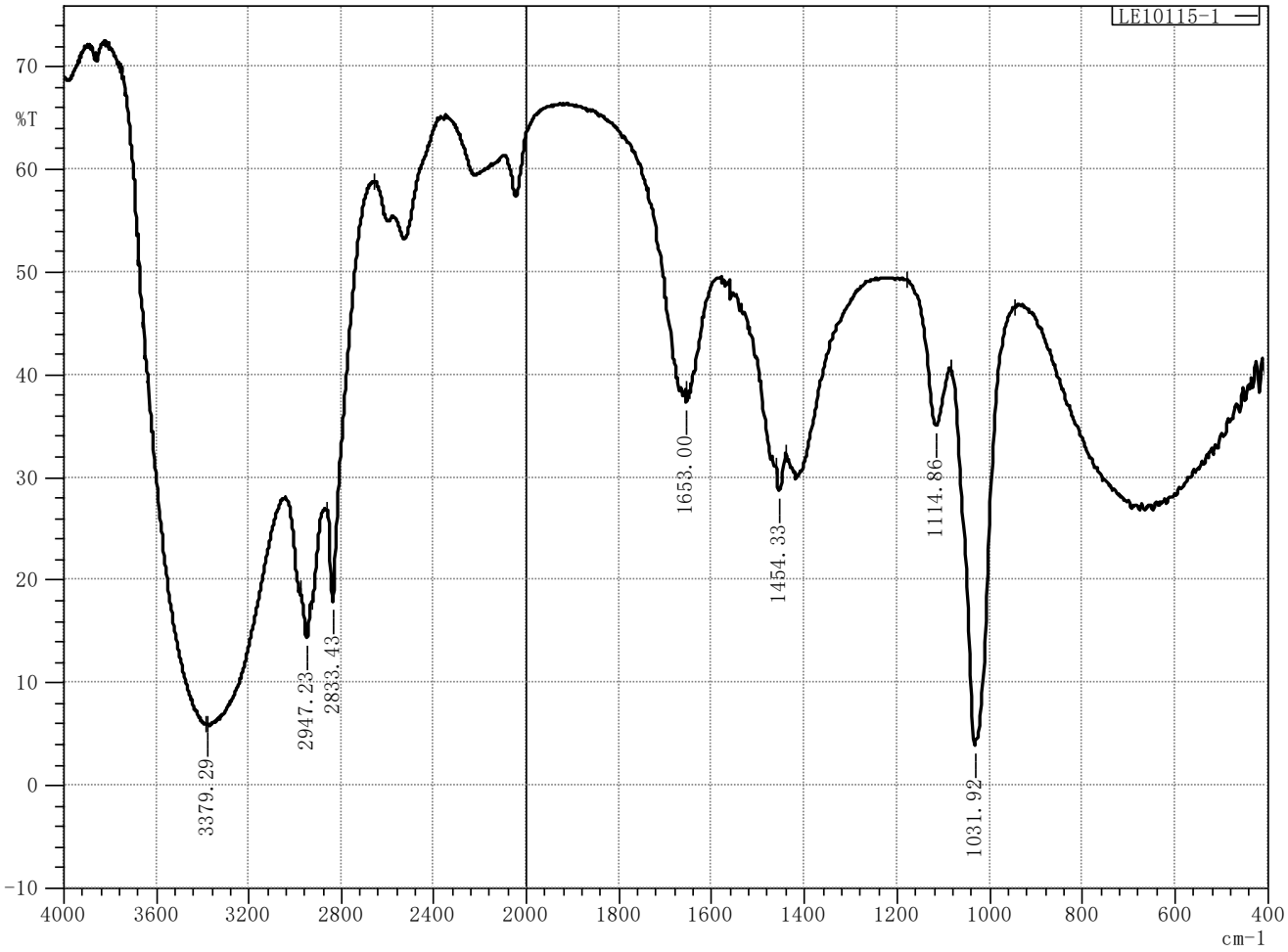

Fig. S49. IR of **5**.

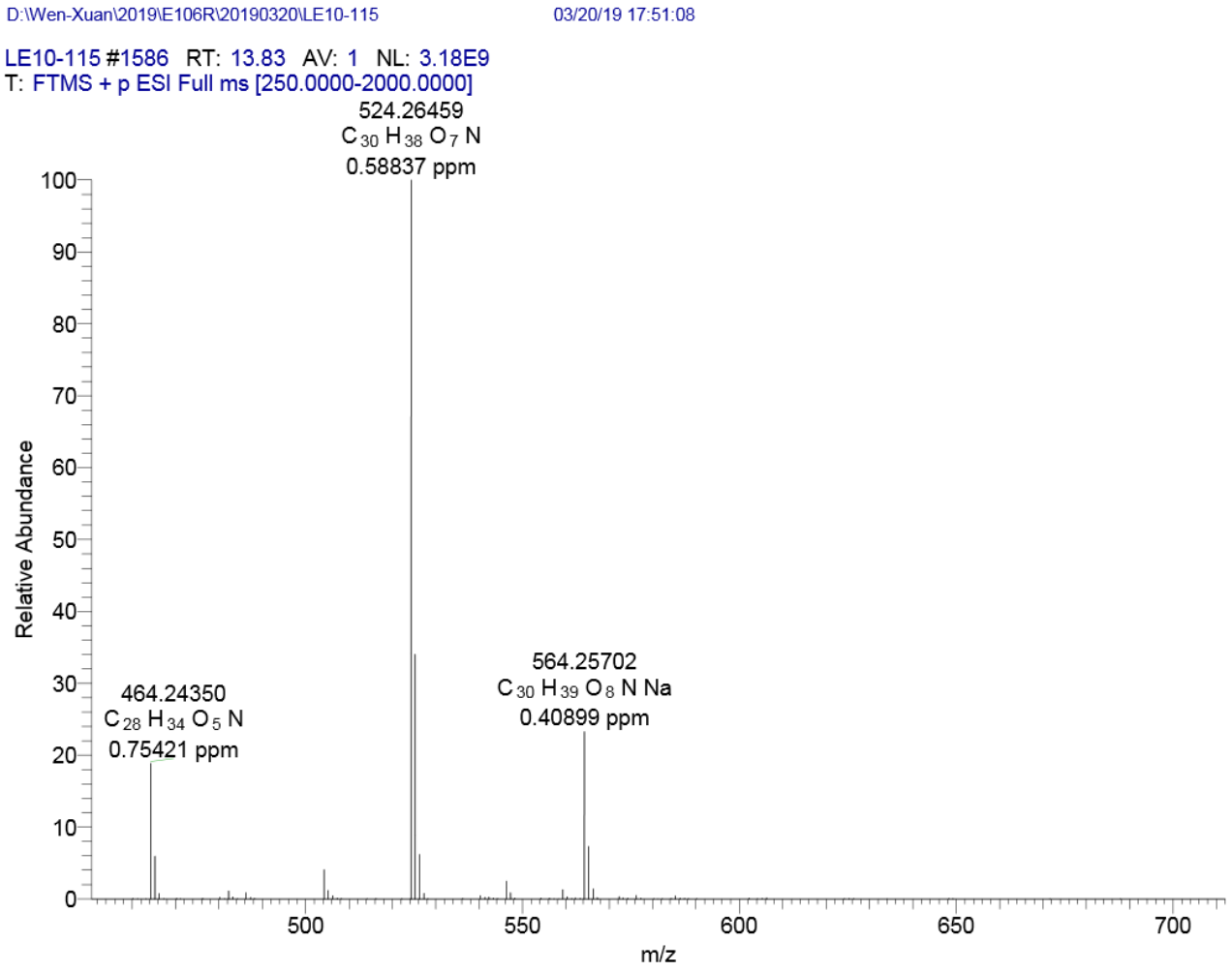

Fig. S50. HRESIMS of **5**.

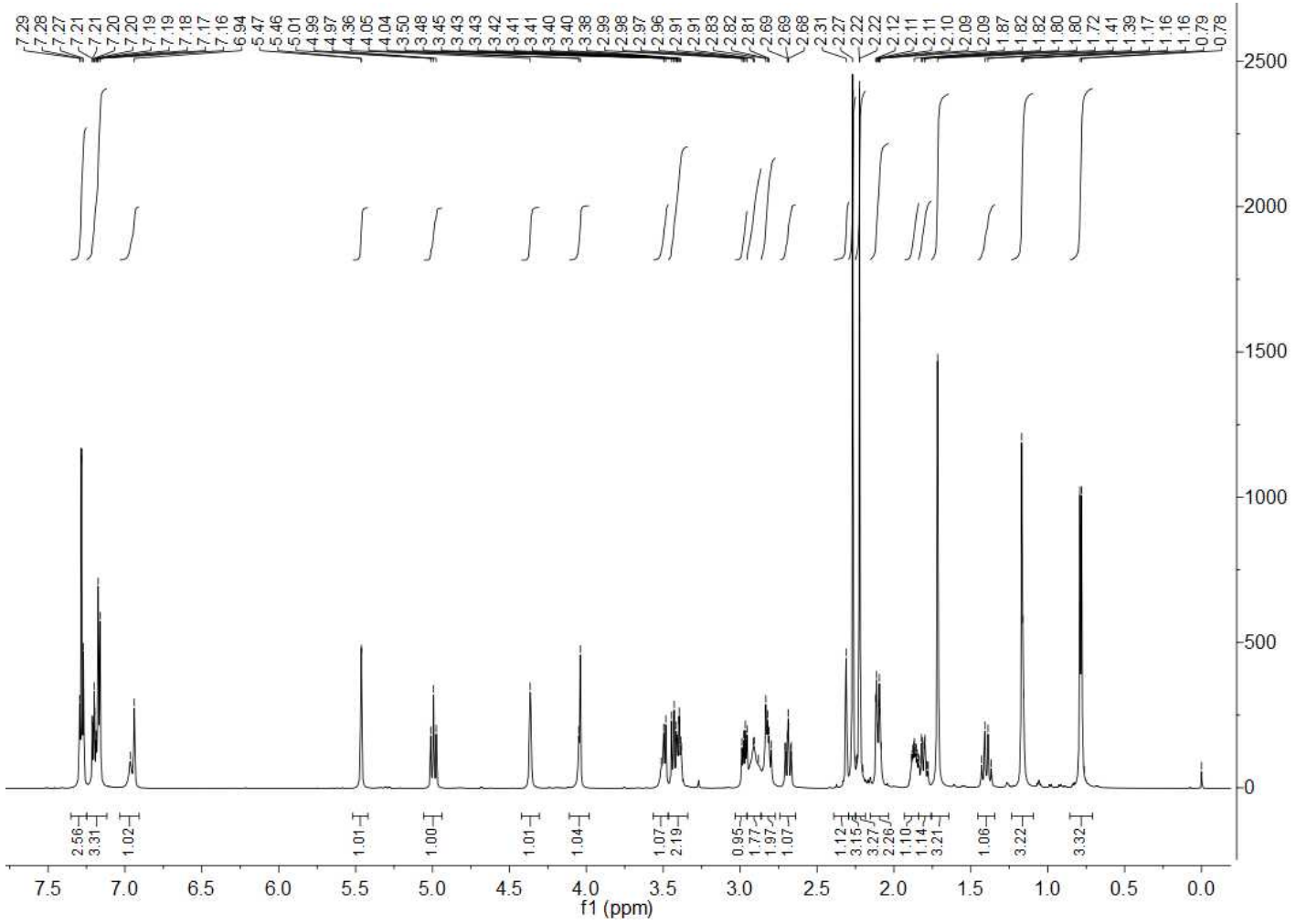

Fig. S51. ^{1}H NMR of **6** ($CDCl_3$, 600 MHz).

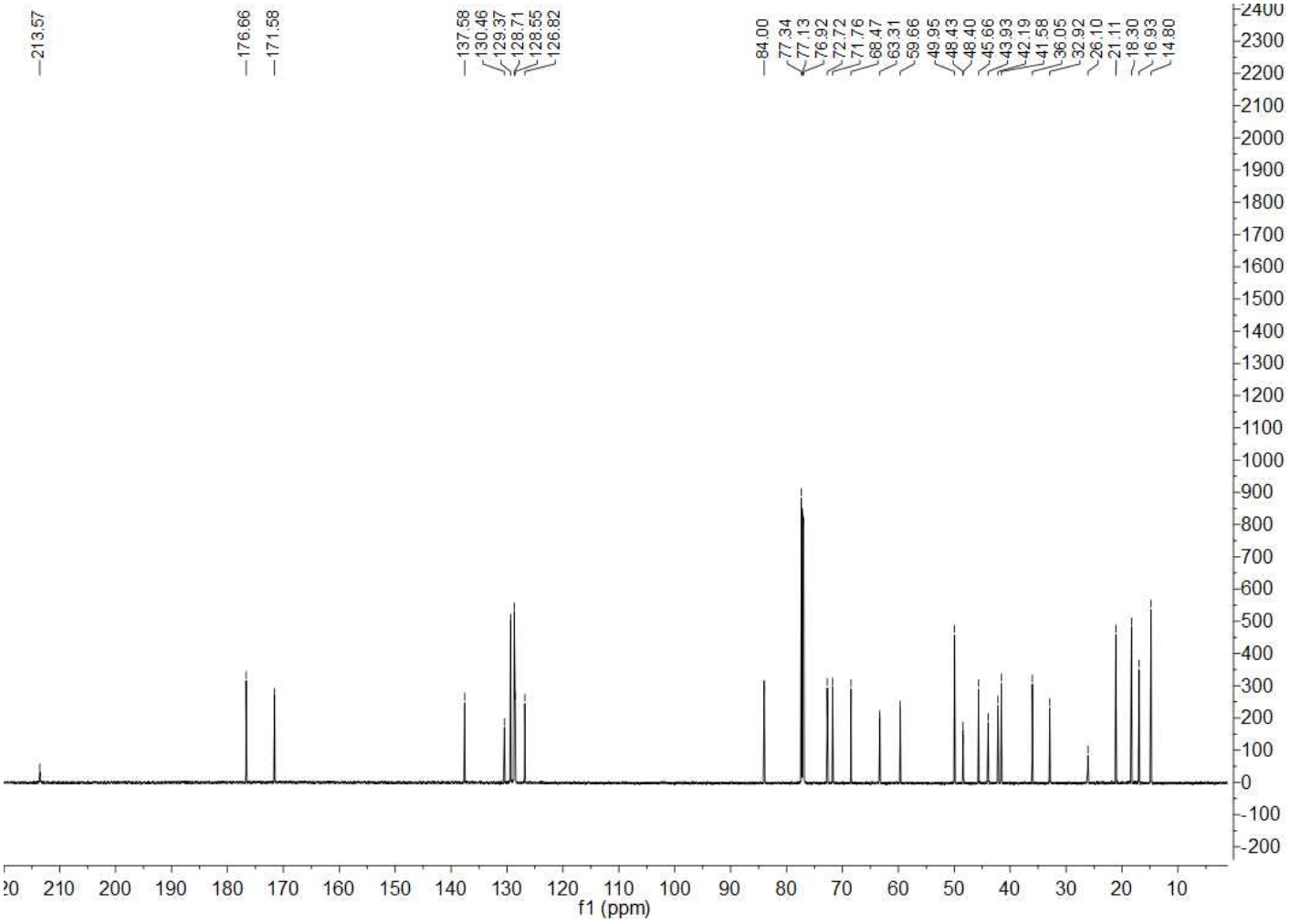

Fig. S52. ^{13}C NMR of **6** ($CDCl_3$, 150 MHz).

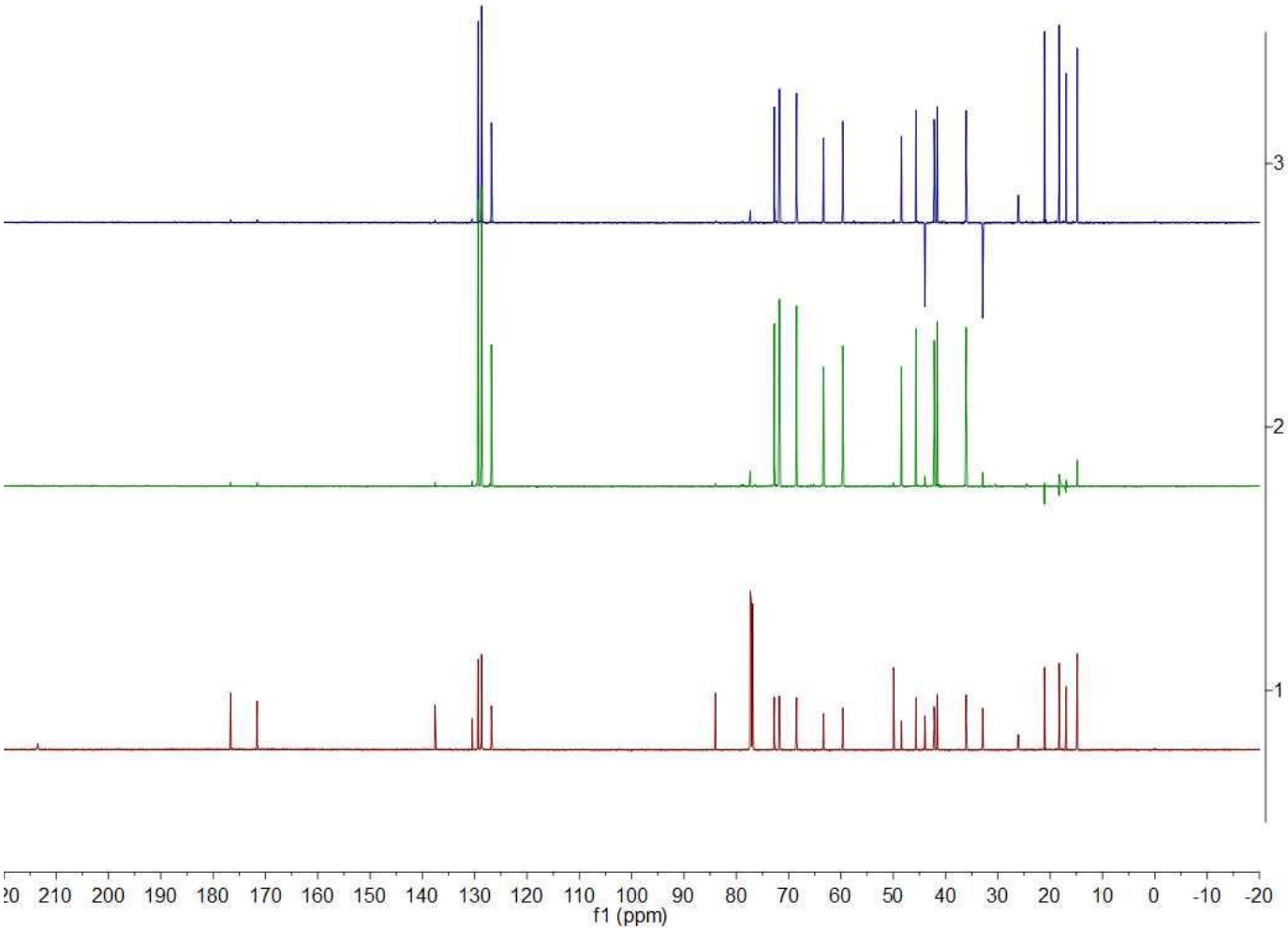

Fig. S53. DEPT of **6**.

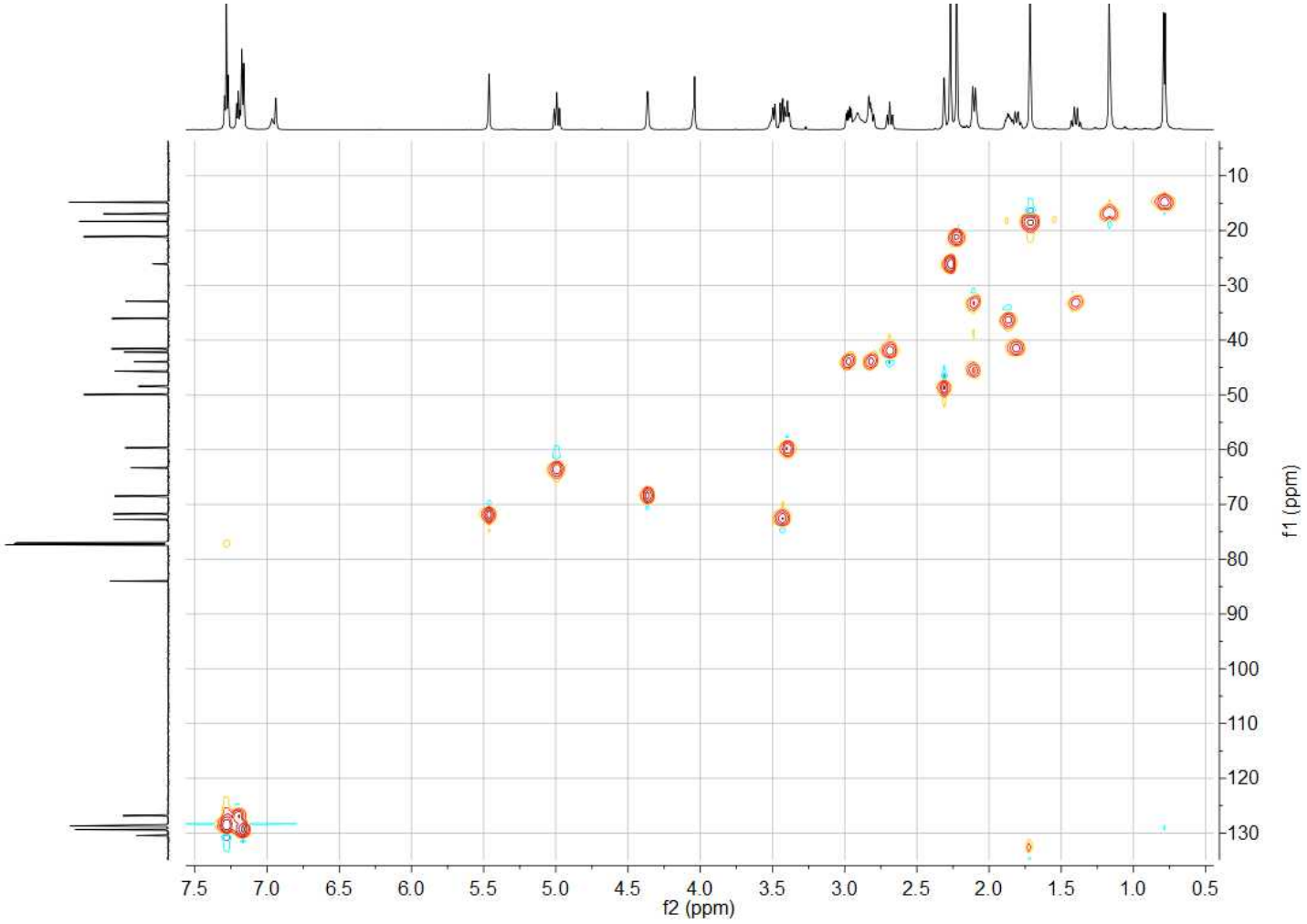

Fig. S54. HSQC of **6**.

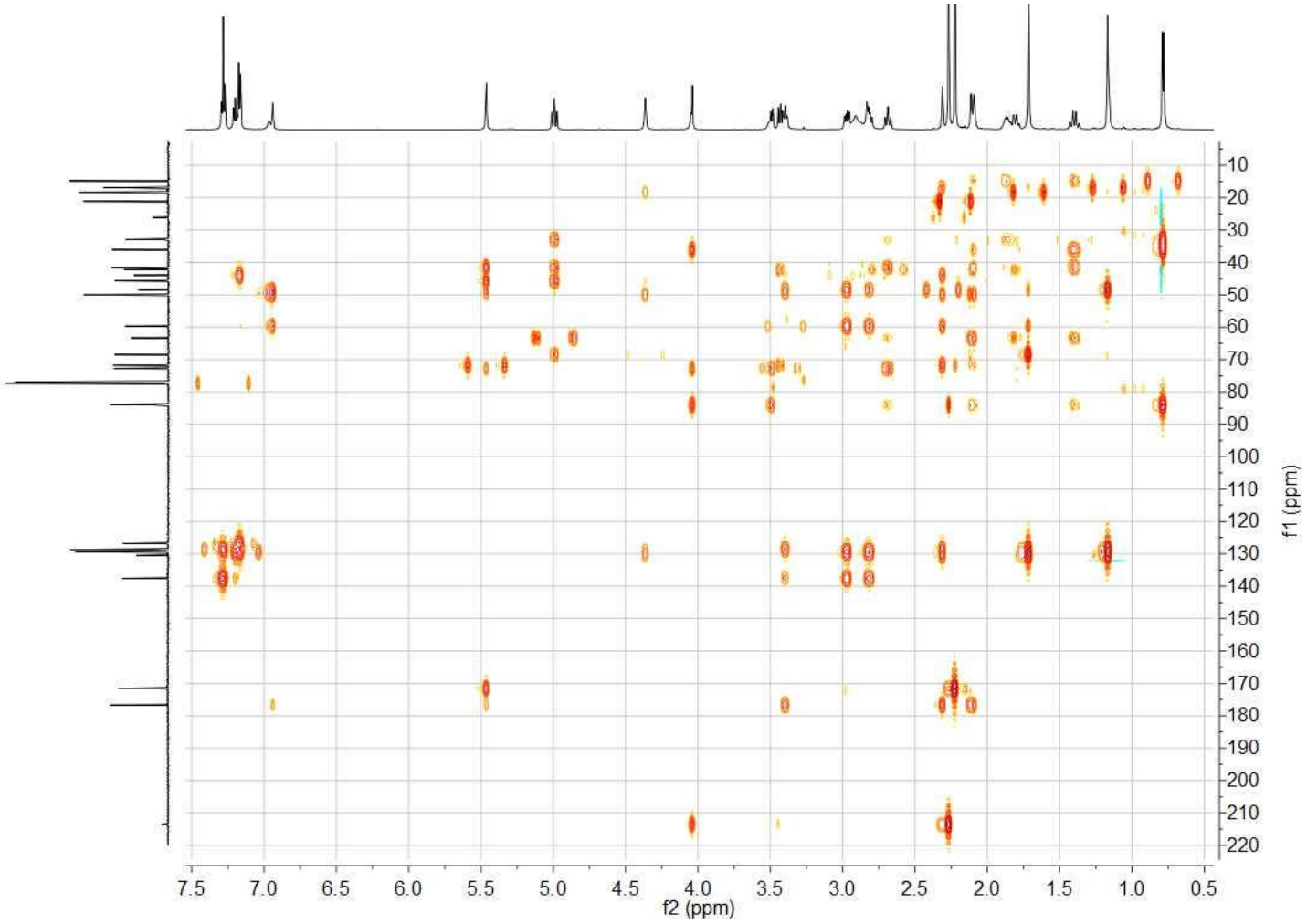

Fig. S55. HMBC of **6**.

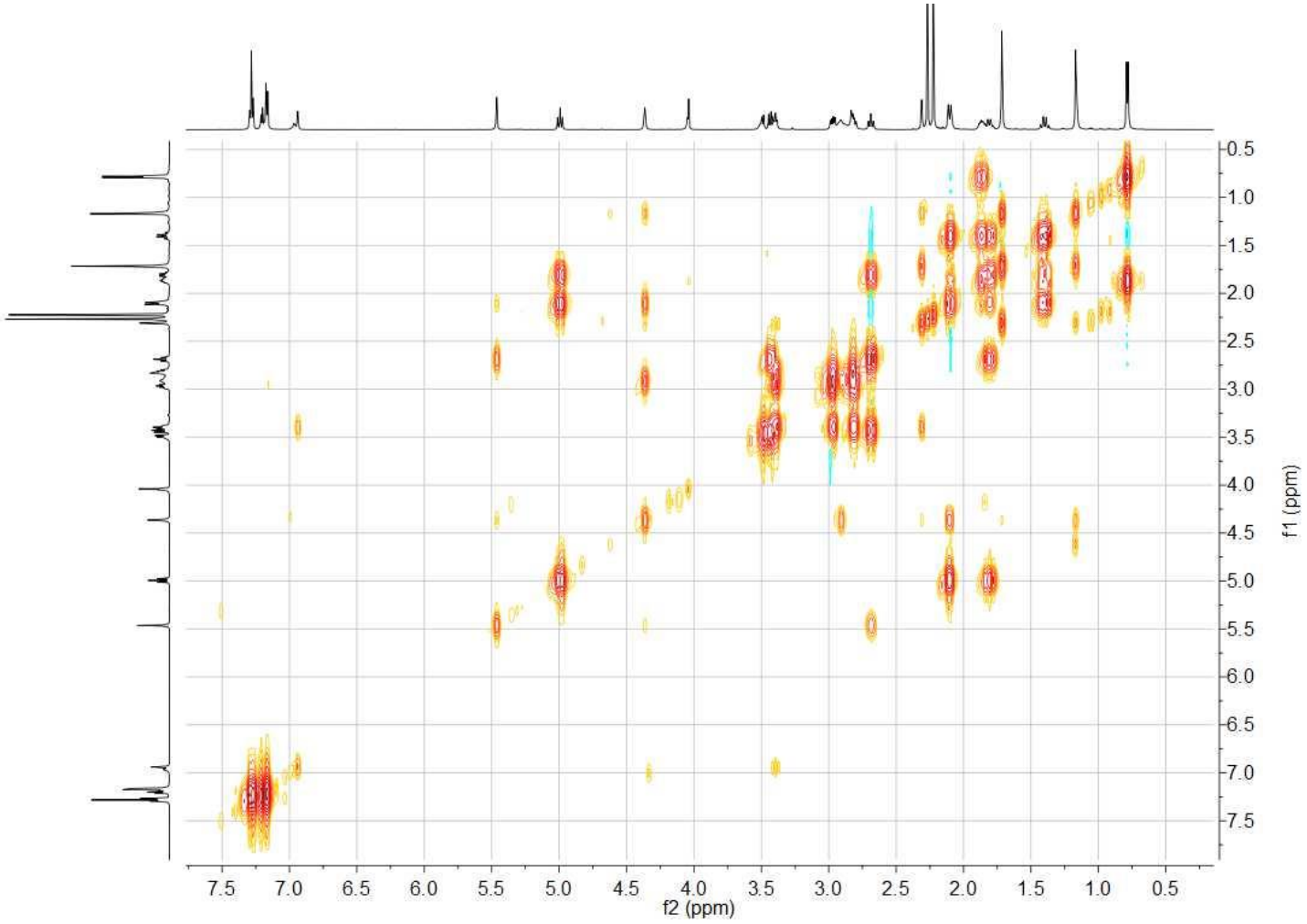

Fig. S56. ^{1}H-^{1}H COSY of **6**.

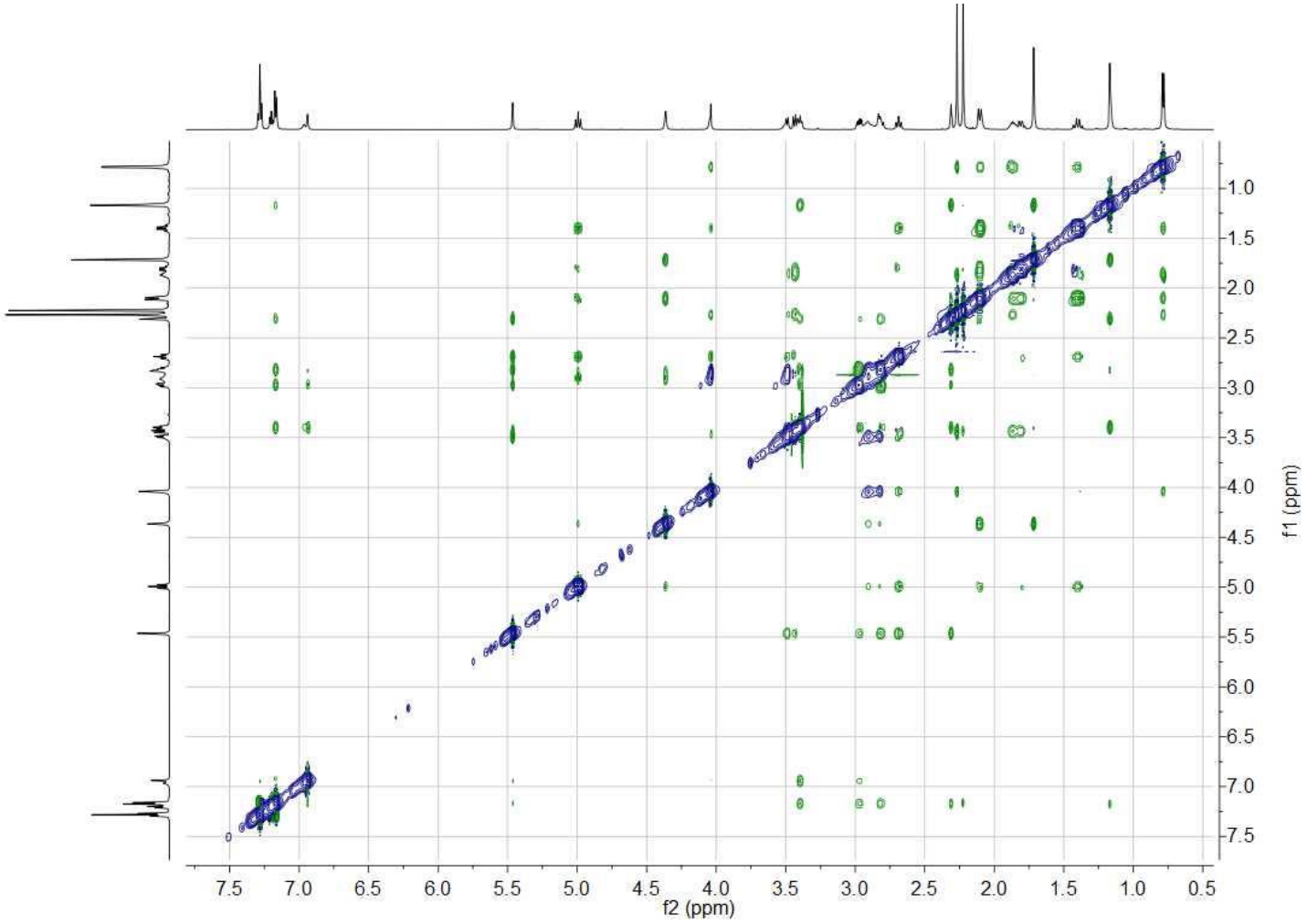

Fig. S57. ROESY of **6**.

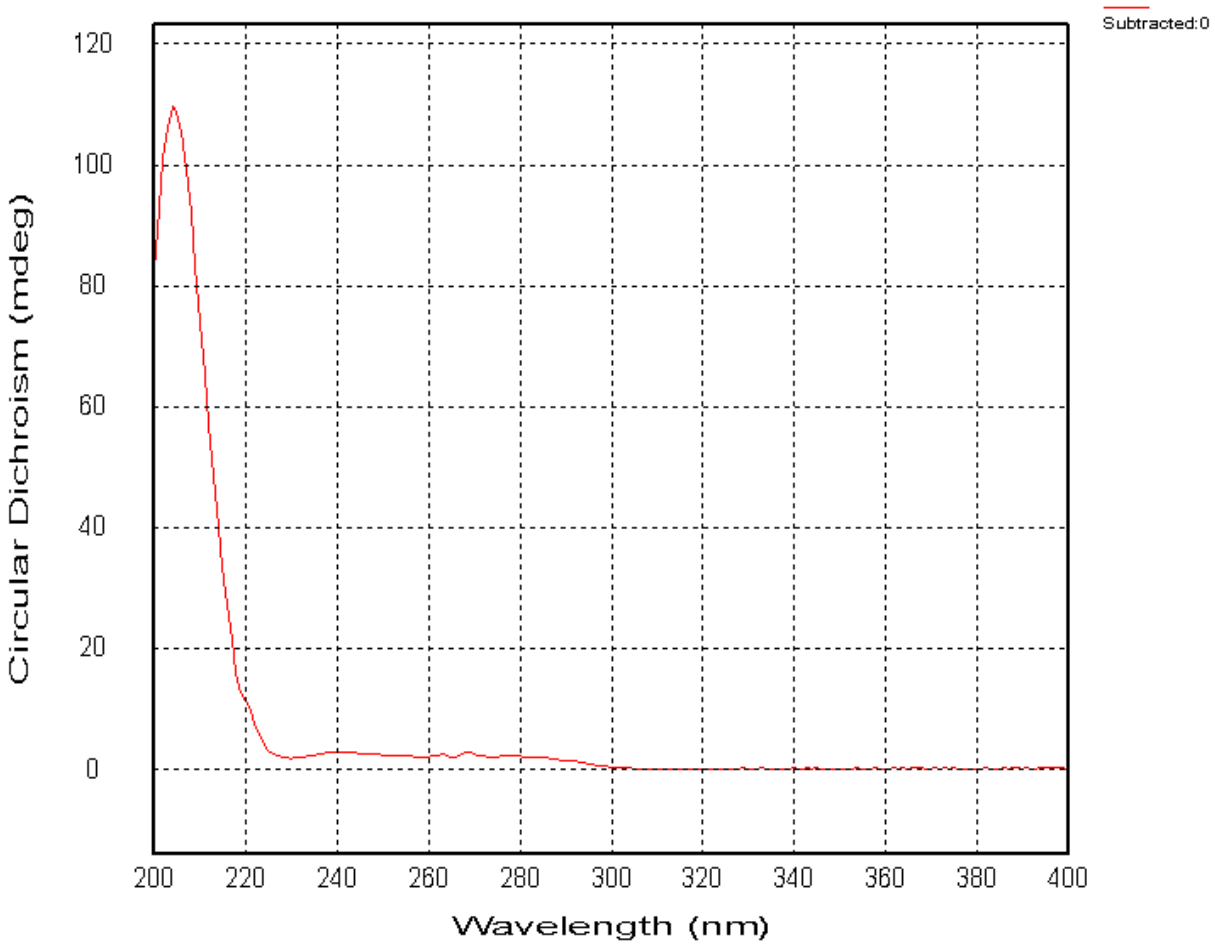

Fig. S58. Experimental ECD of **6**.

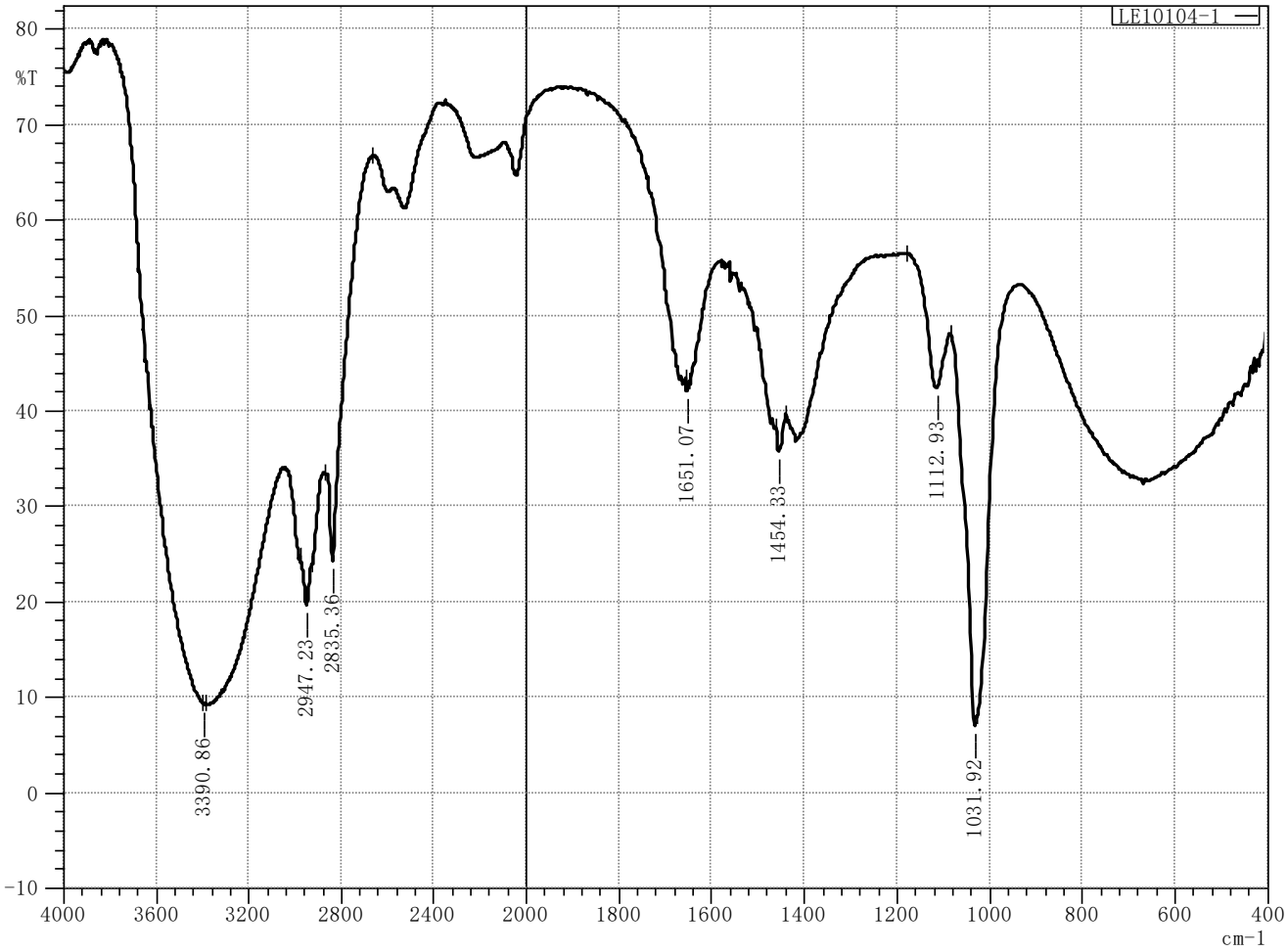

Fig. S59. IR of **6**.

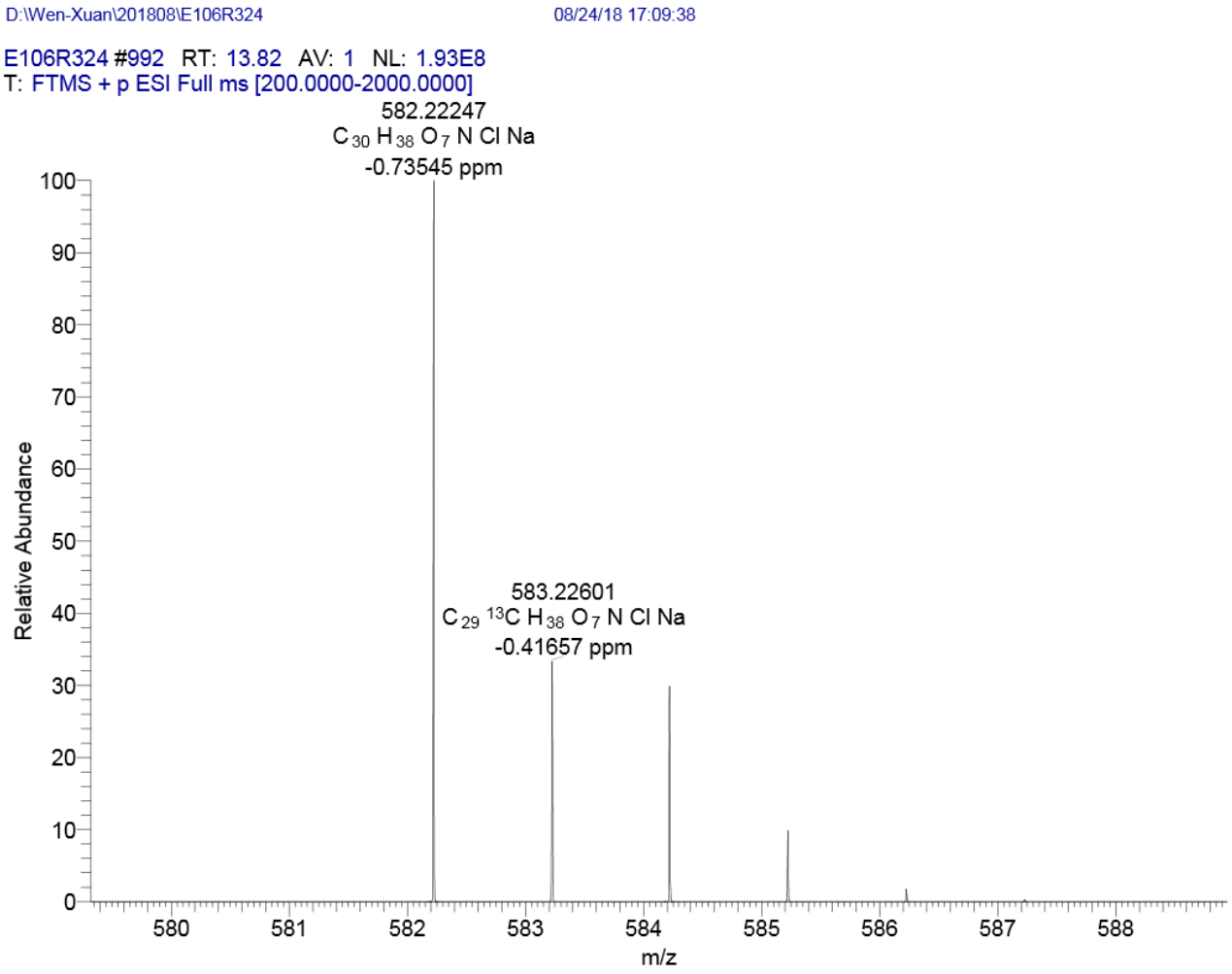

Fig. S60. HRESIMS of **6**.

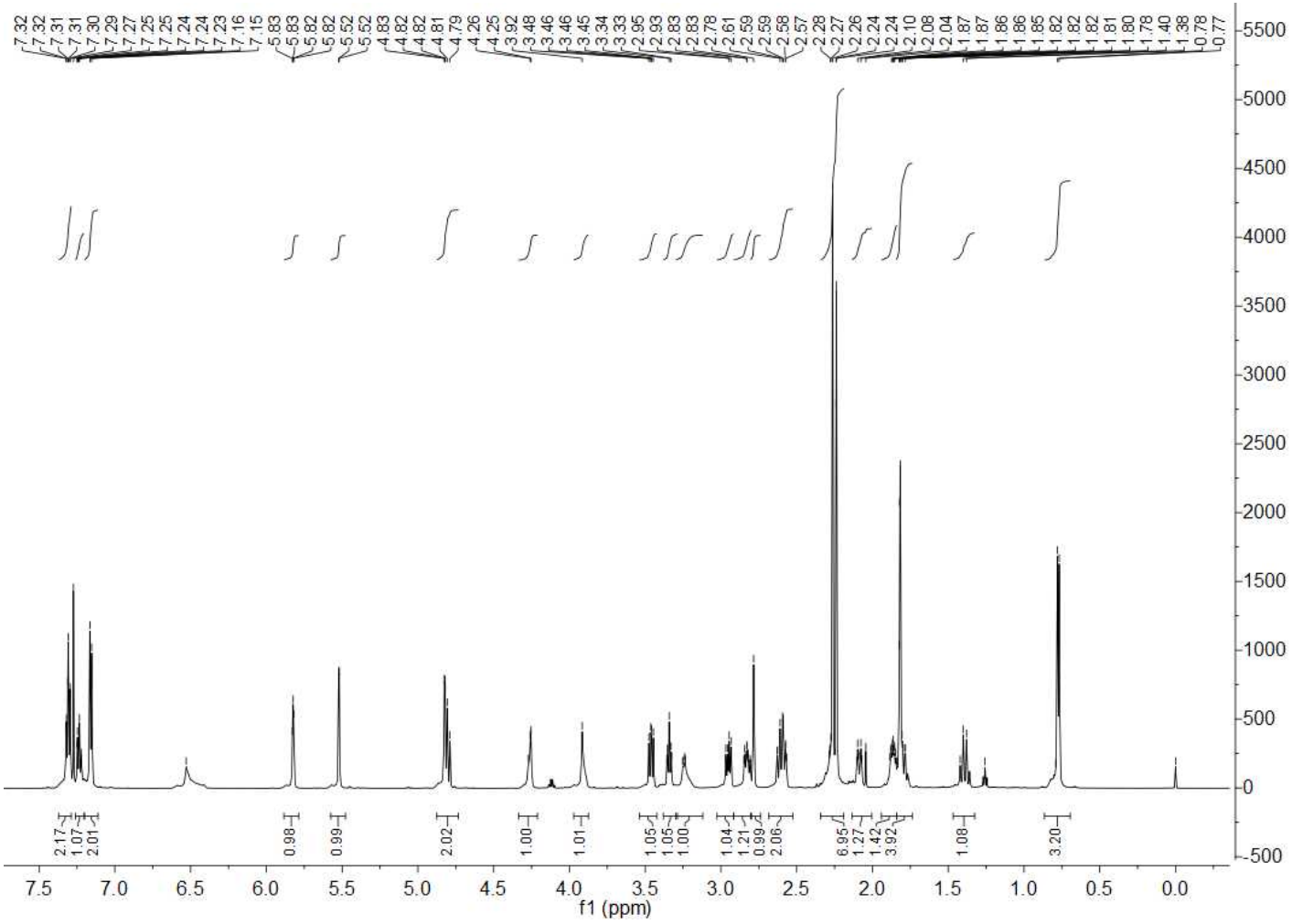

Fig. S61. ^{1}H NMR of **7**.

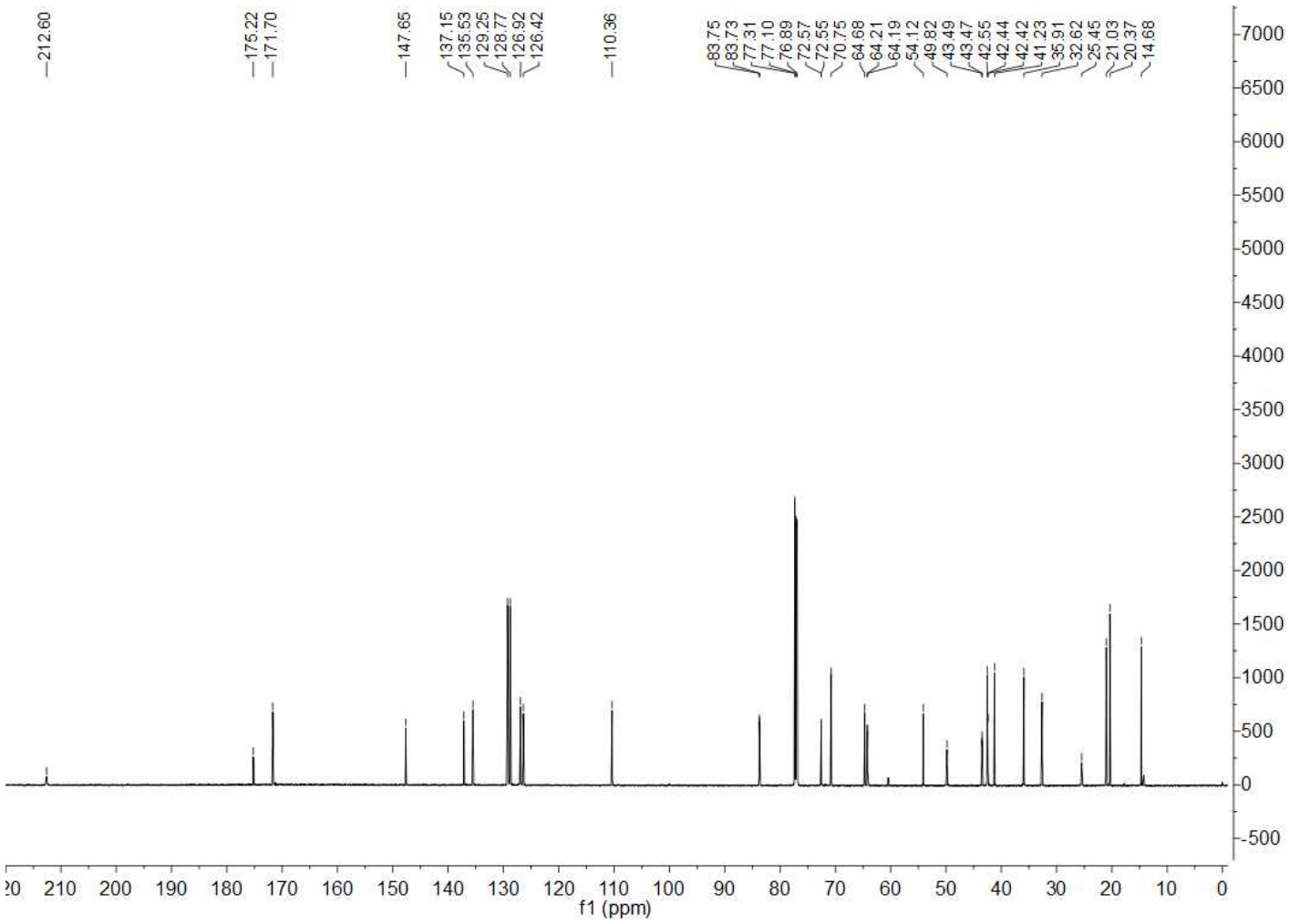

Fig. S62. ^{13}C NMR of **7**.

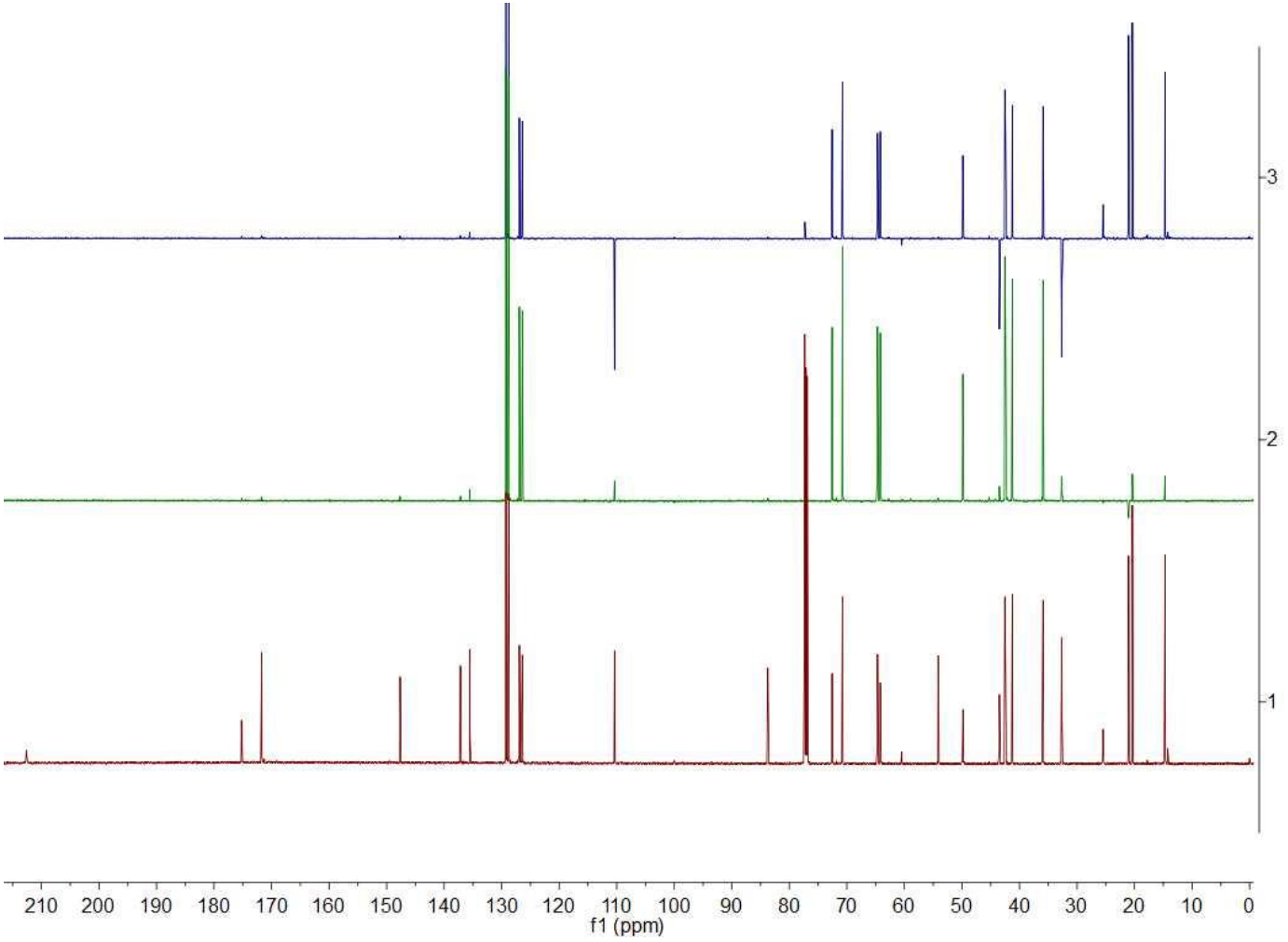

Fig. S63. DEPT of **7**.

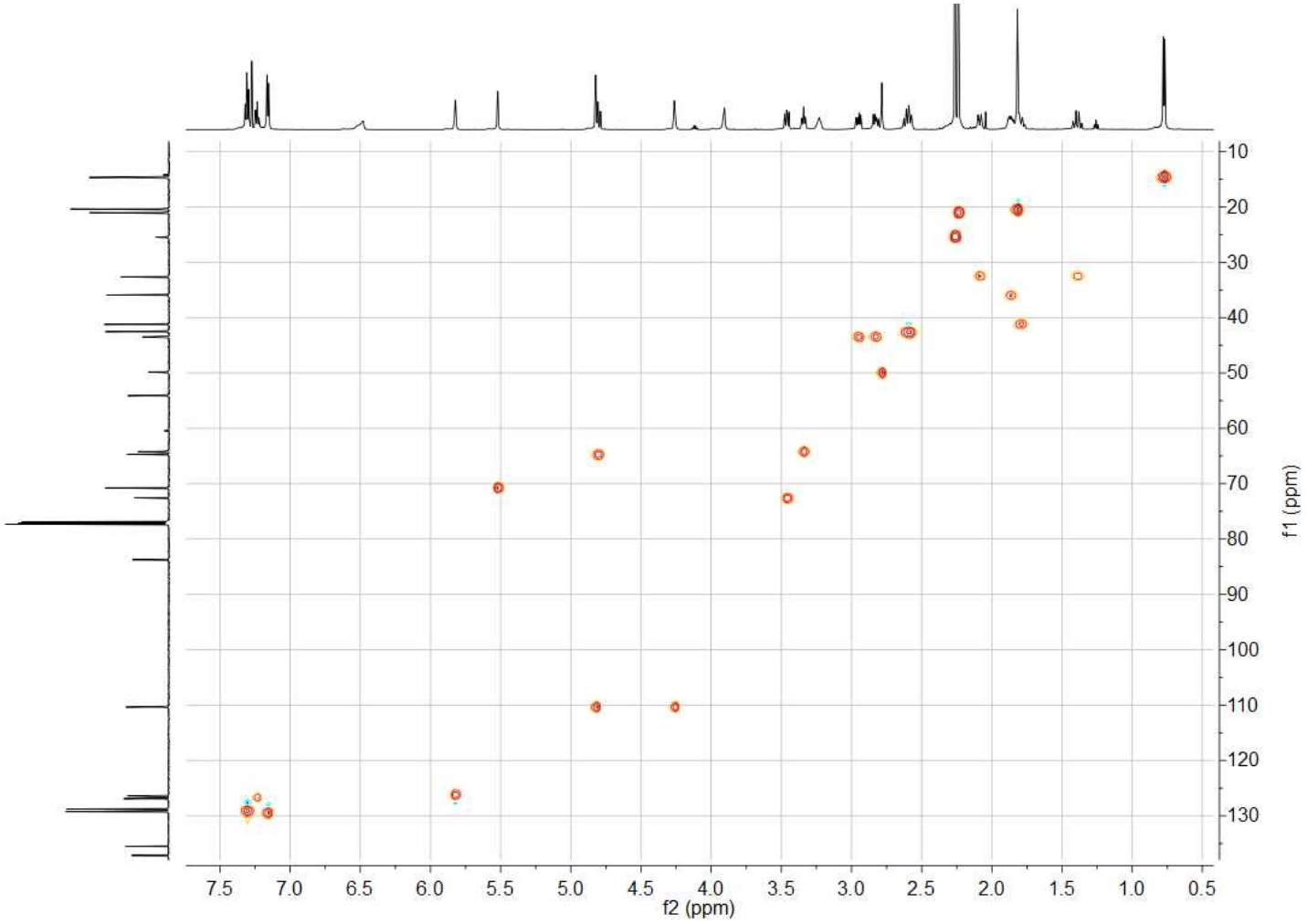

Fig. S64. HSQC of **7**.

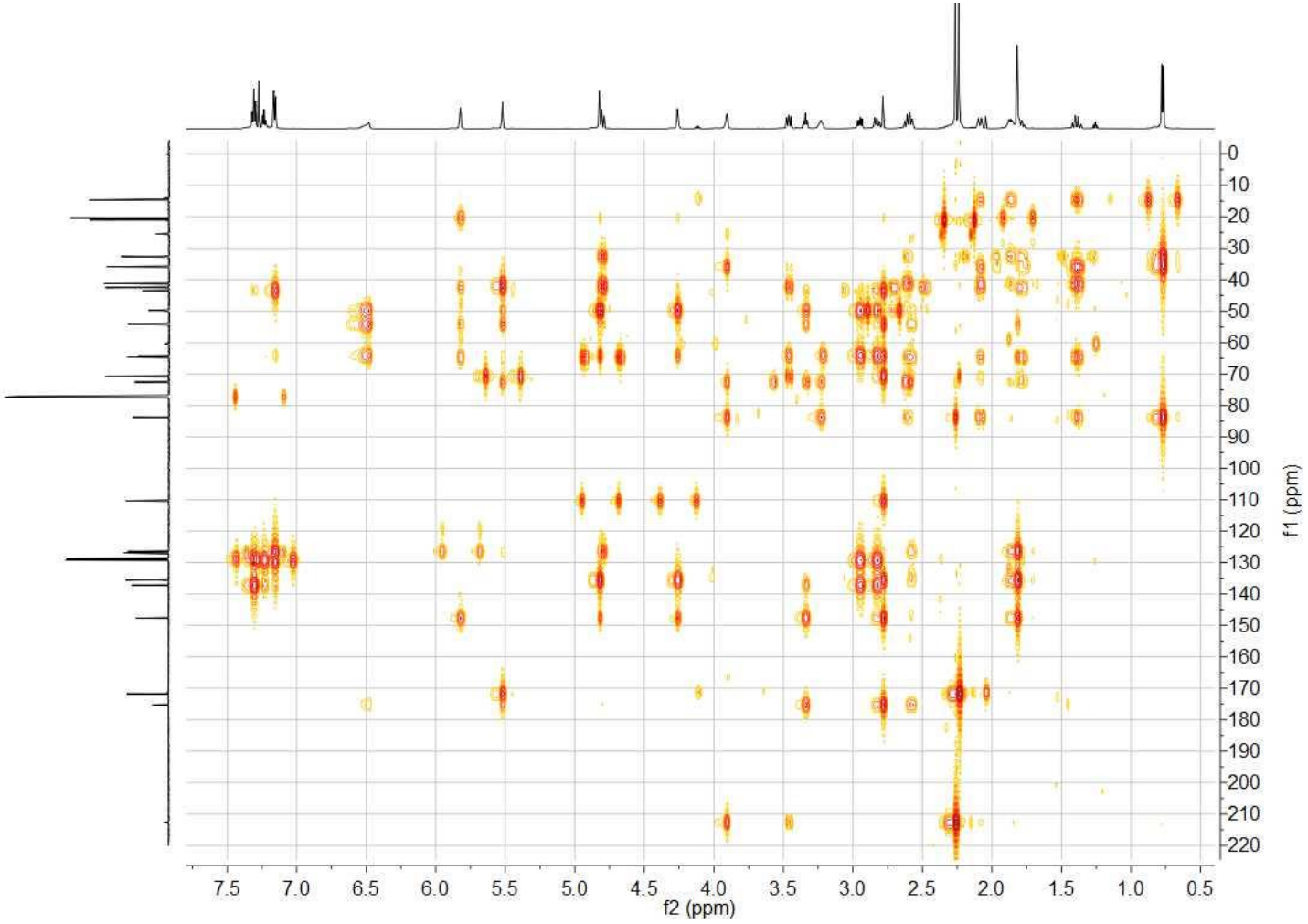

Fig. S65. HMBC of **7**.

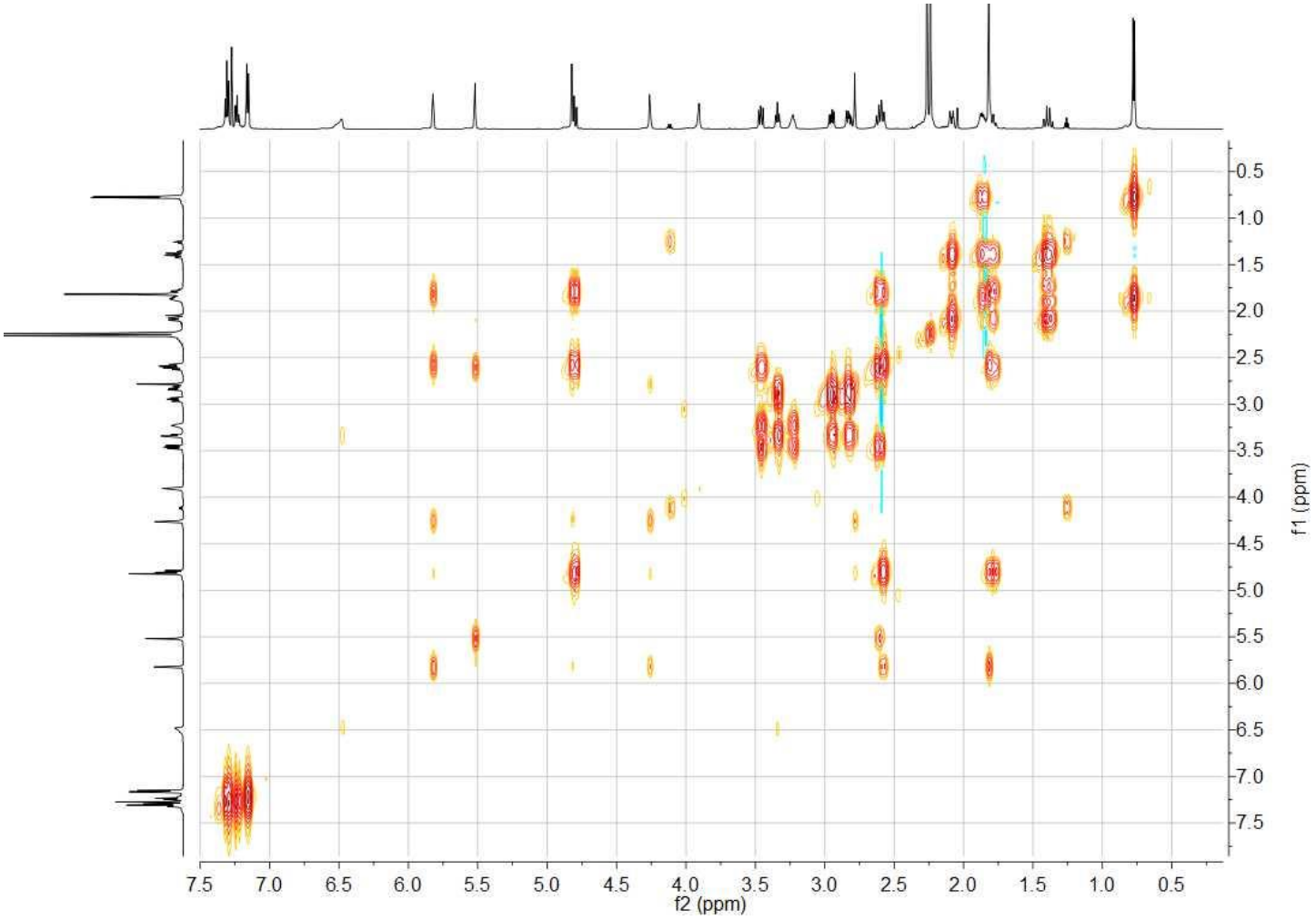

Fig. S66. ^{1}H-^{1}H COSY of **7**.

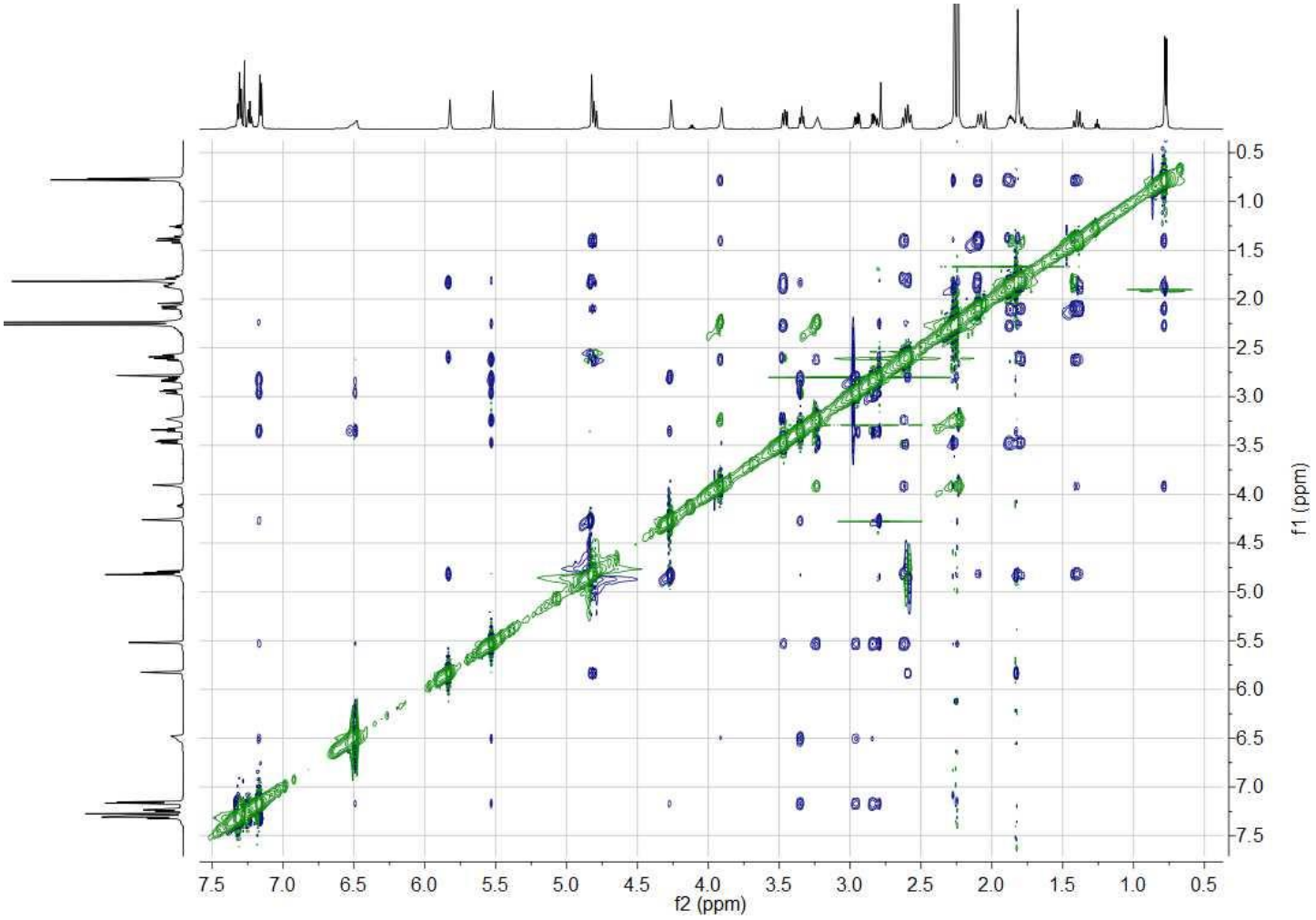

Fig. S67. ROESY of **7**.

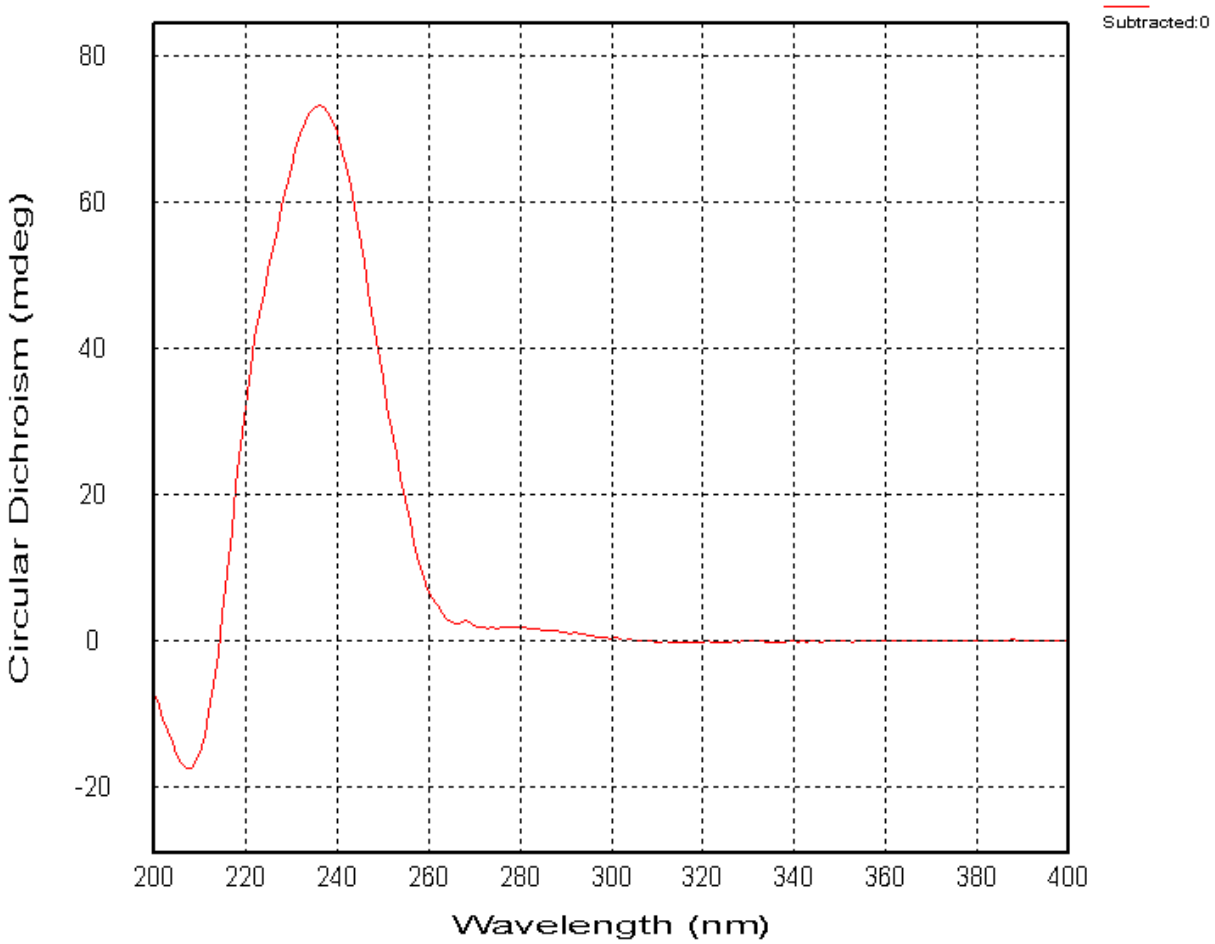

Fig. S68. Experimental ECD of **7**.

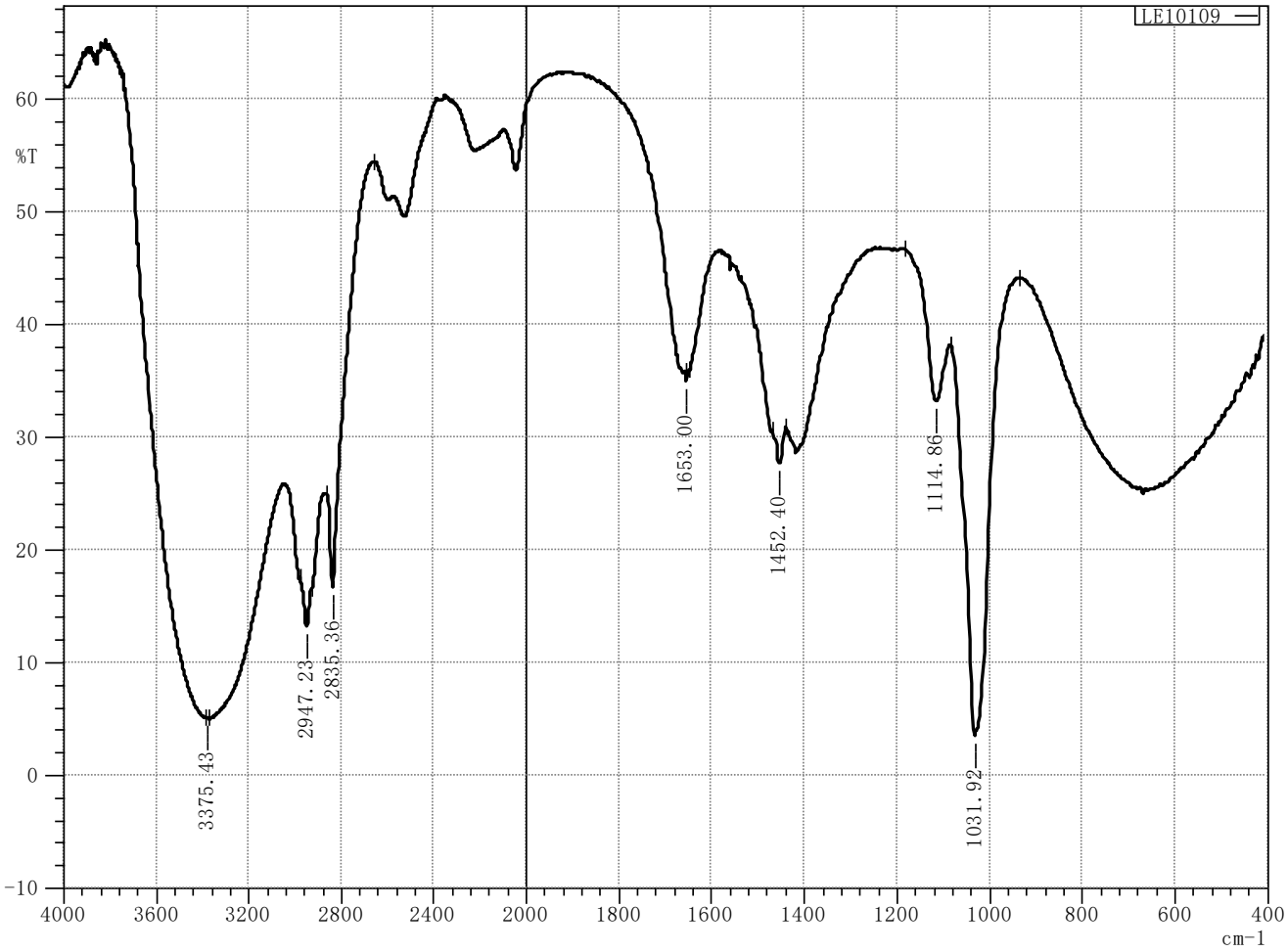

Fig. S69. IR of **7**.

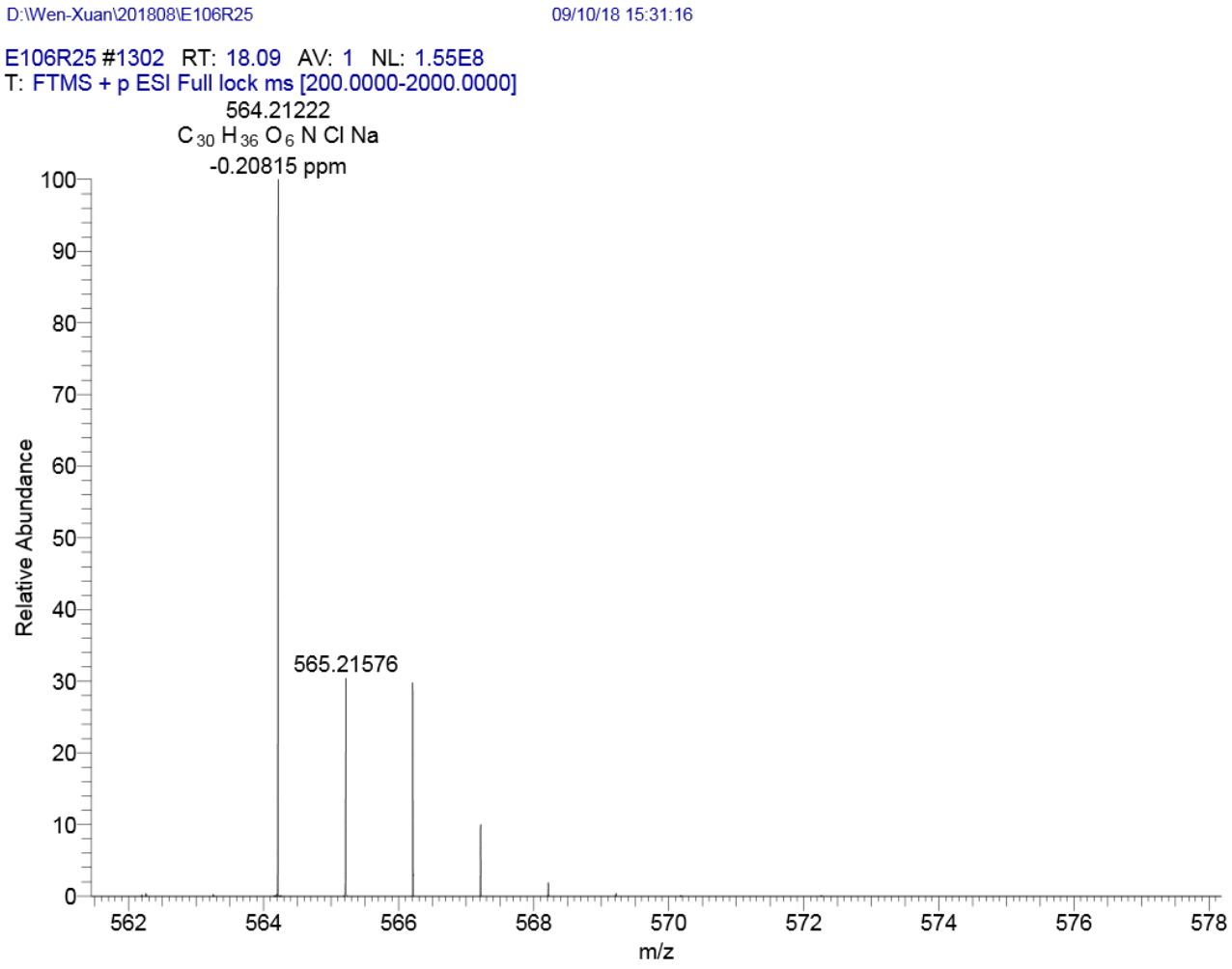

Fig. S70. HRESIMS of **7**.

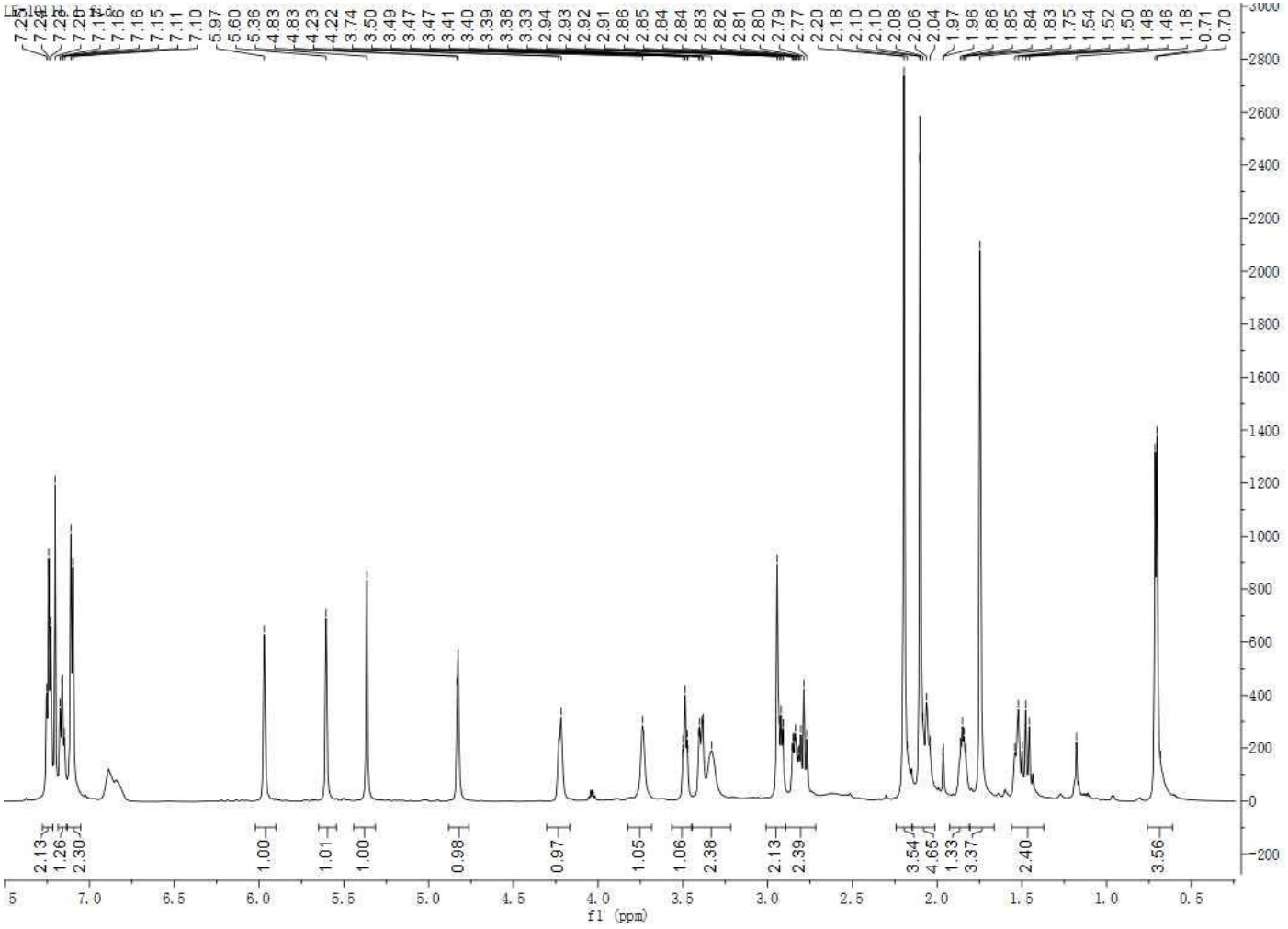

Fig. S71. ^{1}H NMR of **8** ($CDCl_3$, 600 MHz).

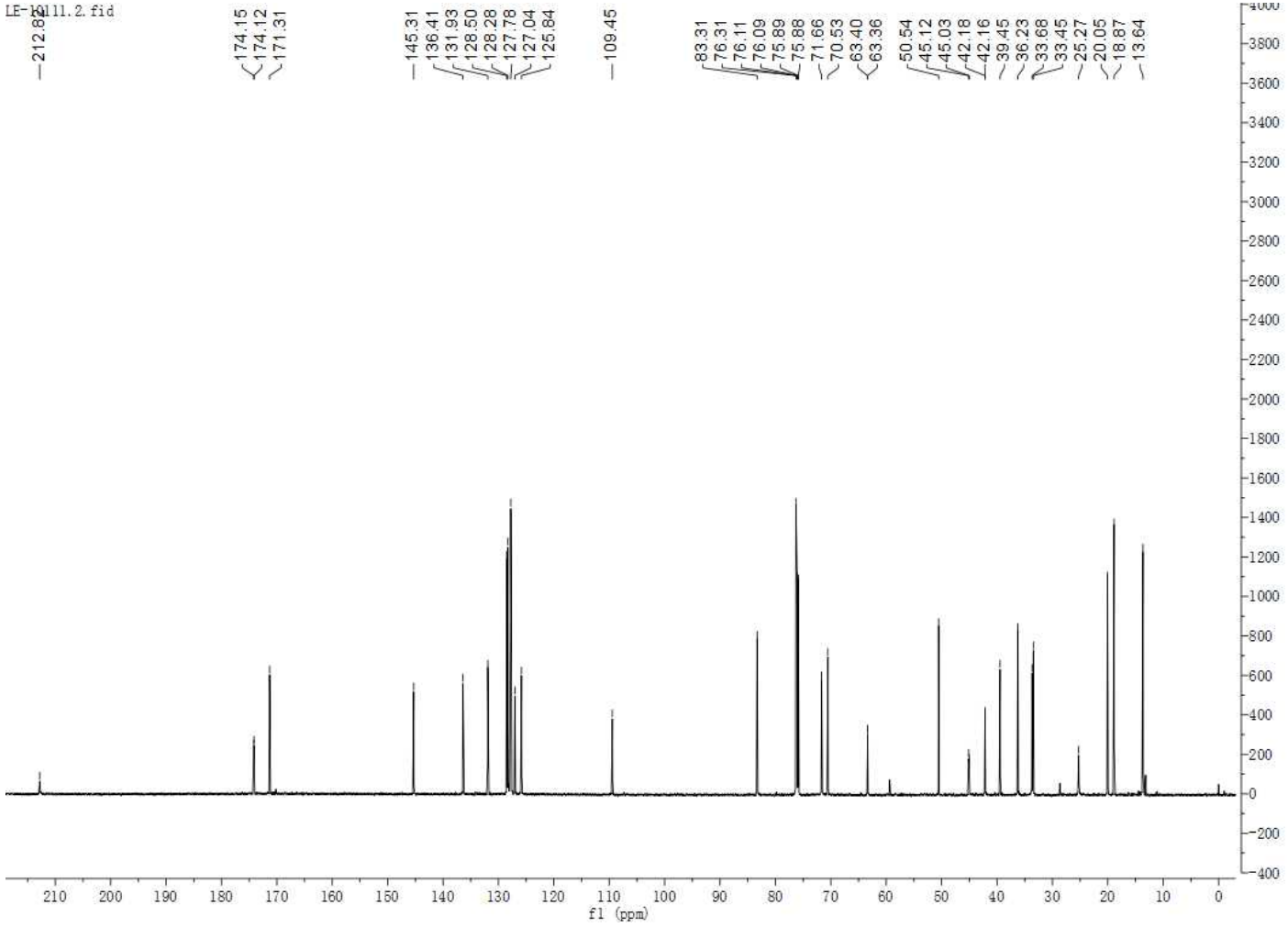

Fig. S72. ^{13}C NMR of **8** ($CDCl_3$, 150 MHz).

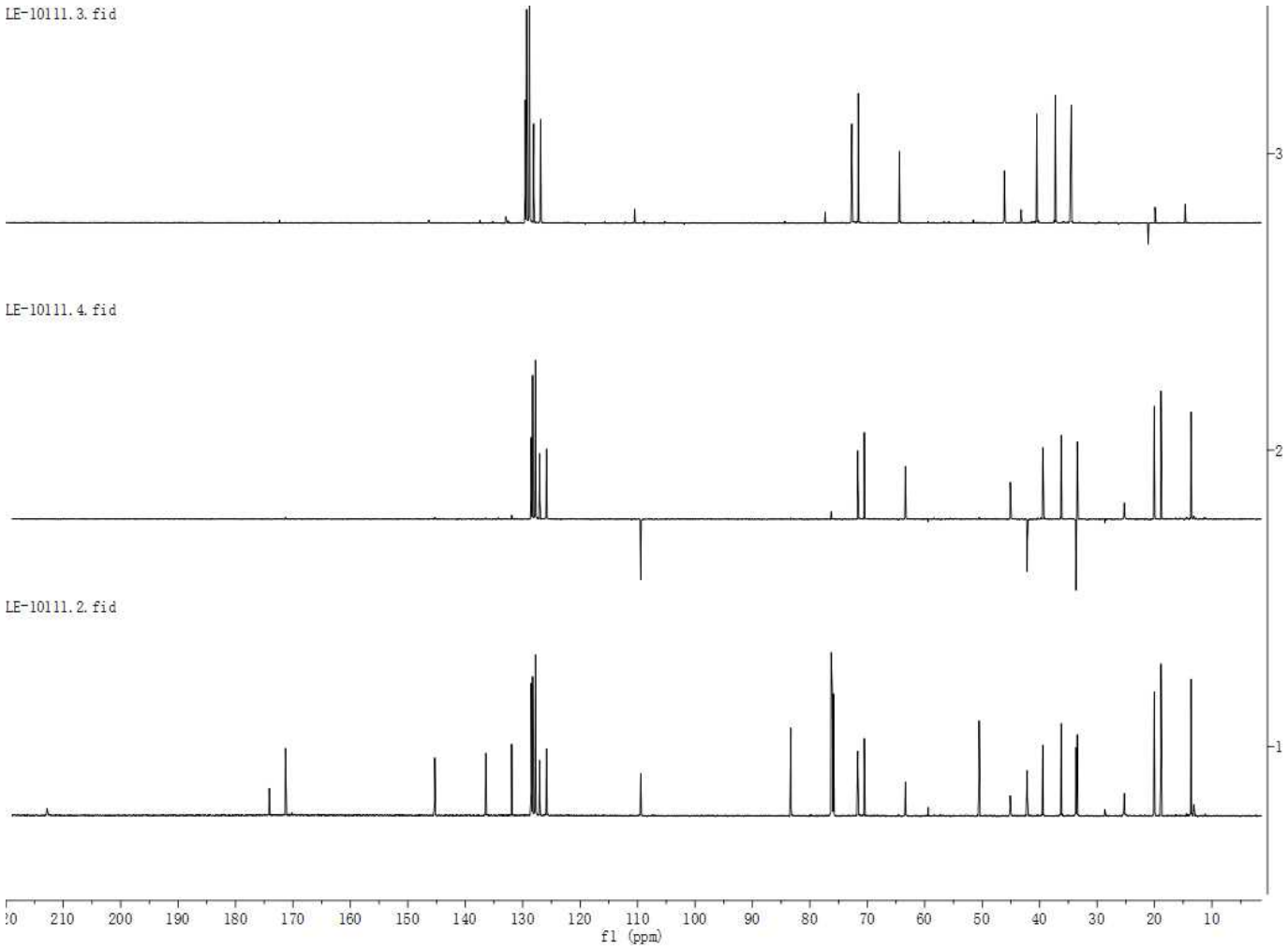

Fig. S73. DEPT of **8**.

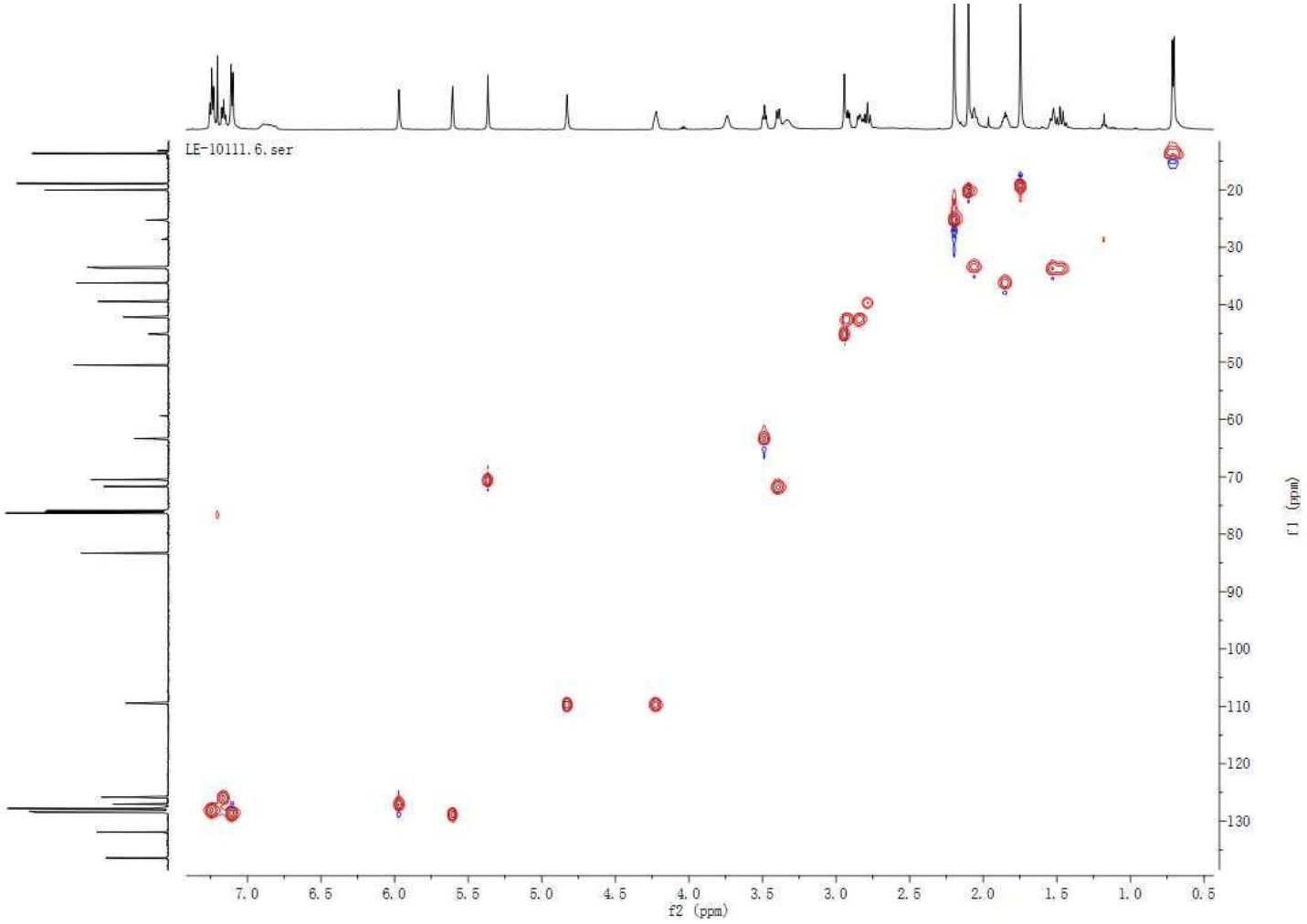

Fig. S74. HSQC of **8**.

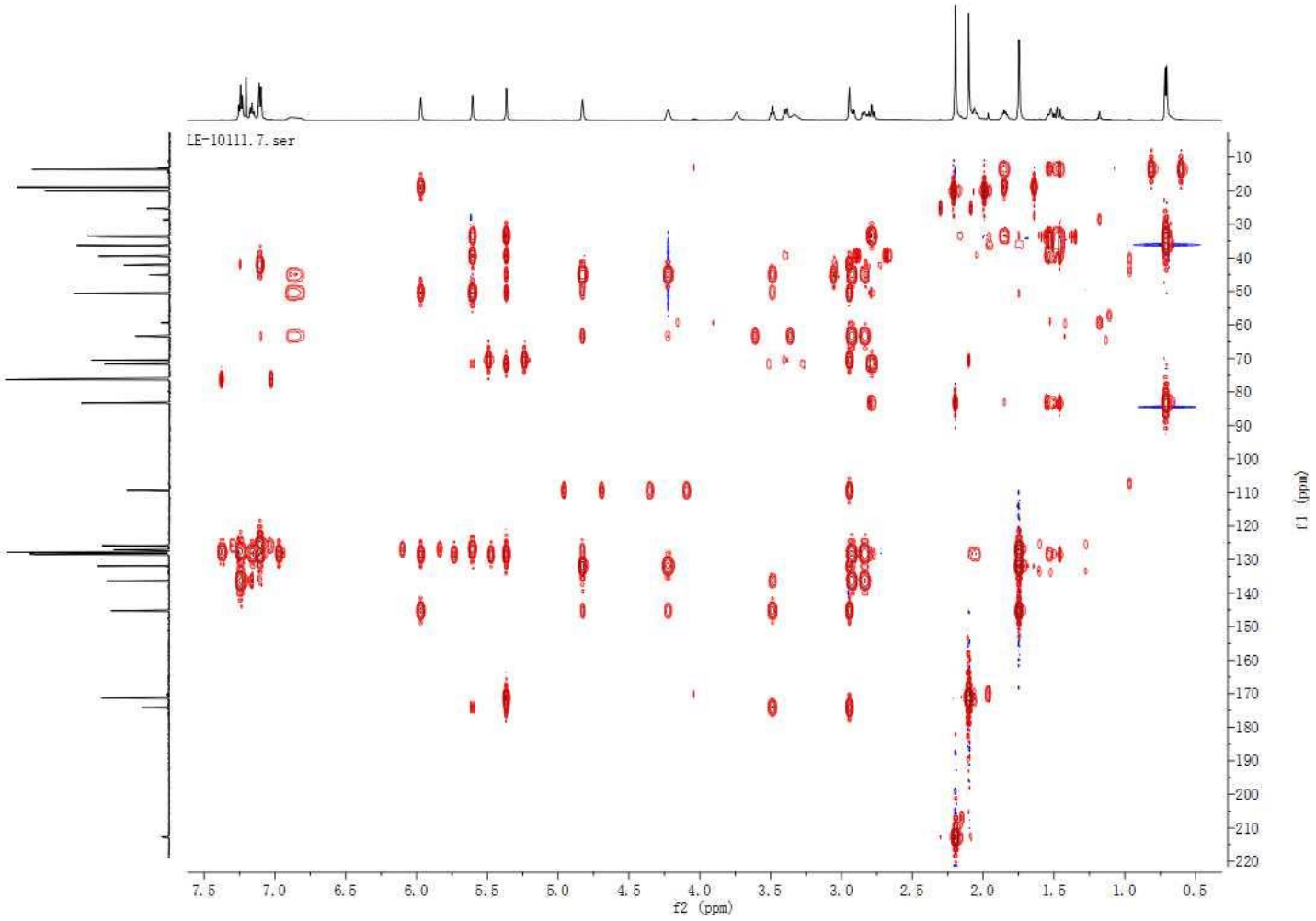

Fig. S75. HMBC of **8**.

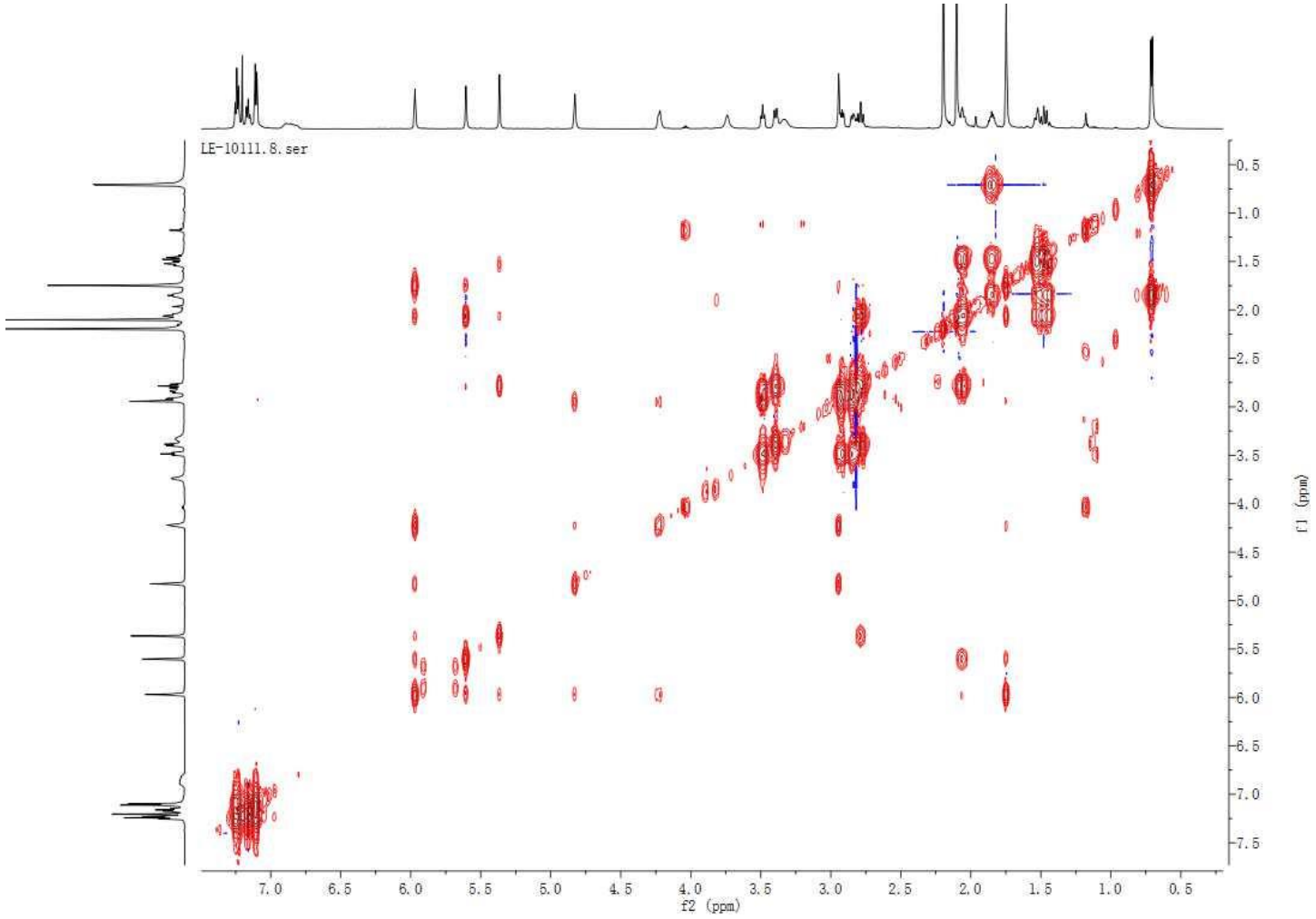

Fig. S76. ^{1}H-^{1}H COSY of **8**.

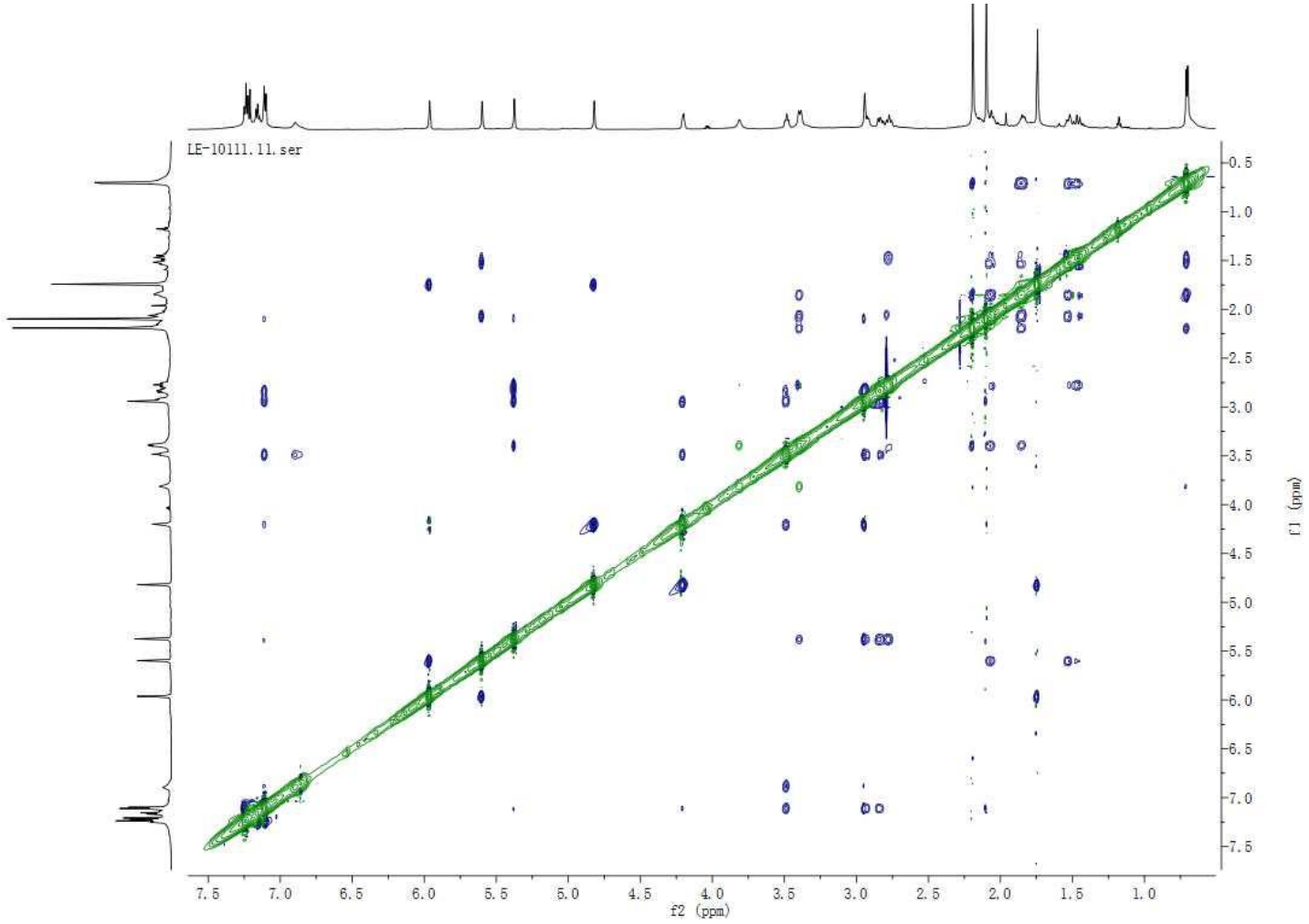

Fig. S77. ROESY of **8**.

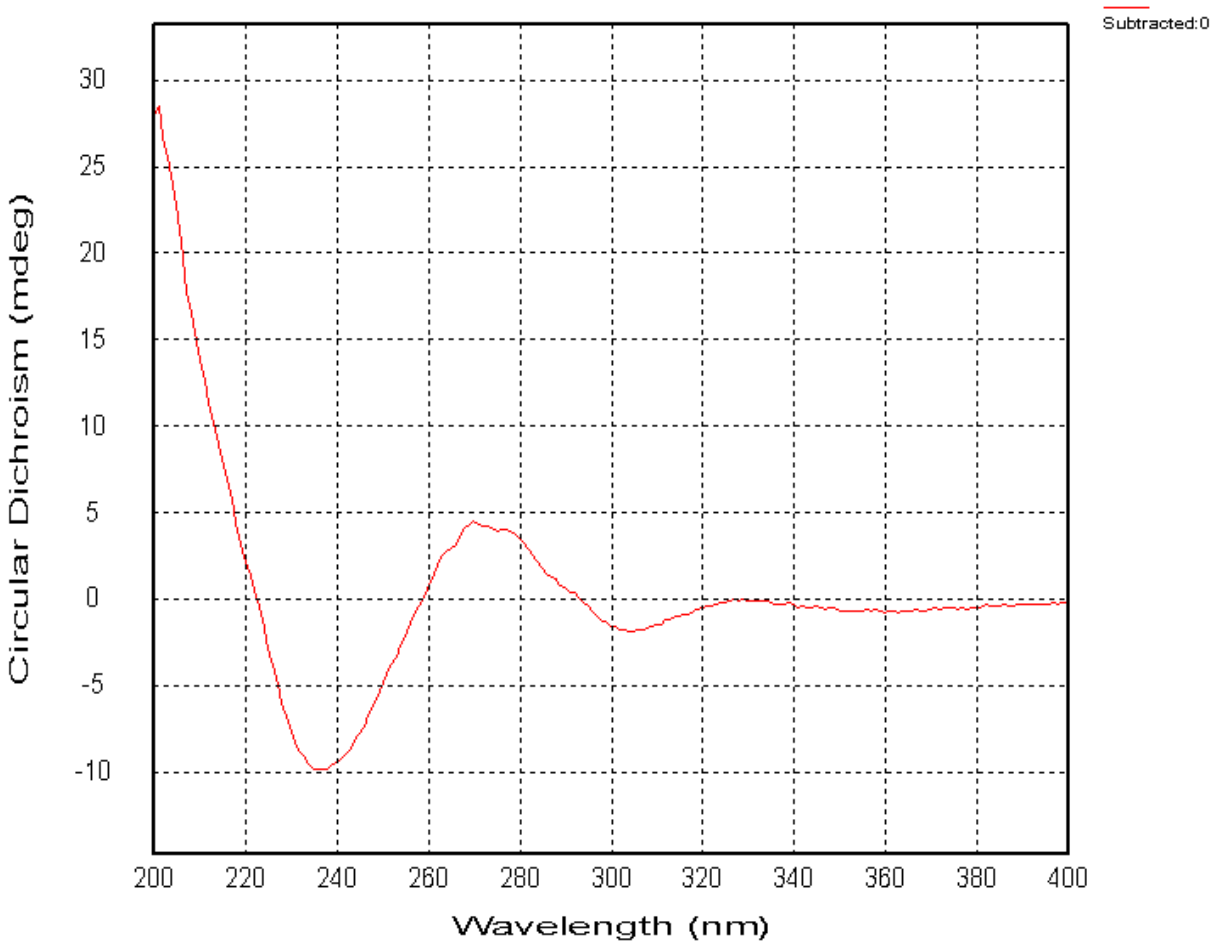

Fig. S78. Experimental ECD of **8**.

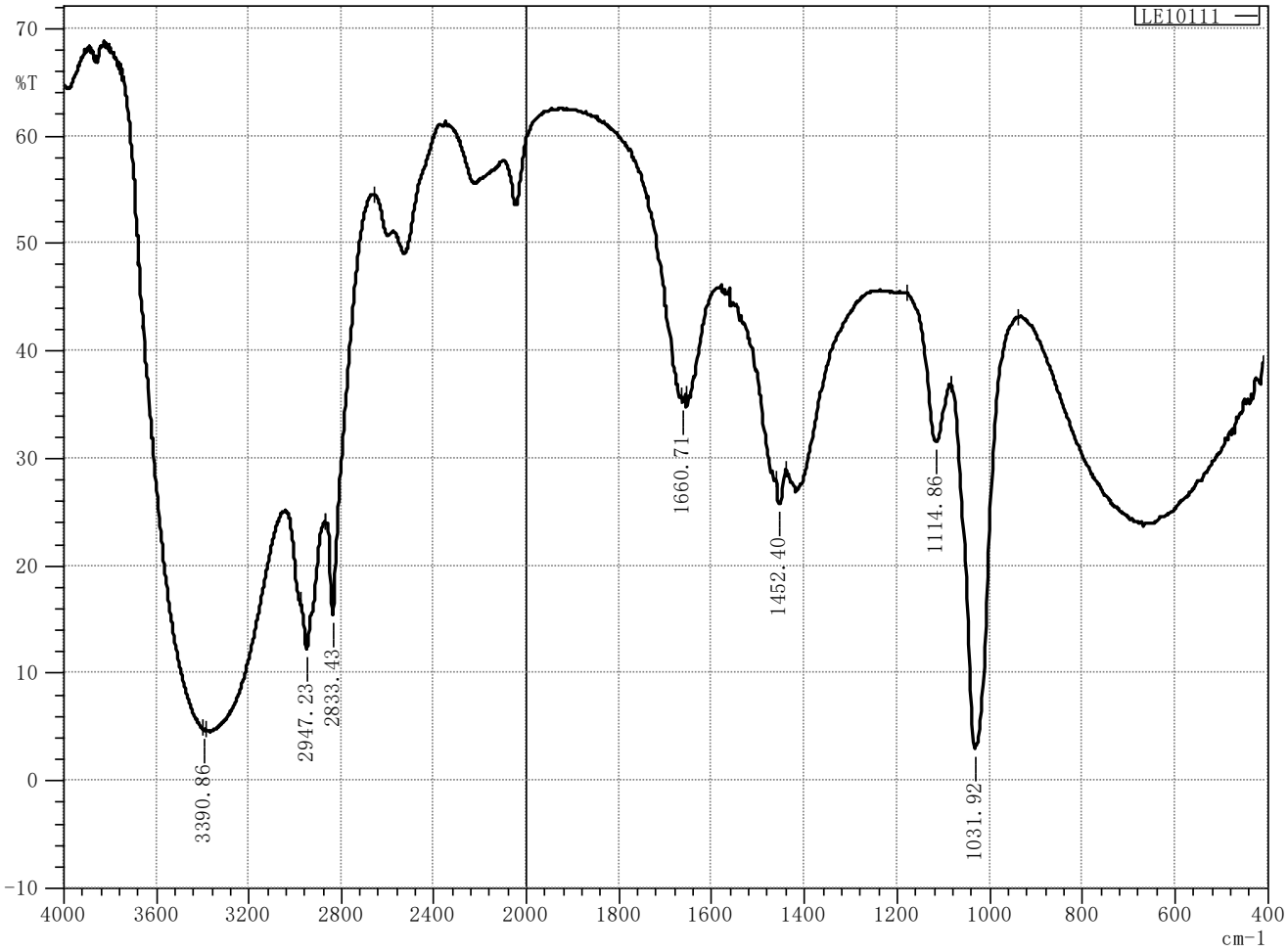

Fig. S79. IR of **8**.

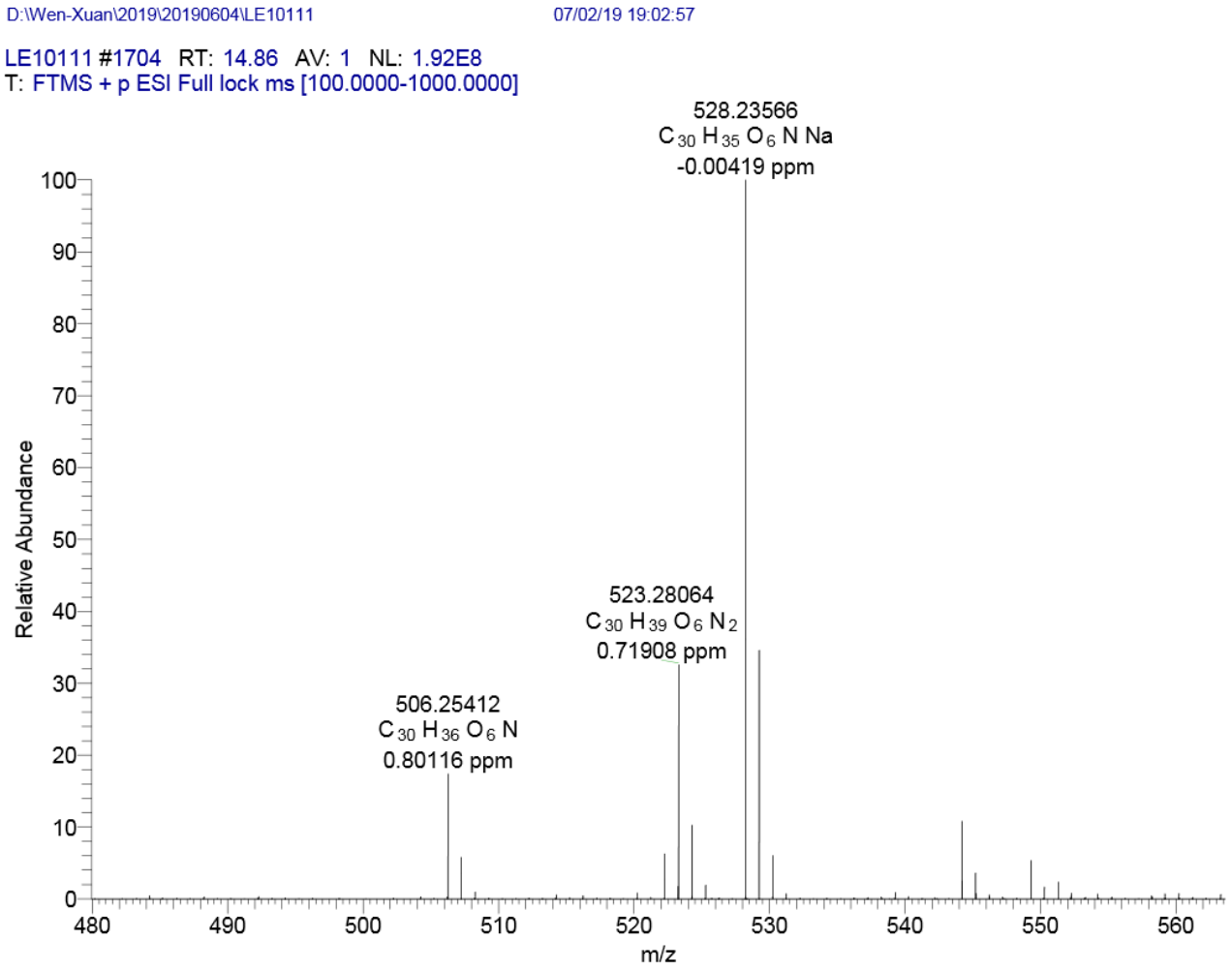

Fig. S80. HRESIMS of **8**.

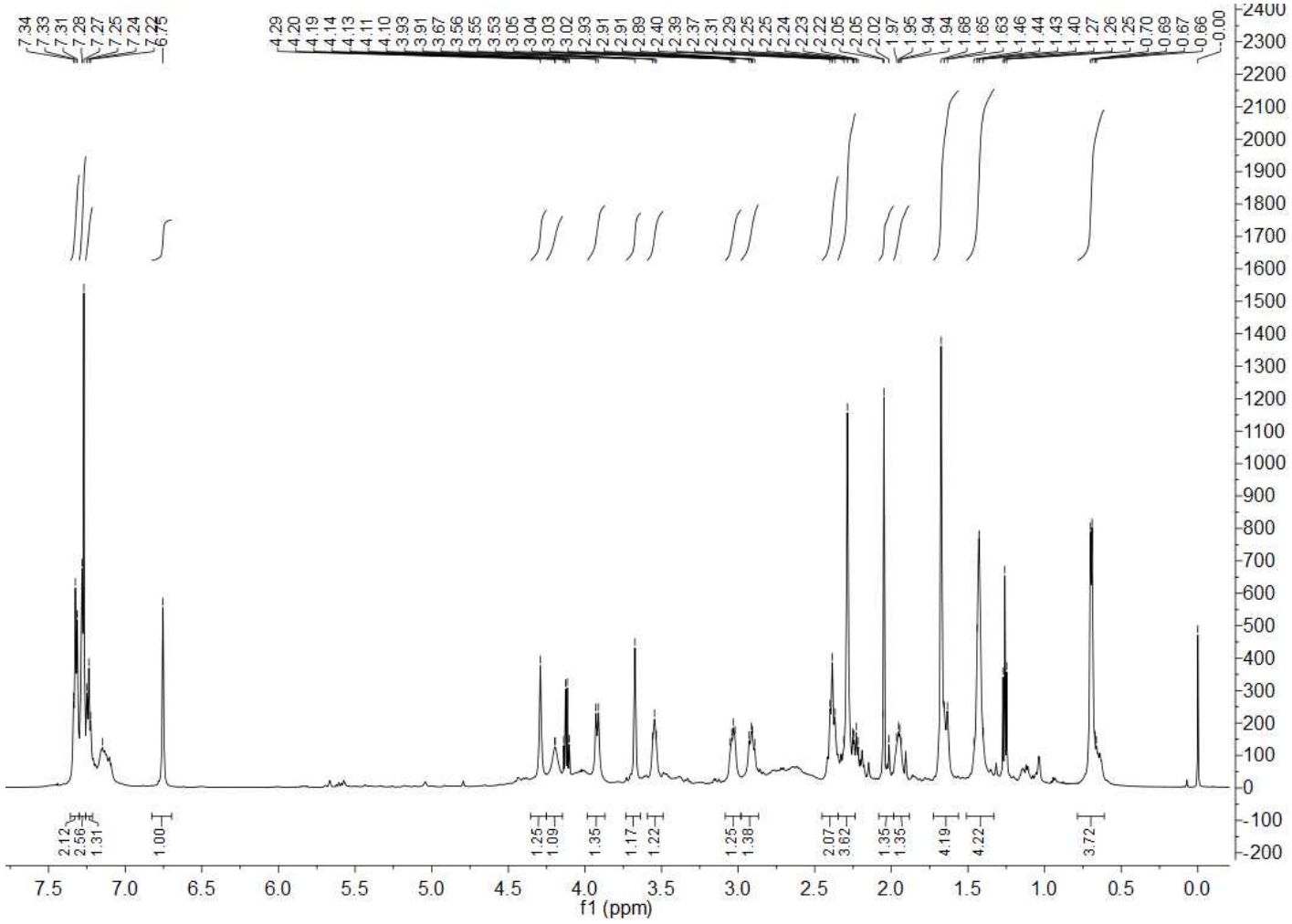

Fig. S81. ^{1}H NMR of **9** ($CDCl_3$, 600 MHz).

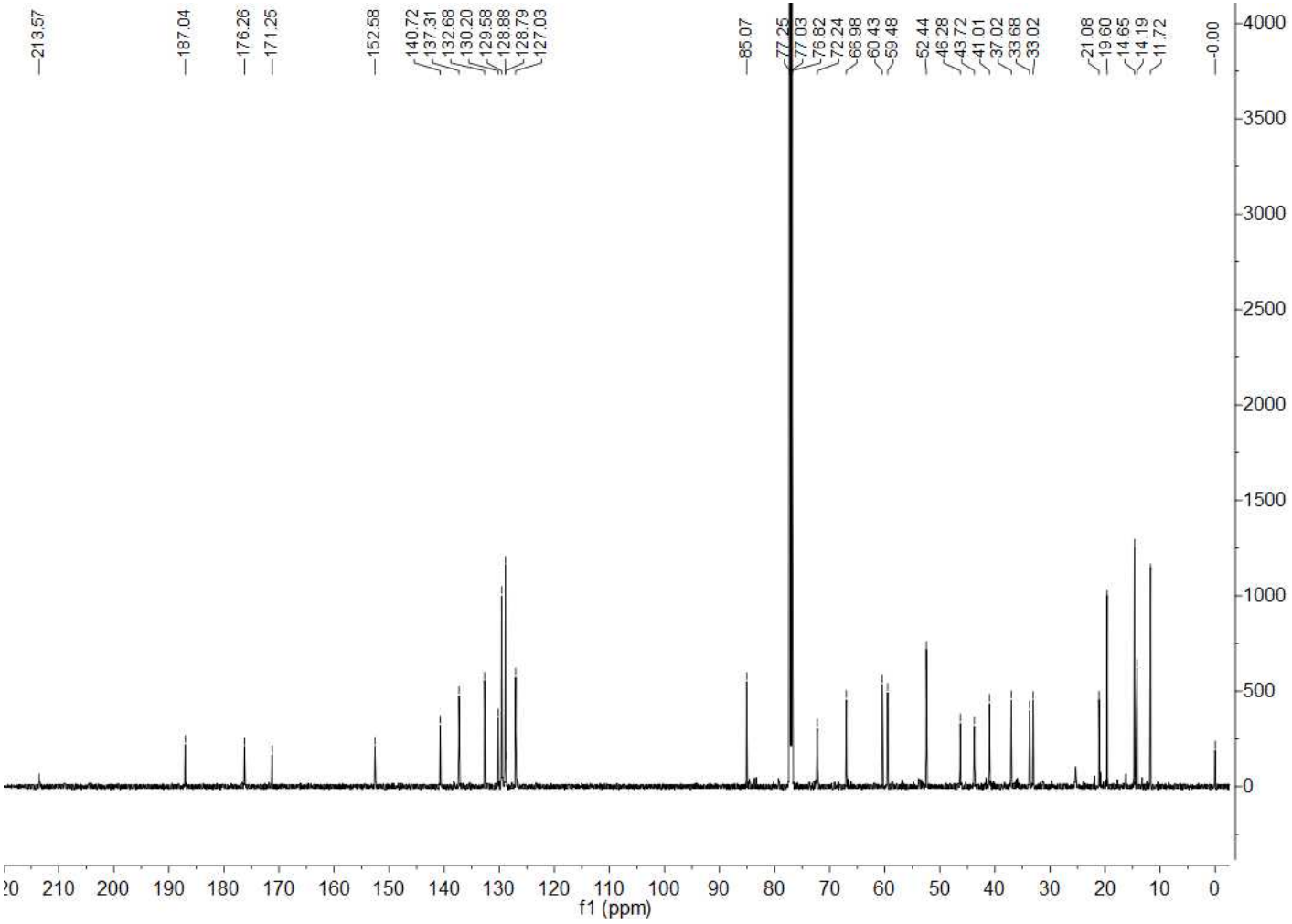

Fig. S82. ^{13}C NMR of **9** ($CDCl_3$, 150 MHz).

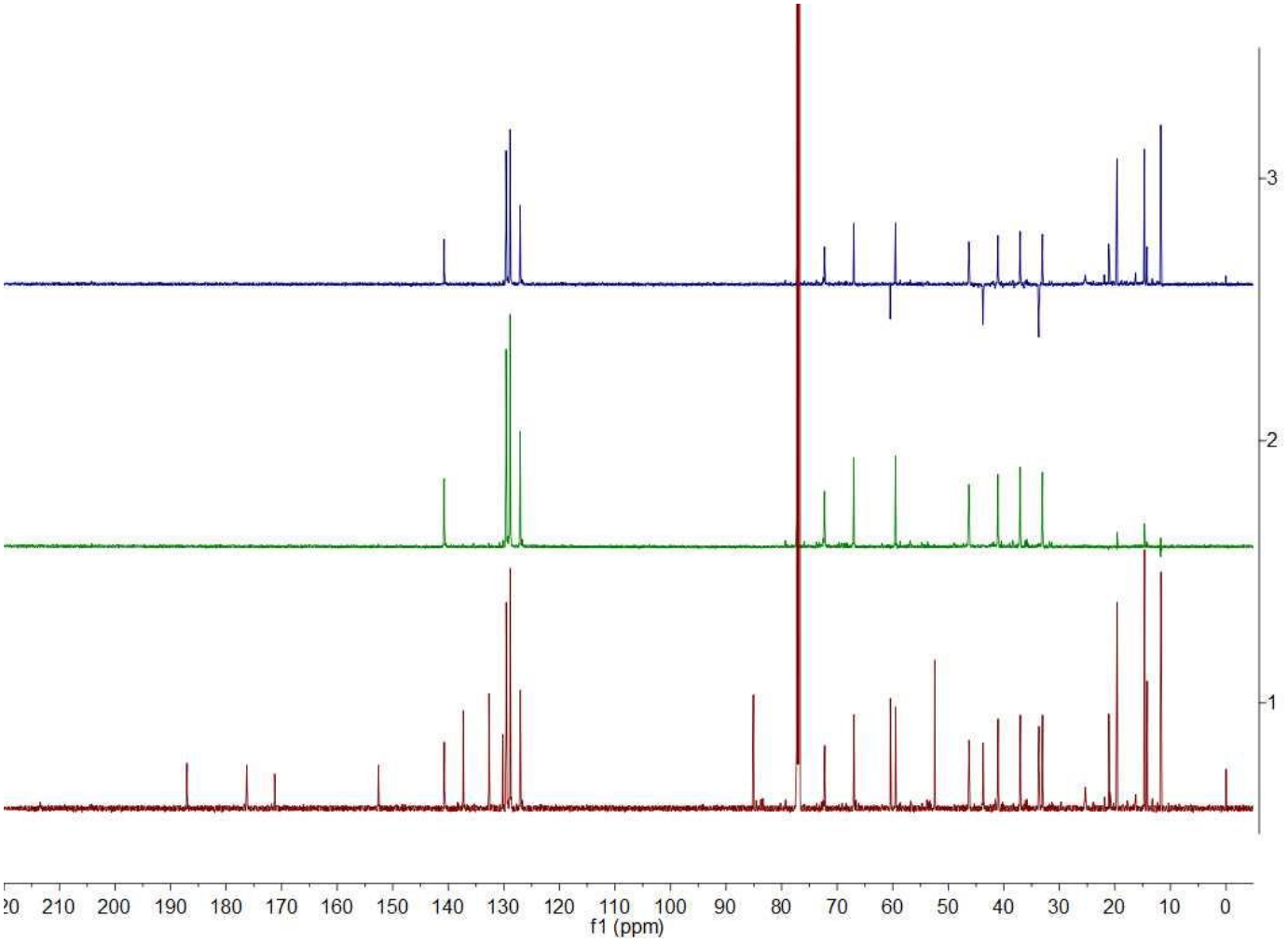

Fig. S83. DEPT of **9**.

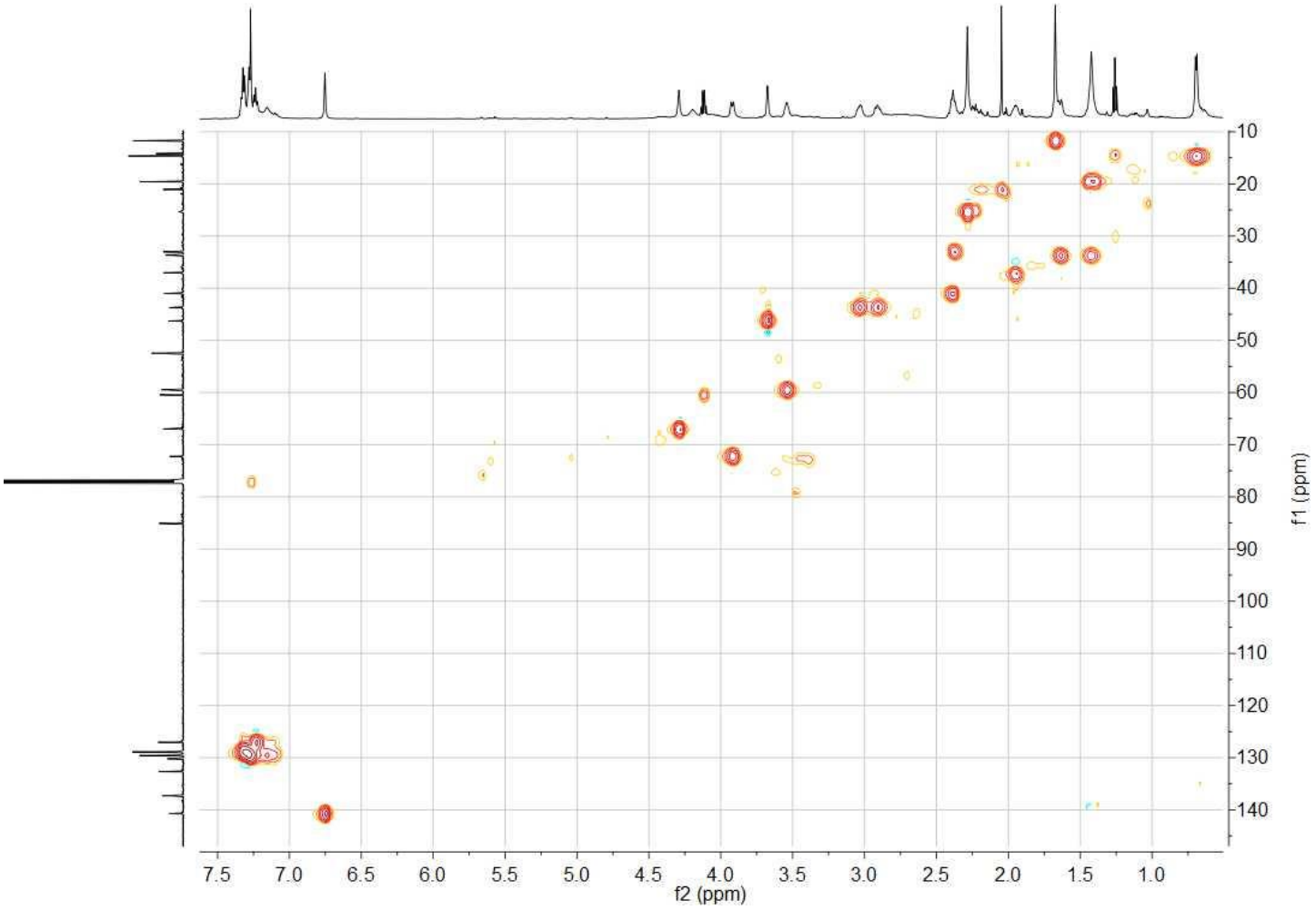

Fig. S84. HSQC of **9**.

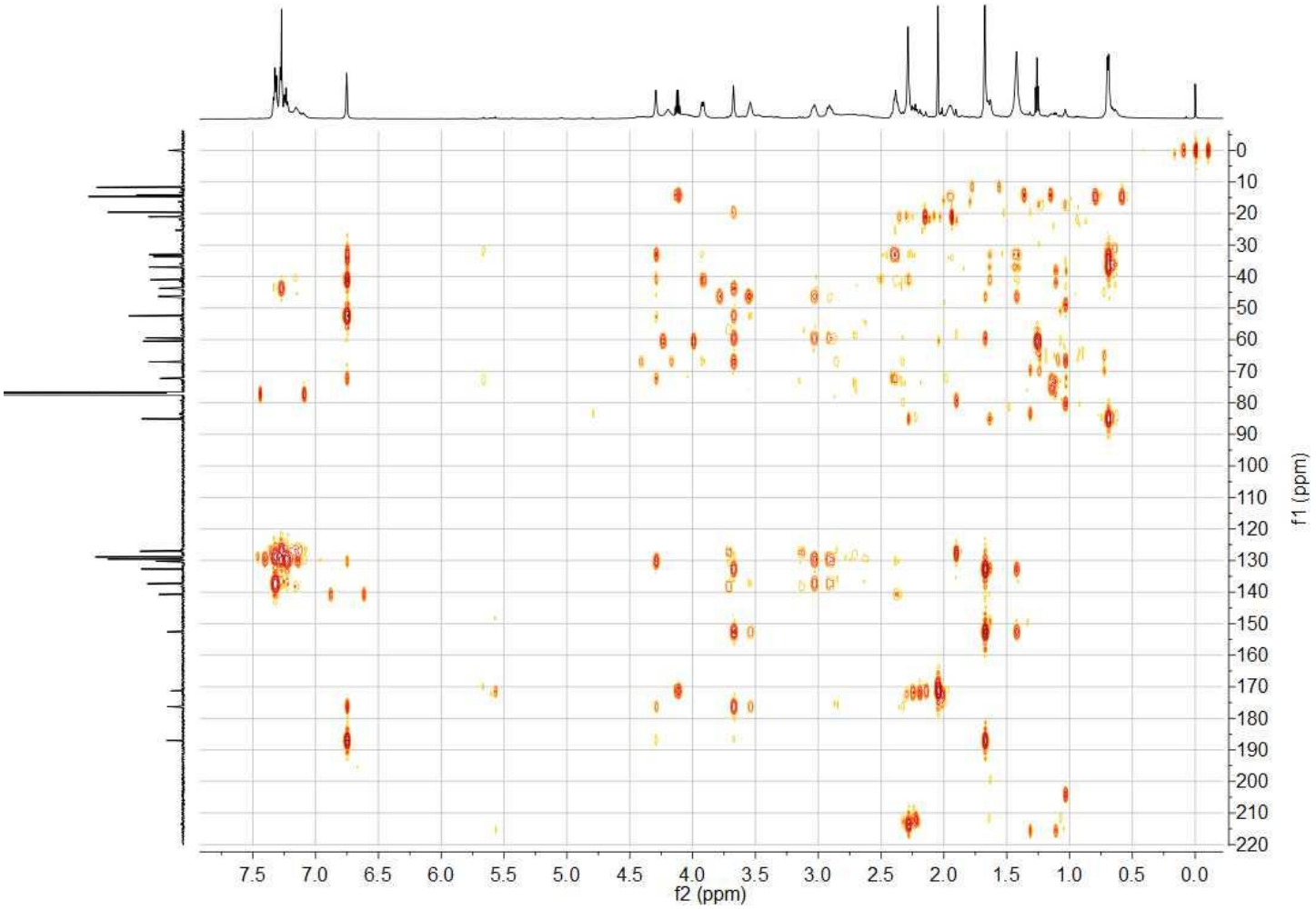

Fig. S85. HMBC of **9**.

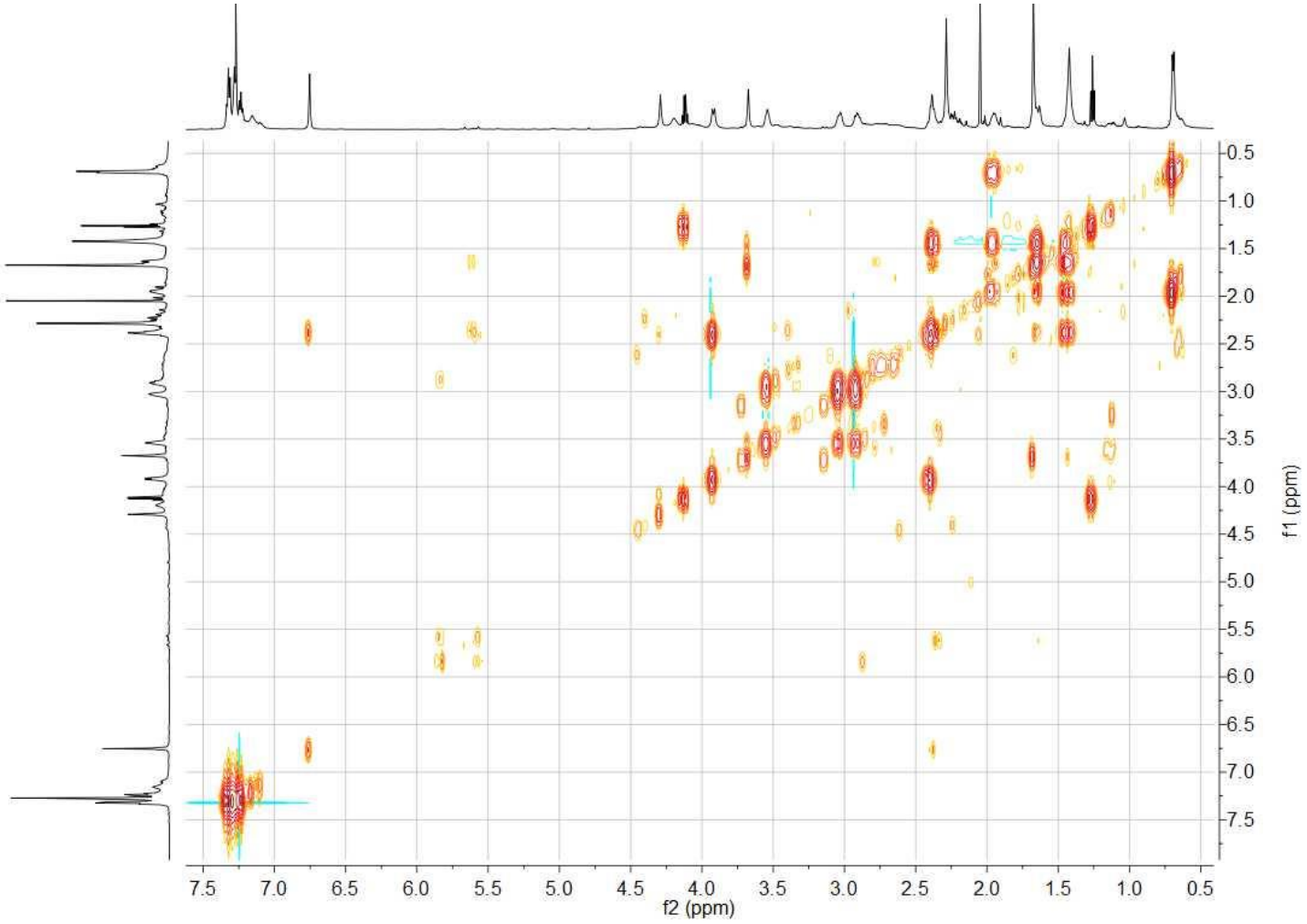

Fig. S86. ^{1}H-^{1}H COSY of **9**.

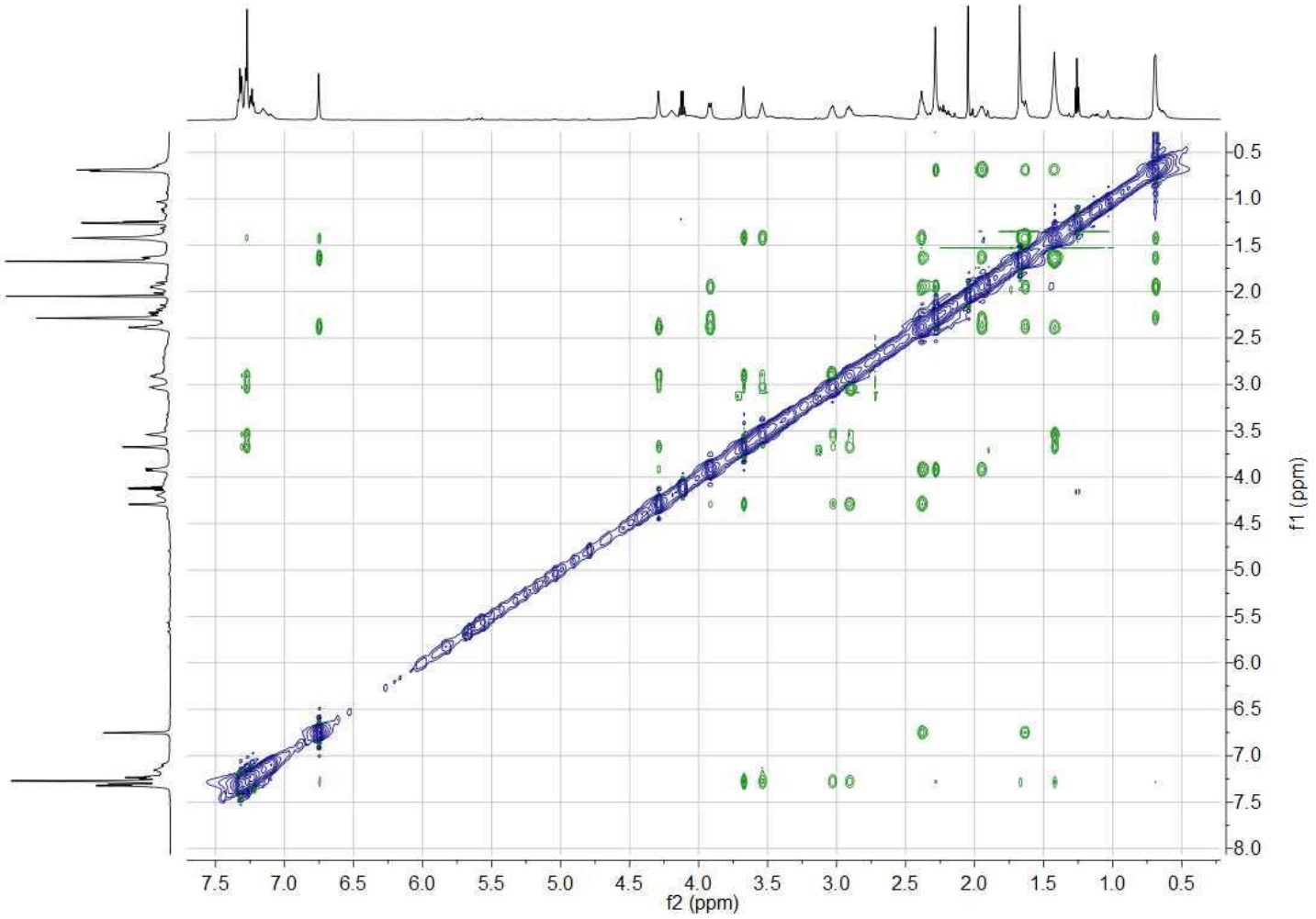

Fig. S87. ROESY of **9**.

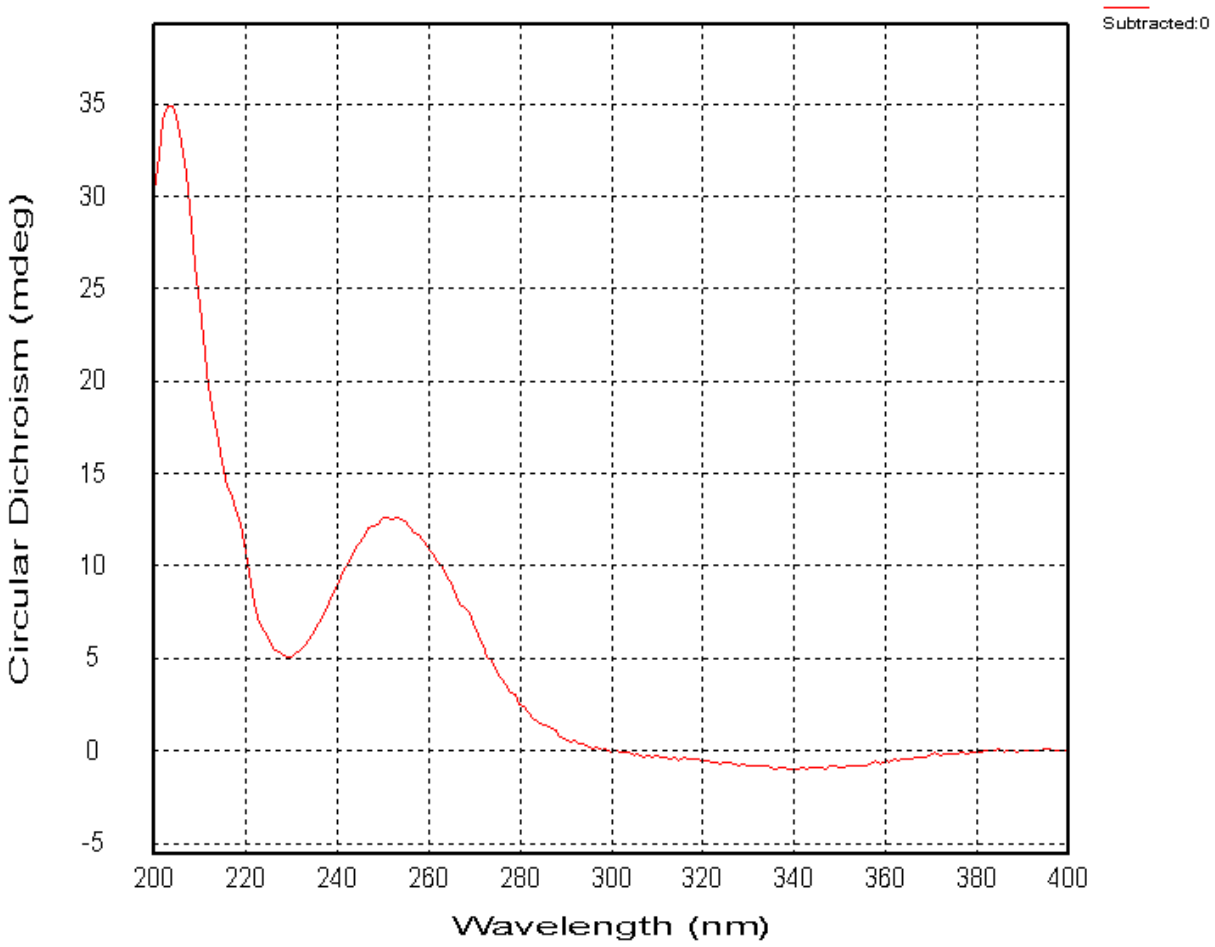

Fig. S88. Experimental ECD of **9**.

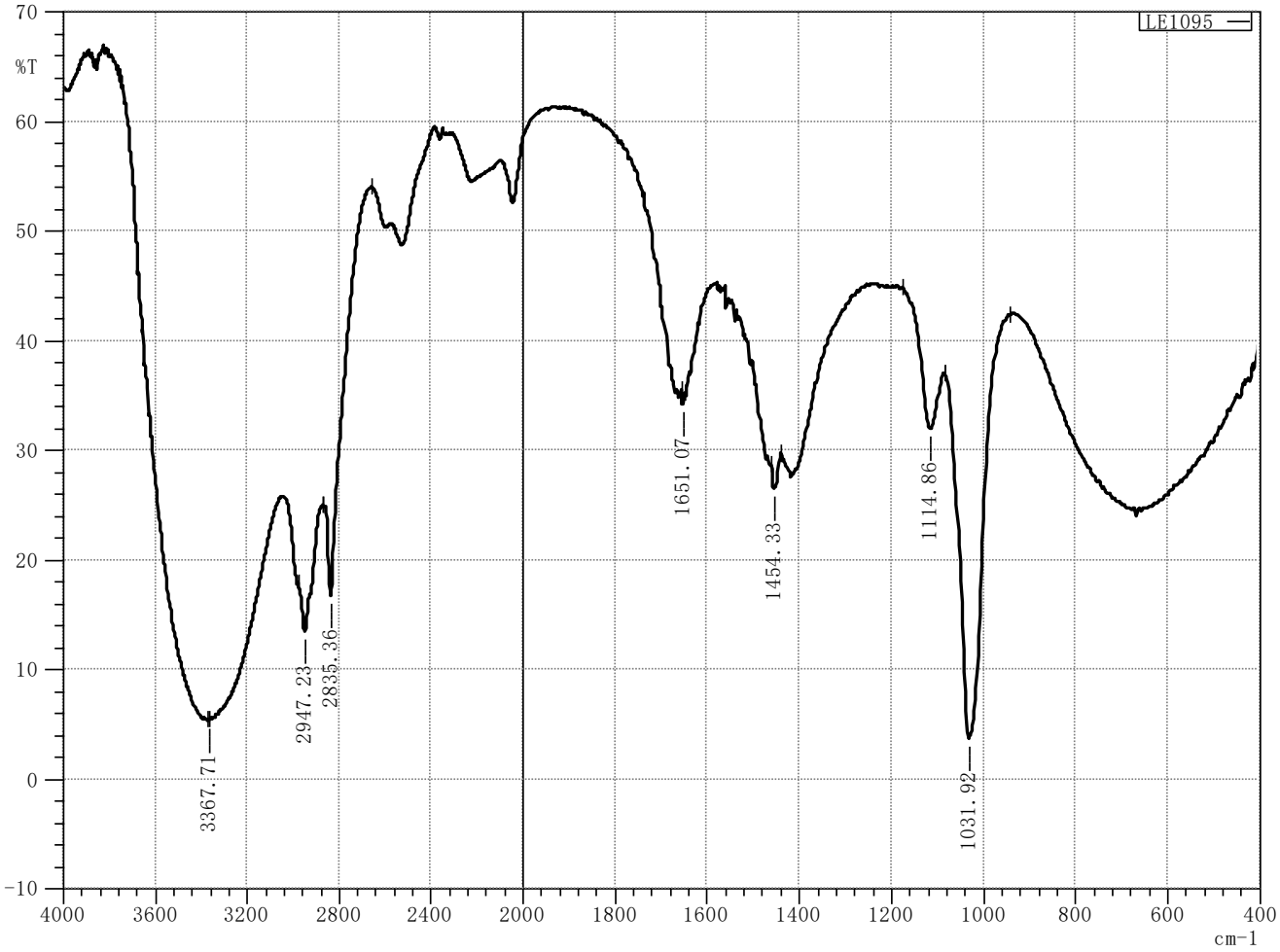

Fig. S89. IR of **9**.

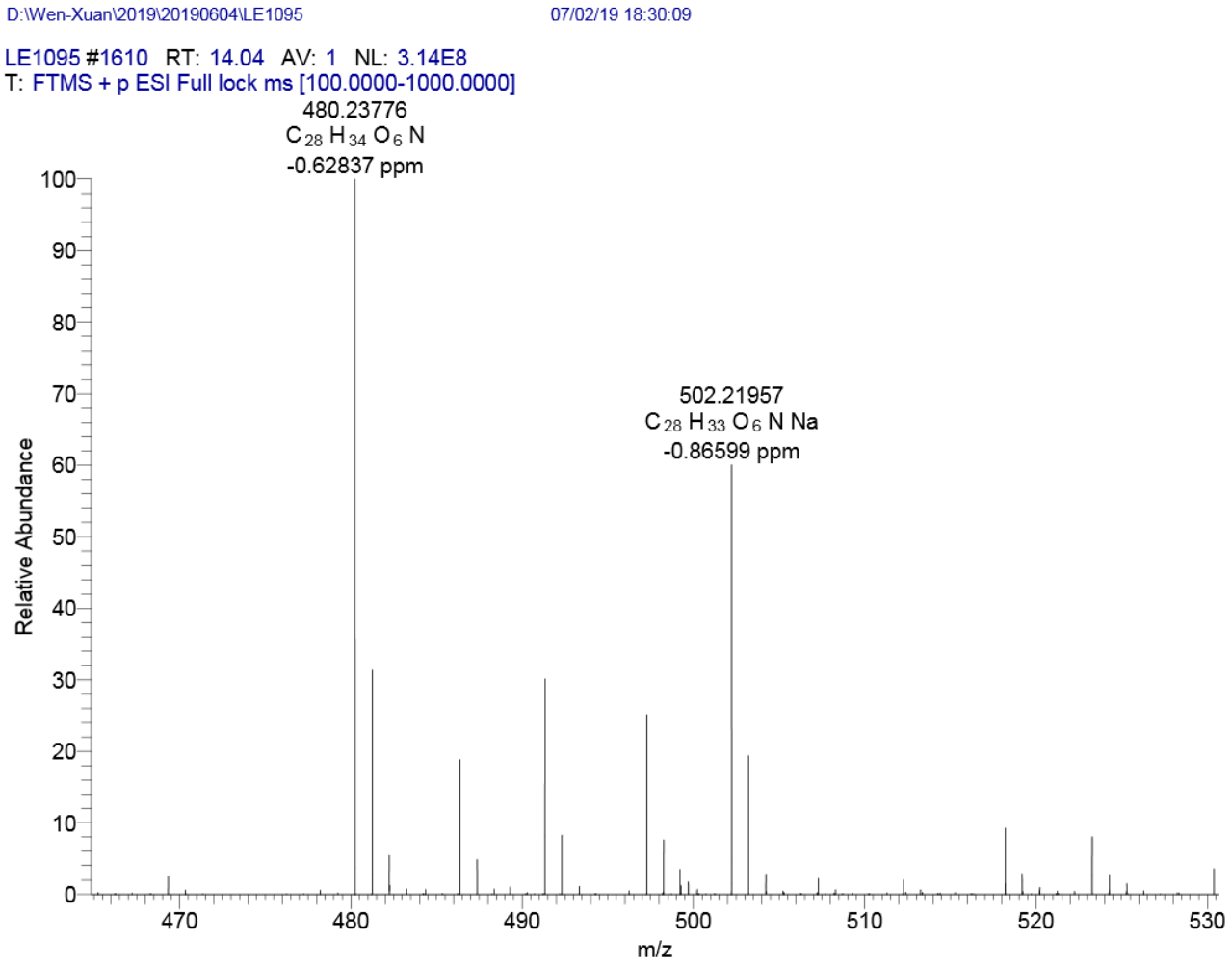

Fig. S90. HRESIMS of **9**.

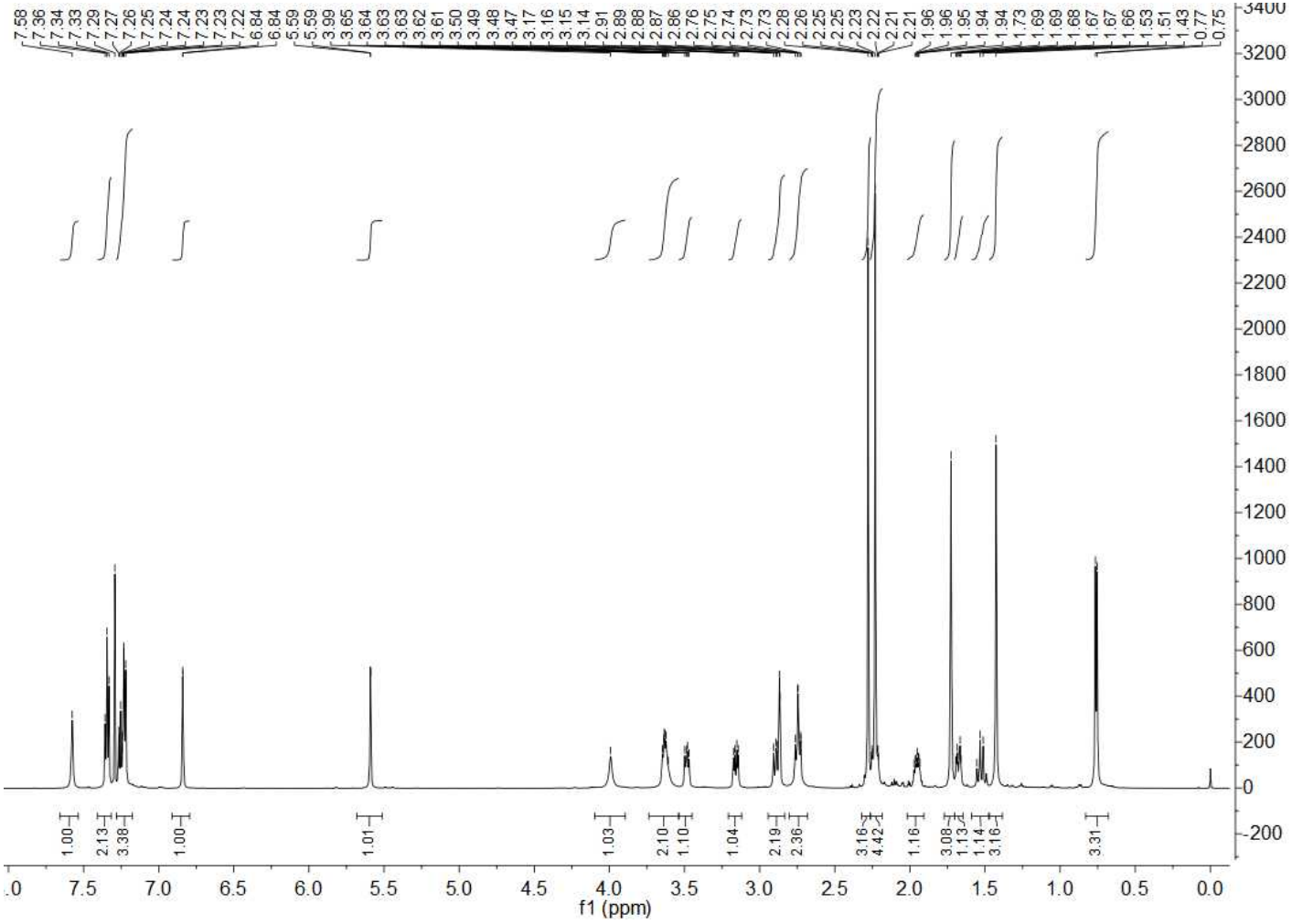

Fig. S91. ^{1}H NMR of **10** ($CDCl_3$, 600 MHz).

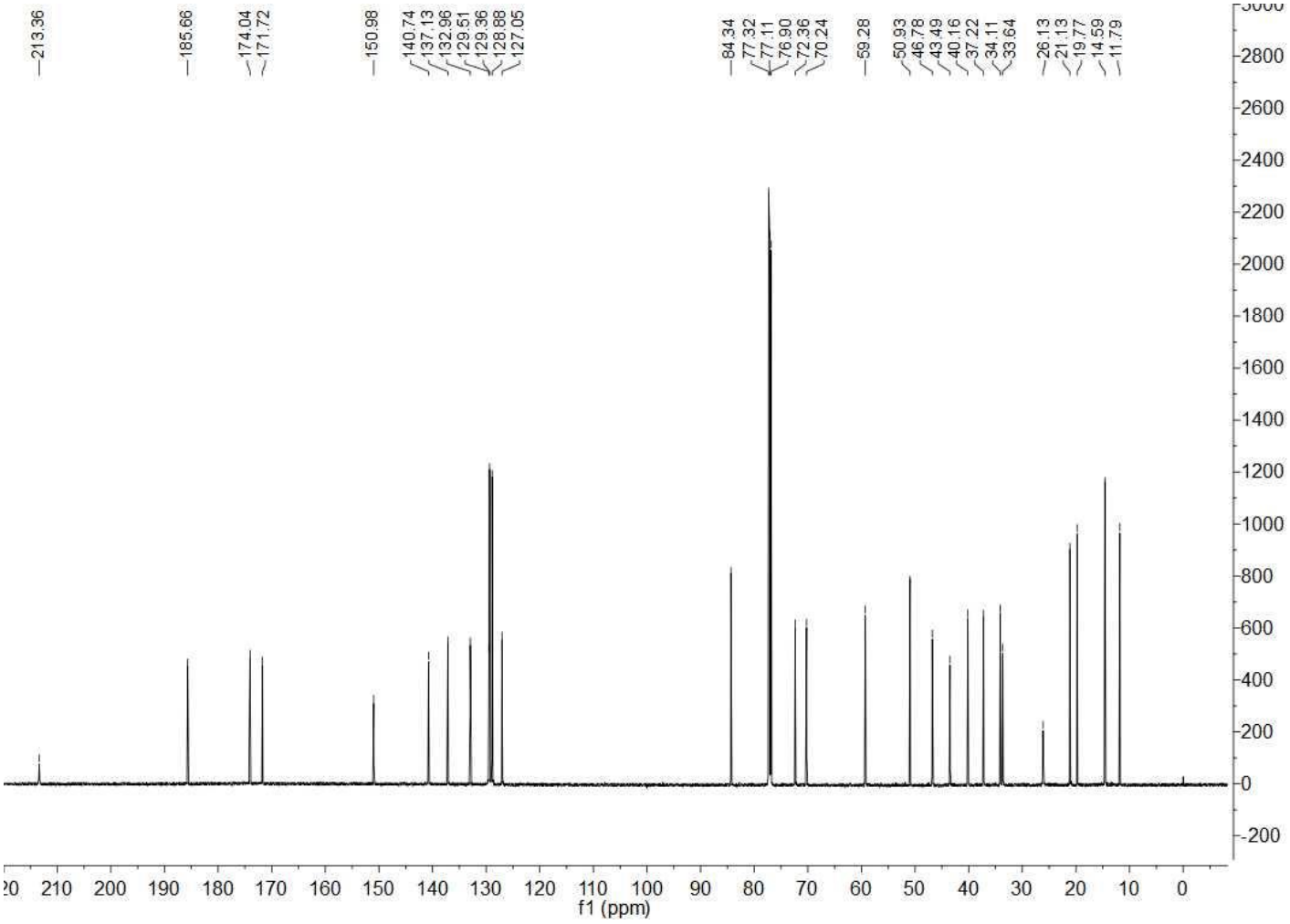

Fig. S92. ^{13}C NMR of **10** ($CDCl_3$, 150 MHz).

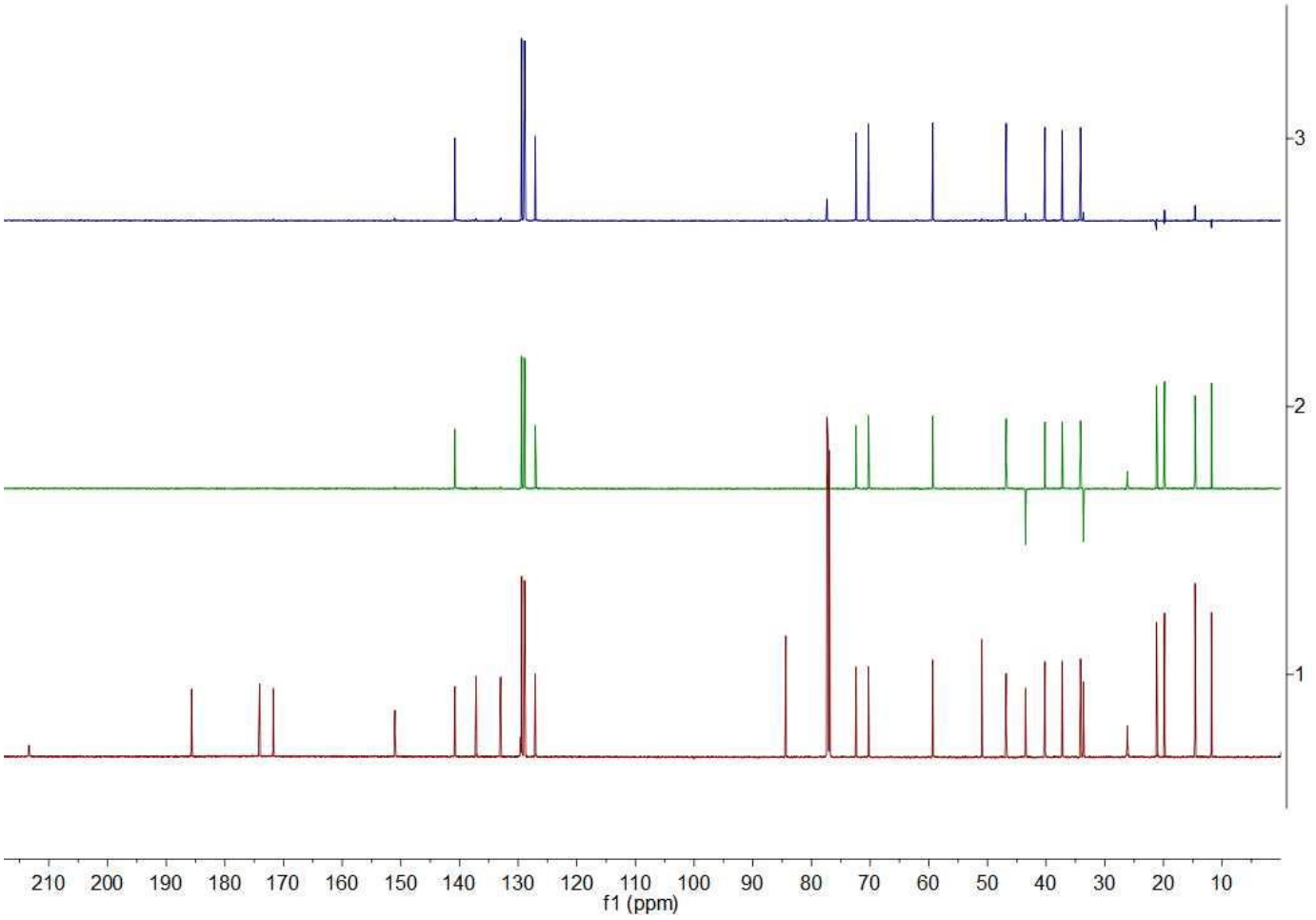

Fig. S93. DEPT of **10**.

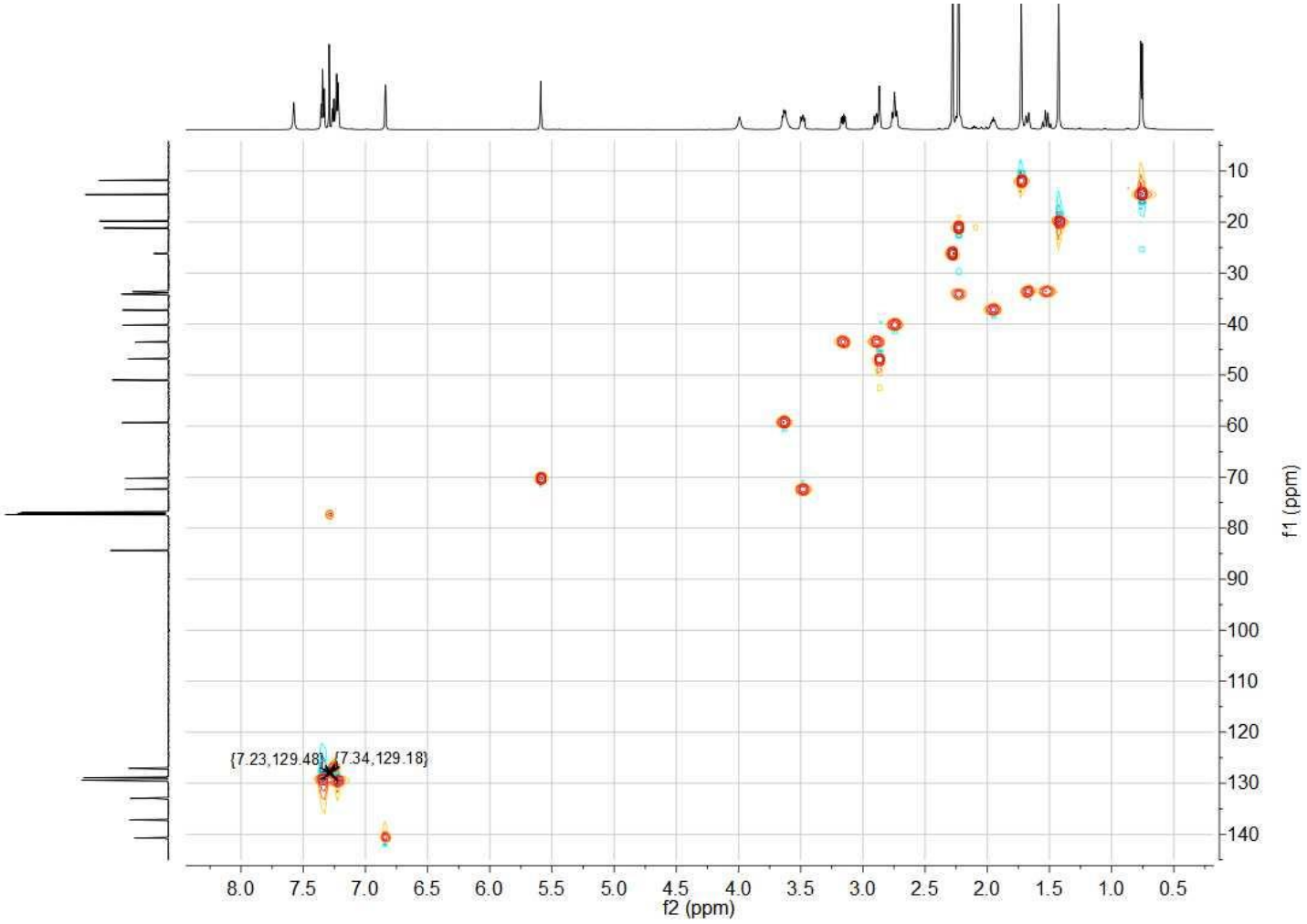

Fig. S94. HSQC of **10**.

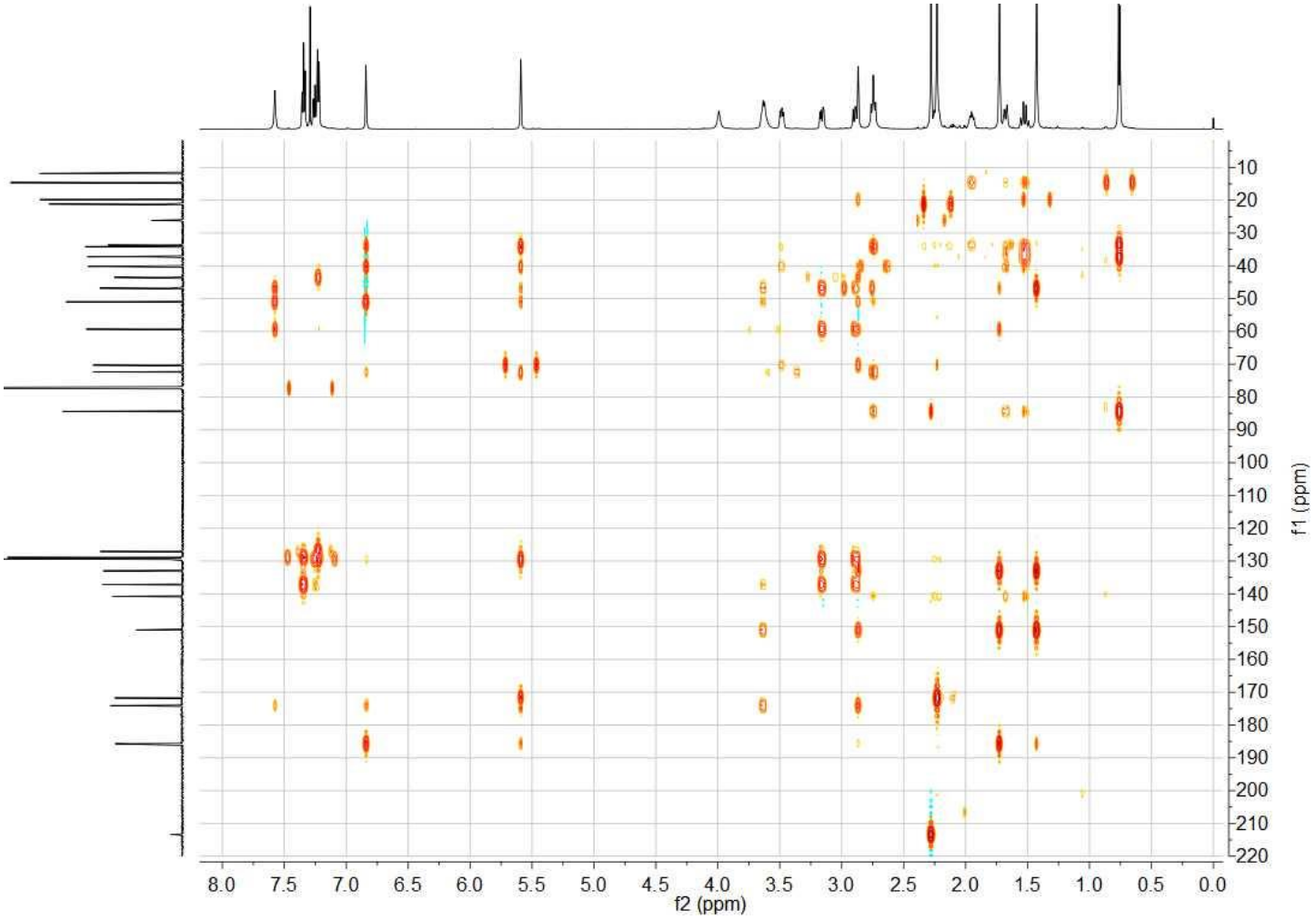

Fig. S95. HMBC of **10**.

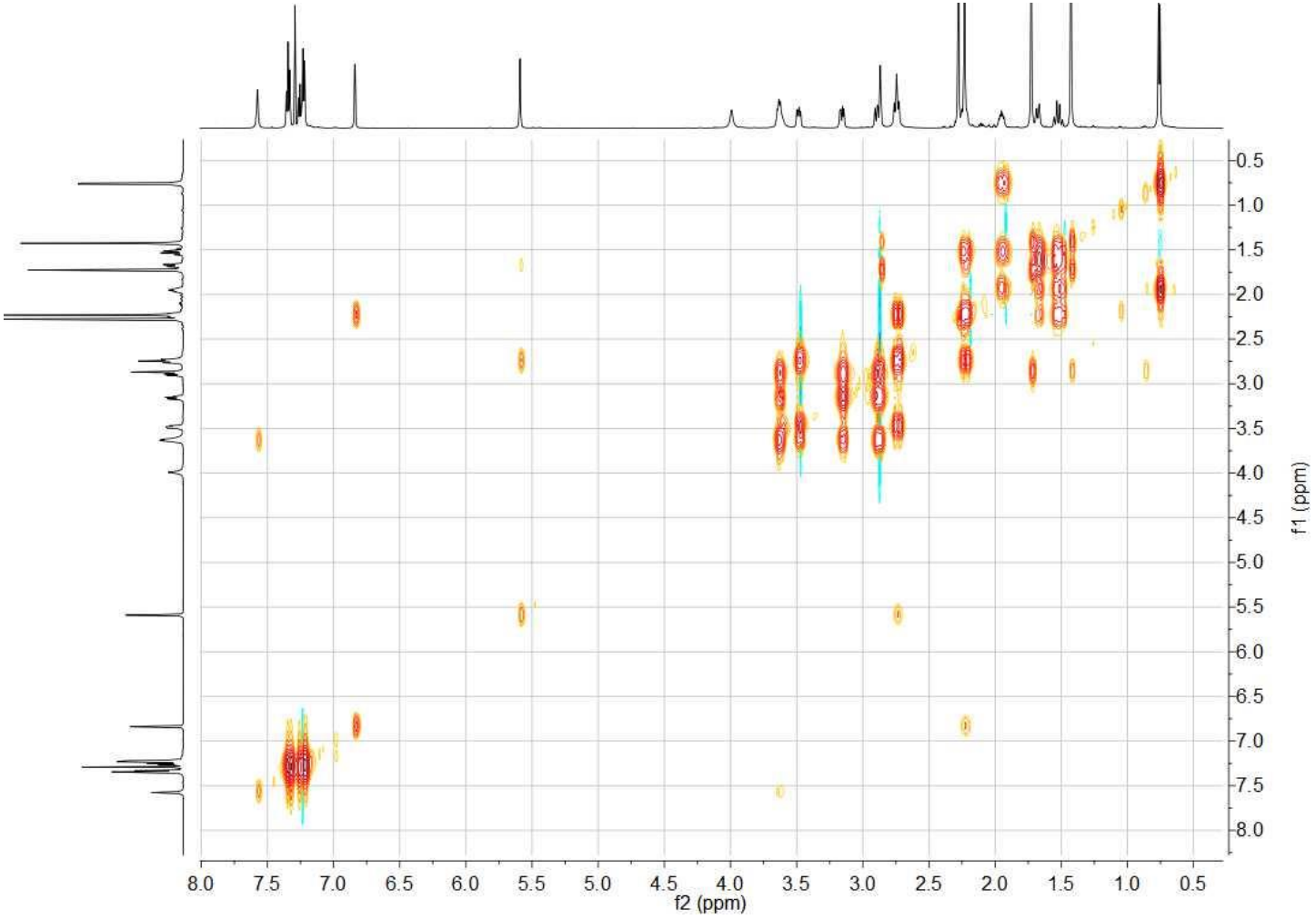

Fig. S96. ^{1}H-^{1}H COSY of **10**.

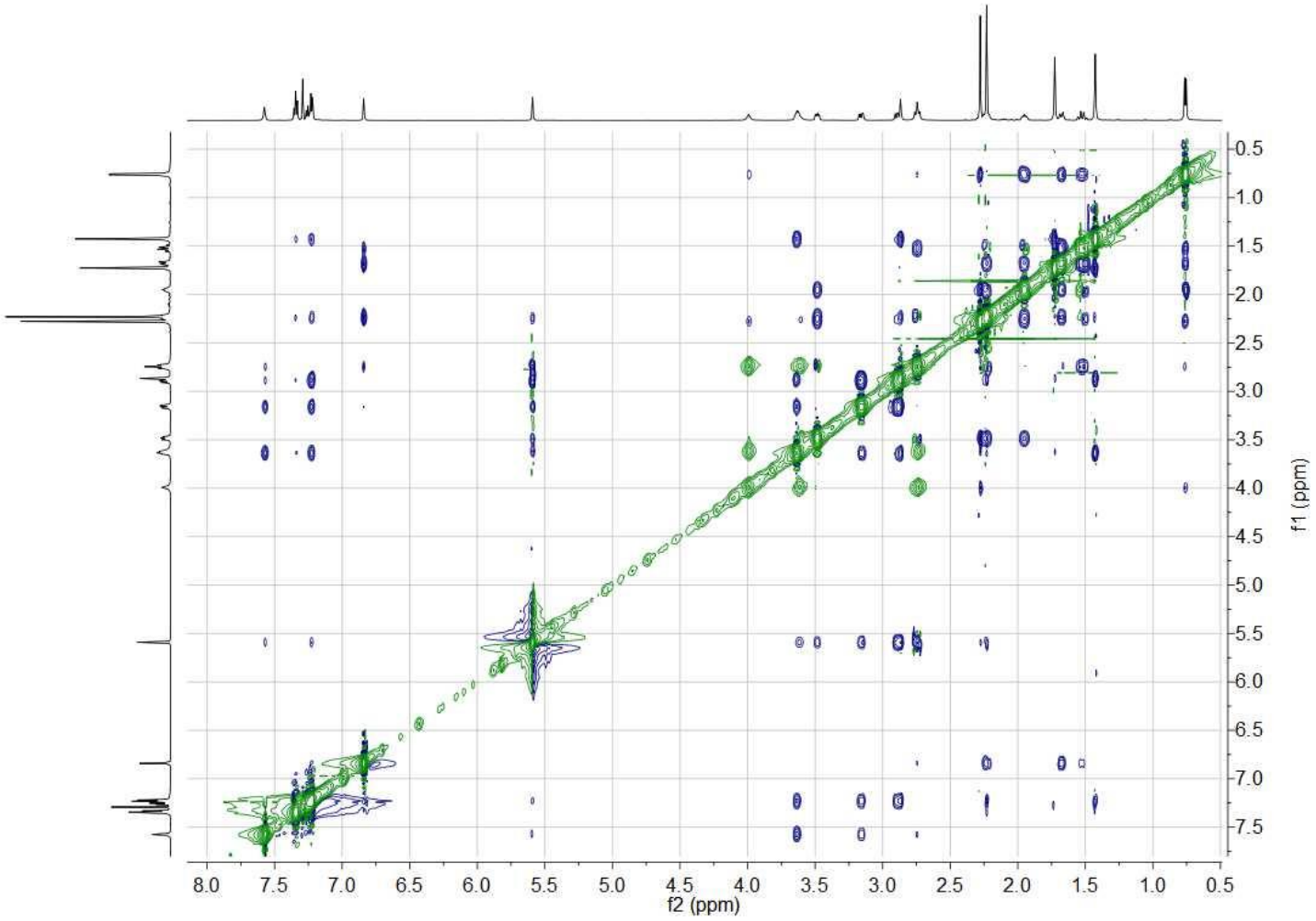

Fig. S97. ROESY of **10**.

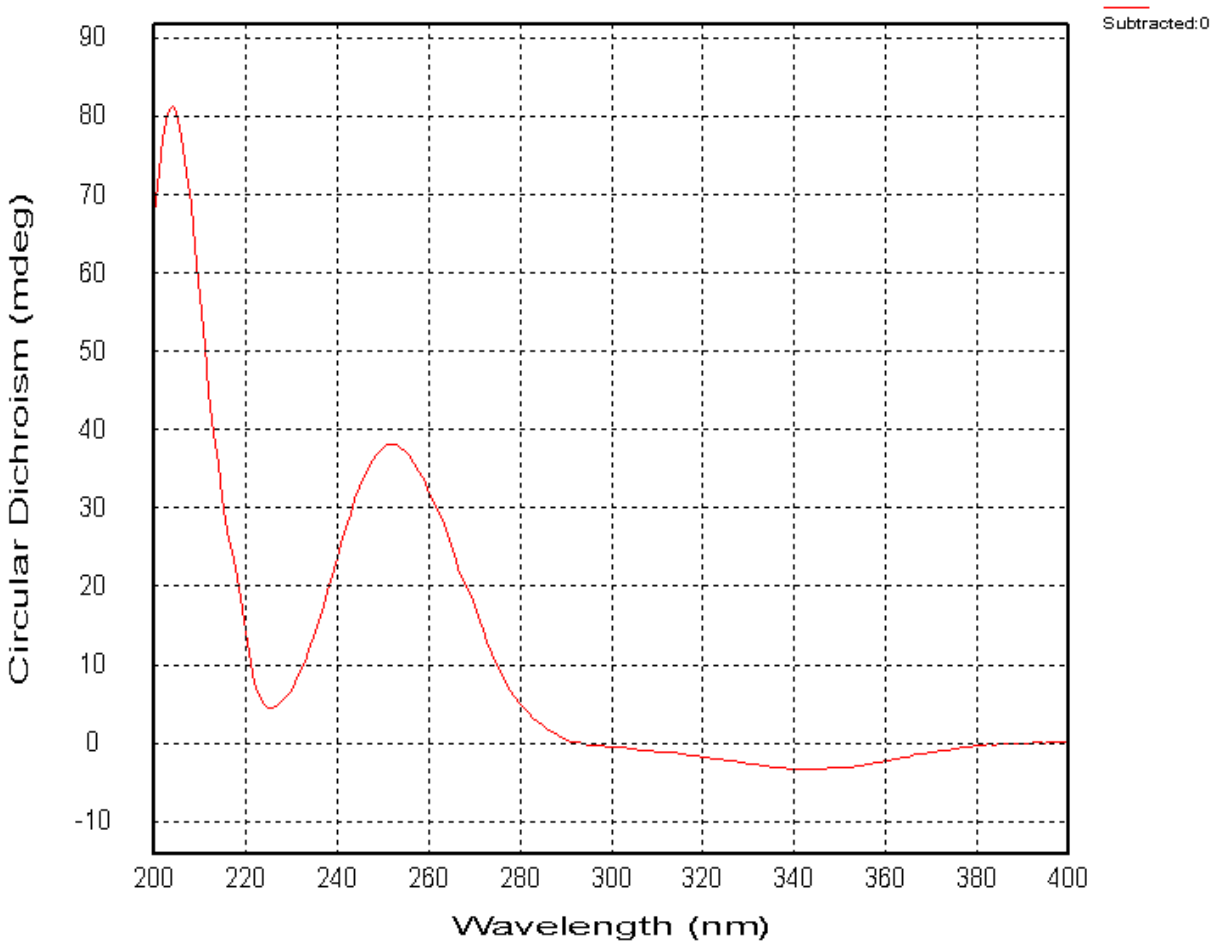

Fig. S98. Experimental ECD of **10**.

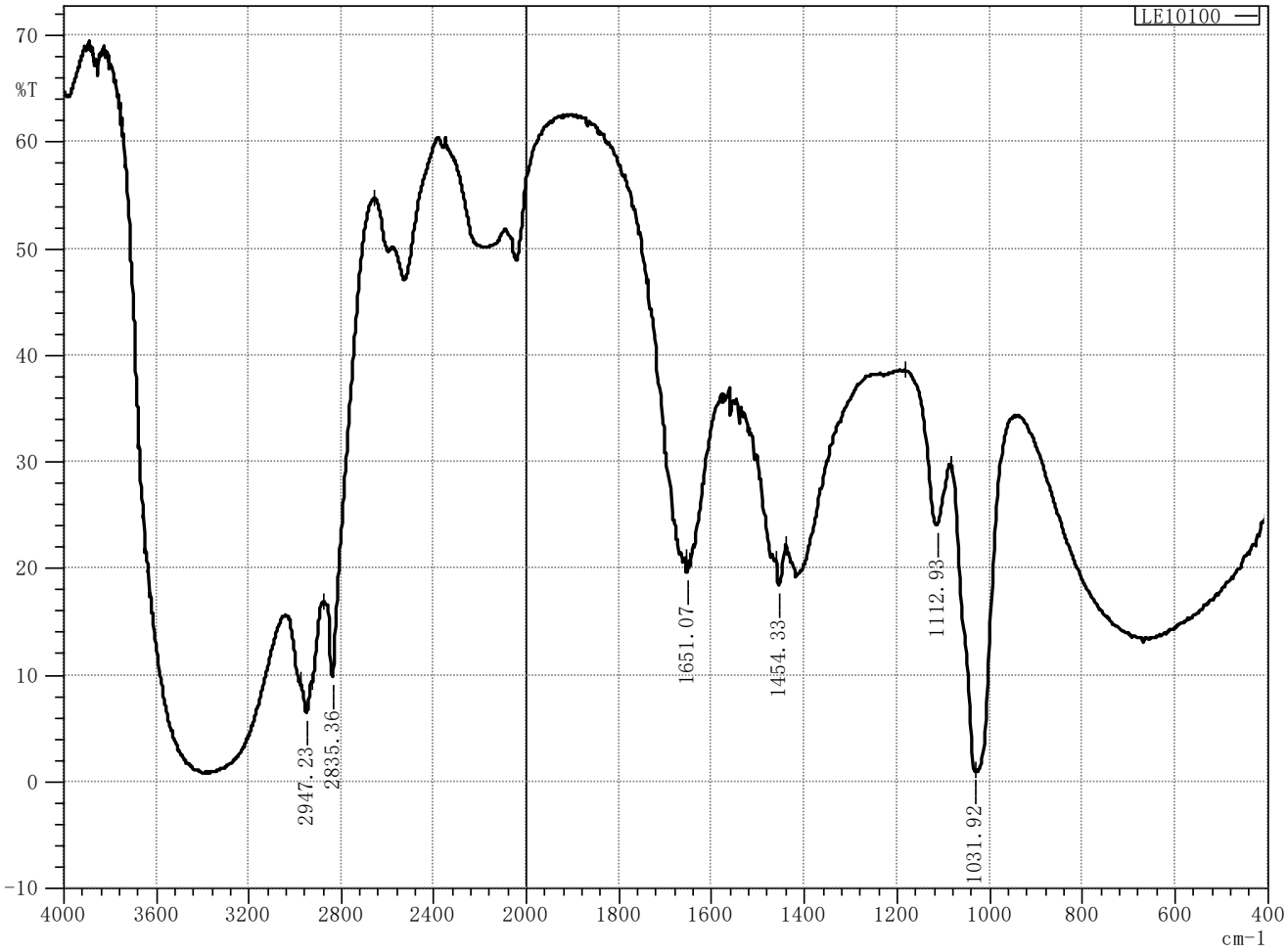

Fig. S99. IR of **10**.

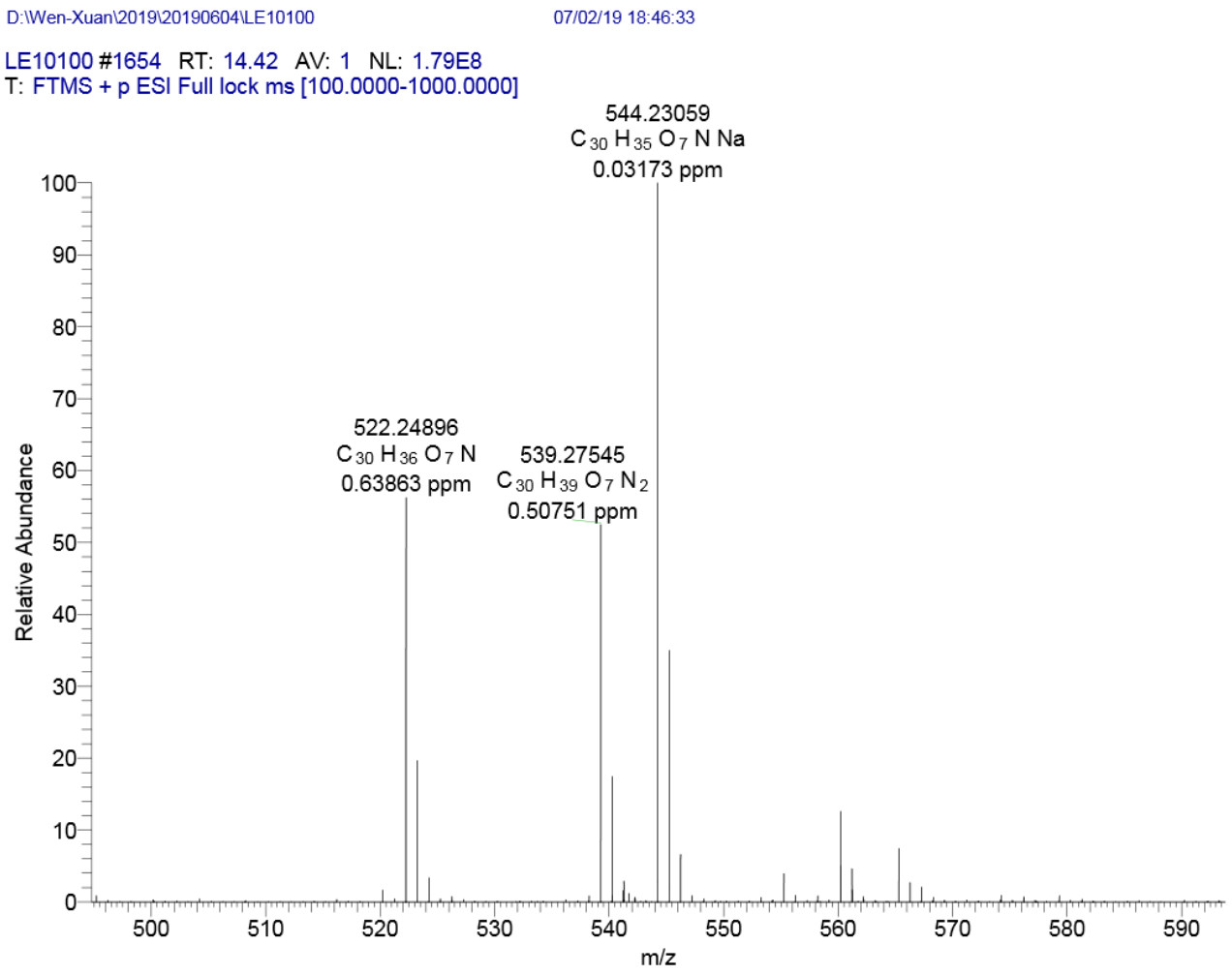

Fig. S100. HRESIMS of **10**.

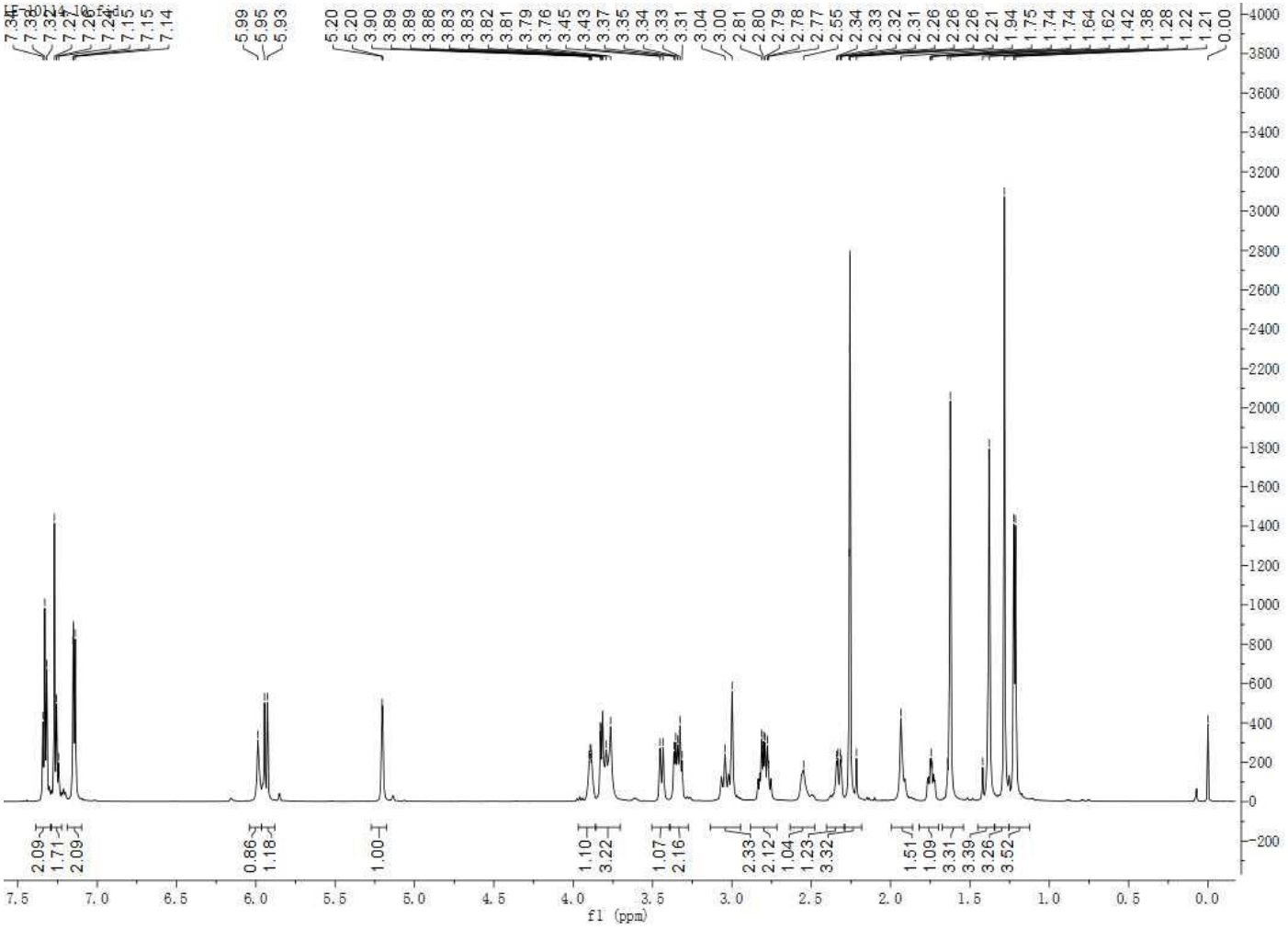

Fig. S101. ^{1}H NMR of **11** ($CDCl_3$, 600 MHz).

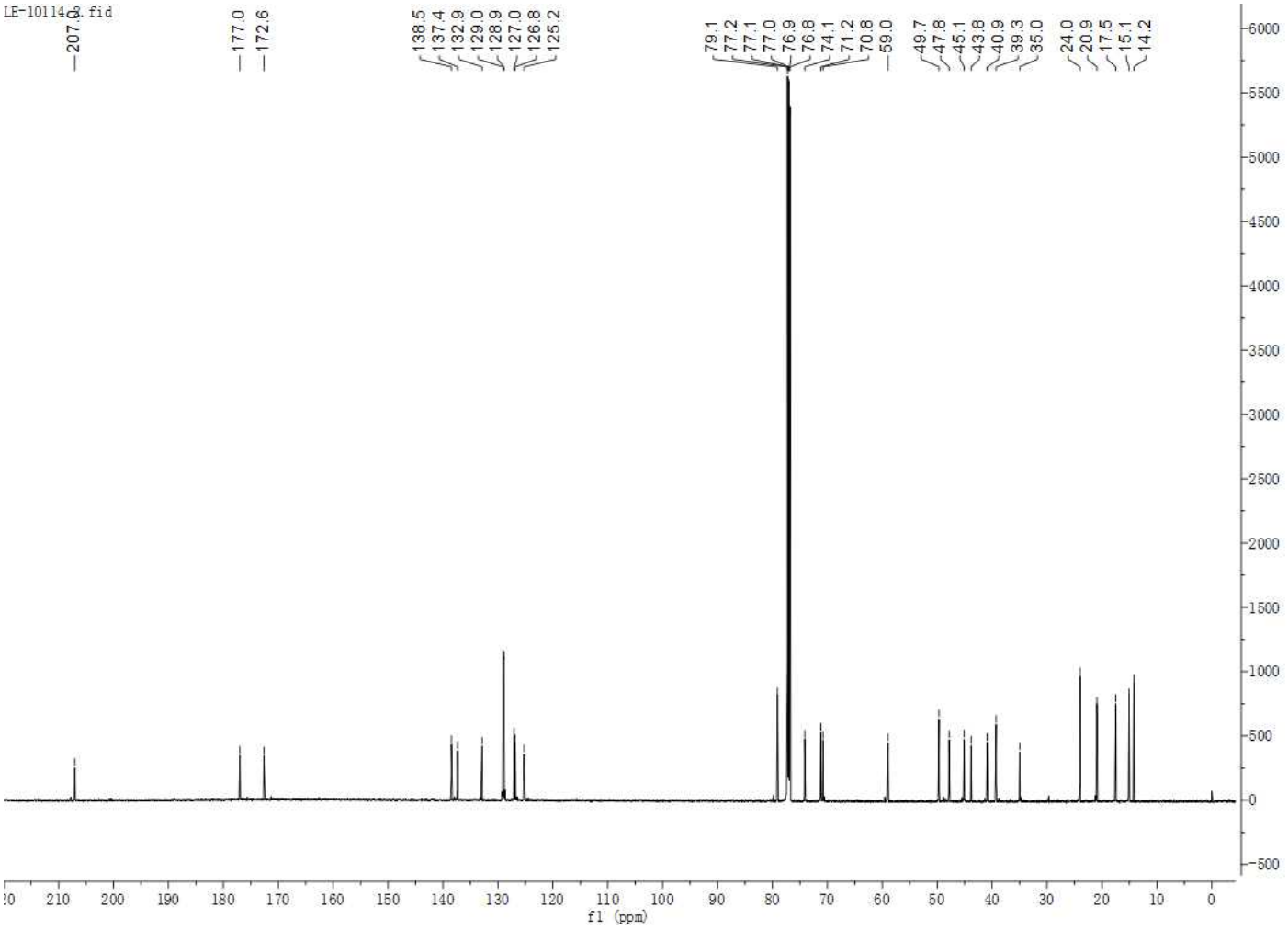

Fig. S102. ^{13}C NMR of **11** ($CDCl_3$, 150 MHz).

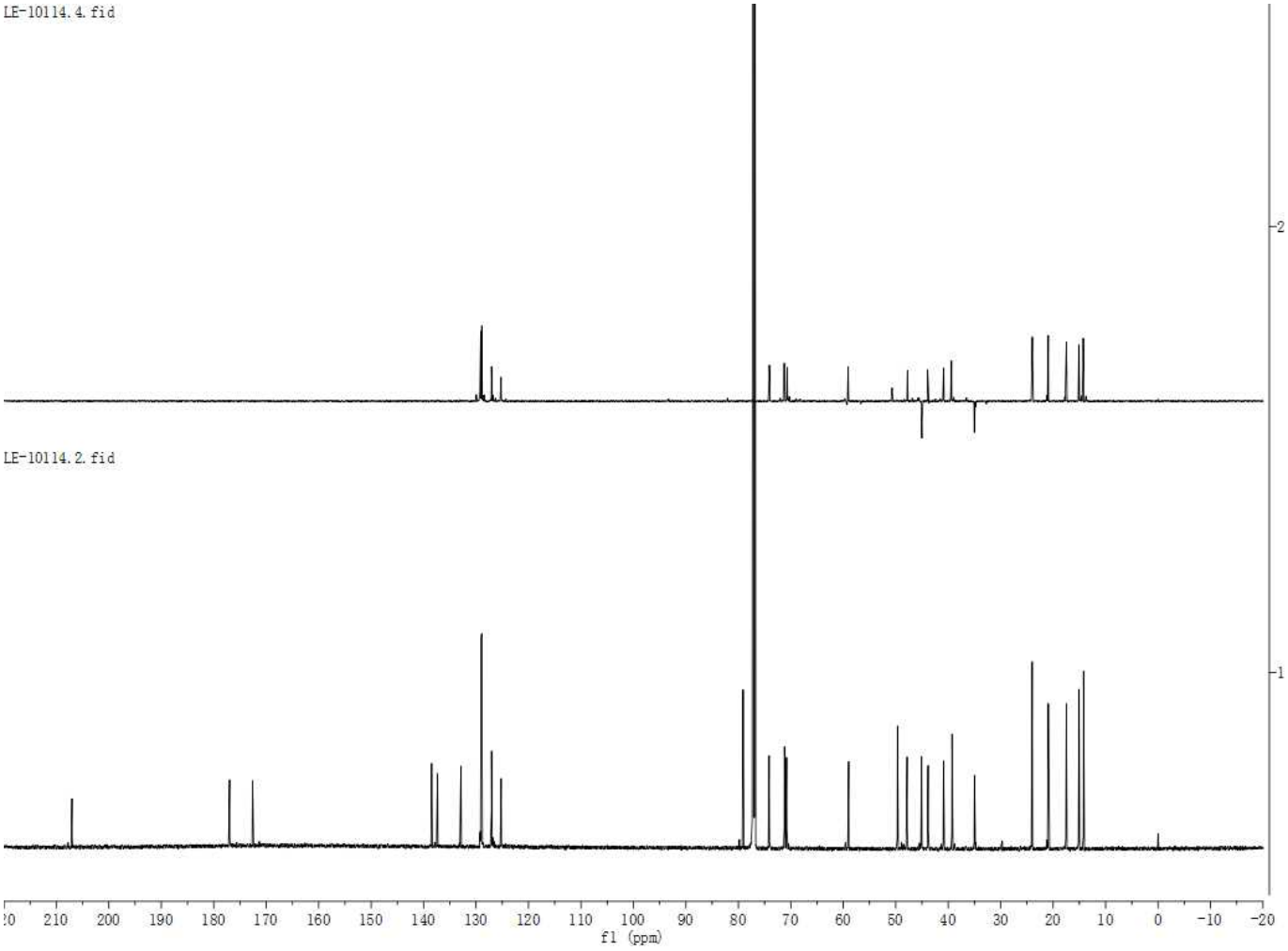

Fig. S103. DEPT of **11**.

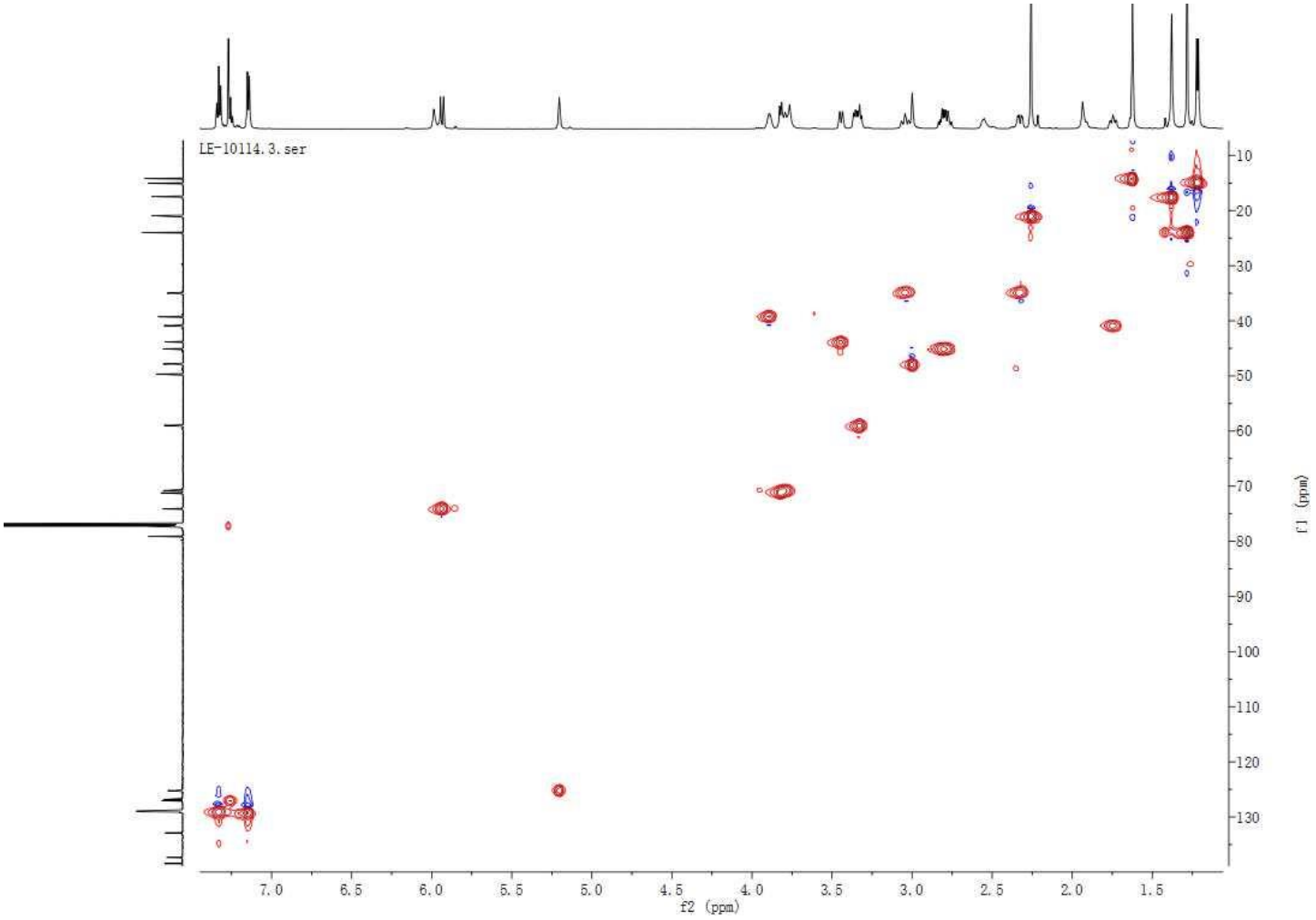

Fig. S104. HSQC of **11**.

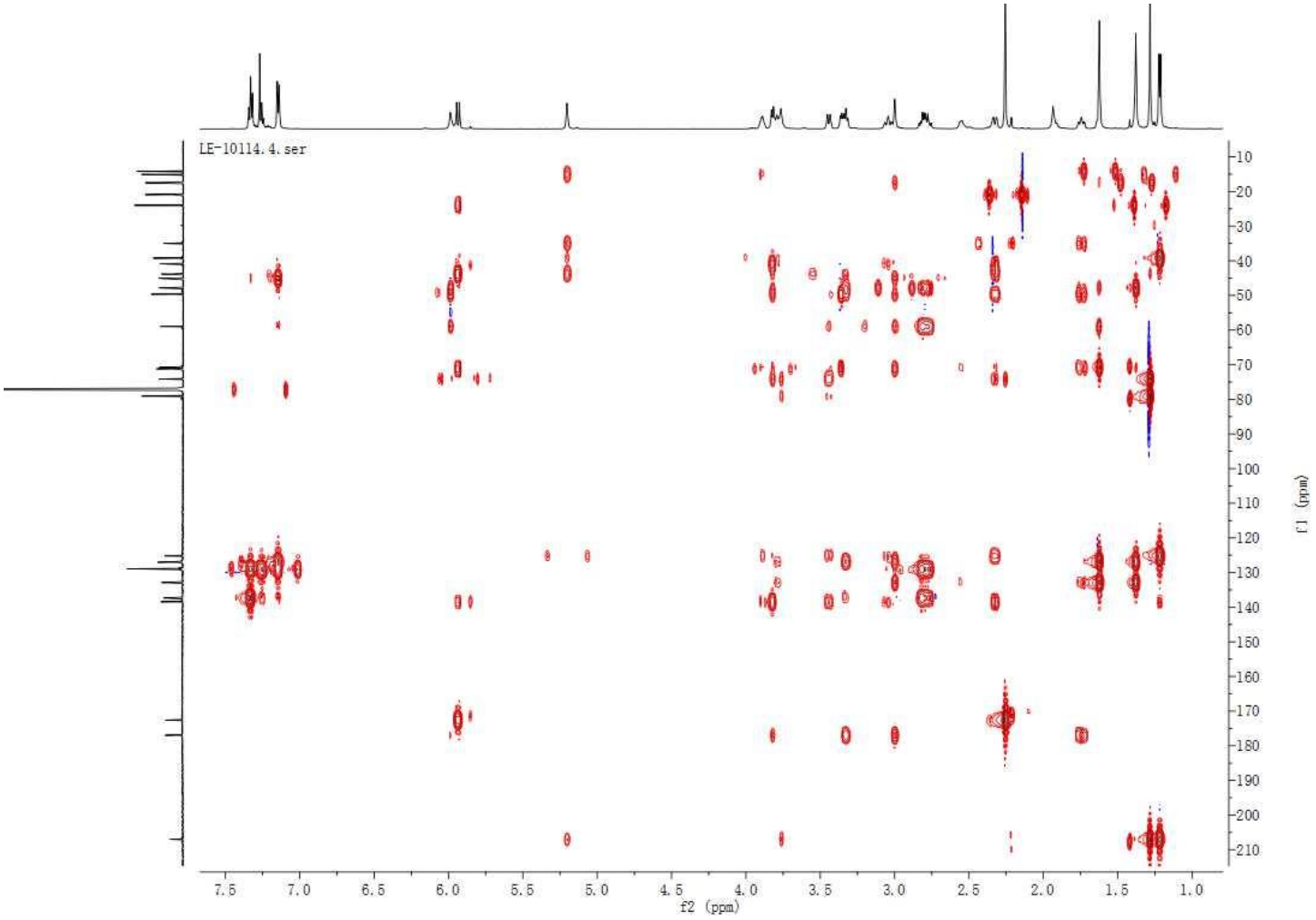

Fig. S105. HMBC of **11**.

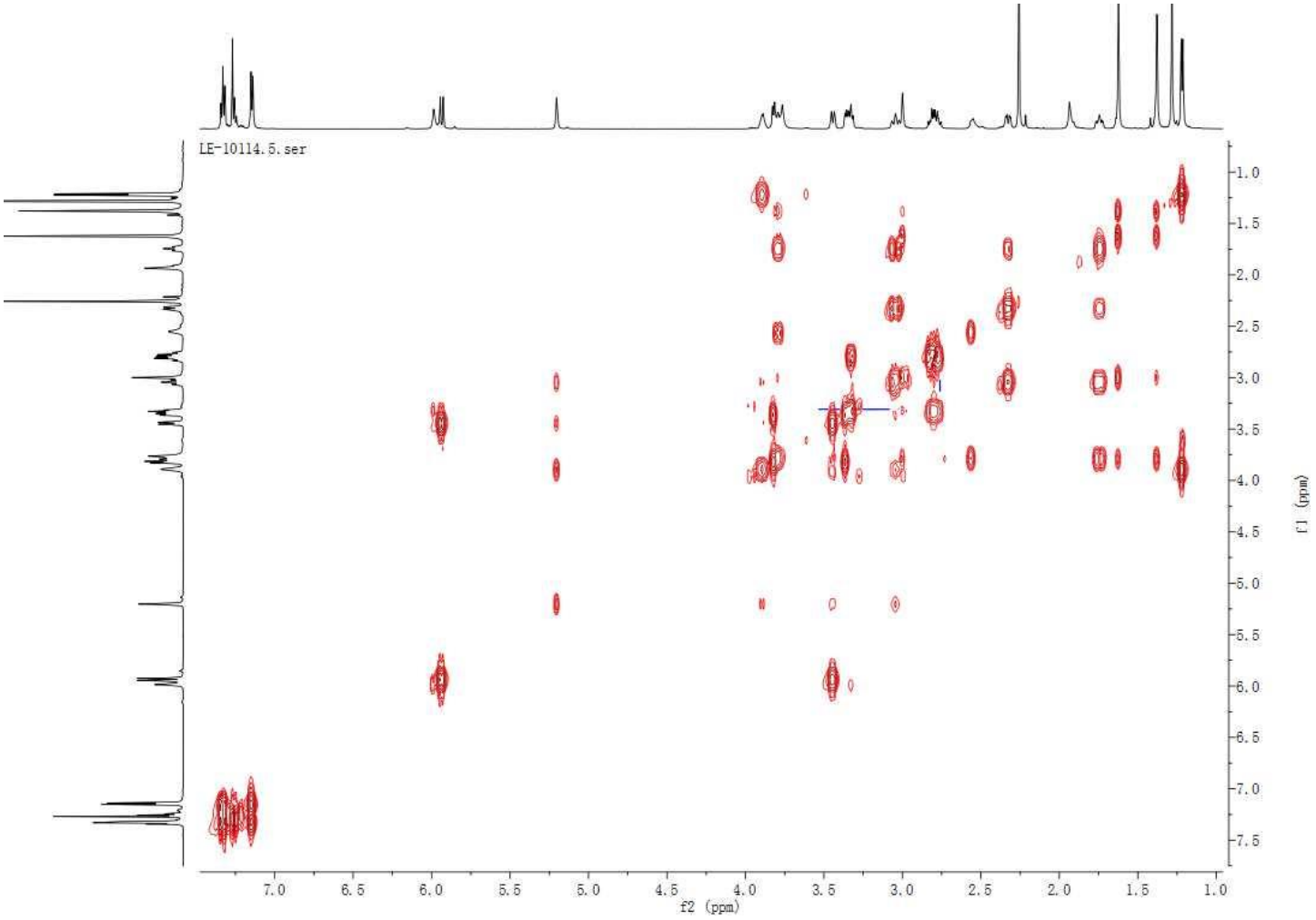

Fig. S106. ^{1}H-^{1}H COSY of **11**.

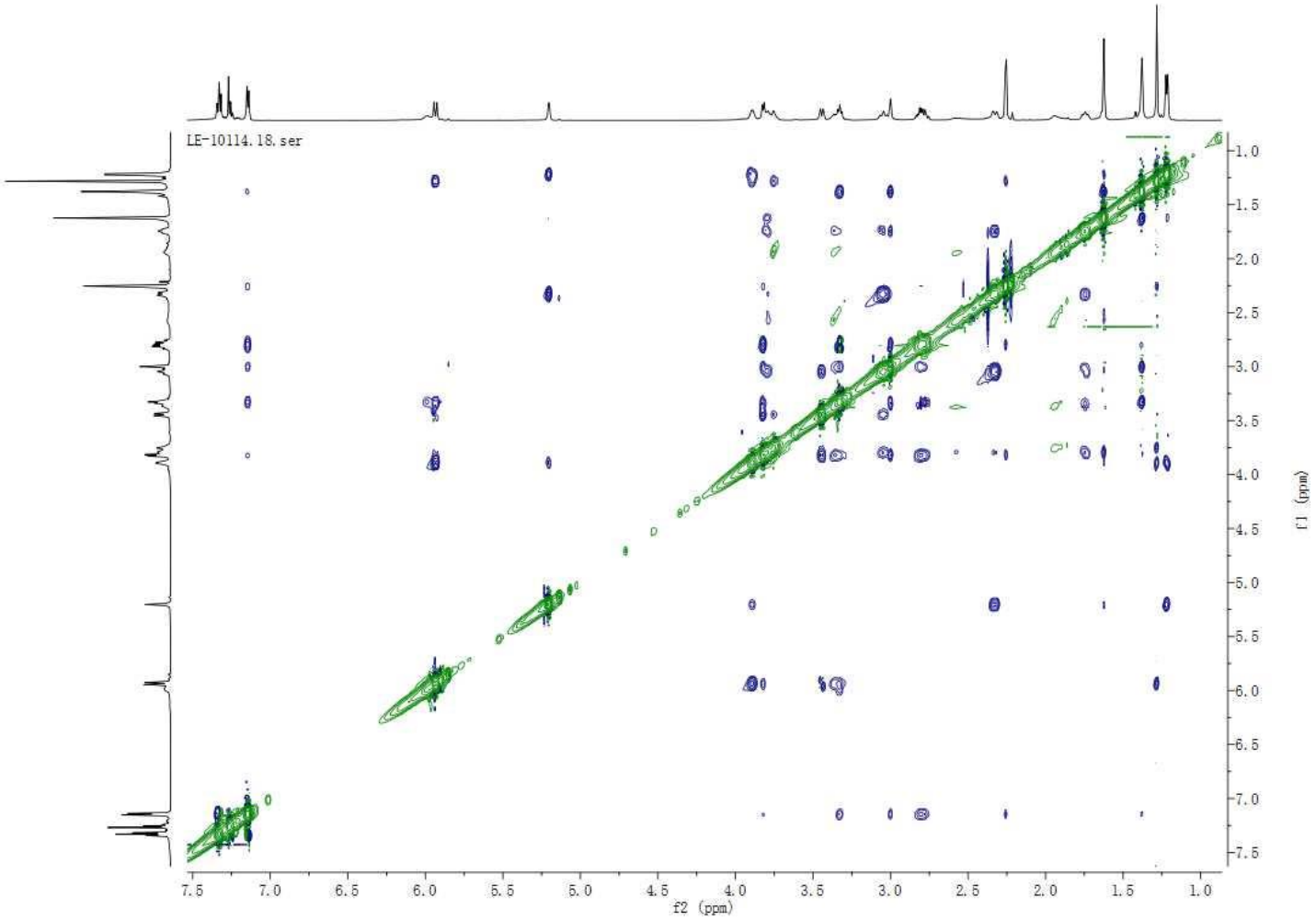

Fig. S107. ROESY of **11**.

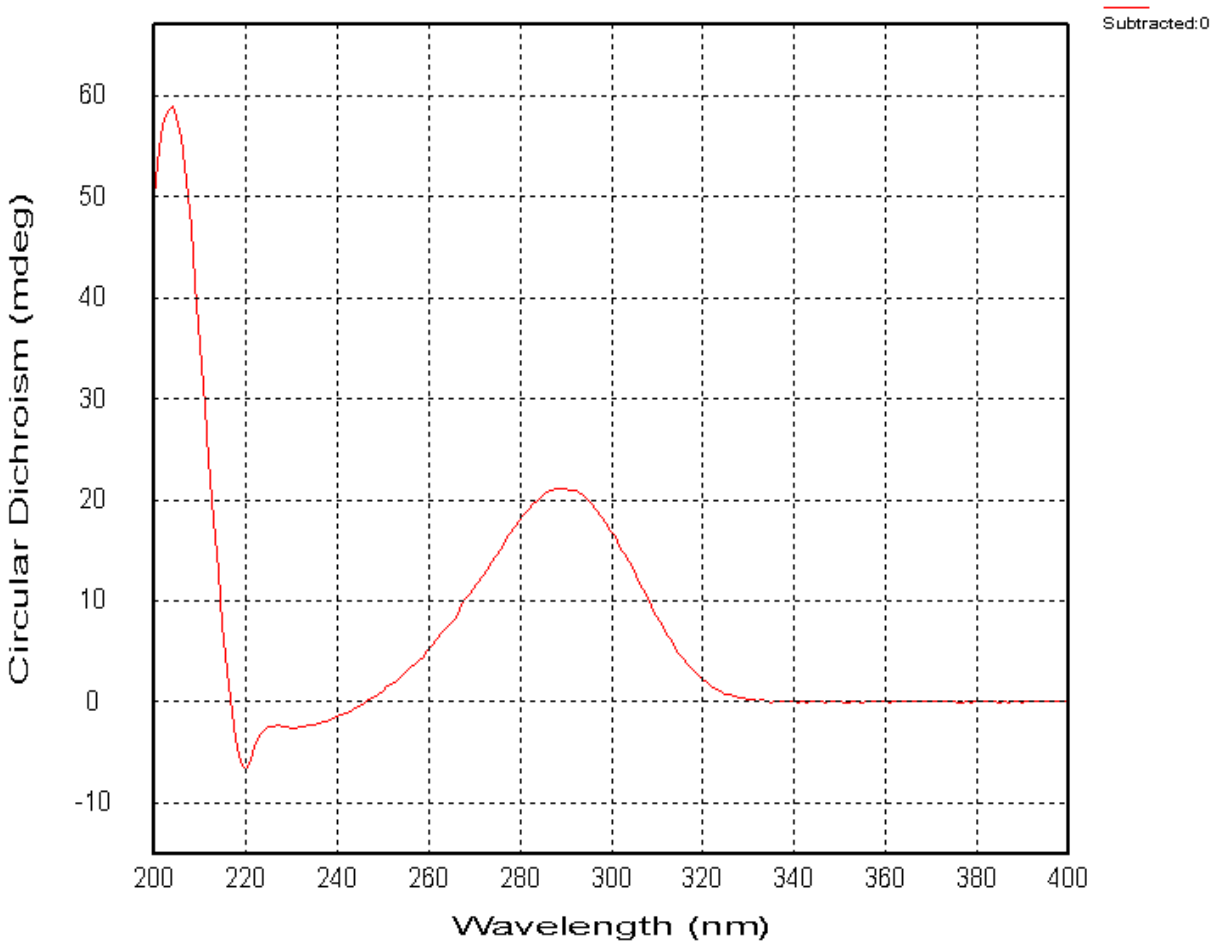

Fig. S108. Experimental ECD of **11**.

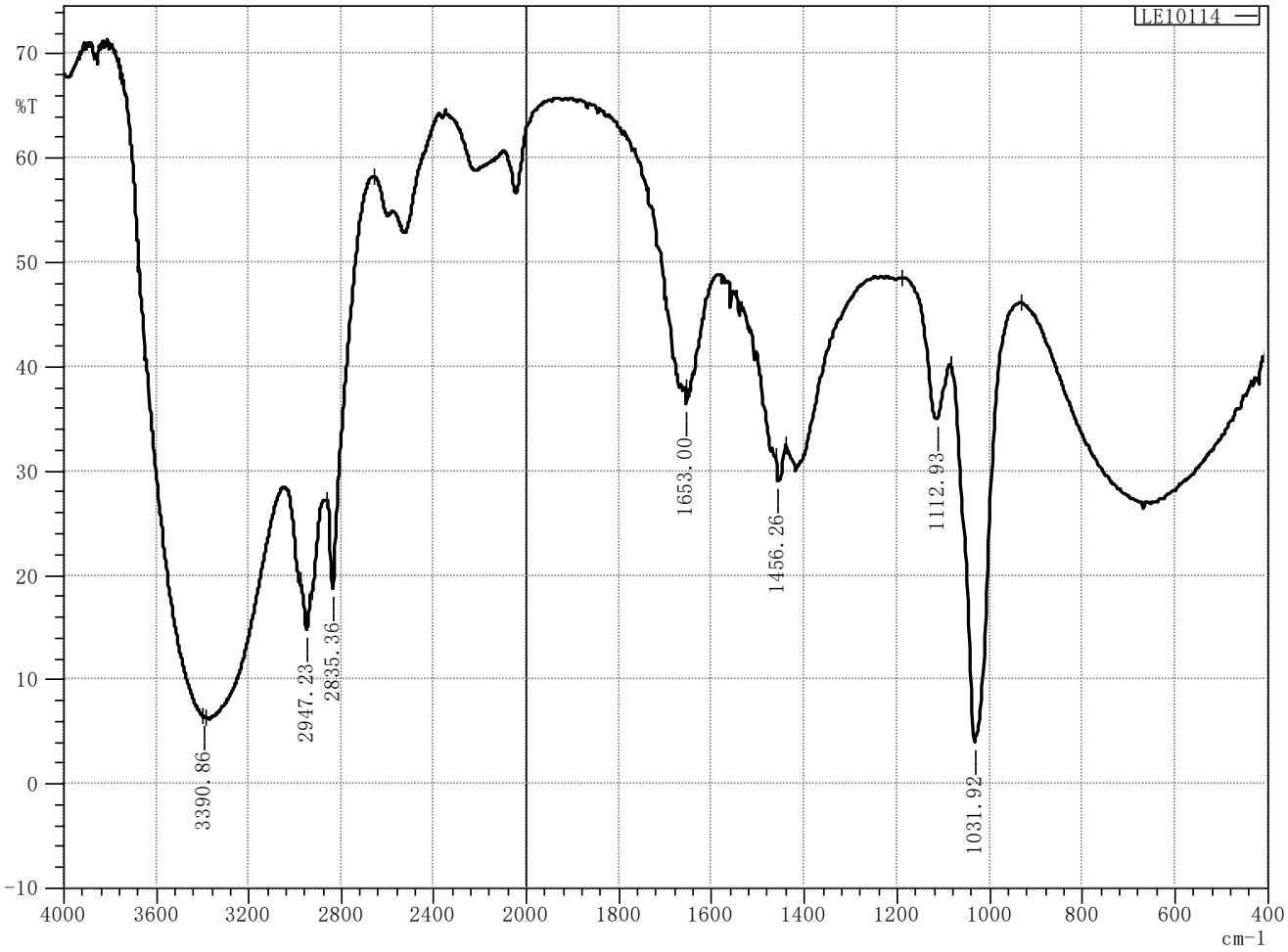

Fig. S109. IR of **11**.

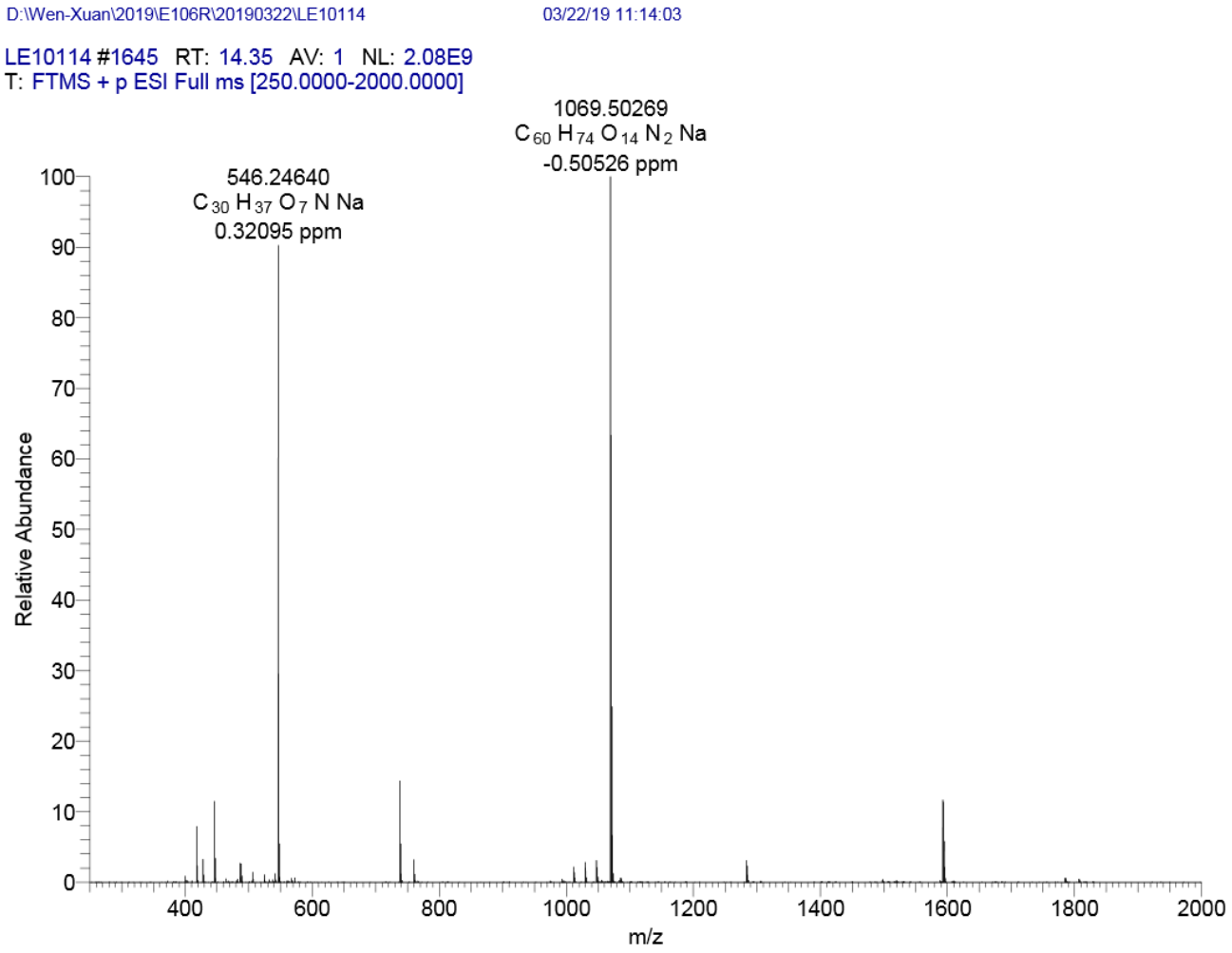

Fig. S110. HRESIMS of **11**.