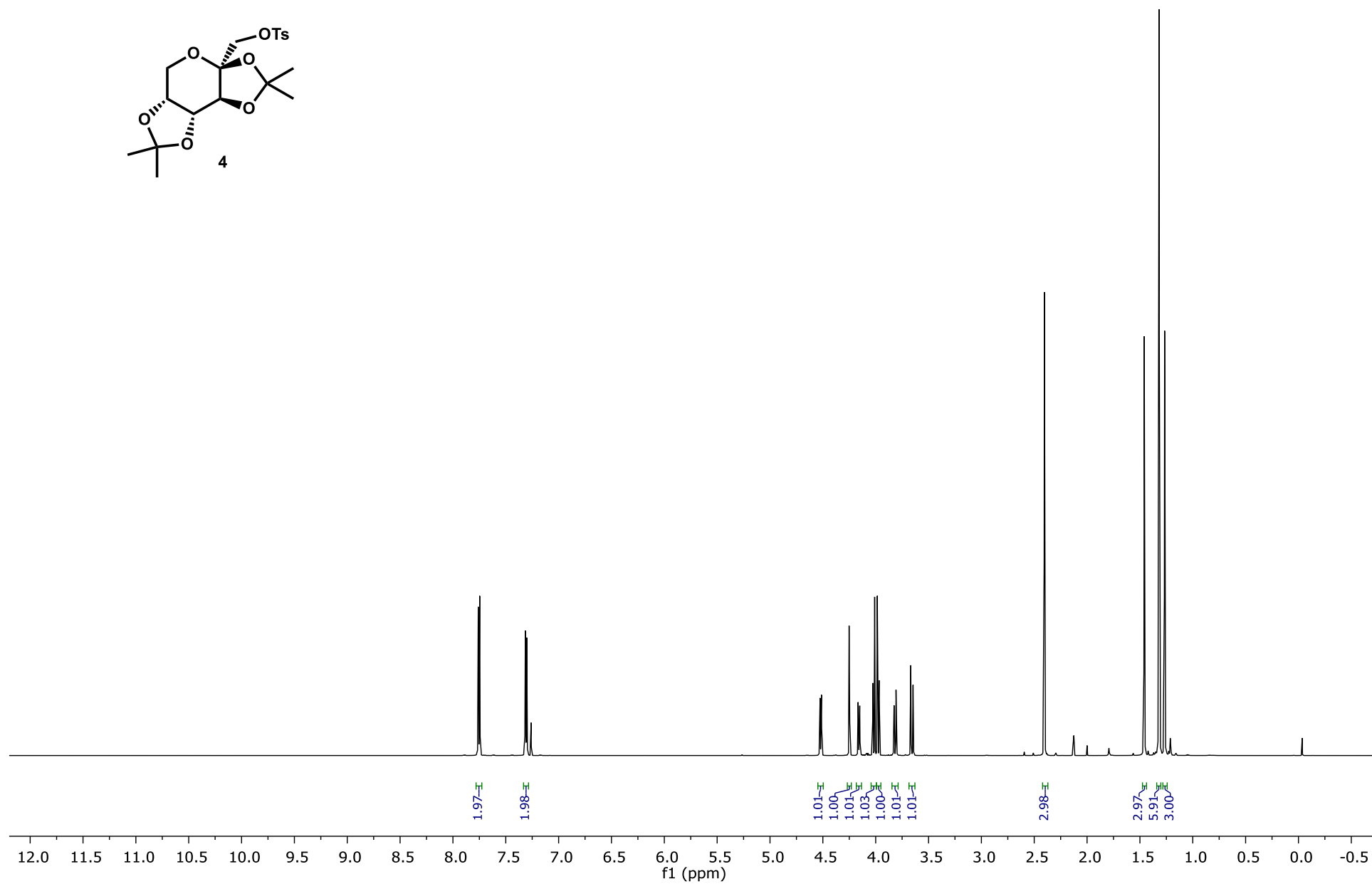
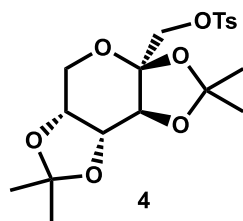


Carbohydrate-Small Molecule Hybrids as Lead Compounds Targeting IL-6 Signaling

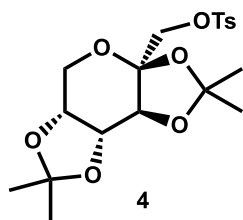
Daniel C. Schultz ¹, Li Pan ², Tiffany Wang ², Conner Booker ¹, Iram Hyder ¹, Laura Hanold ¹, Garret Rubin ¹, Yousong Ding ¹, Jiayuh Lin ², and Chenglong Li ^{1,*}

Supplementary Information:

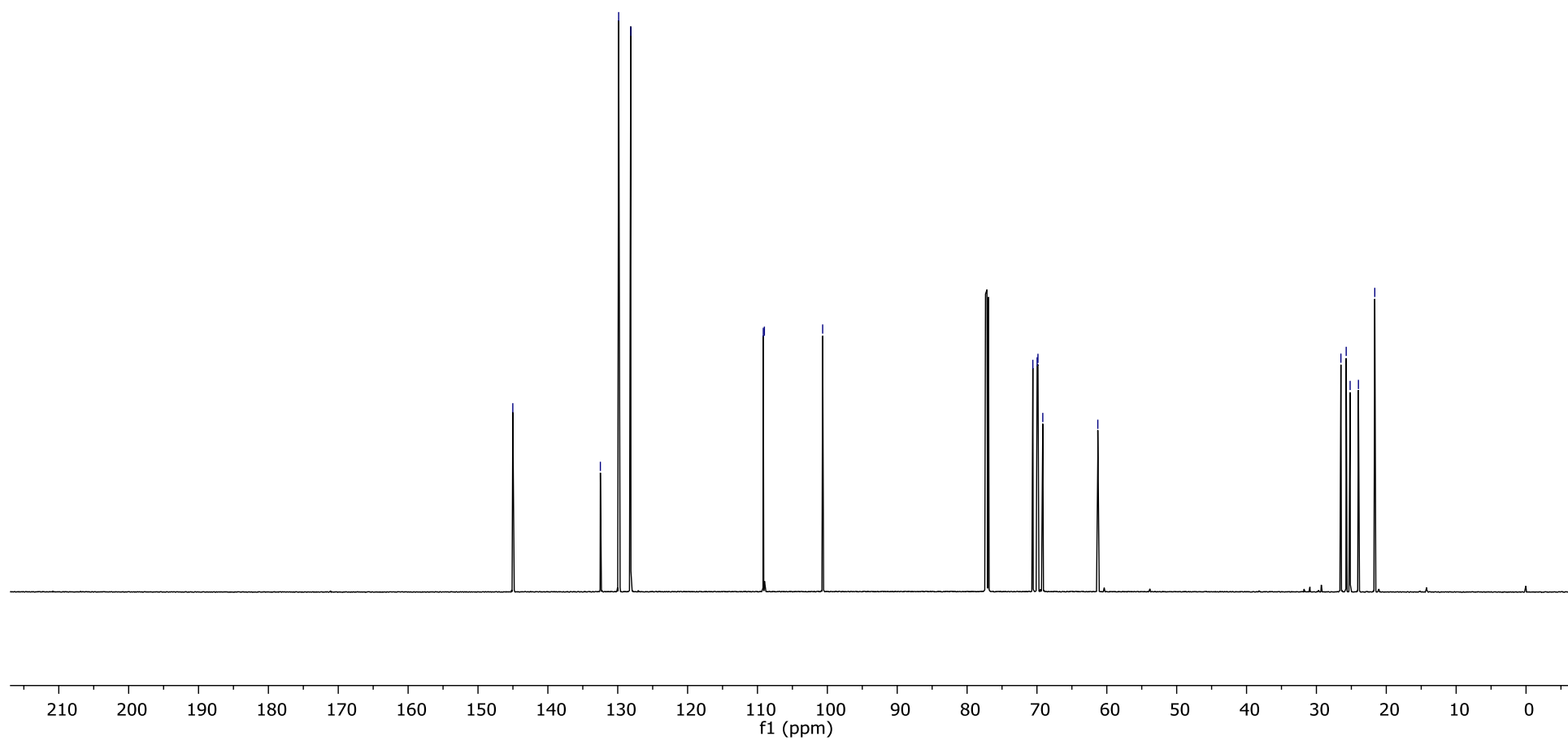
¹H, ¹³C, and 2D NMR Spectra



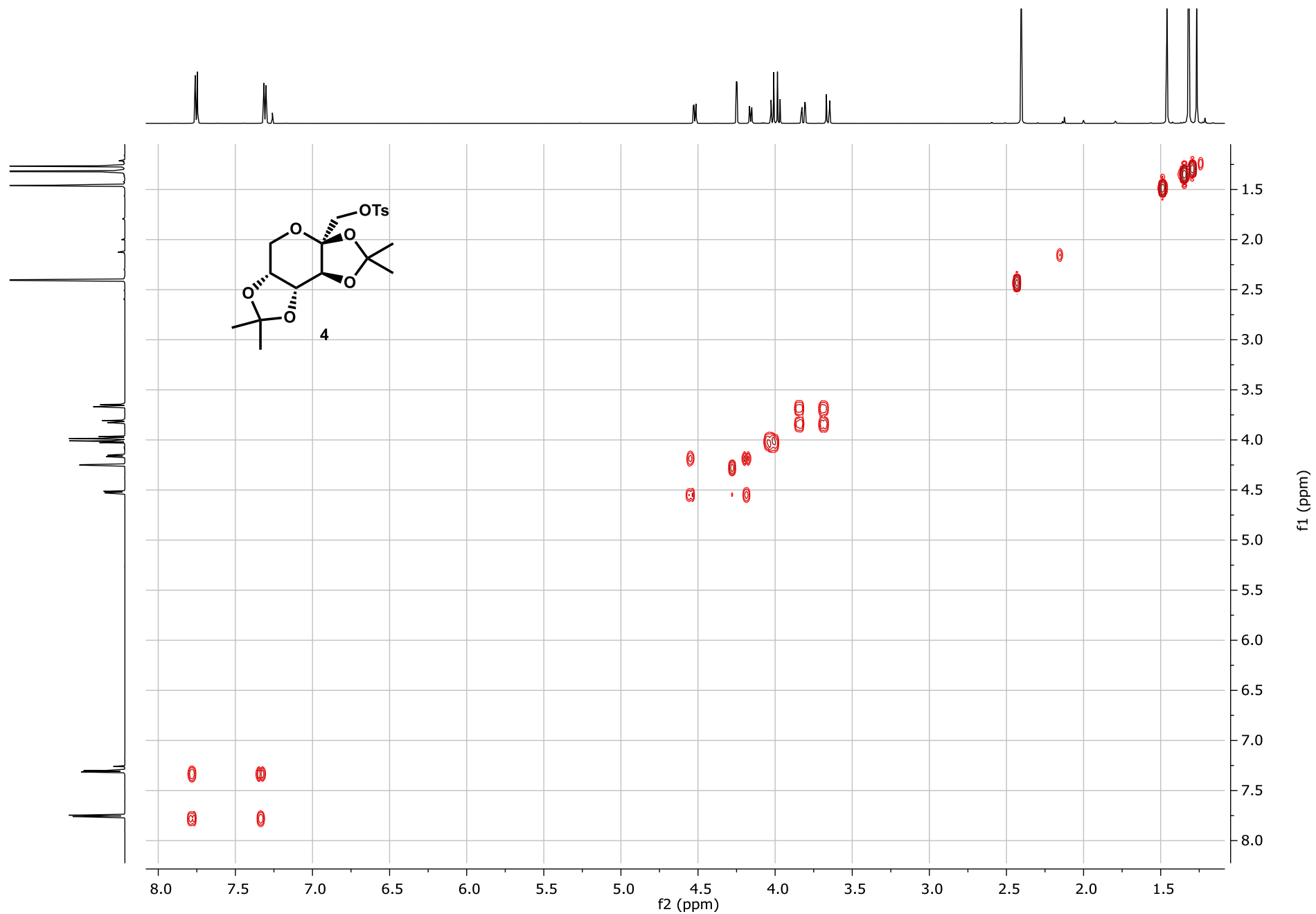
¹H NMR Spectrum for Compound 4 (CDCl₃, 600 MHz).



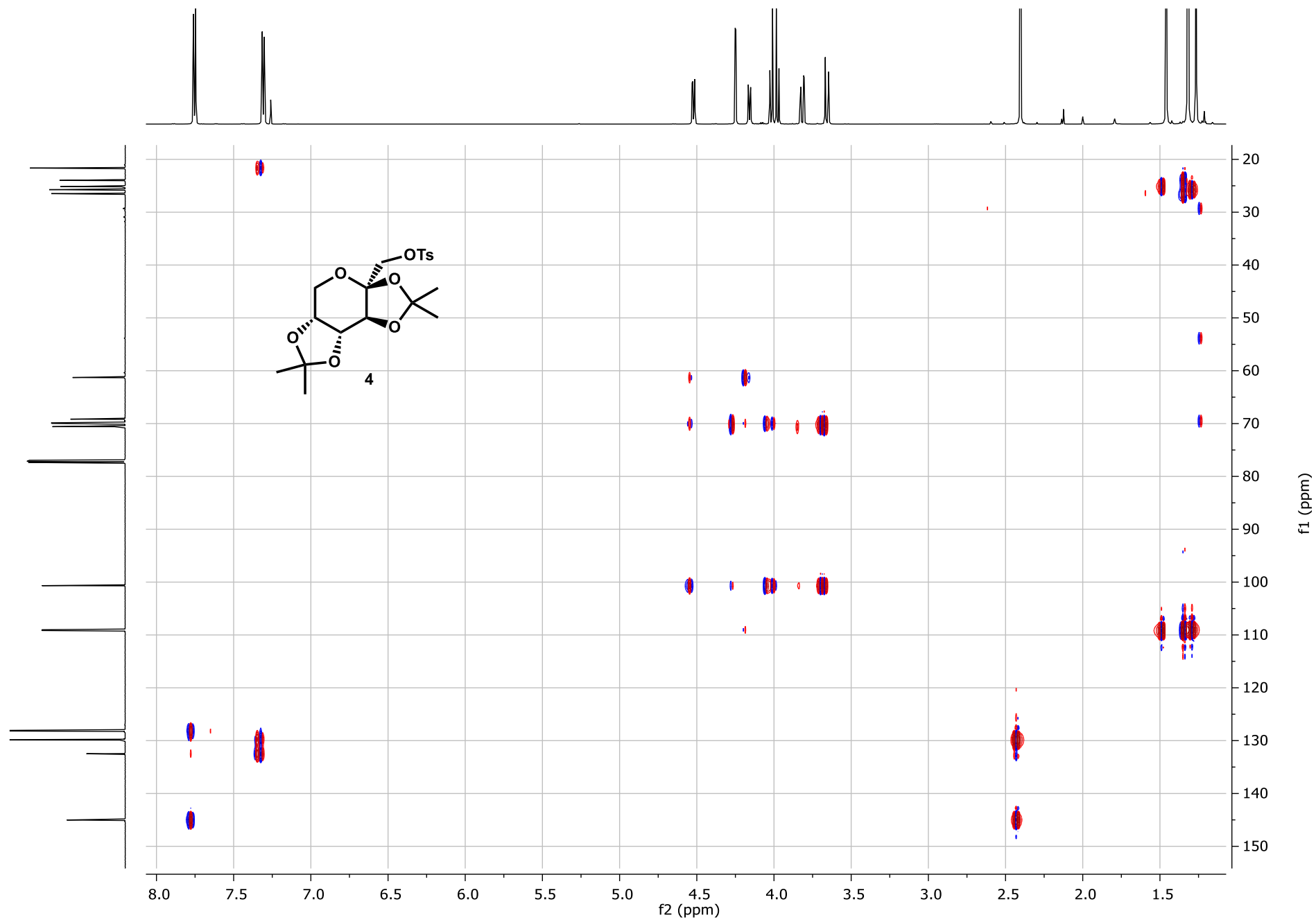
¹³C NMR chemical shifts (ppm):
 145.02, 132.49, 129.87, 128.14, 109.17, 109.01, 100.67, 70.59, 69.97, 69.86, 69.16, 61.29, 26.50, 25.73, 25.17, 23.99, 21.65



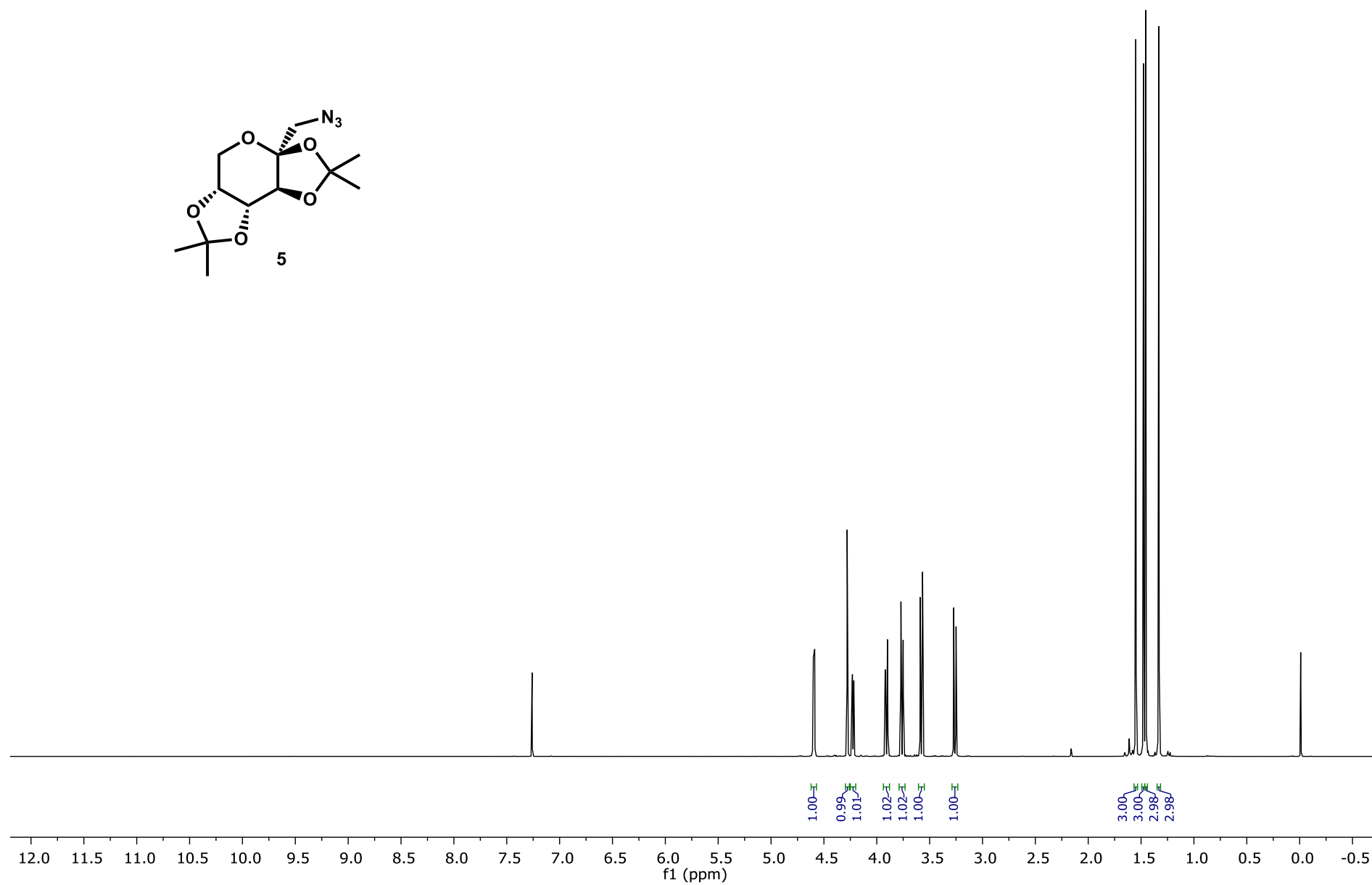
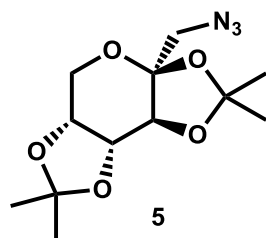
¹³C NMR Spectrum for Compound **4** (CDCl₃, 151 MHz).



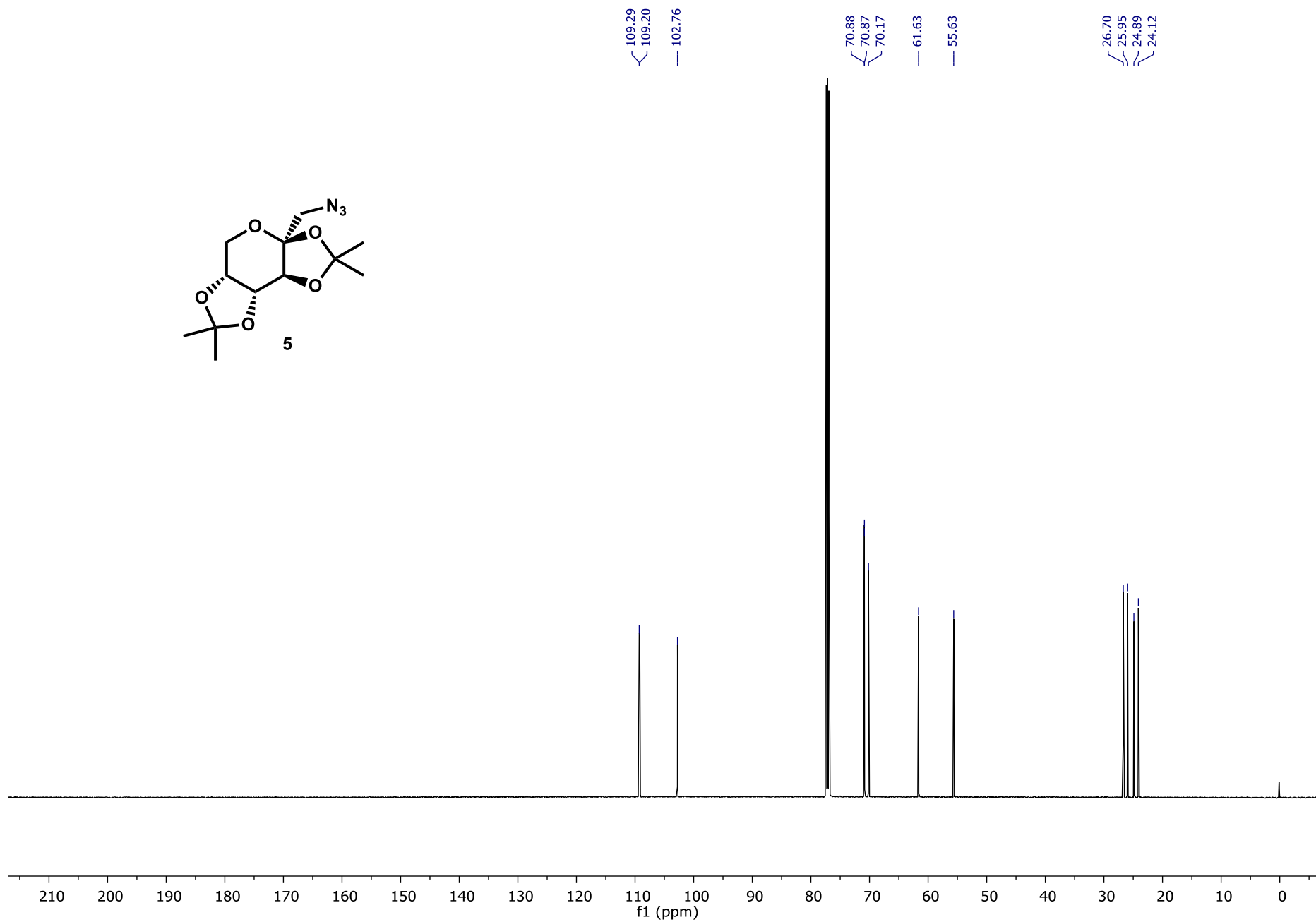
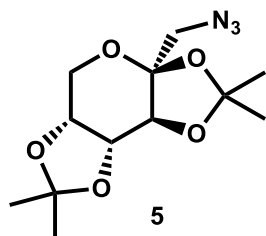
COSY Spectrum for Compound 4 (CDCl₃).



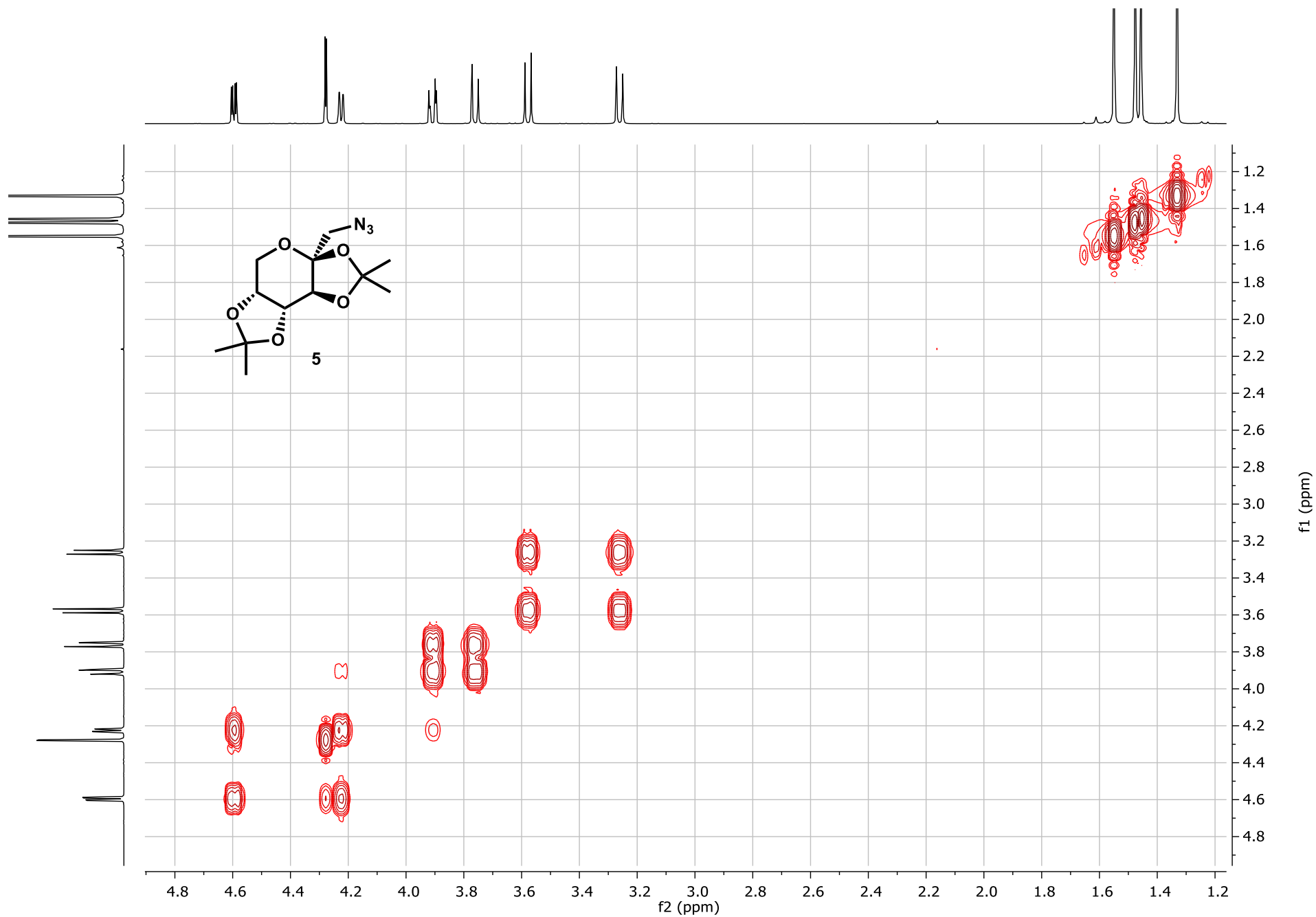
HMBC Spectrum for Compound **4** (CDCl_3).



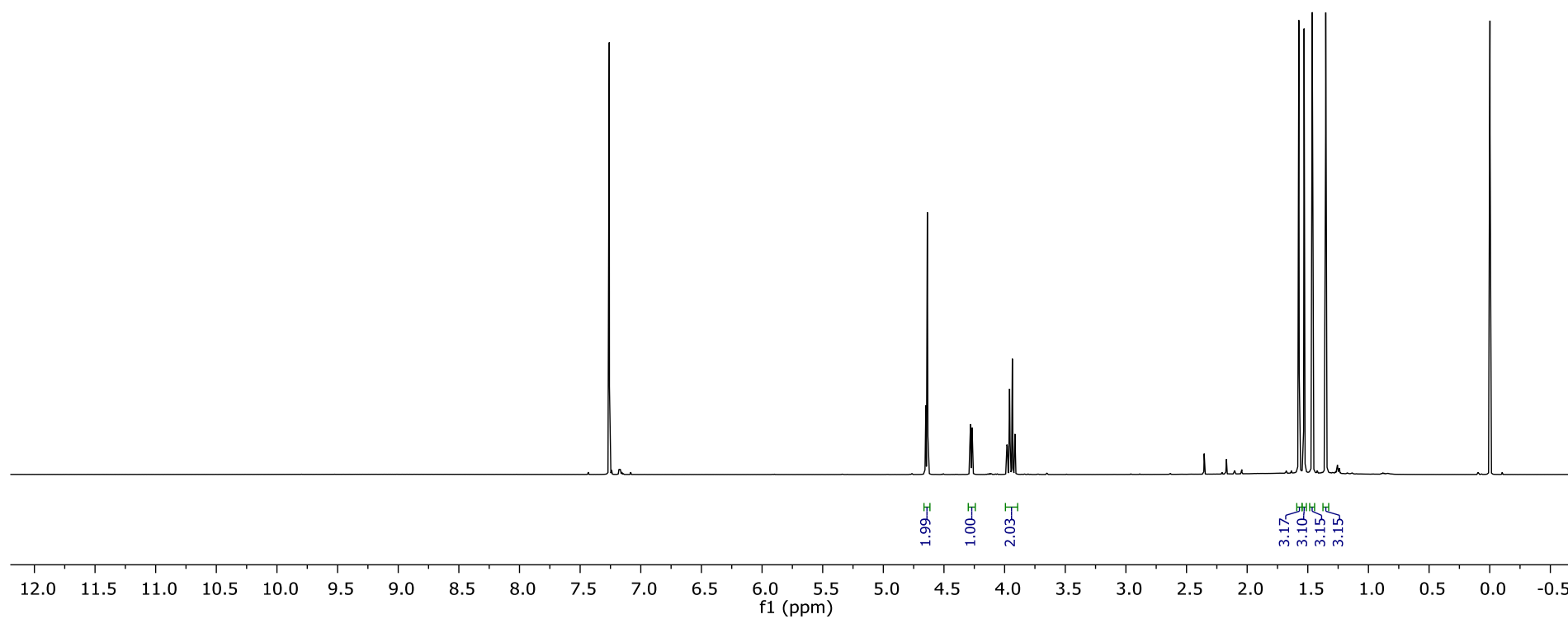
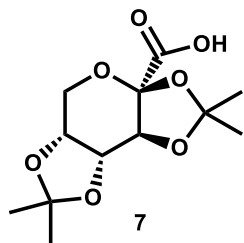
¹H NMR Spectrum for Compound 5 (CDCl₃, 600 MHz).



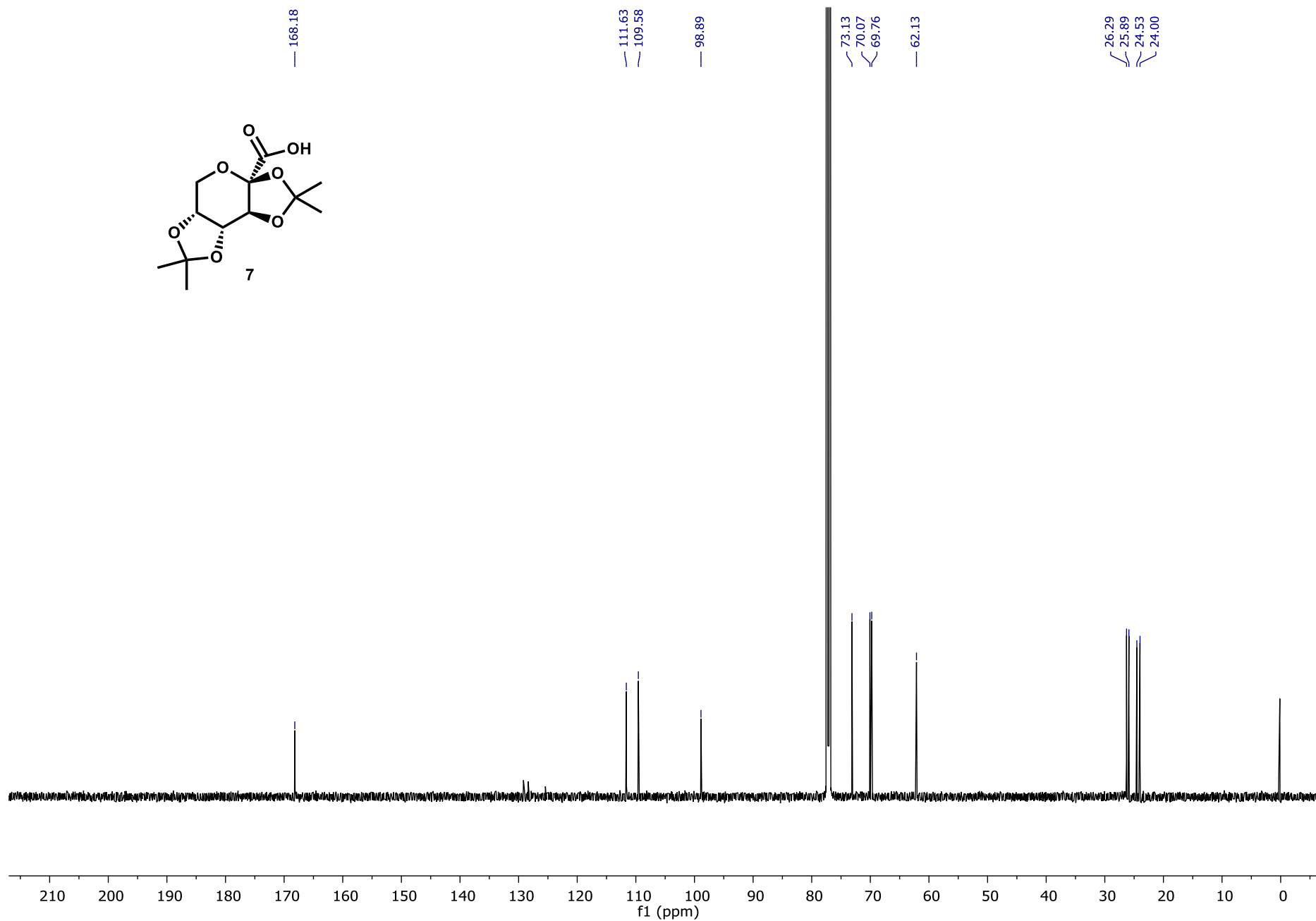
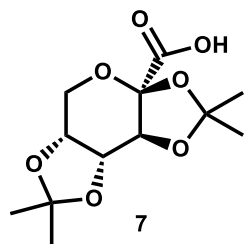
^{13}C NMR Spectrum for Compound 5 ($CDCl_3$, 151 MHz).



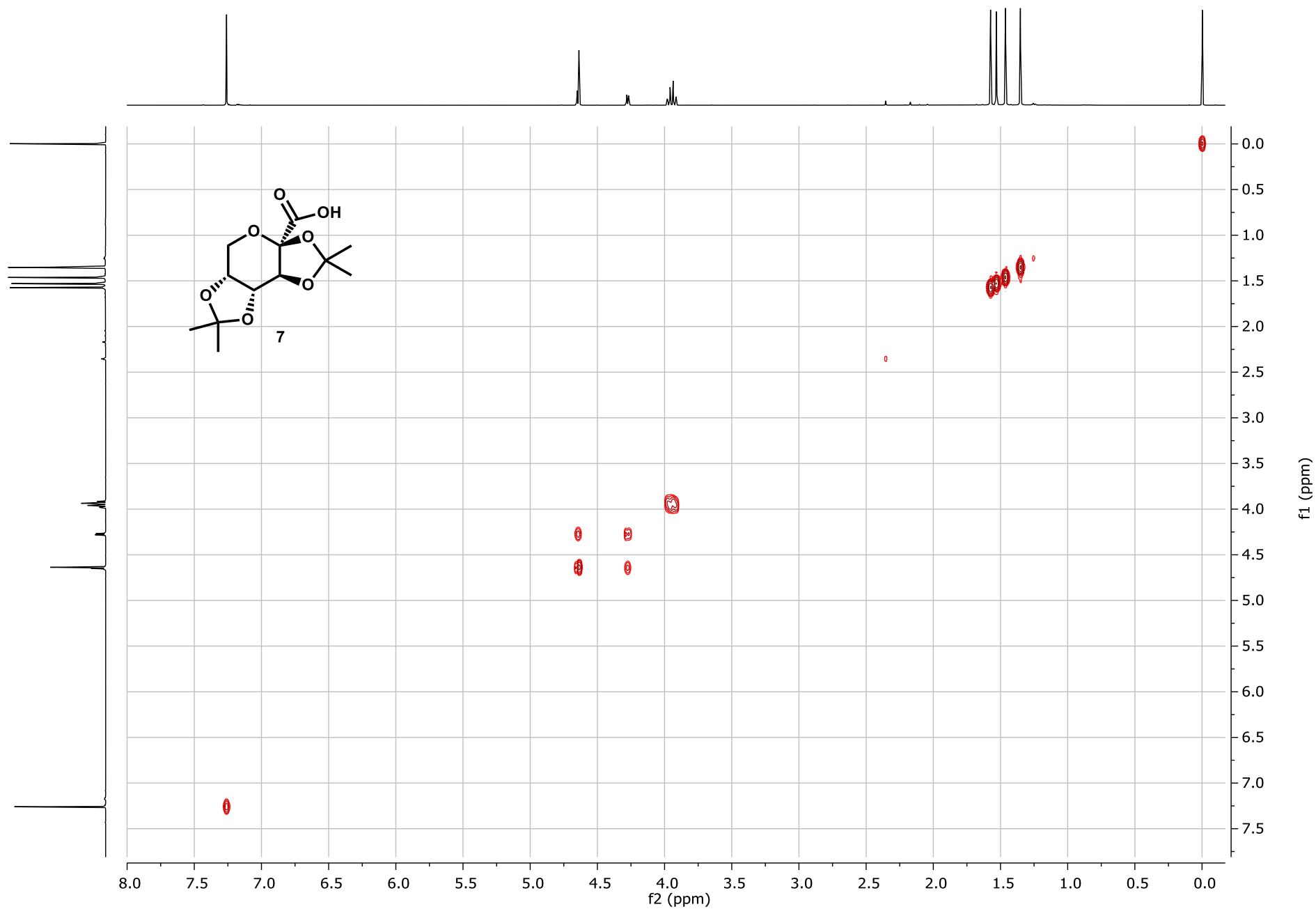
COSY Spectrum for Compound 5 (CDCl_3).



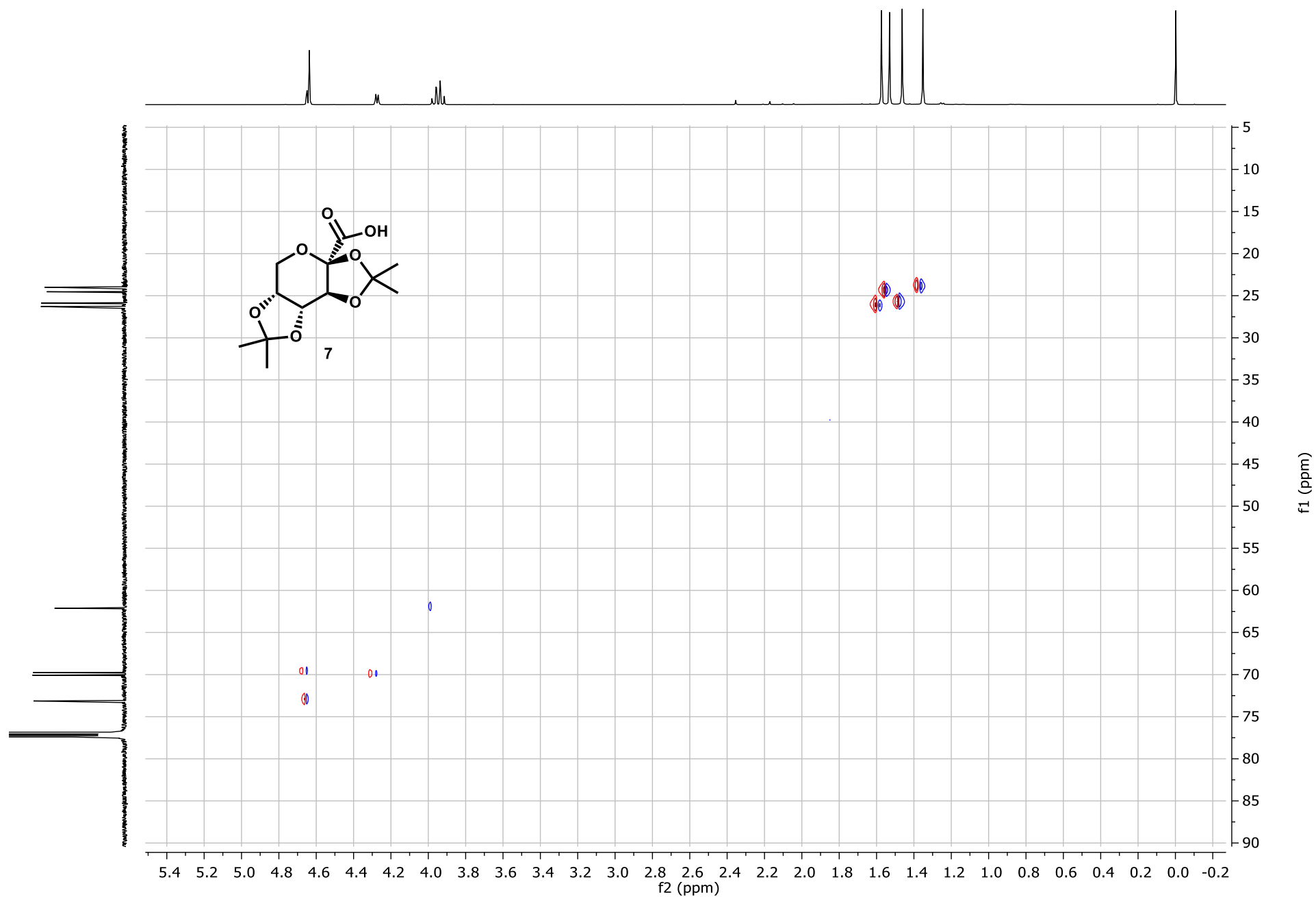
^1H NMR Spectrum for Compound 7 (CDCl_3 , 600 MHz).



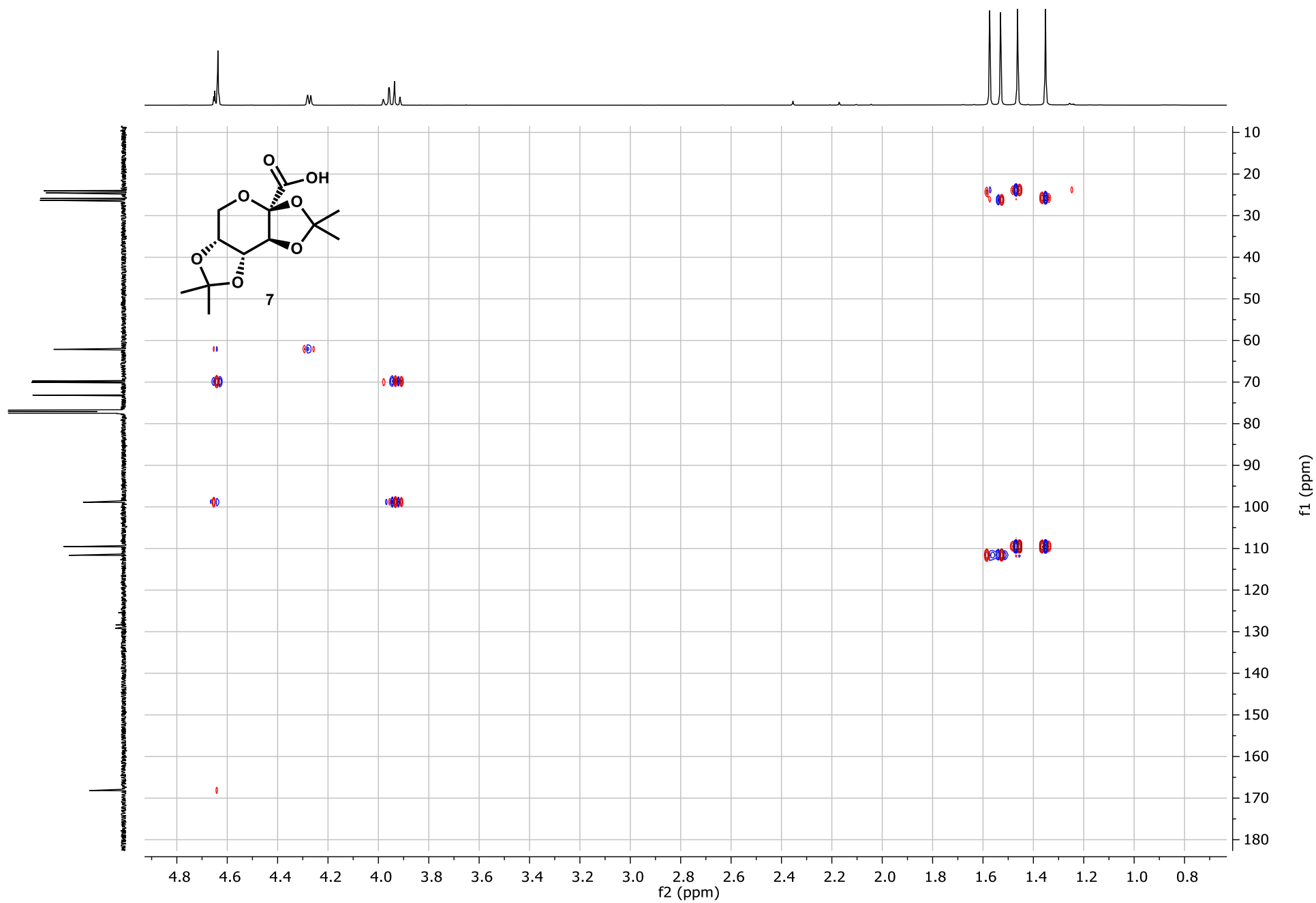
¹³C NMR Spectrum for Compound 7 (CDCl₃, 151 MHz).



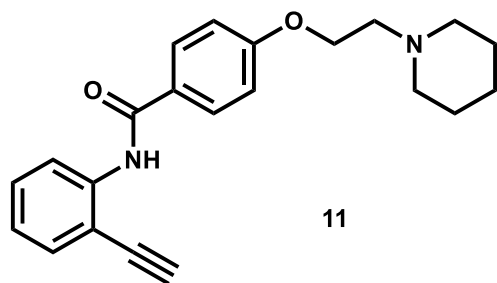
COSY Spectrum for Compound 7 (CDCl_3).



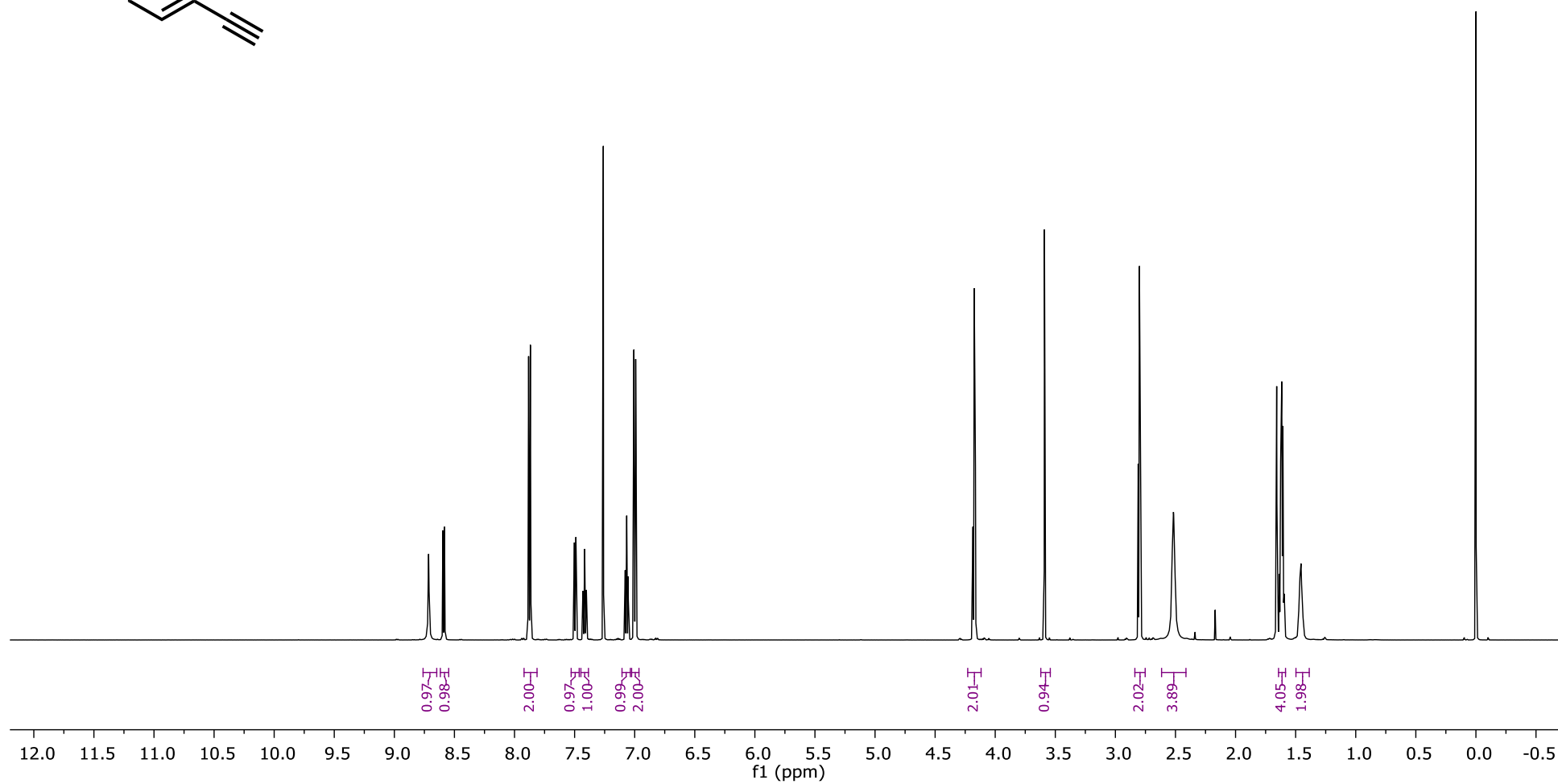
HSQC Spectrum for Compound 7 (CDCl₃).



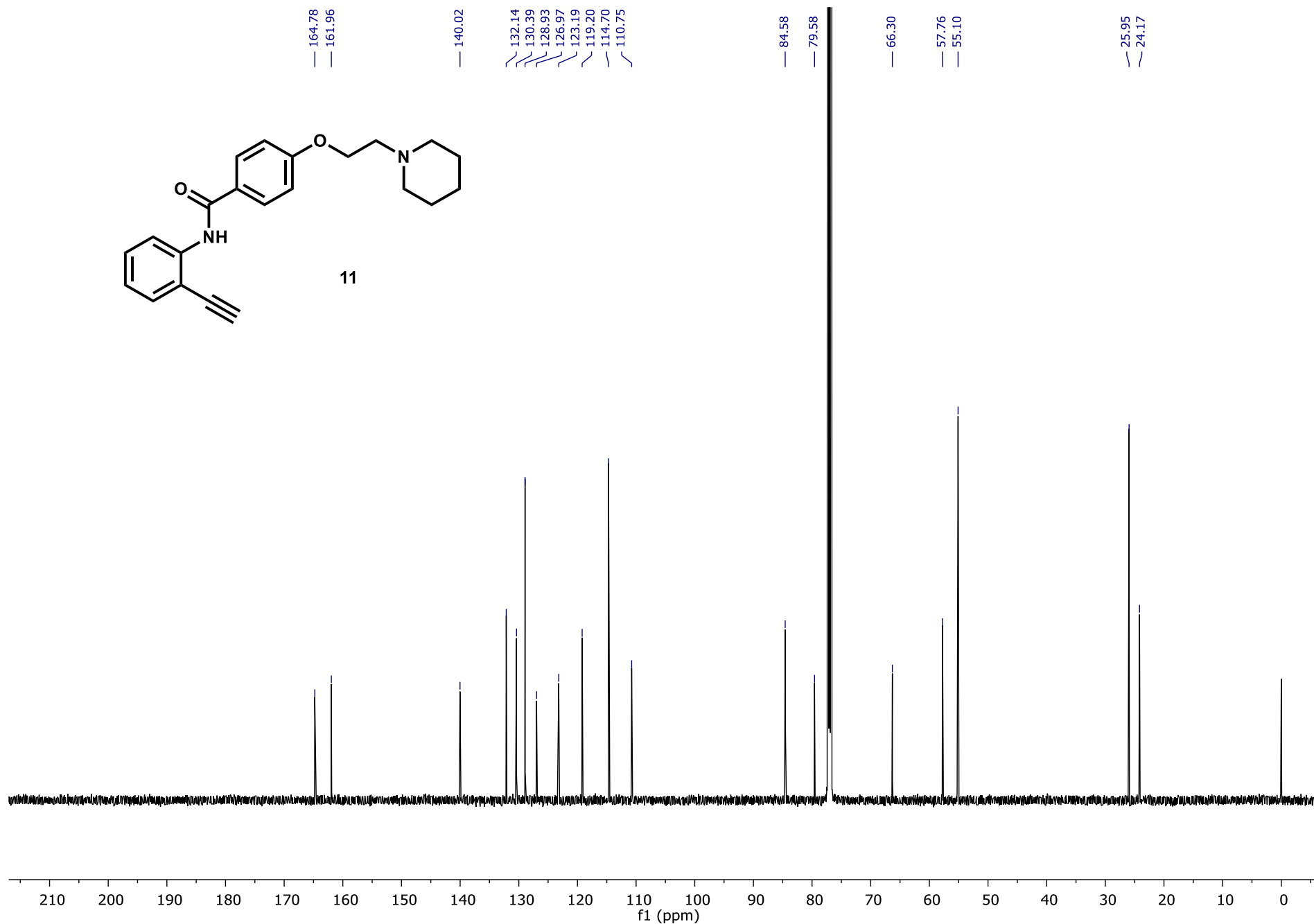
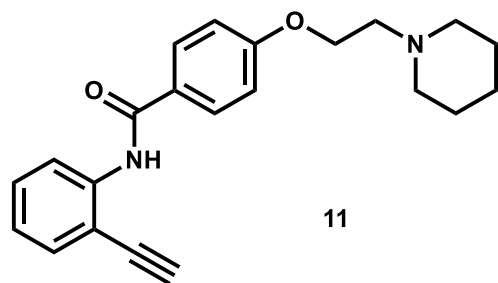
HMBC Spectrum for Compound 7 (CDCl_3).



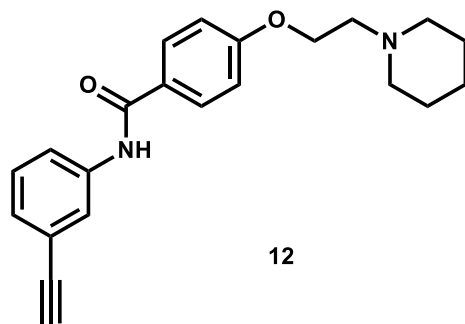
11



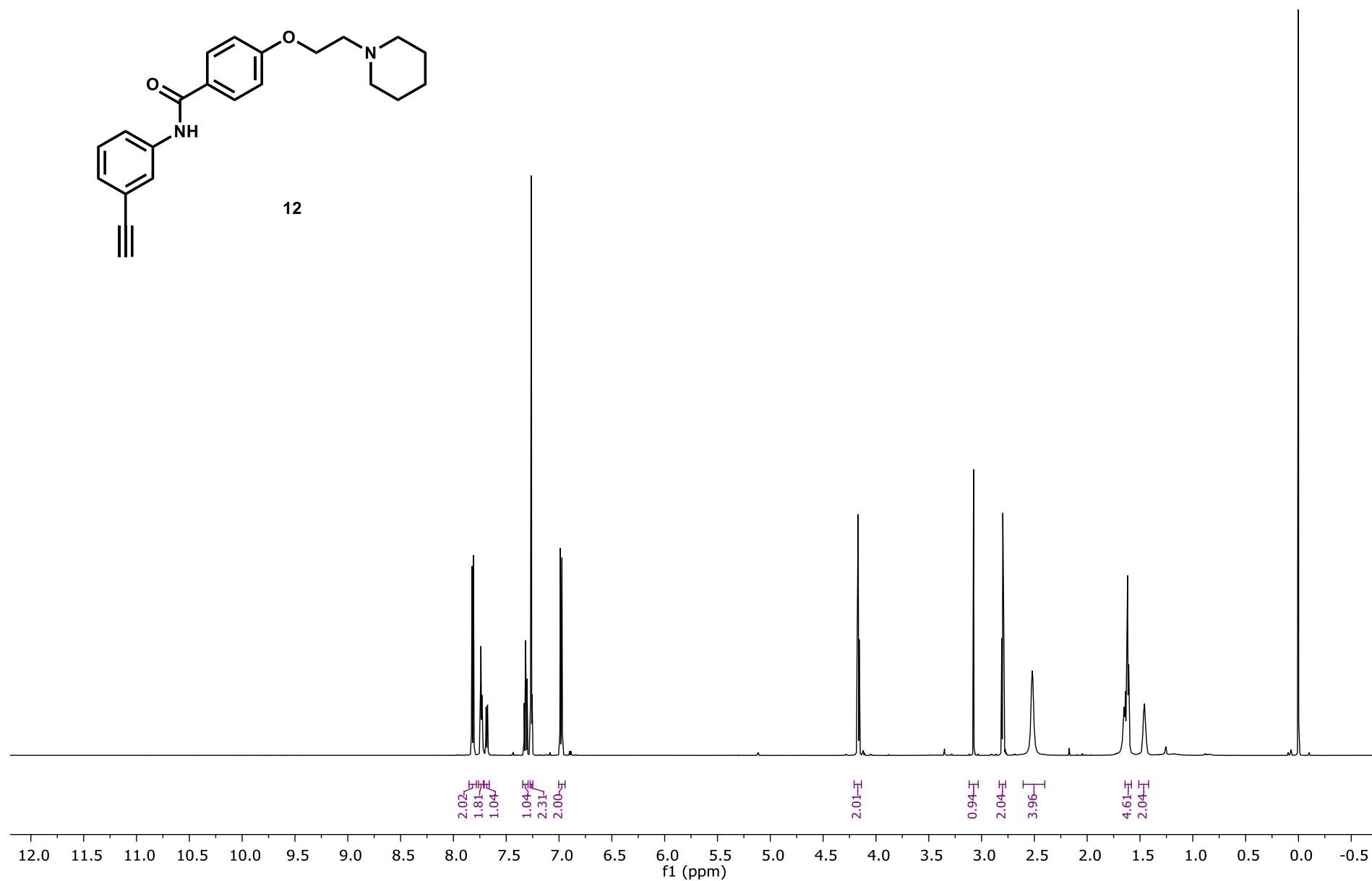
¹H NMR Spectrum for Compound **11** (CDCl₃, 600 MHz).



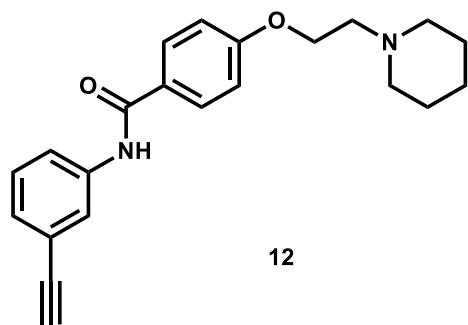
¹³C NMR Spectrum for Compound **11** (CDCl₃, 151 MHz).



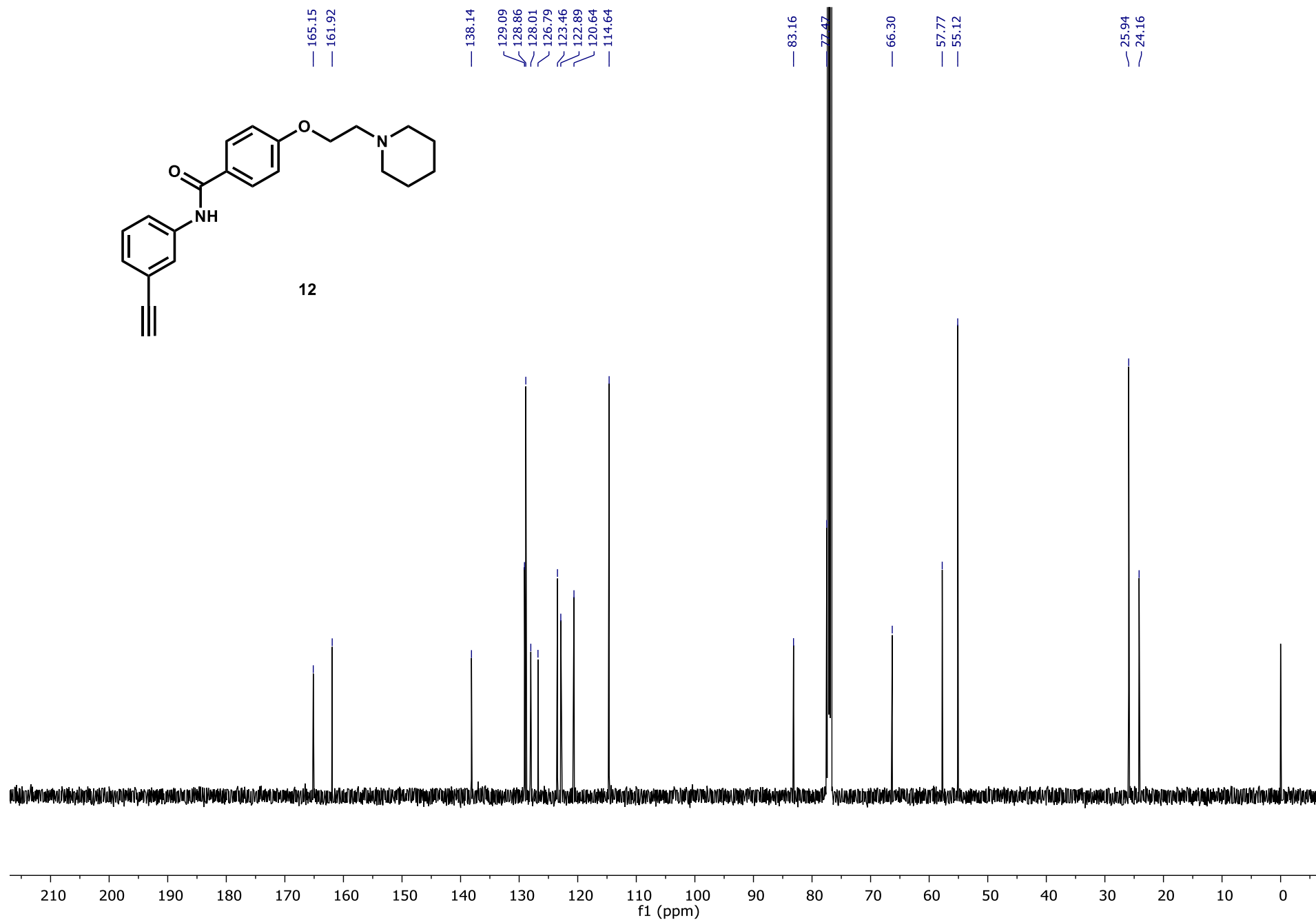
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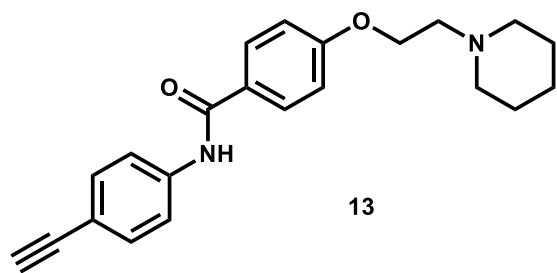


¹H NMR Spectrum for Compound **12** (CDCl₃, 600 MHz).

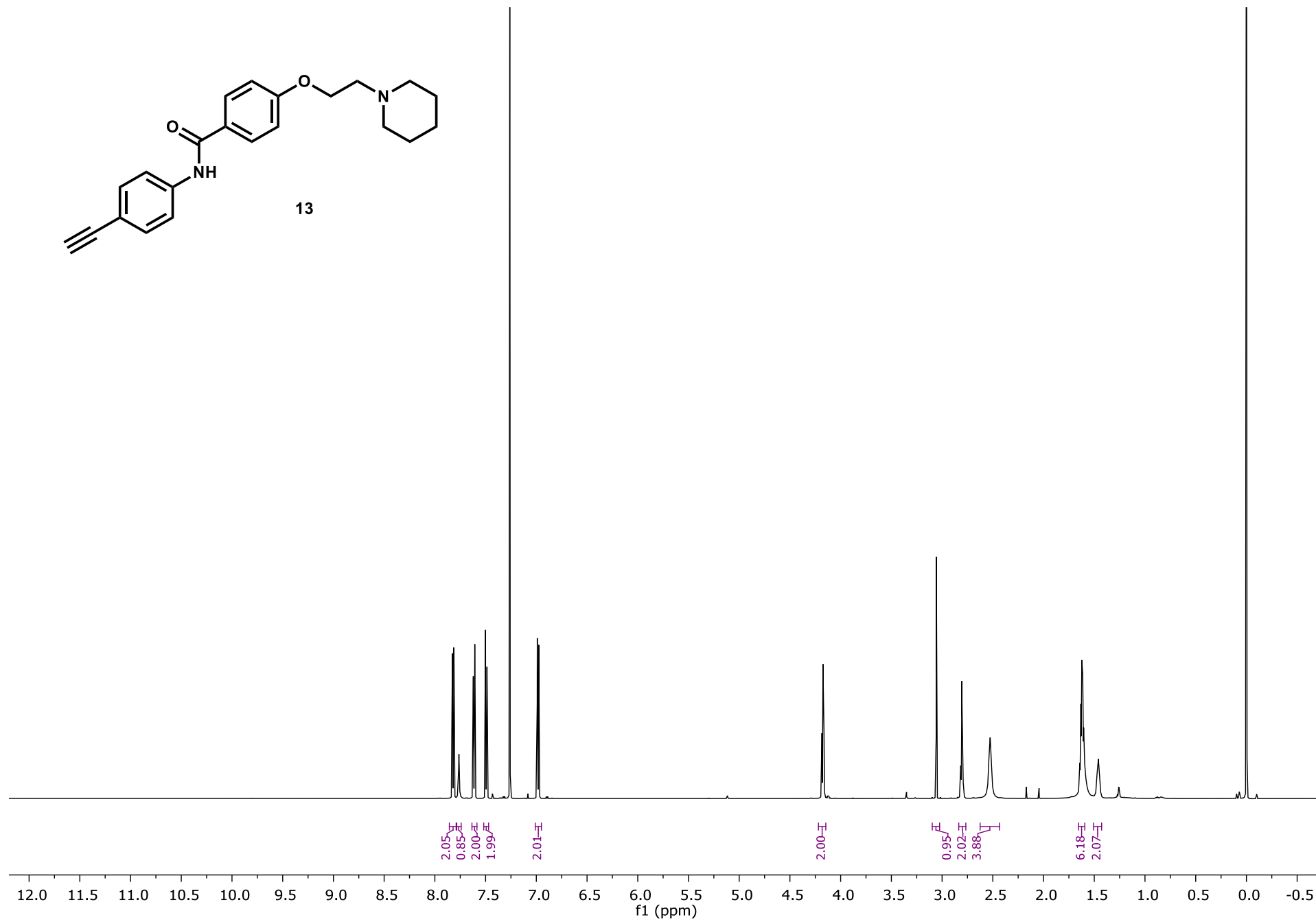


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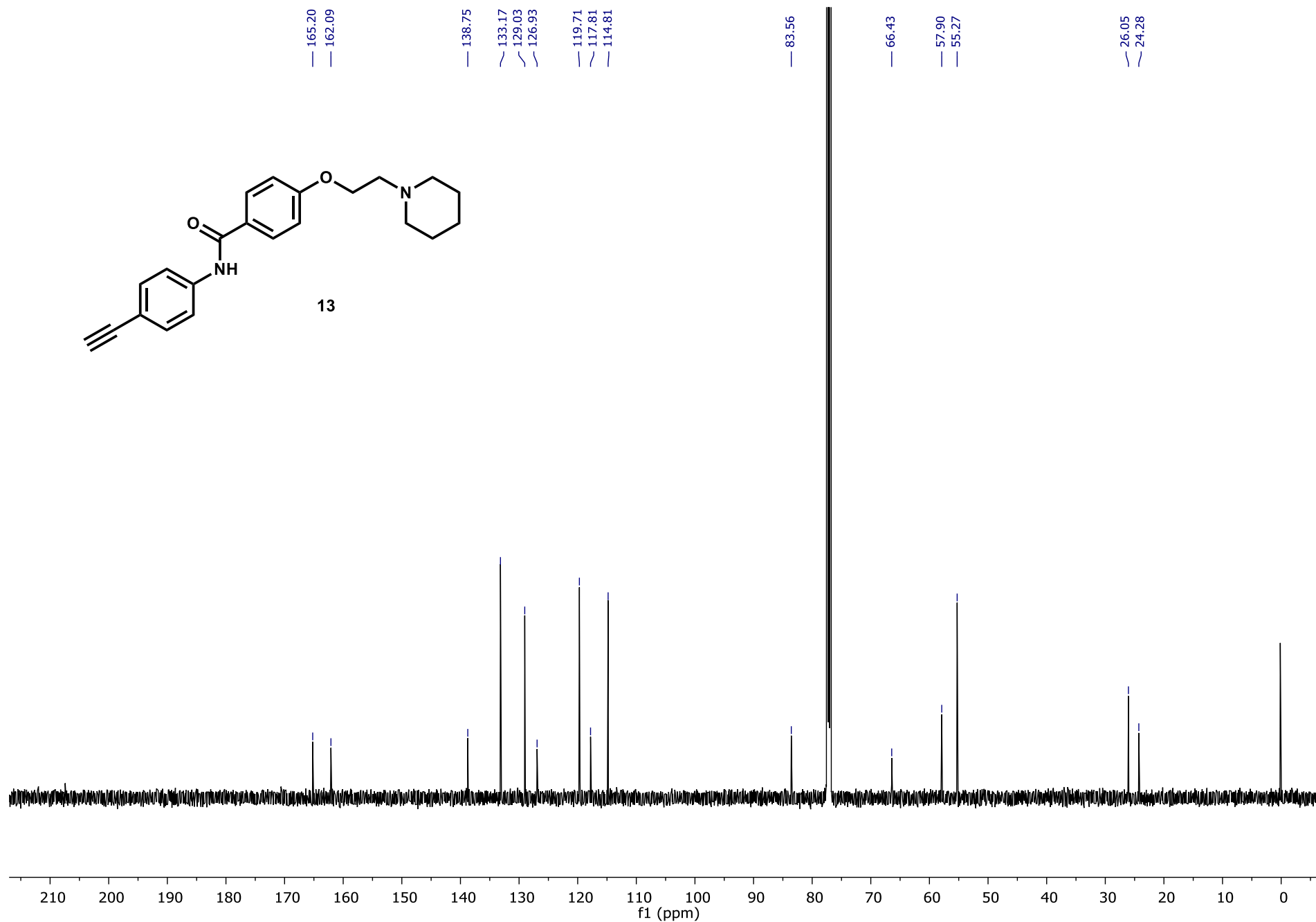




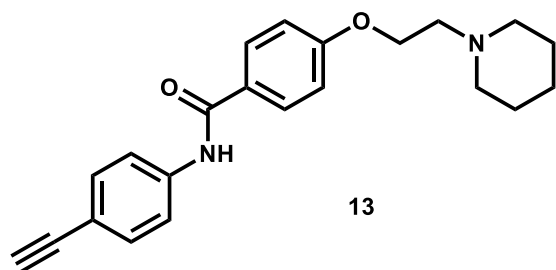
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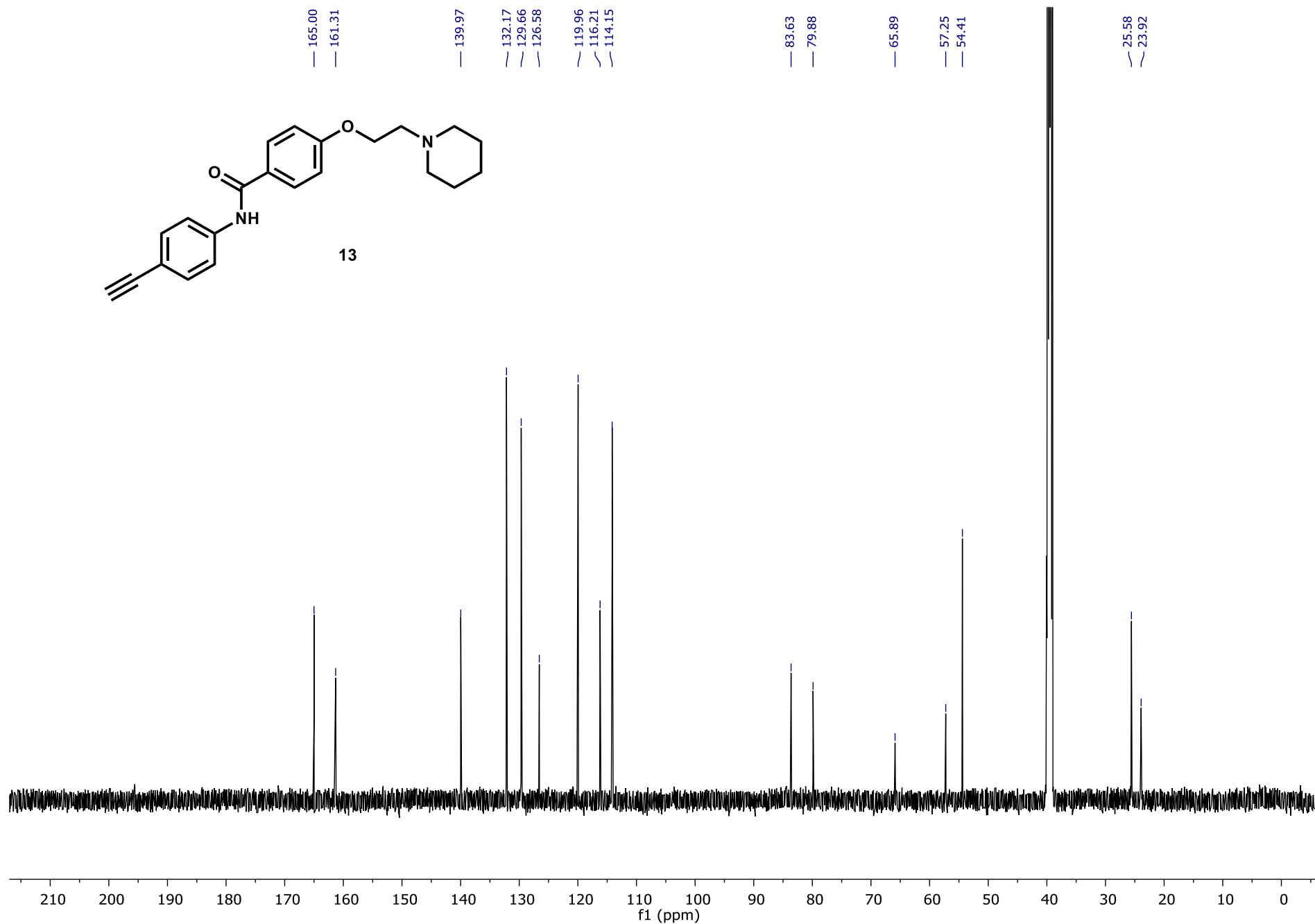
¹H NMR Spectrum for Compound 13 (CDCl₃, 600 MHz).



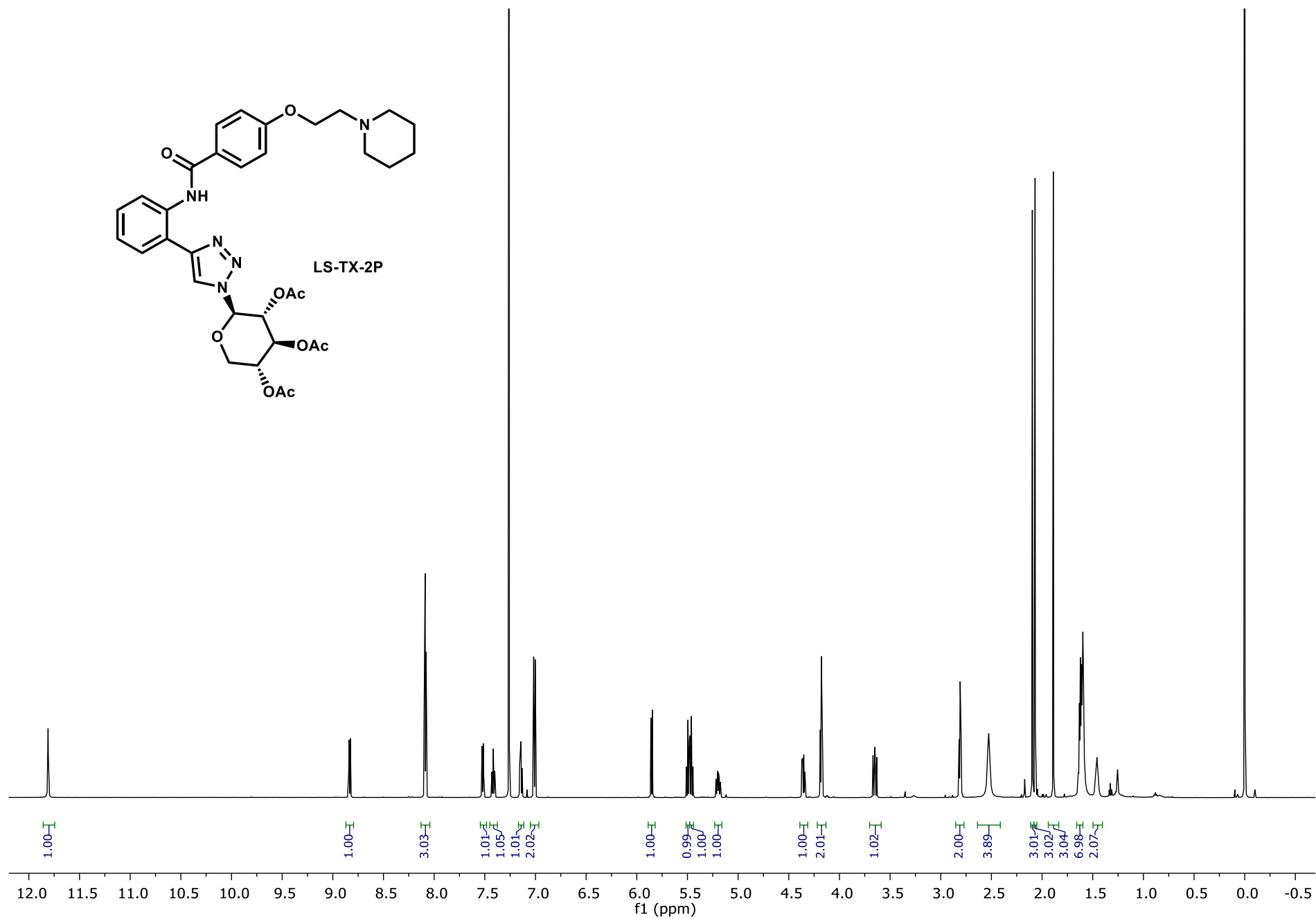
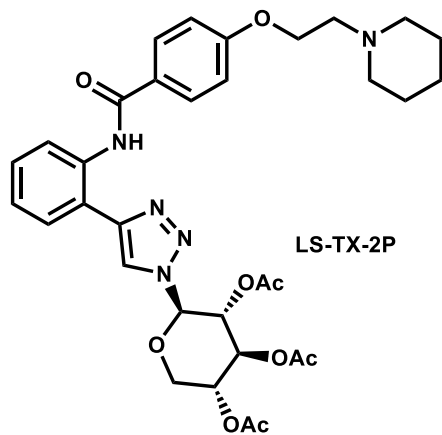
¹³C NMR Spectrum for Compound **13** (CDCl₃, 151 MHz).



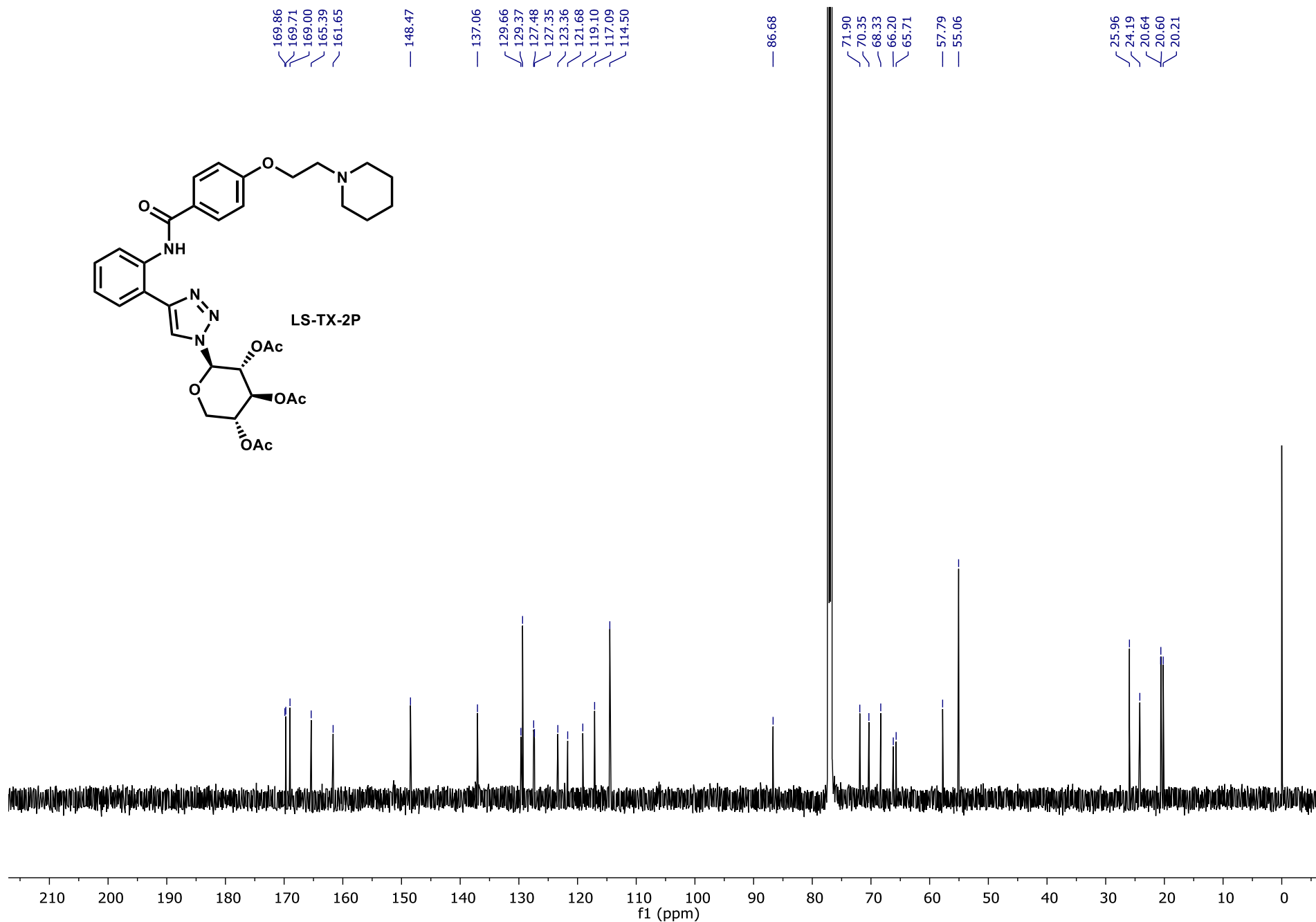
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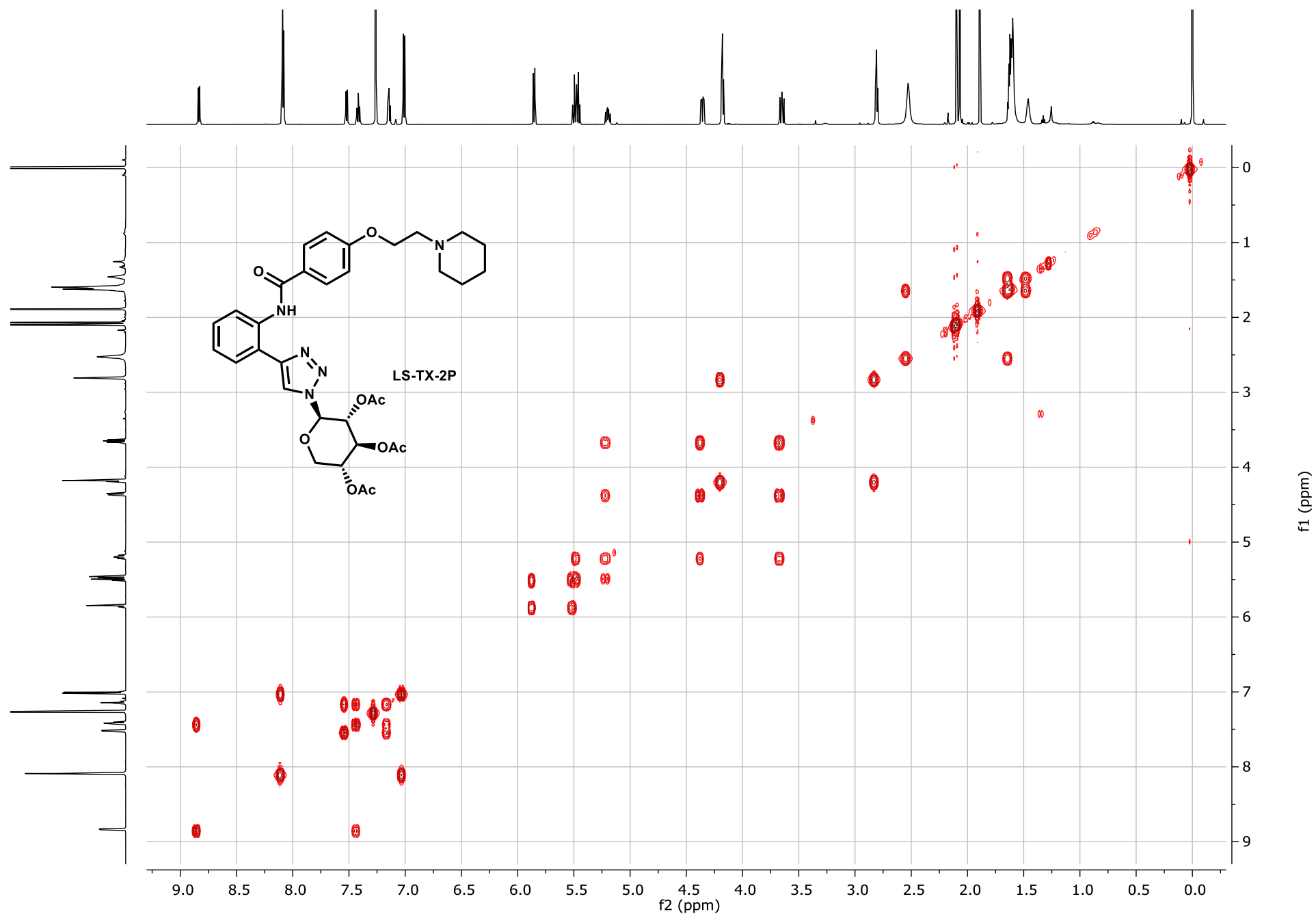
¹³C NMR Spectrum for Compound 13 (DMSO-*d*₆, 151 MHz).



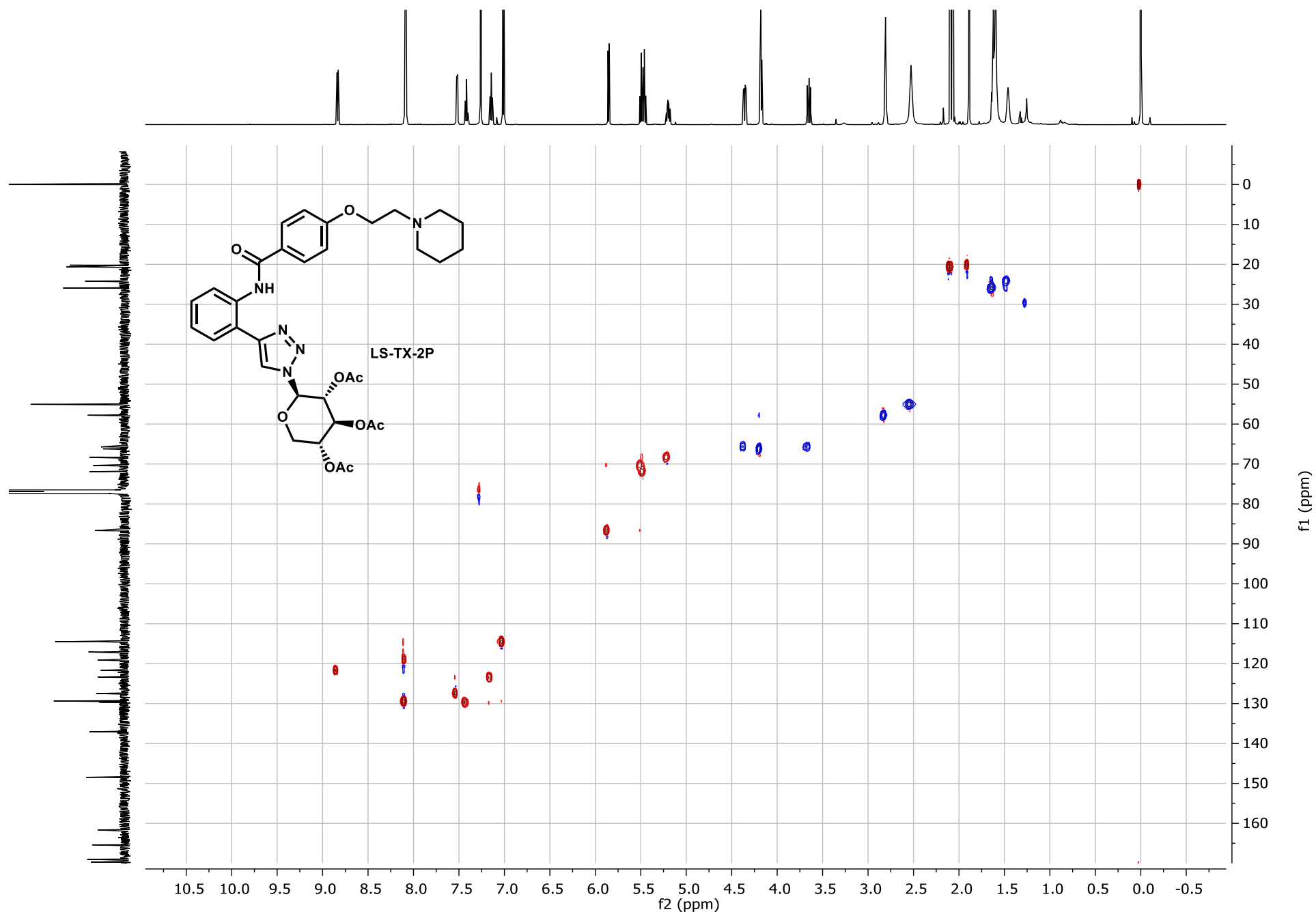
¹H NMR Spectrum for LS-TX-2P (CDCl₃, 600 MHz).

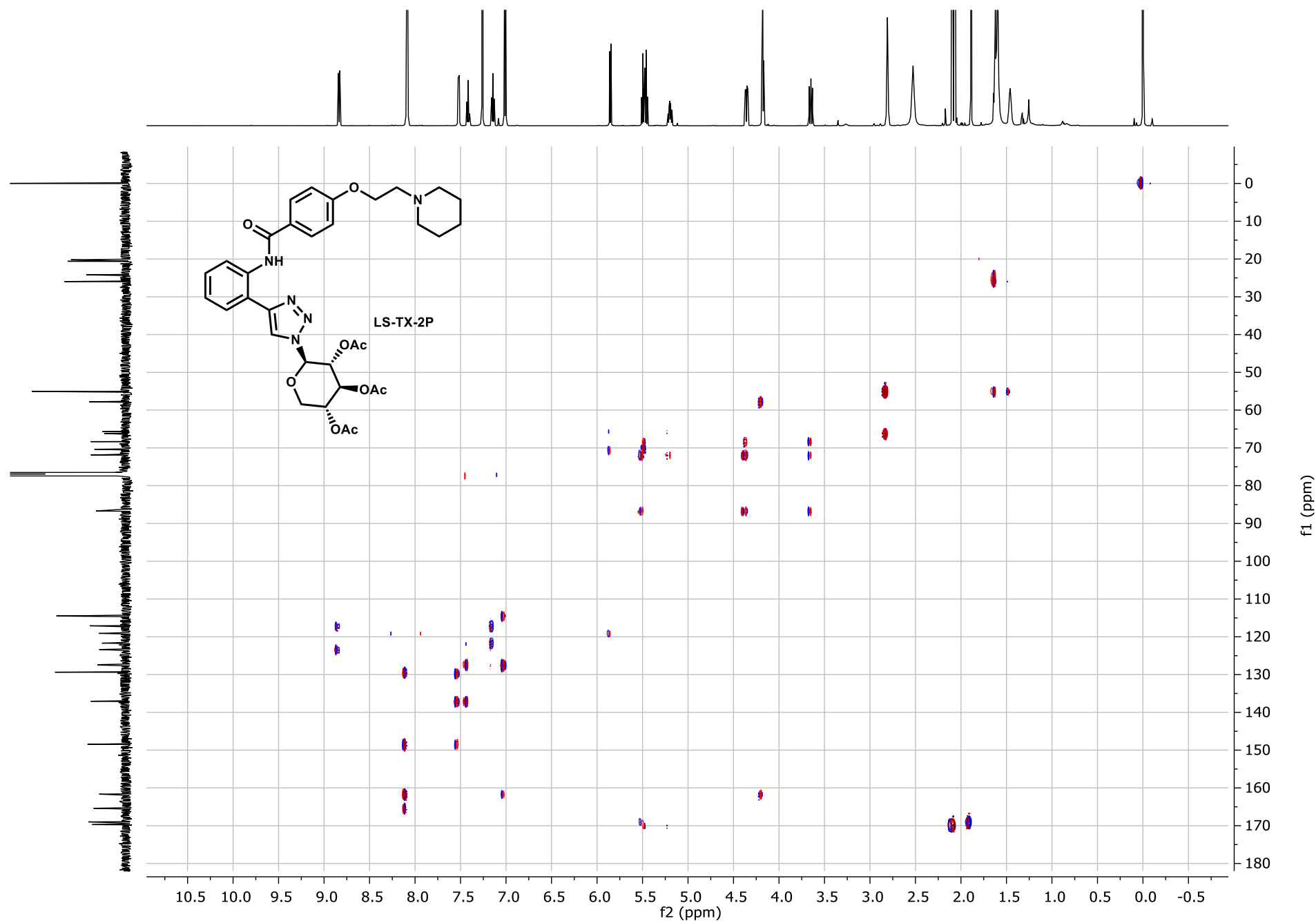


¹³C NMR Spectrum for **LS-TX-2P** (CDCl₃, 151 MHz).

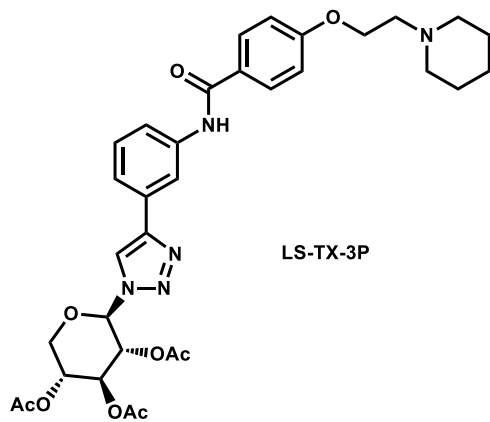


COSY Spectrum for **LS-TX-2P** (CDCl₃).

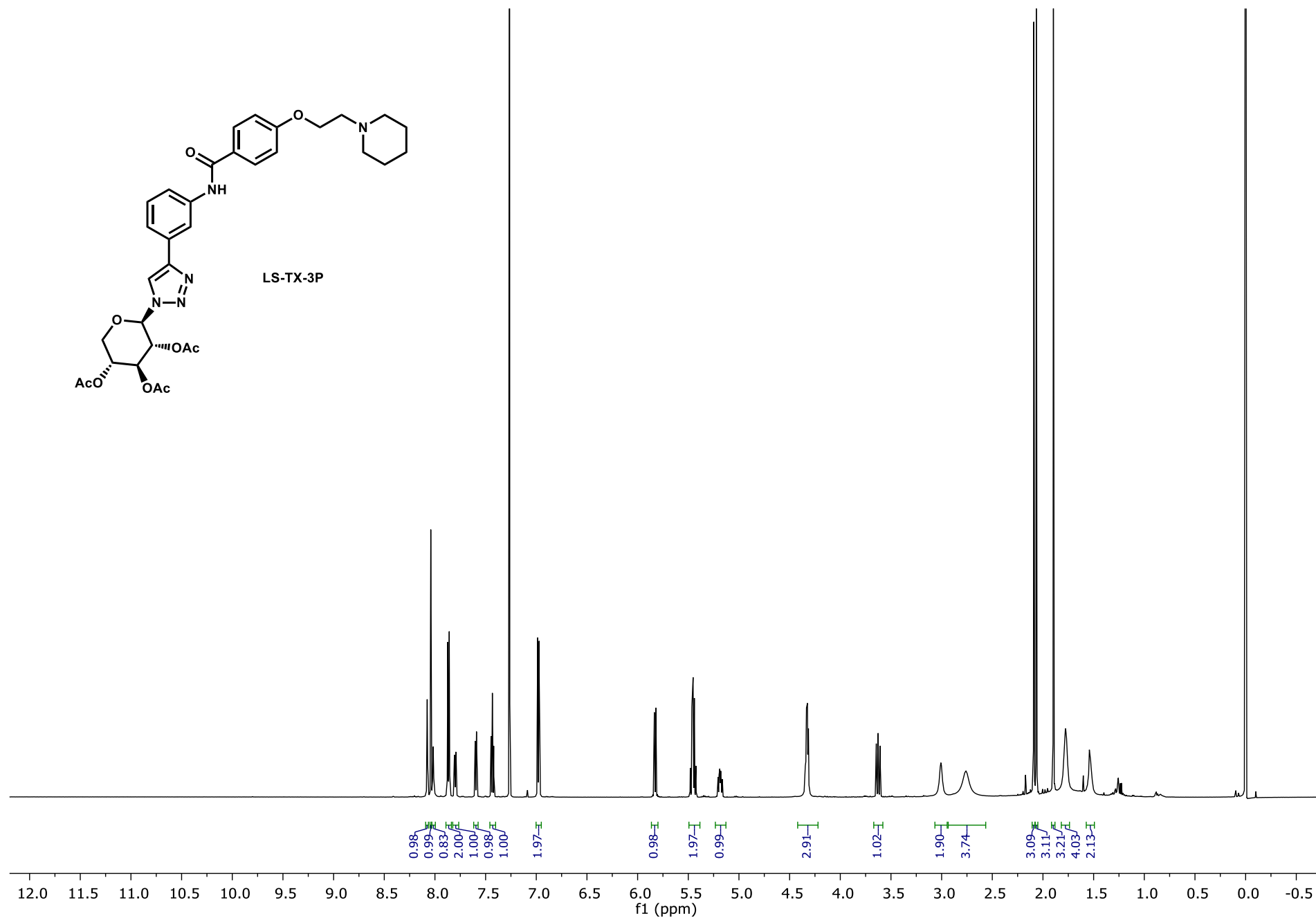




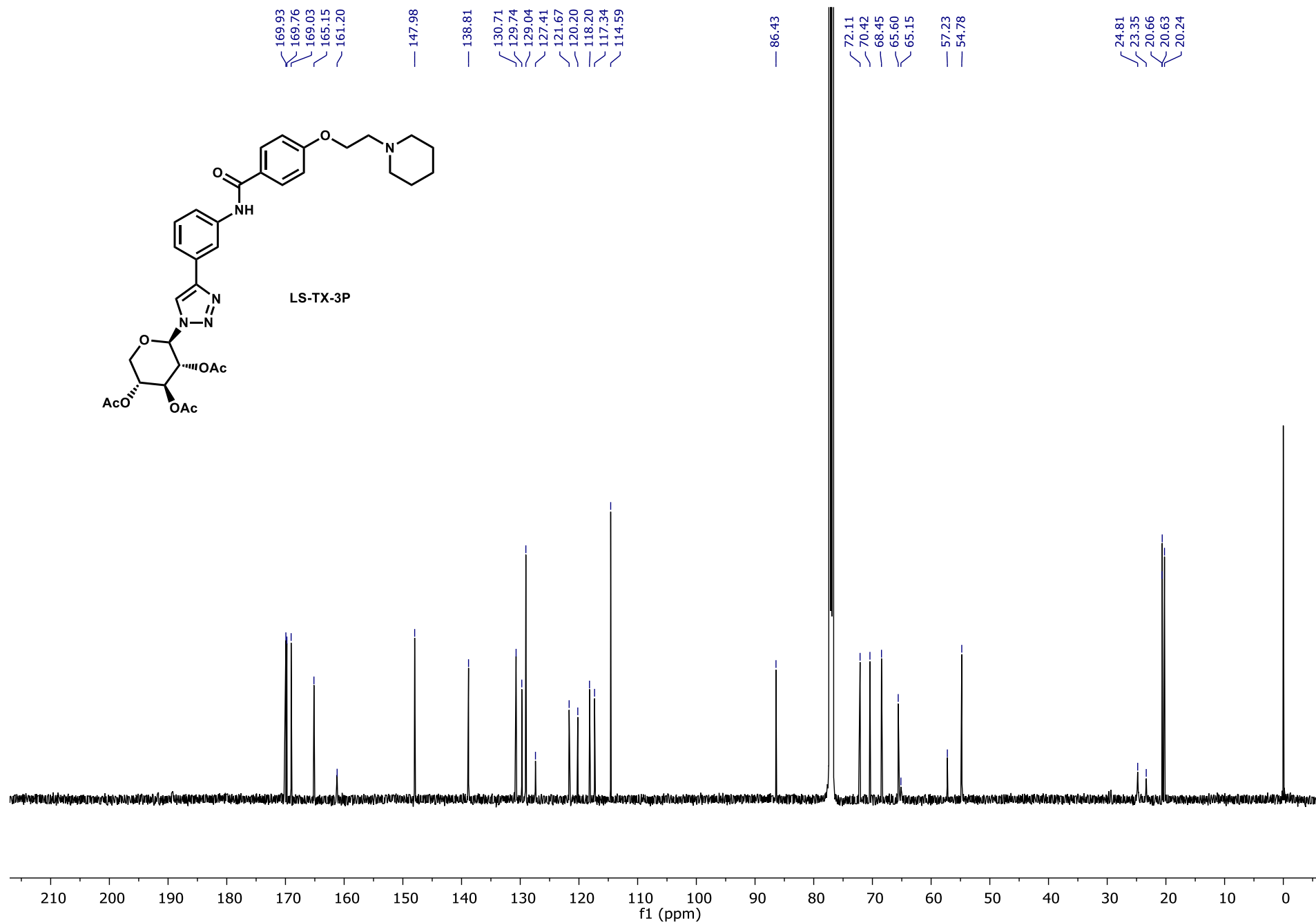
HMBC Spectrum for **LS-TX-2P** (CDCl_3).



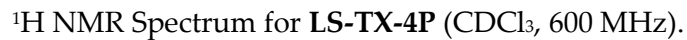
LS-TX-3P

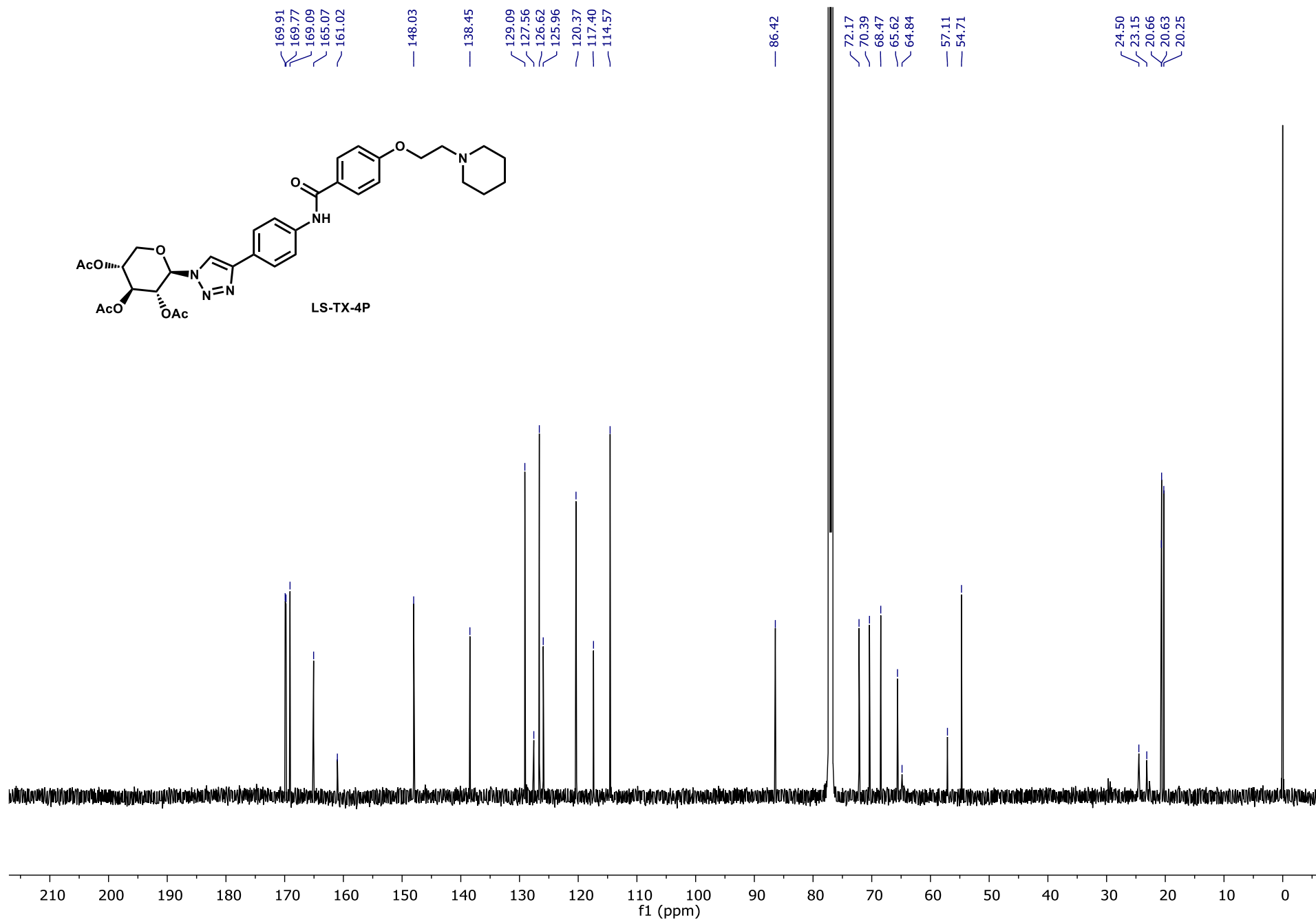


¹H NMR Spectrum for LS-TX-3P (CDCl₃, 600 MHz).

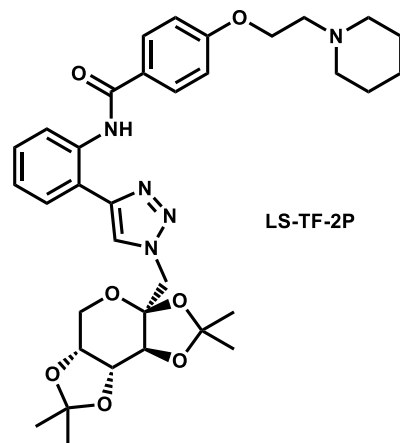


¹³C NMR Spectrum for **LS-TX-3P** (CDCl₃, 151 MHz).

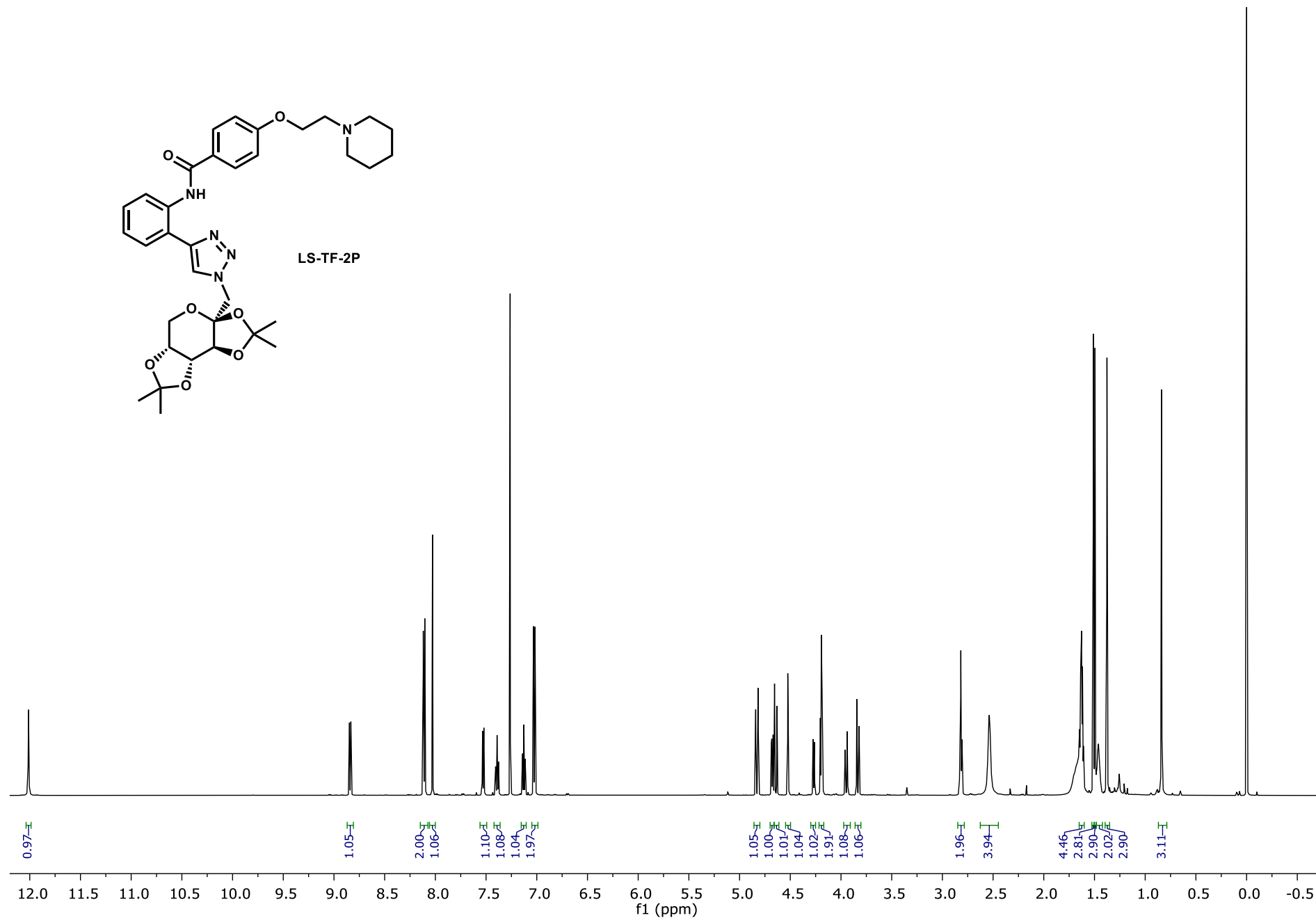




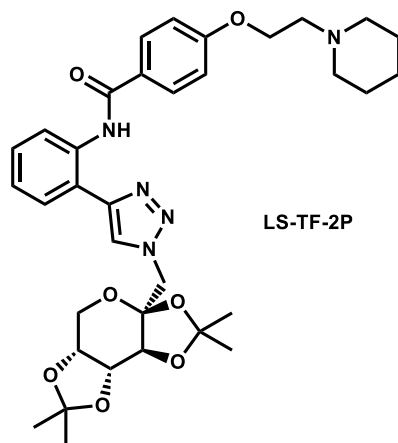
¹³C NMR Spectrum for **LS-TX-4P** (CDCl₃, 151 MHz).



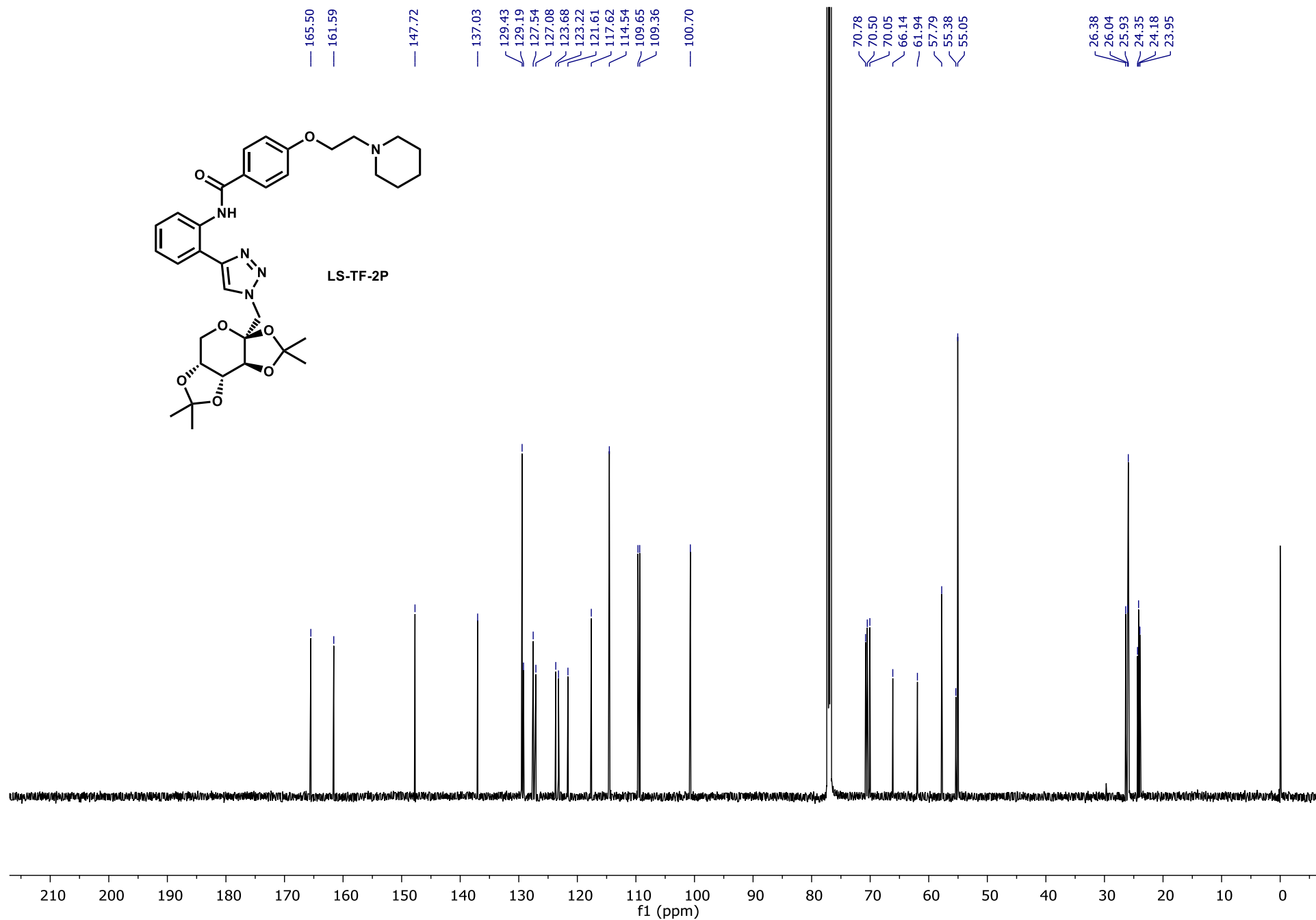
LS-TF-2P



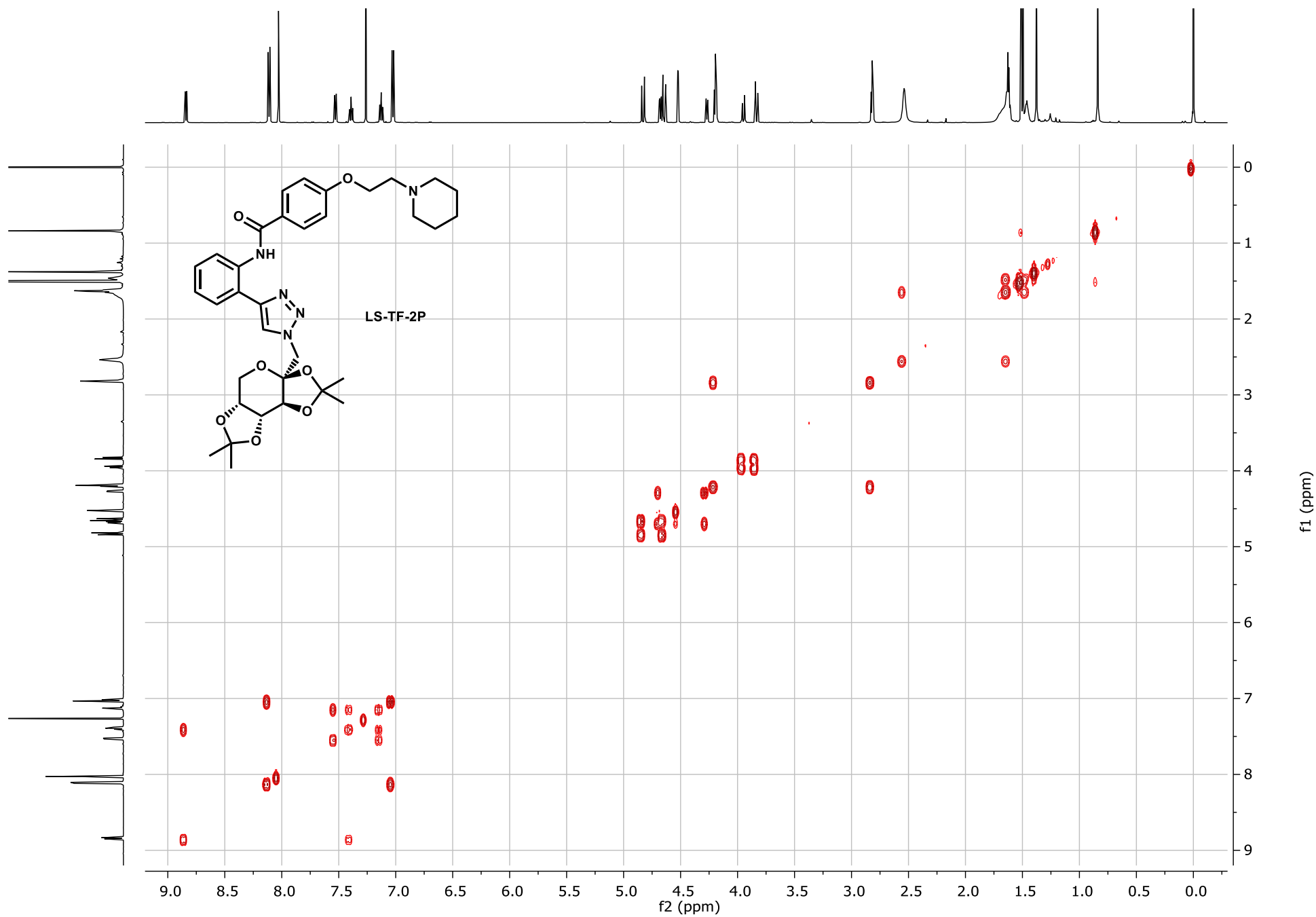
¹H NMR Spectrum for LS-TF-2P (CDCl₃, 600 MHz).



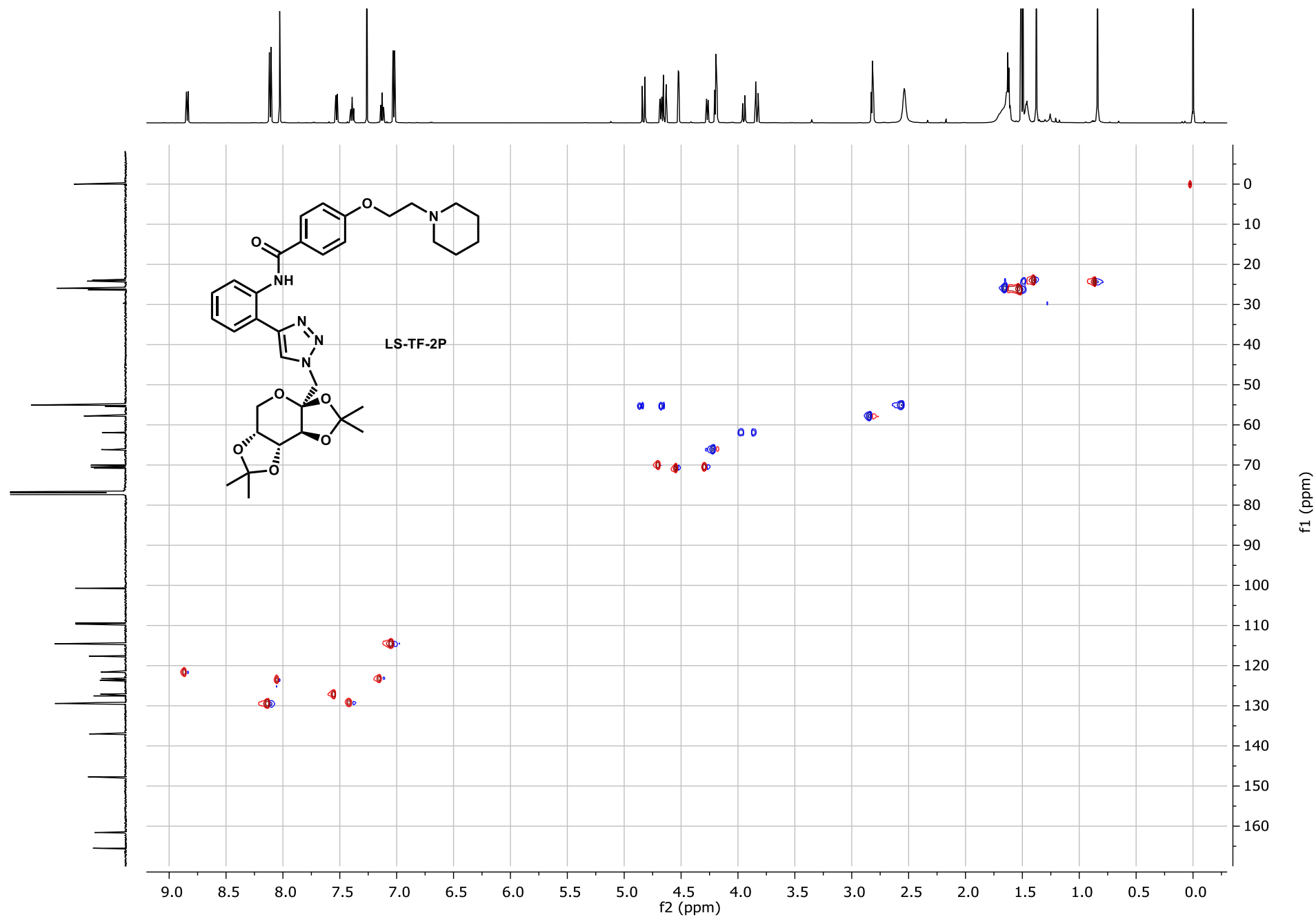
LS-TF-2P



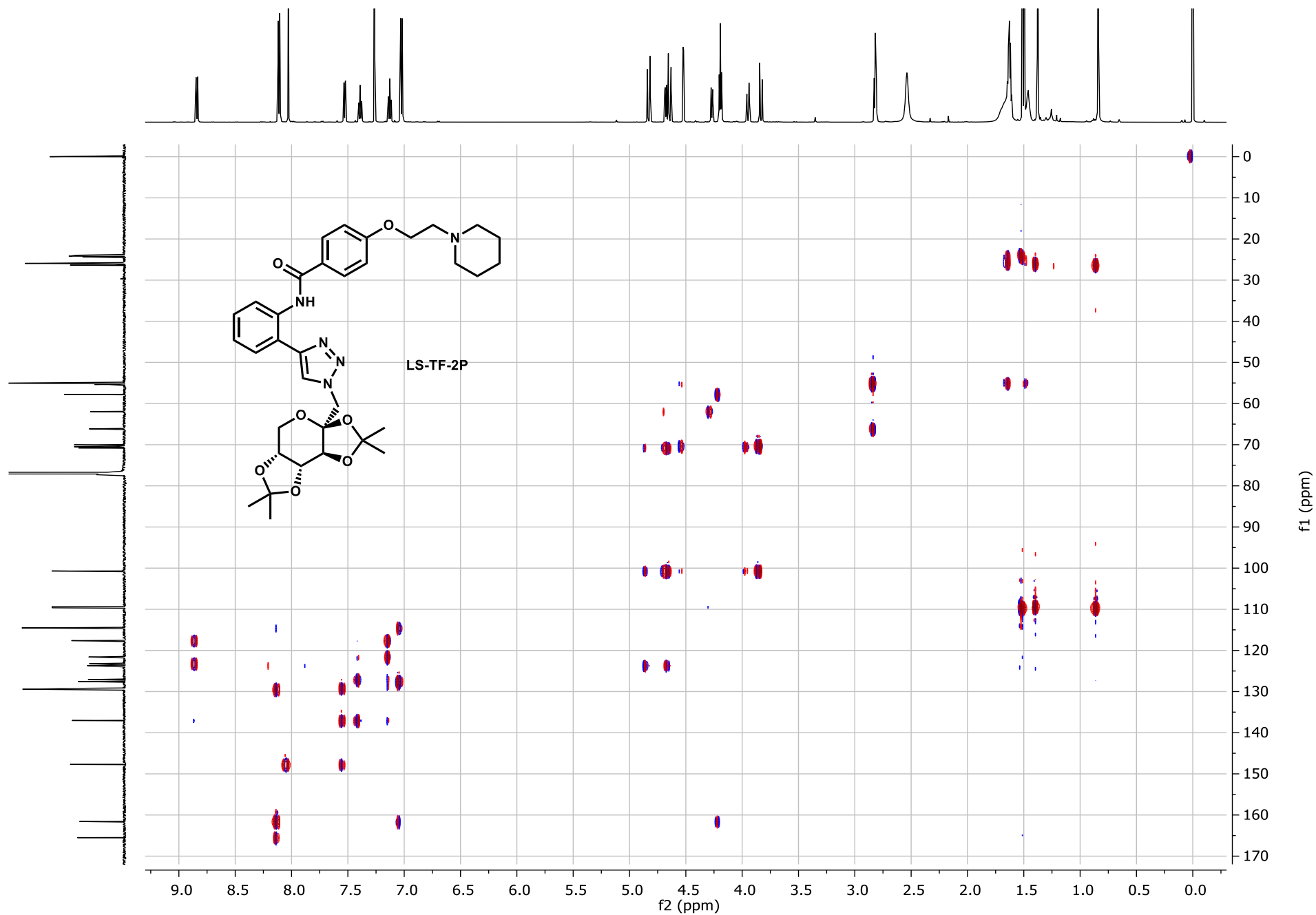
¹³C NMR Spectrum for LS-TF-2P (CDCl₃, 151 MHz).



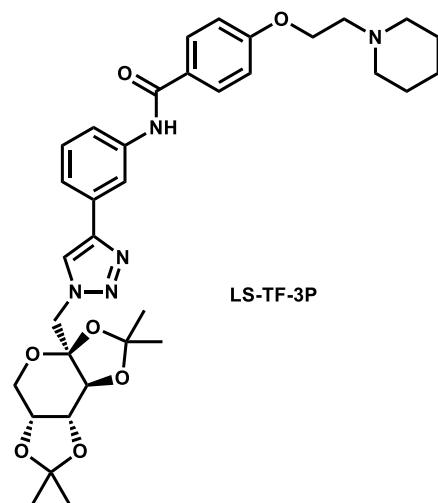
COSY Spectrum for **LS-TF-2P** (CDCl_3).



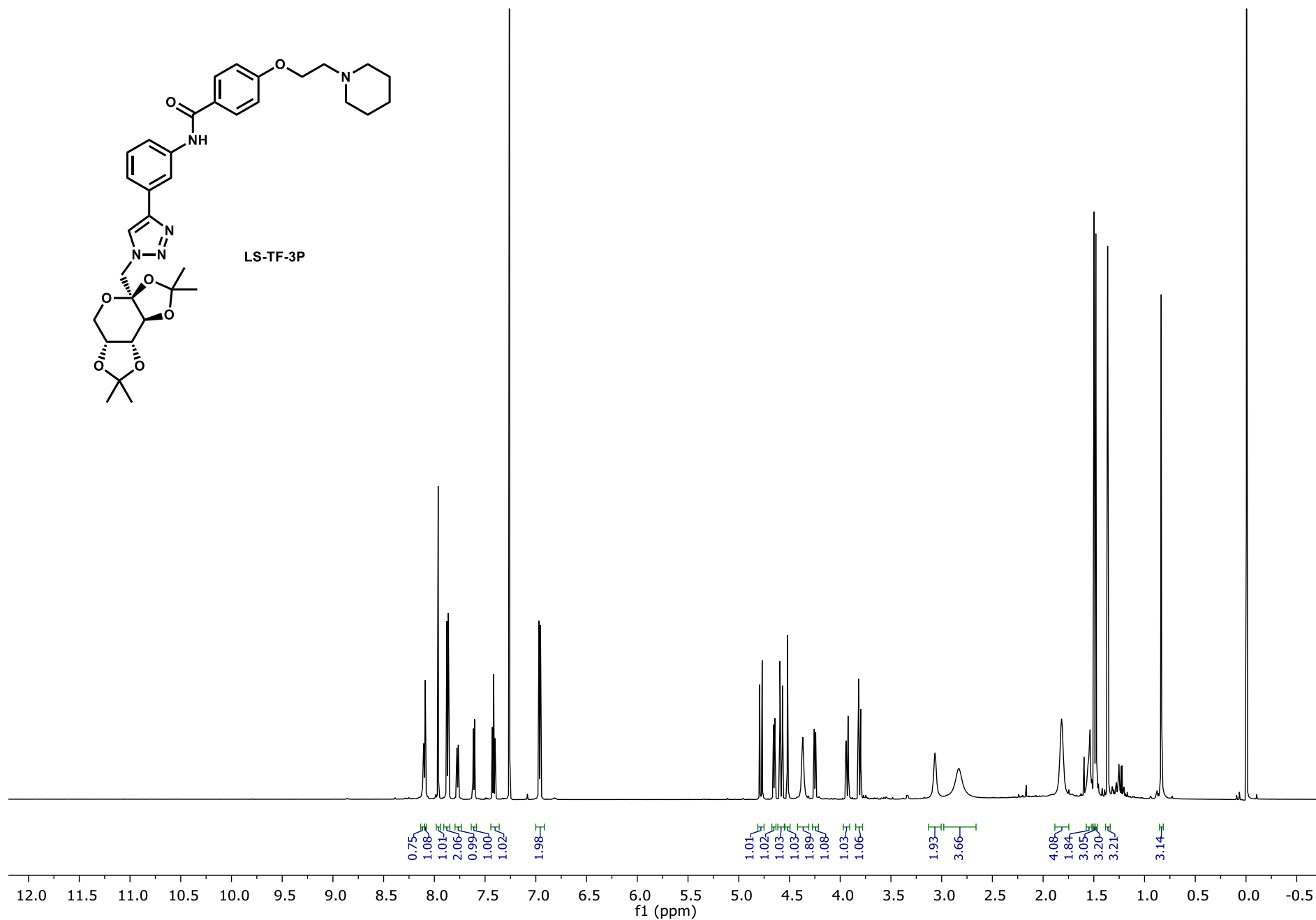
HSQC Spectrum for **LS-TF-2P** (CDCl_3).



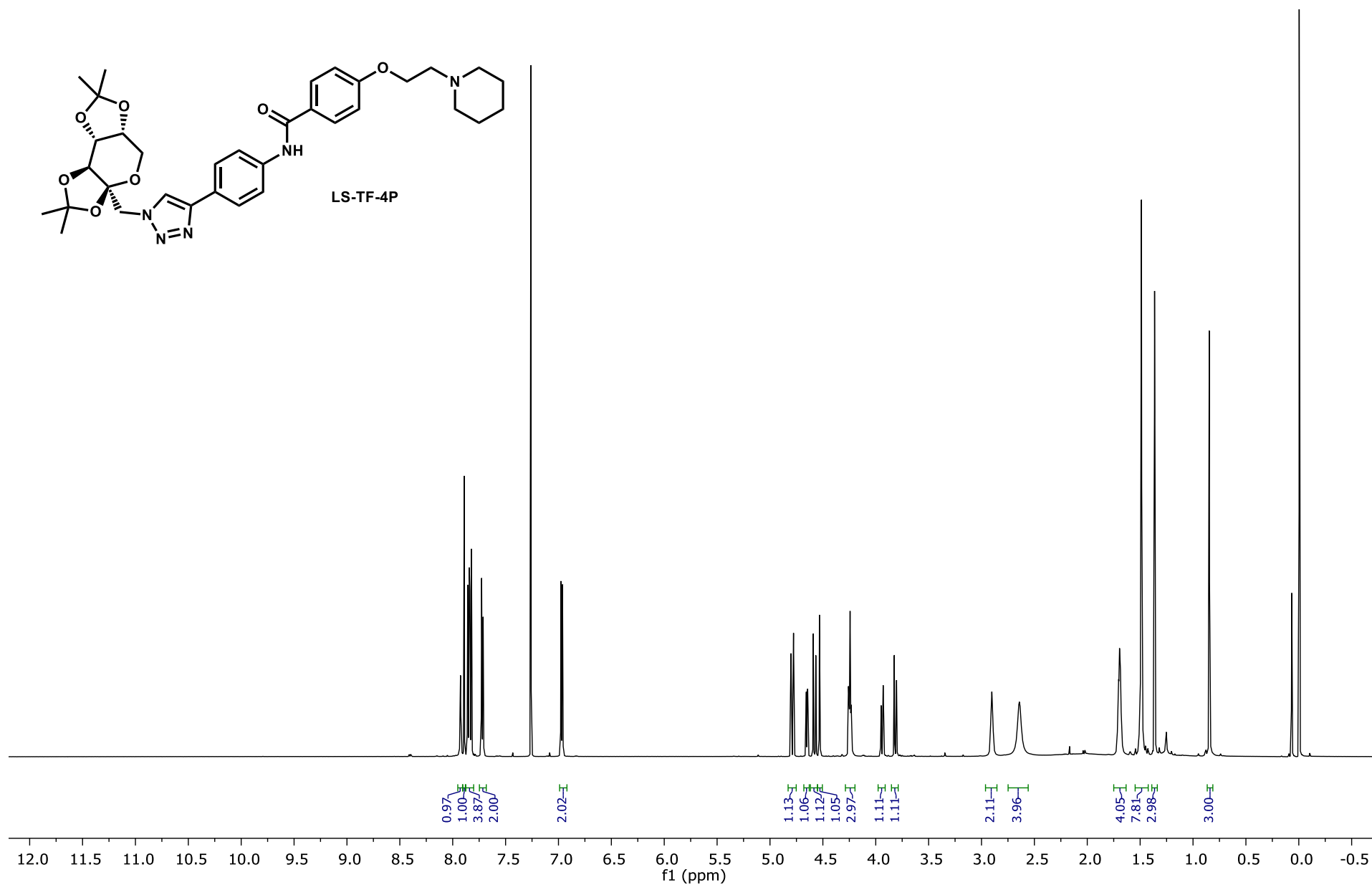
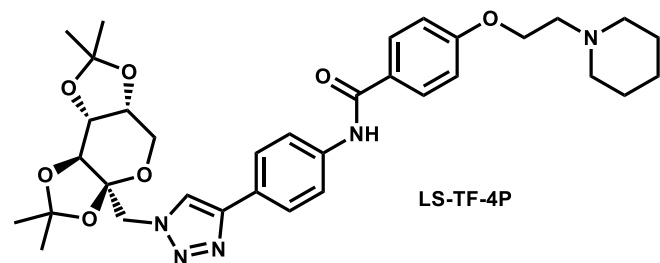
HMBC Spectrum for LS-TF-2P (CDCl_3).



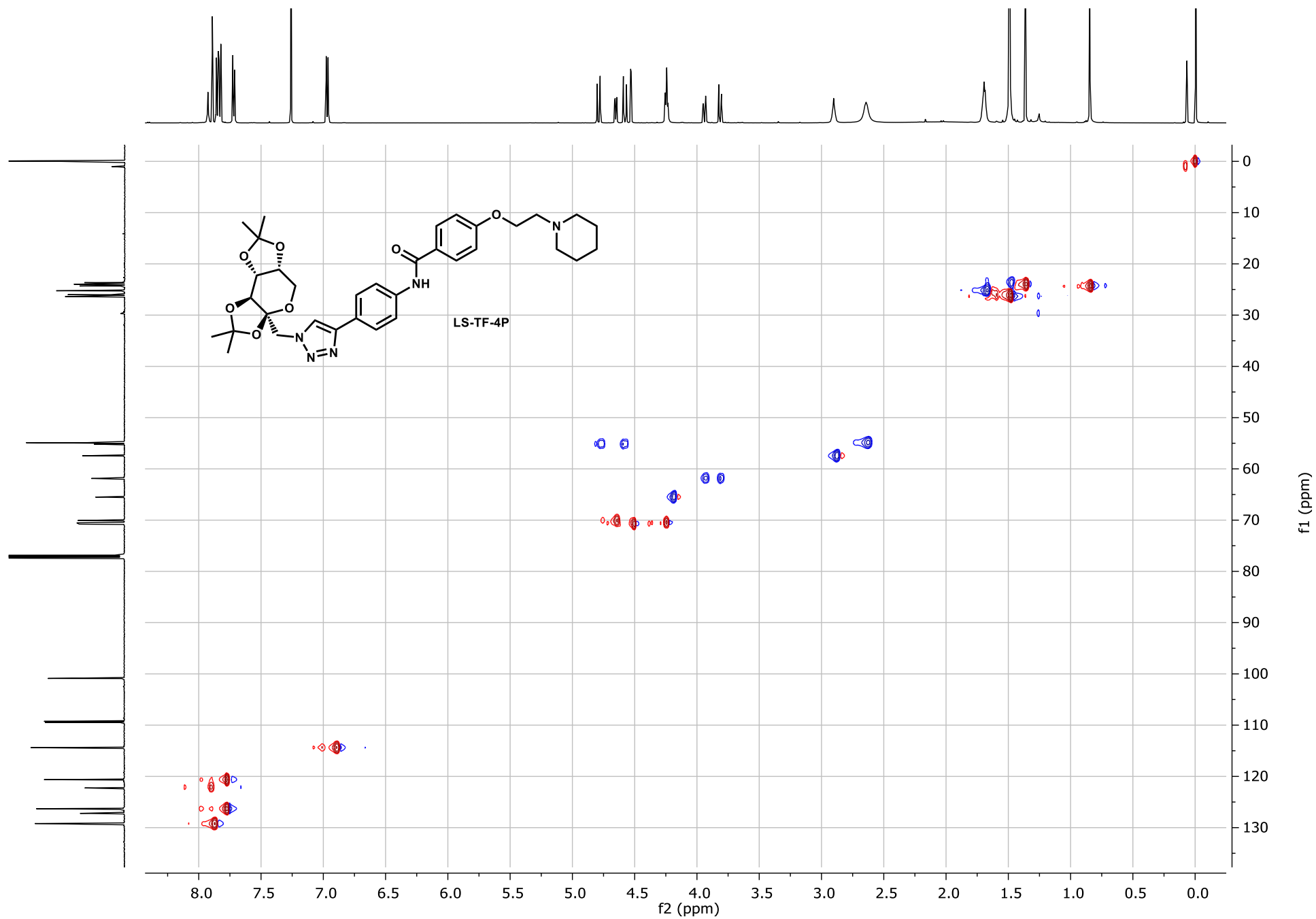
LS-TF-3P



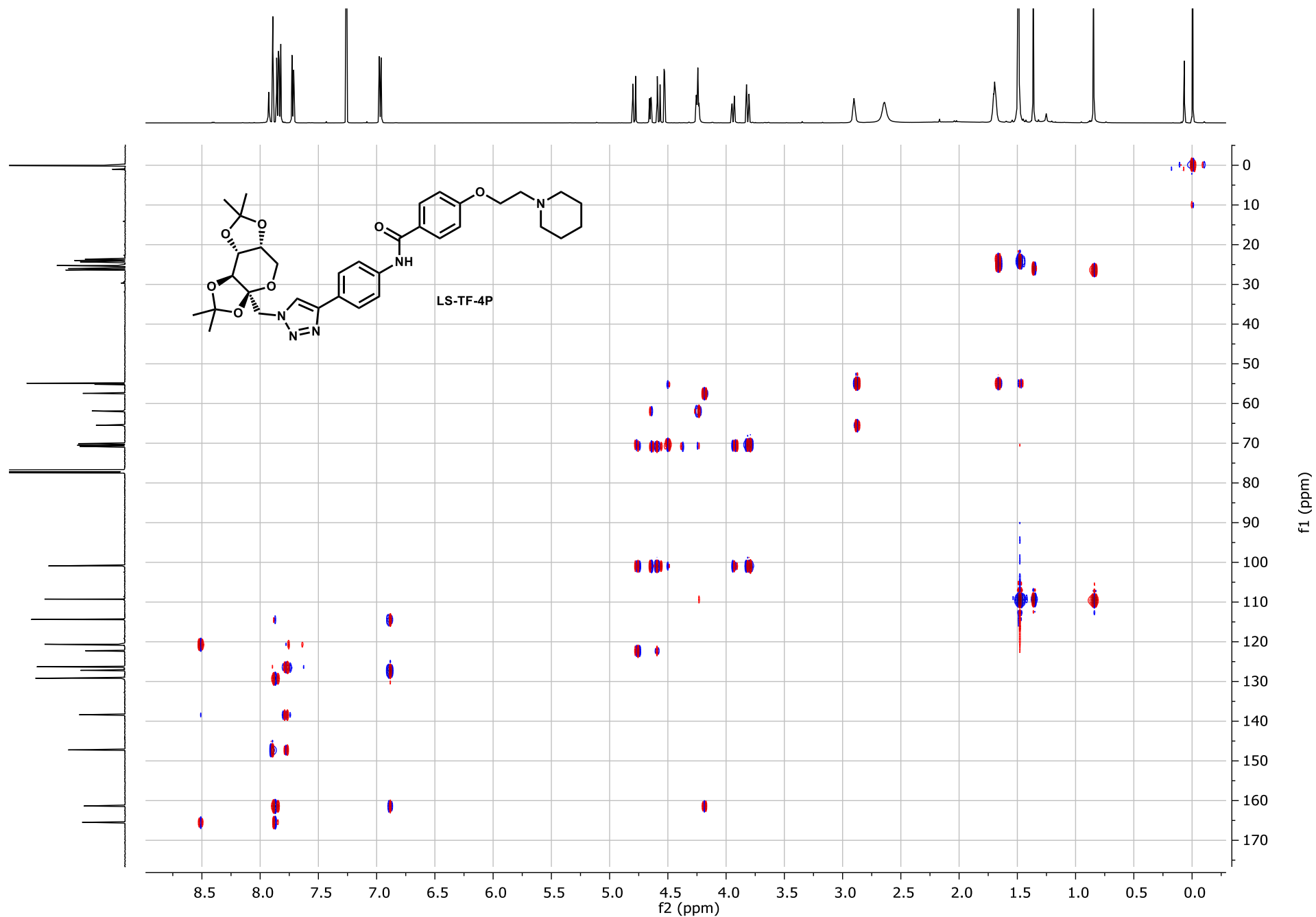
^1H NMR Spectrum for **LS-TF-3P** (CDCl_3 , 600 MHz).



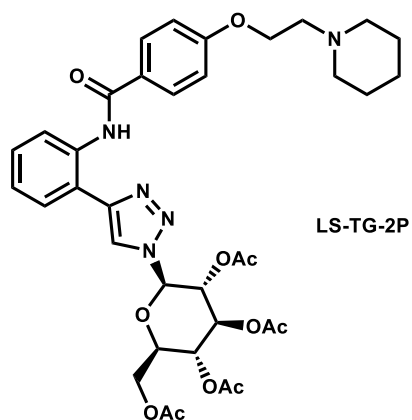
^1H NMR Spectrum for **LS-TF-4P** (CDCl_3 , 600 MHz).



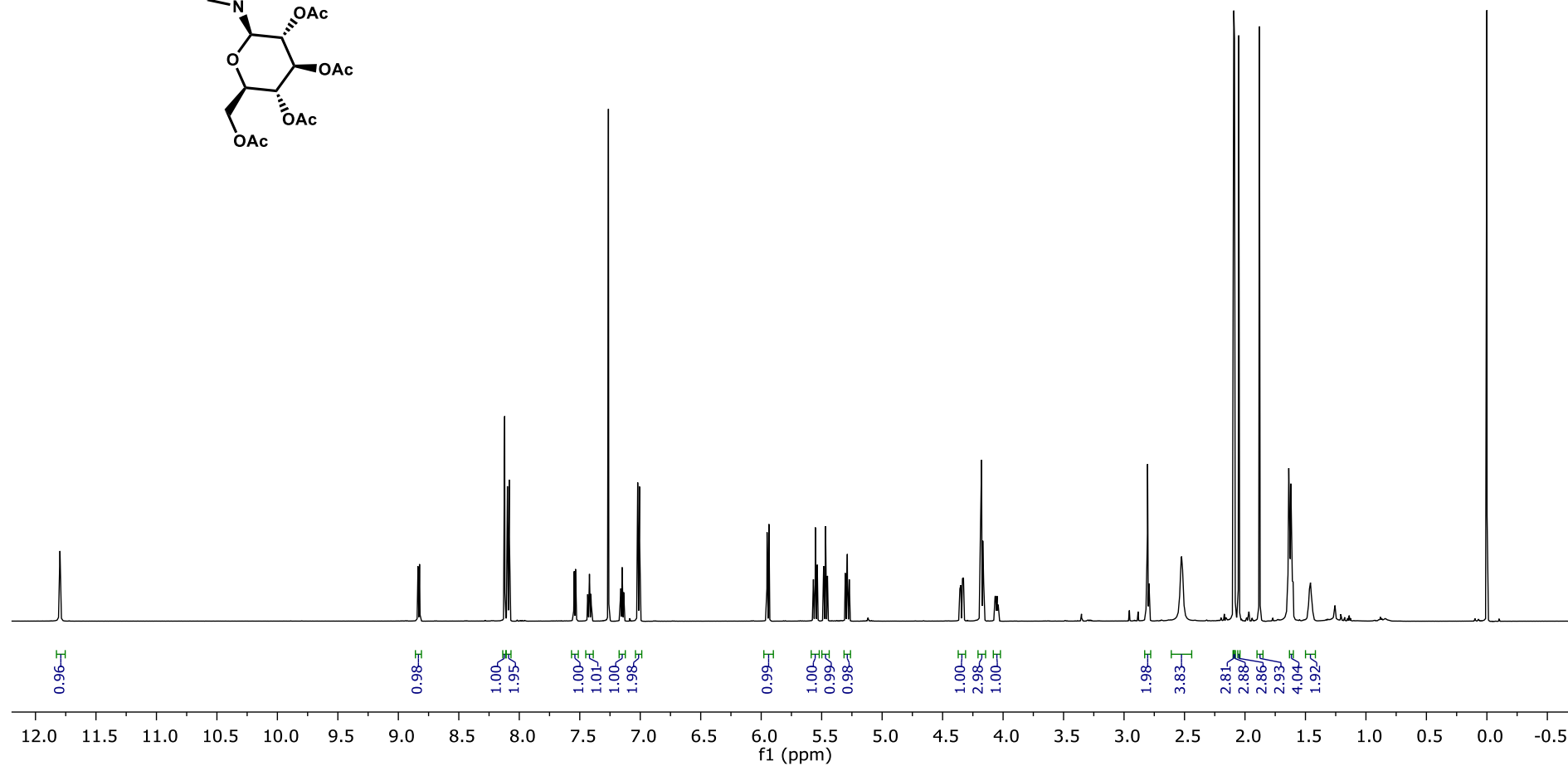
HSQC Spectrum for LS-TF-4P (CDCl₃).



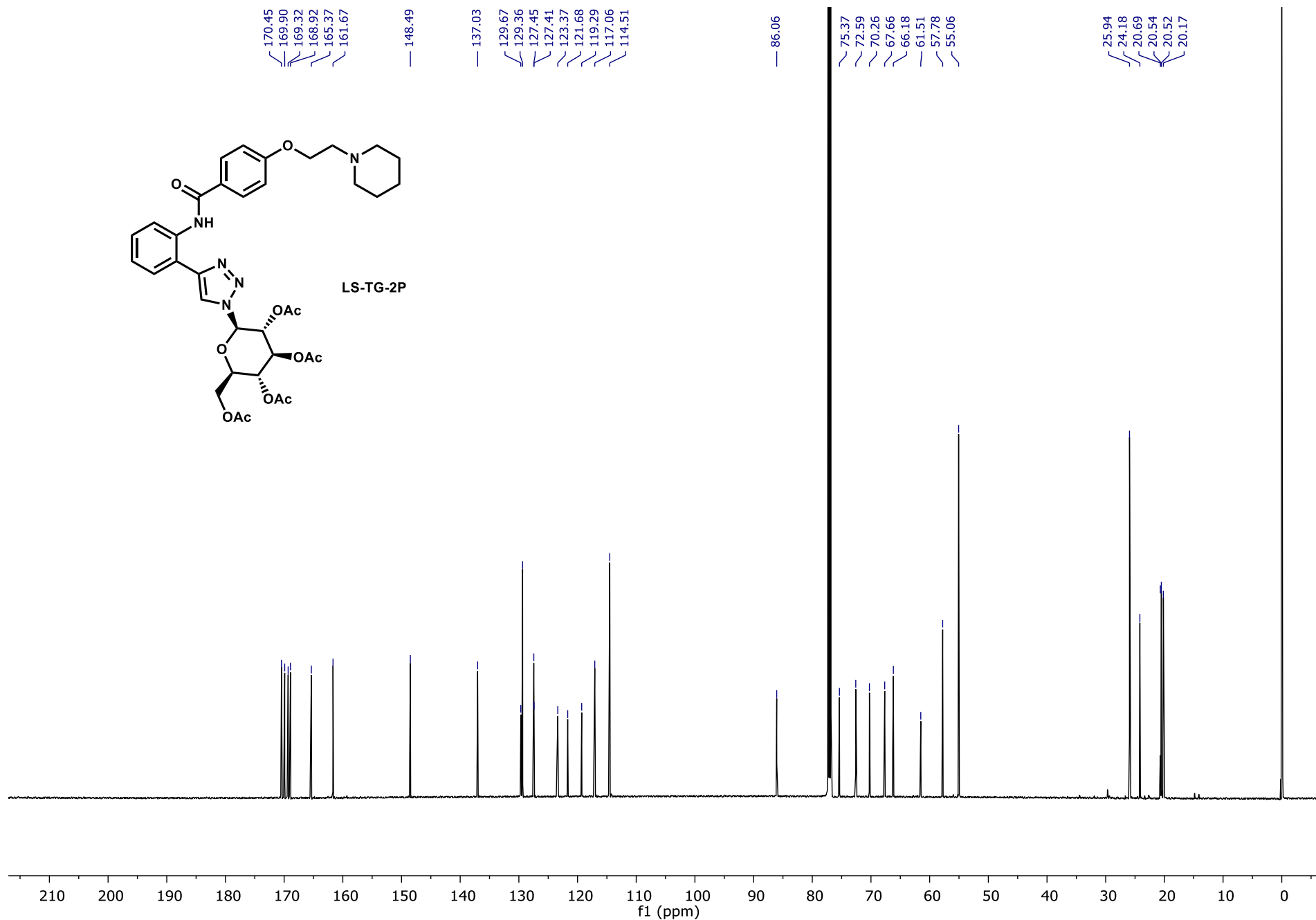
HMBC Spectrum for **LS-TF-4P** (CDCl_3).



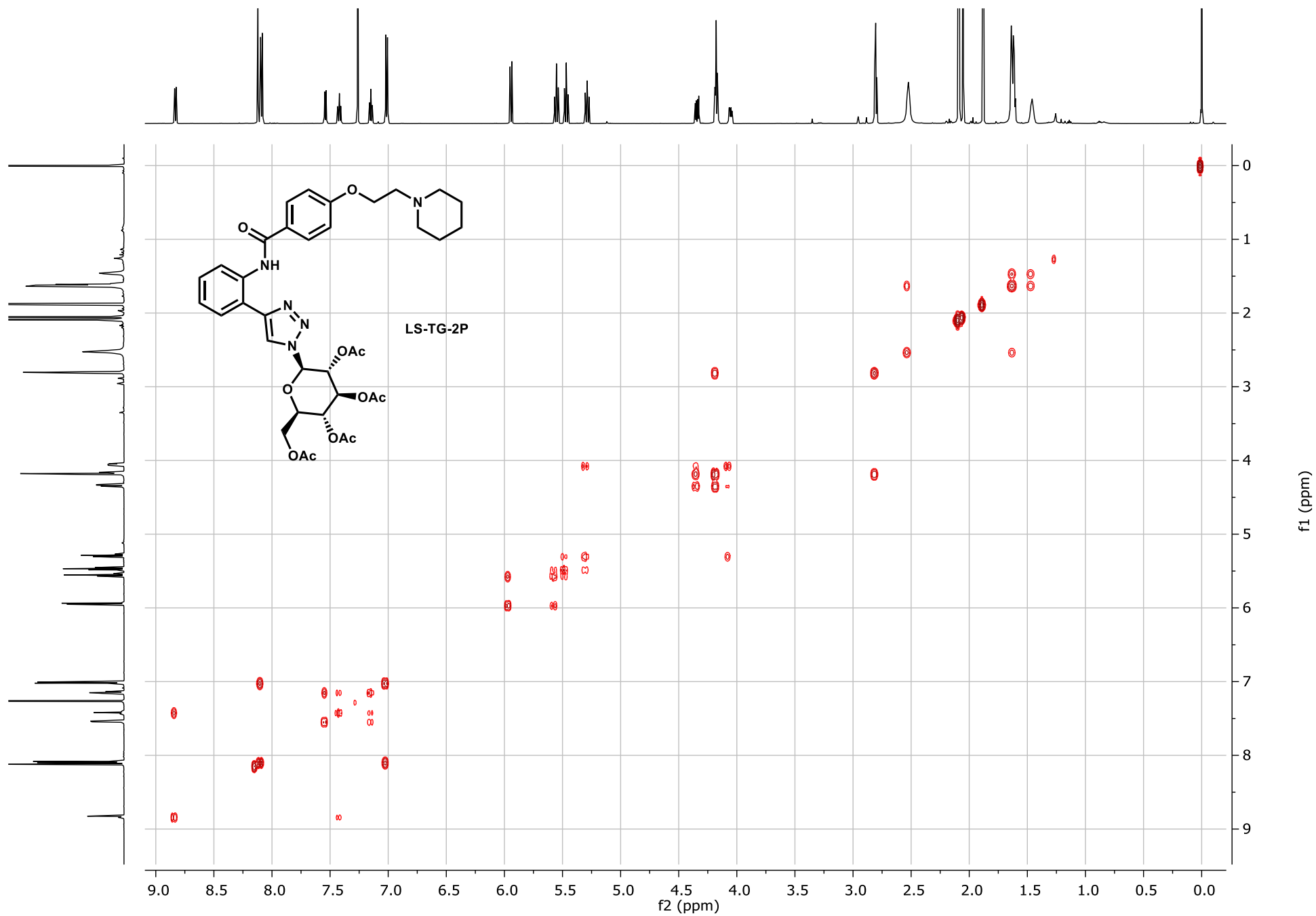
LS-TG-2P



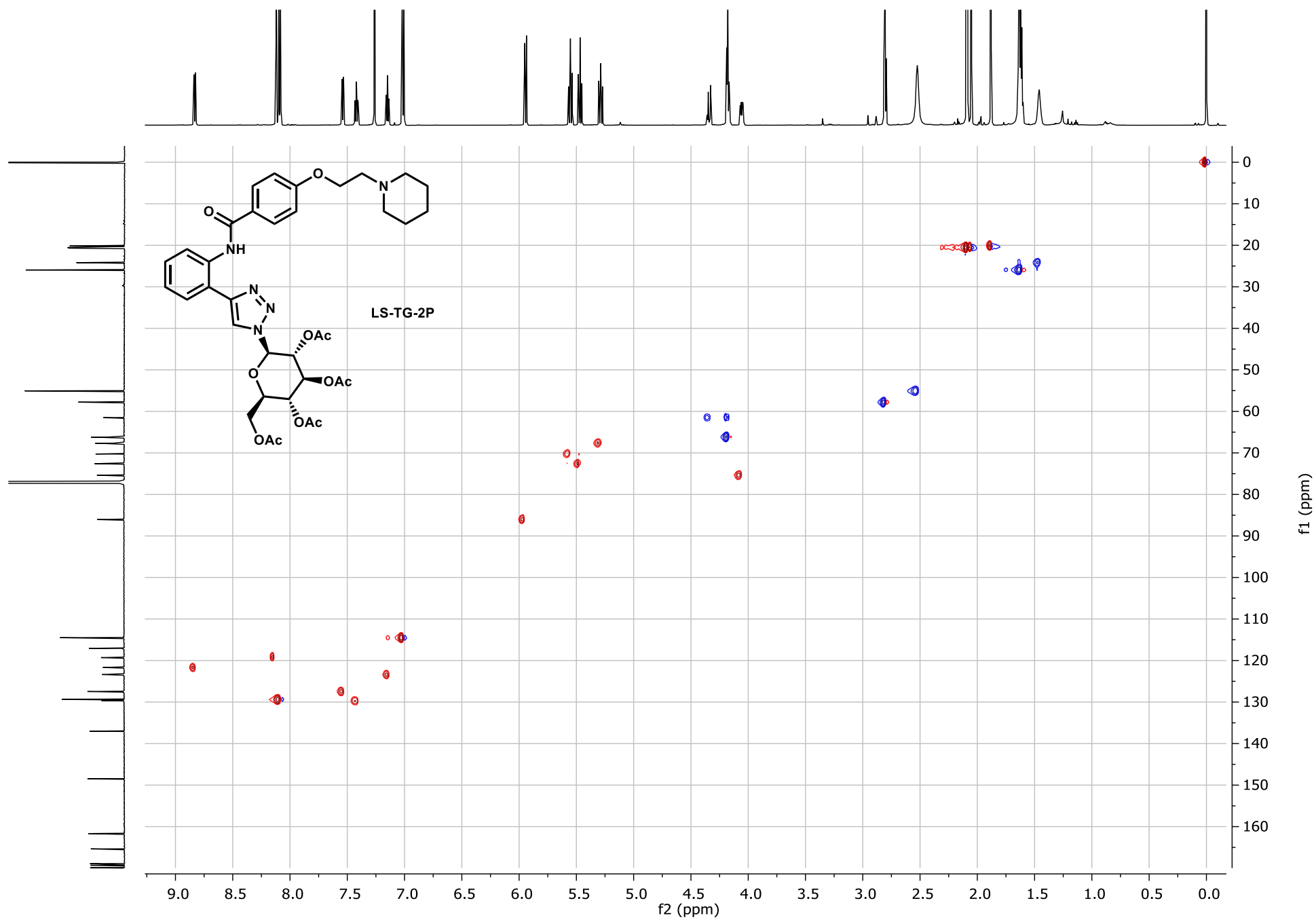
¹H NMR Spectrum for LS-TG-2P (CDCl₃, 600 MHz).

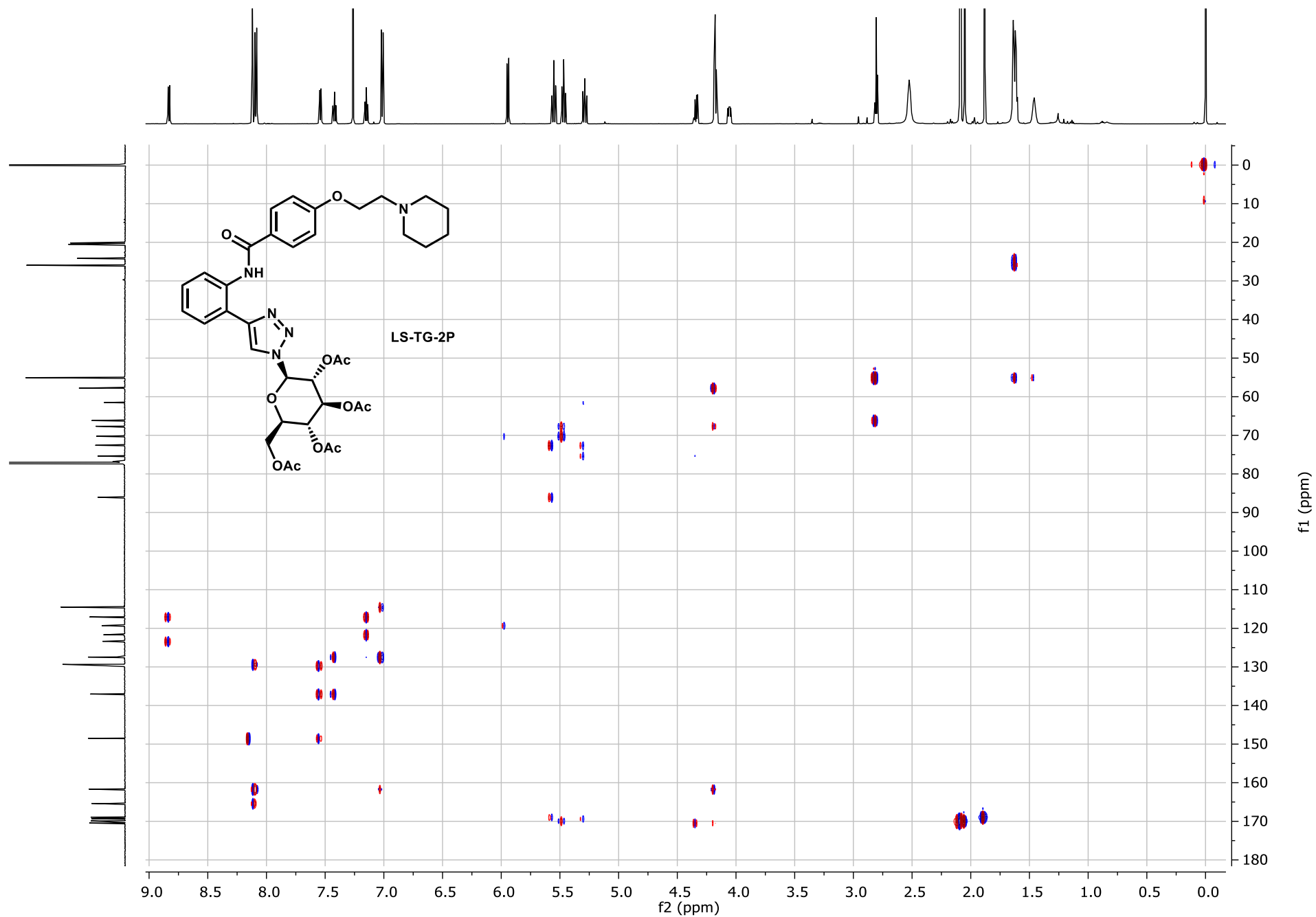


¹³C NMR Spectrum for **LS-TG-2P** (CDCl₃, 151 MHz).

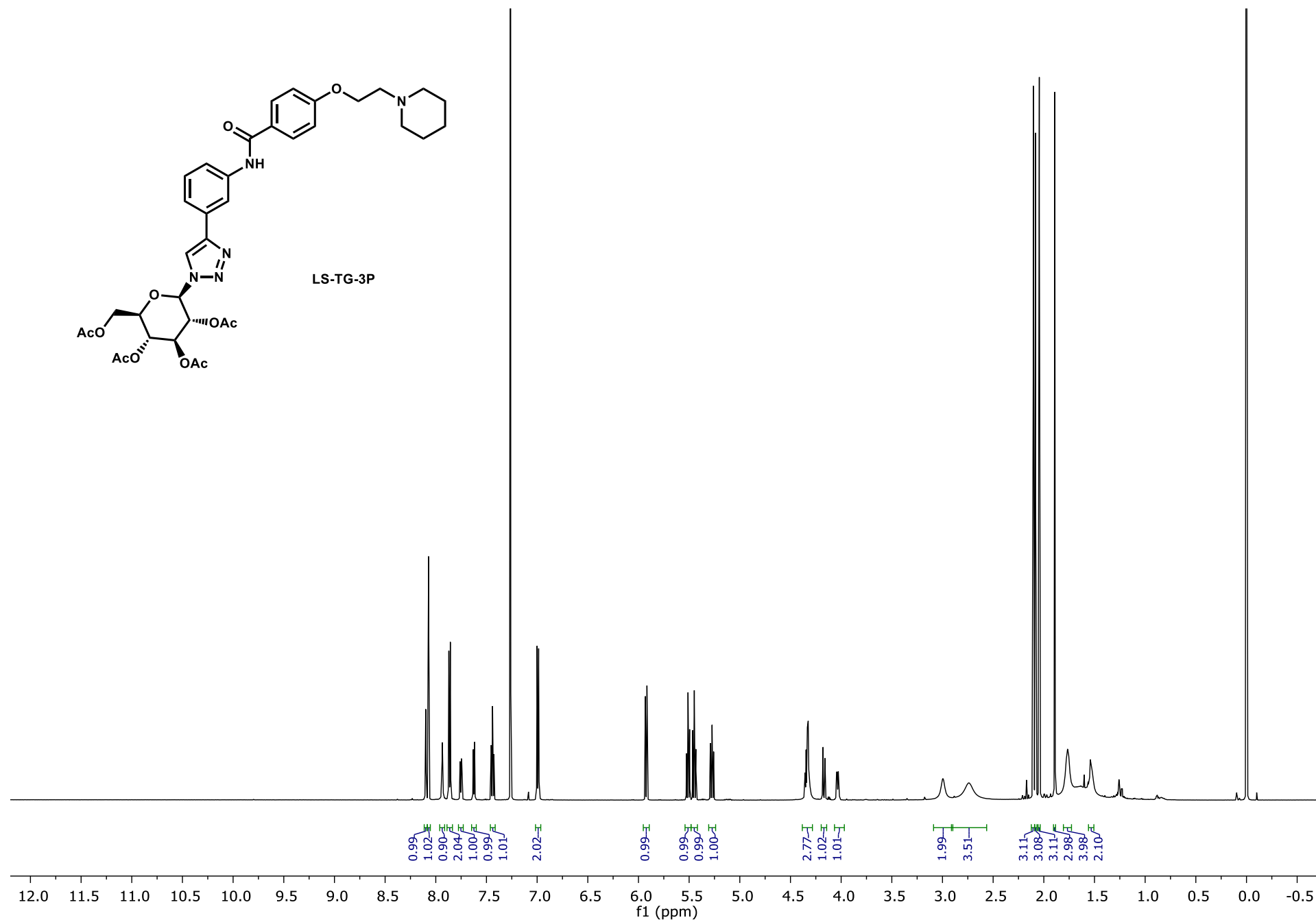


COSY Spectrum for **LS-TG-2P** (CDCl₃).

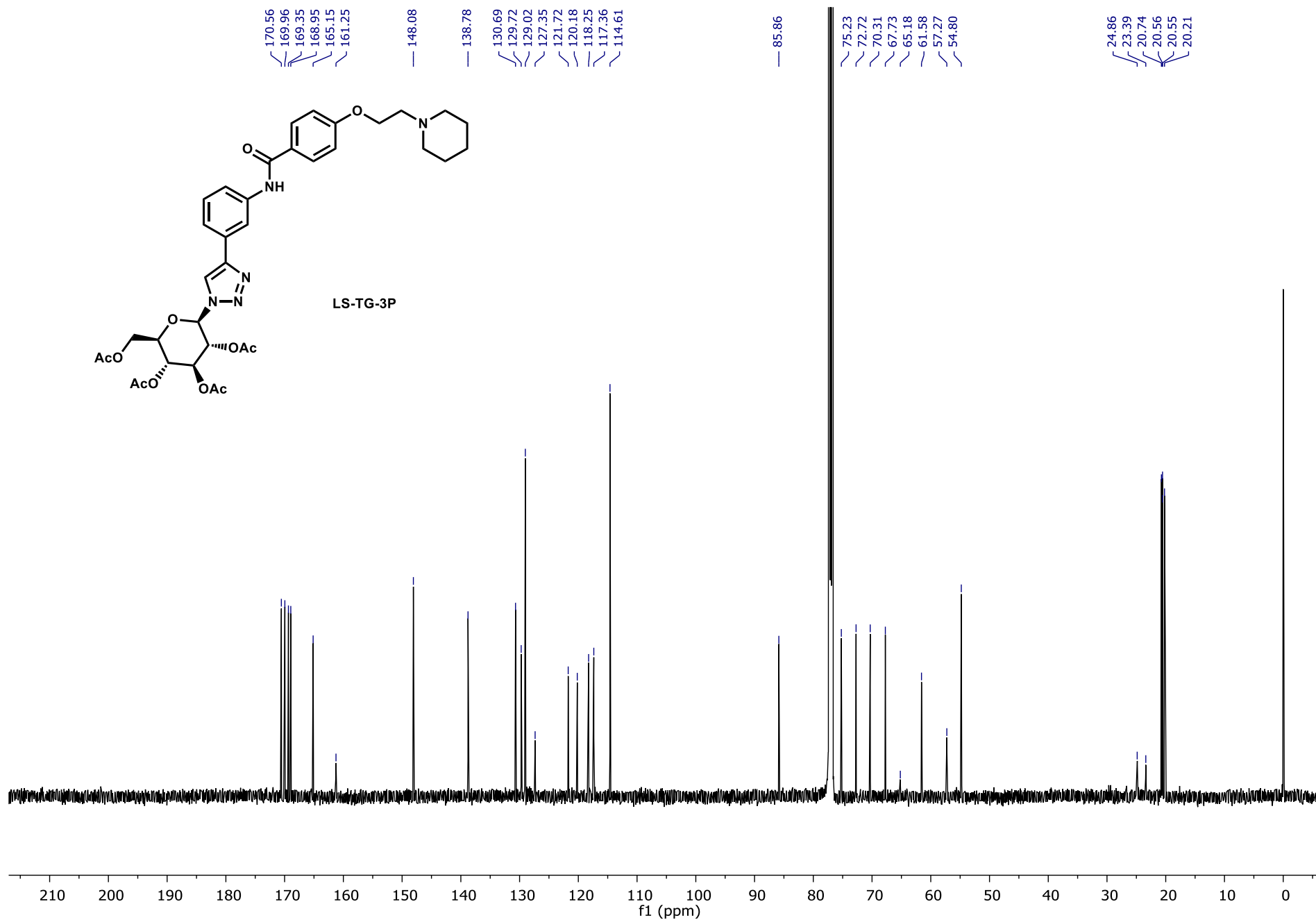




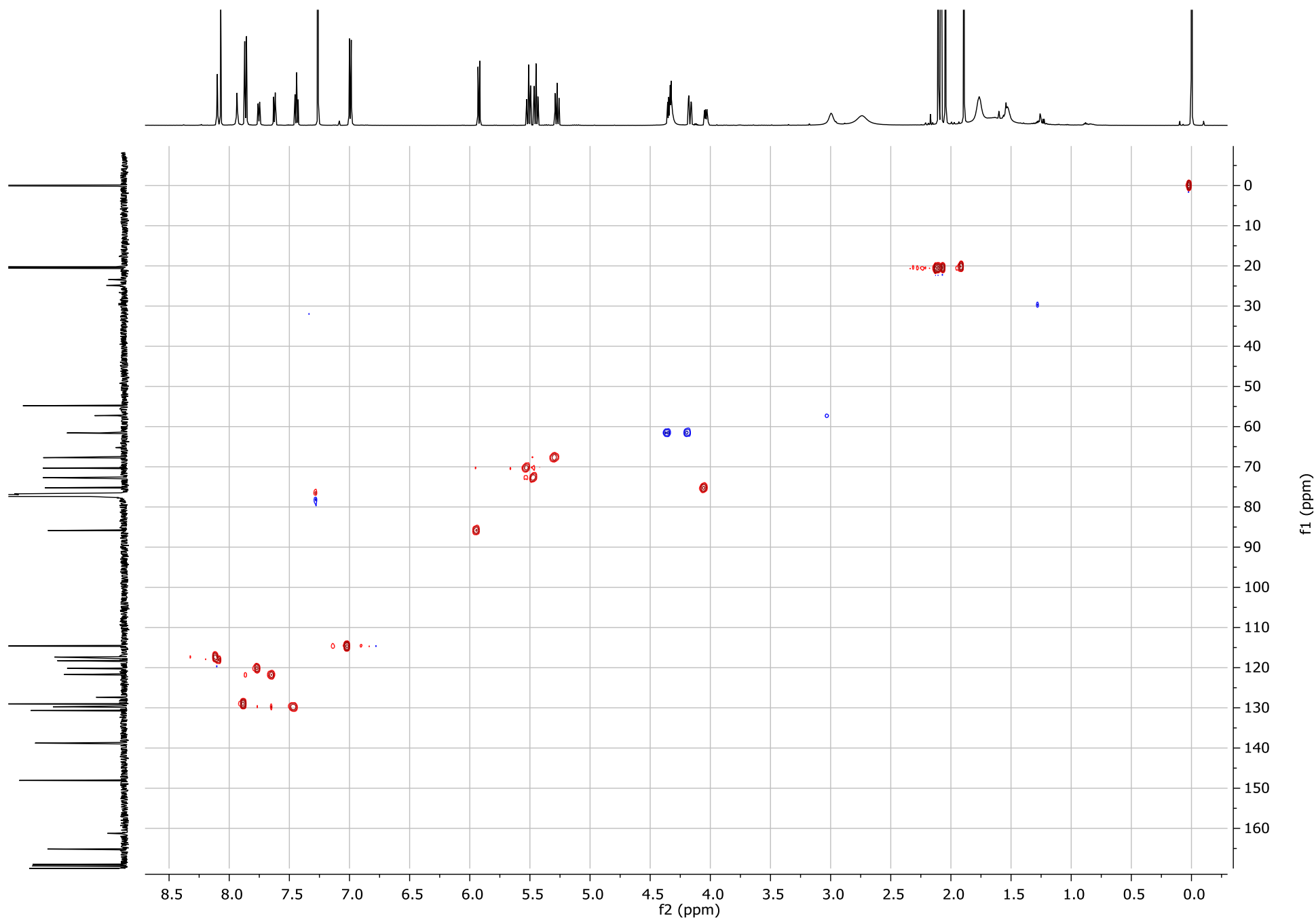
HMBC Spectrum for **LS-TG-2P** (CDCl_3).



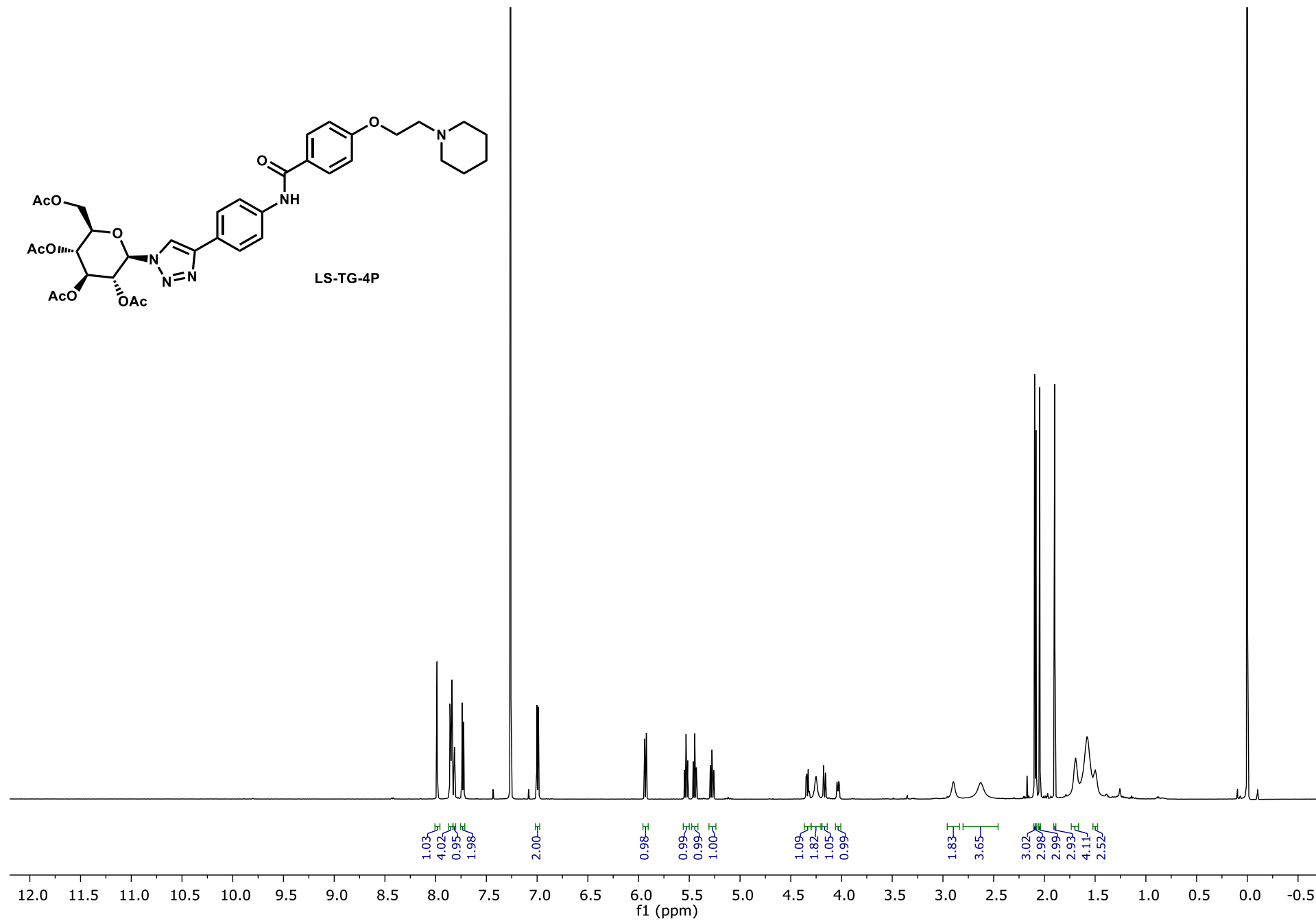
¹H NMR Spectrum for **LS-TG-3P** (CDCl₃, 600 MHz).



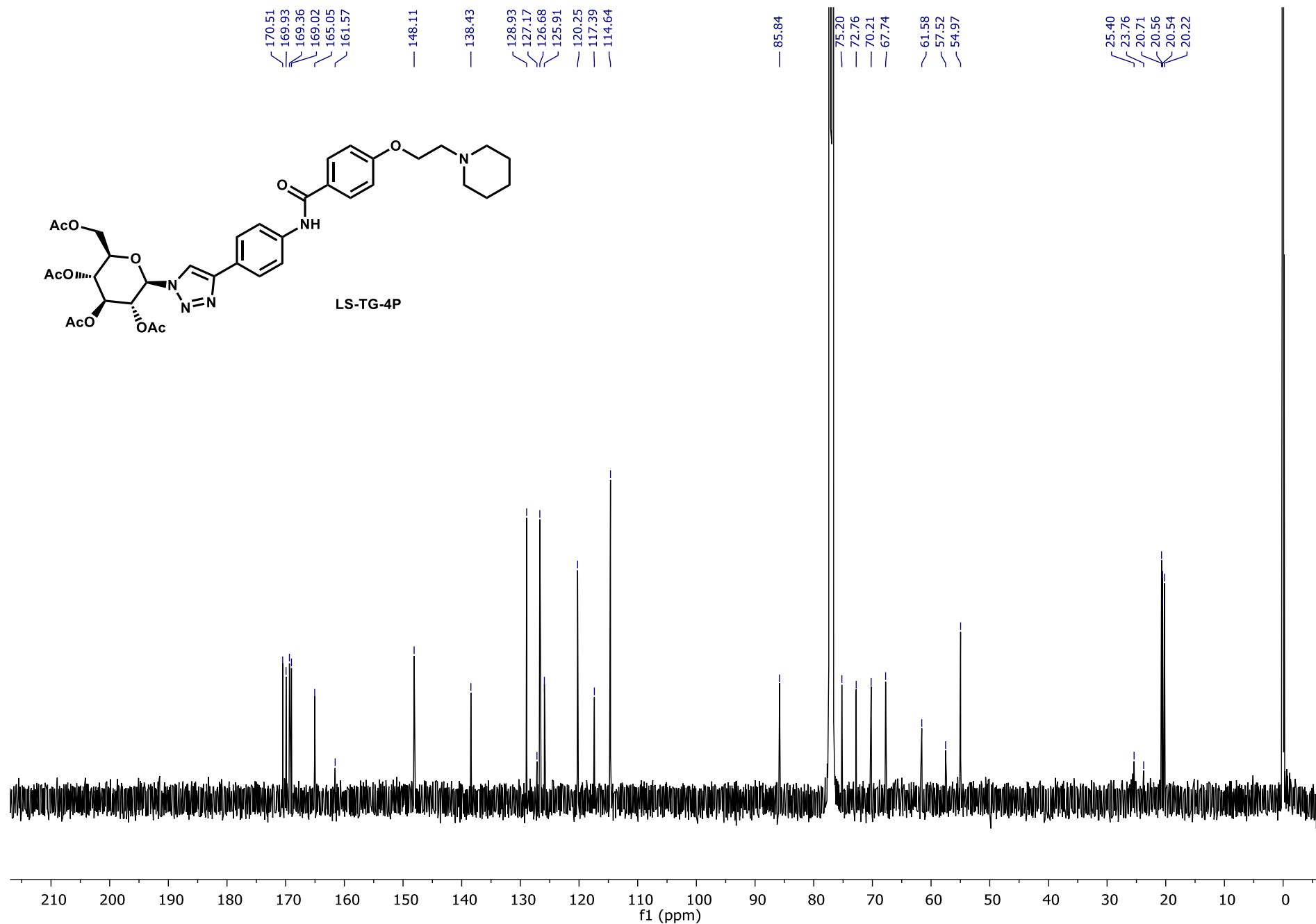
^{13}C NMR Spectrum for **LS-TG-3P** (CDCl_3 , 151 MHz).



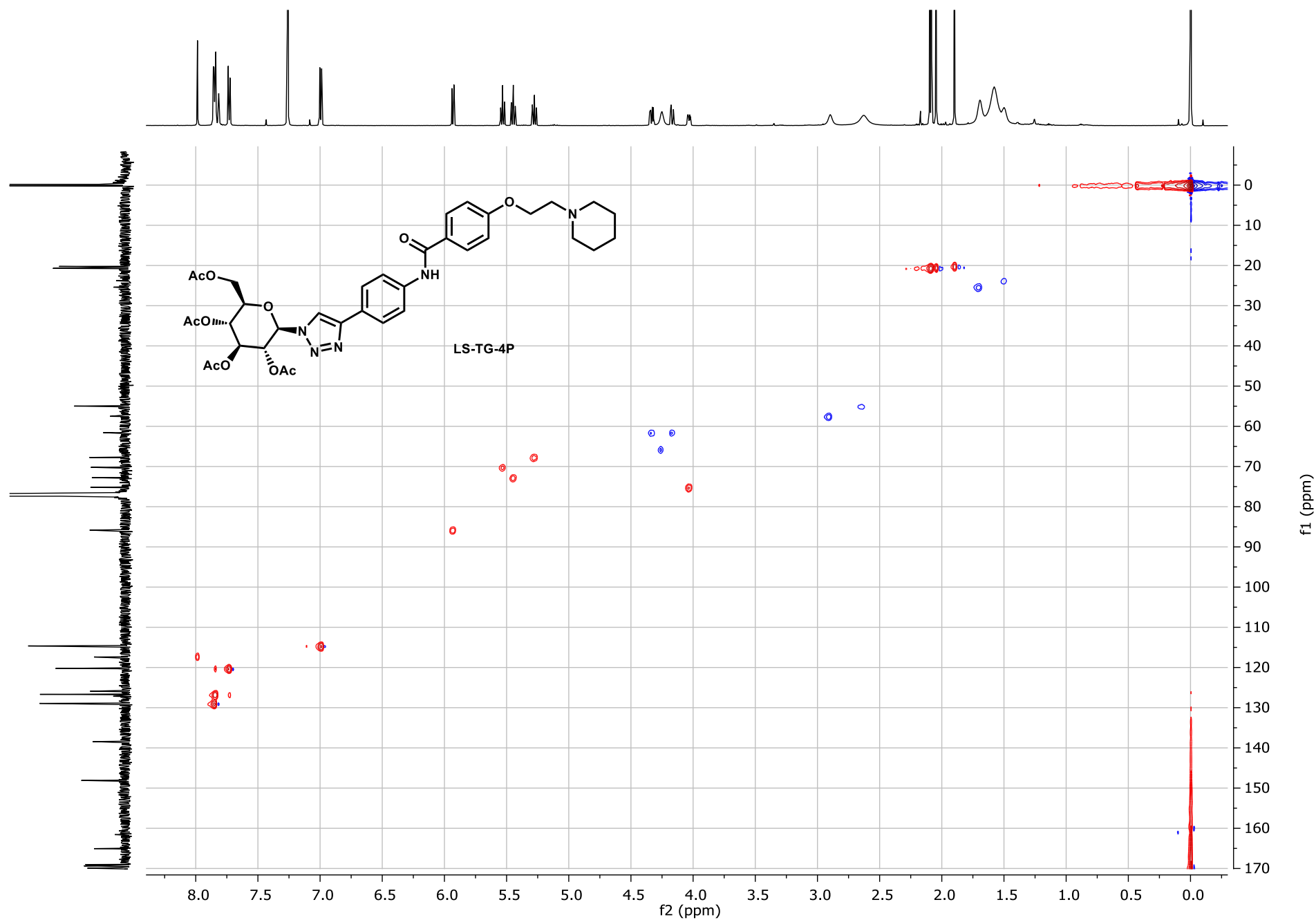
HSQC Spectrum for LS-TG-3P (CDCl_3).



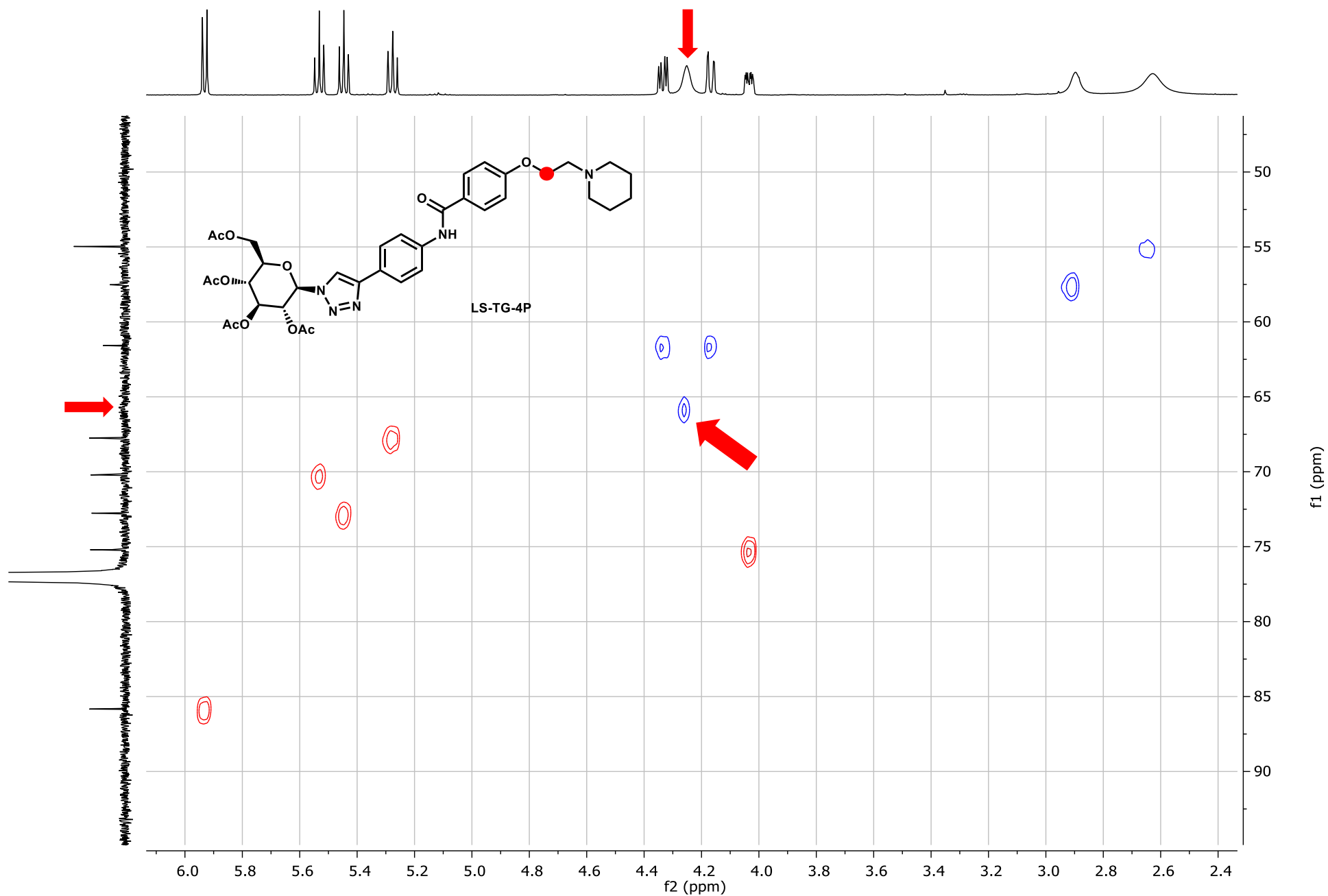
^1H NMR Spectrum for **LS-TG-4P** (CDCl_3 , 600 MHz).

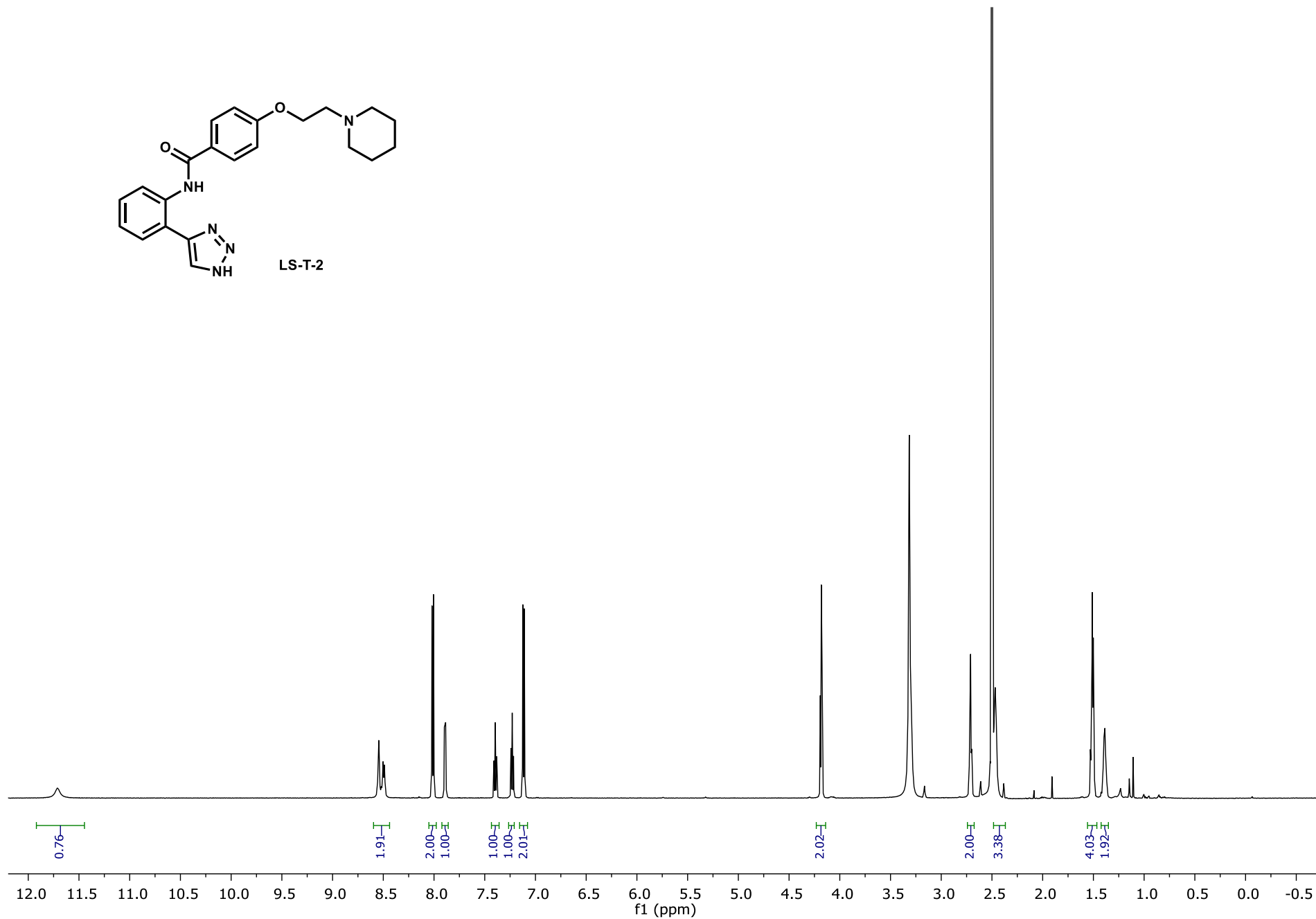
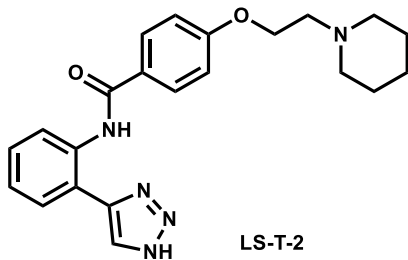


^{13}C NMR Spectrum for **LS-TG-4P** (CDCl_3 , 151 MHz).

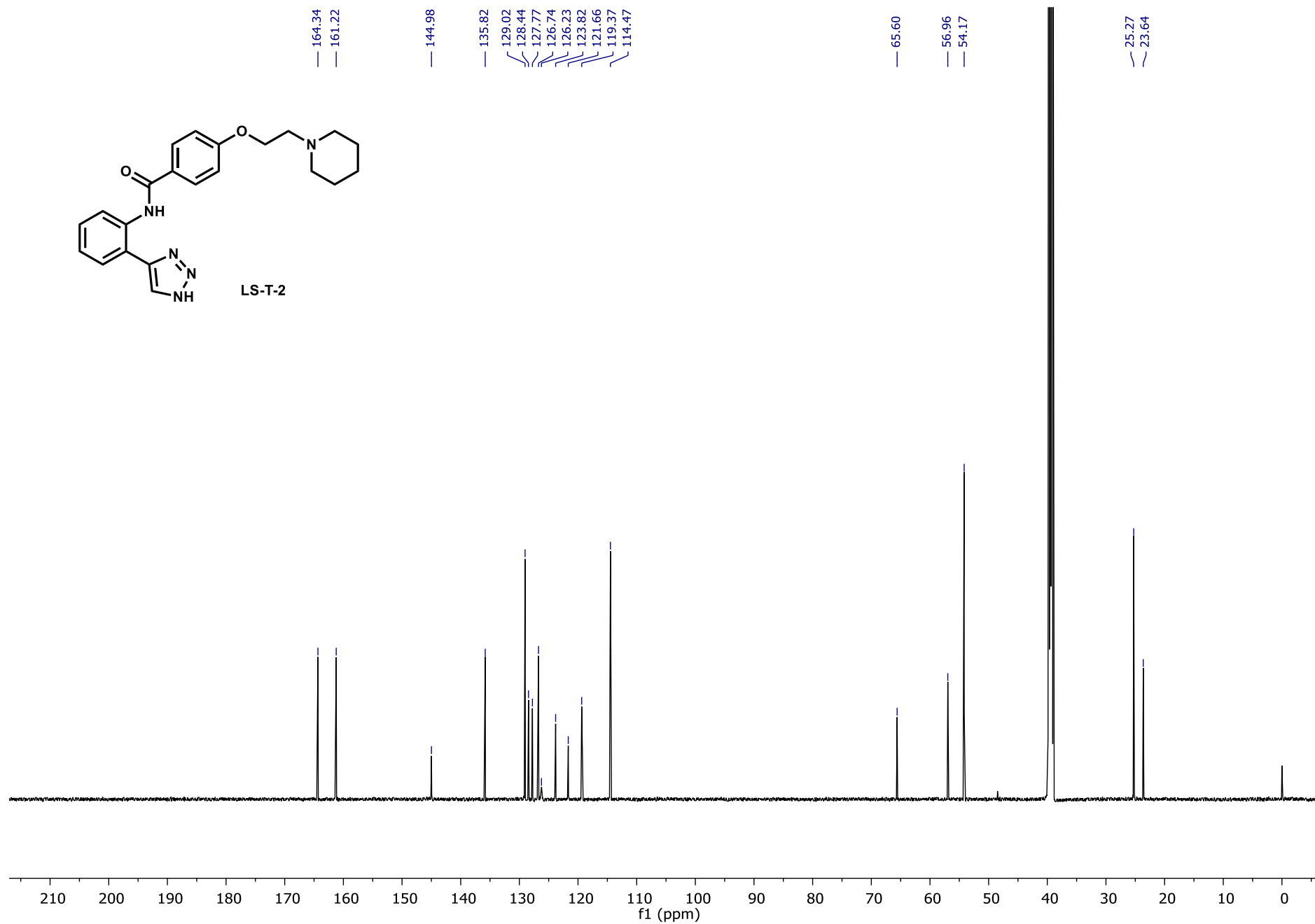
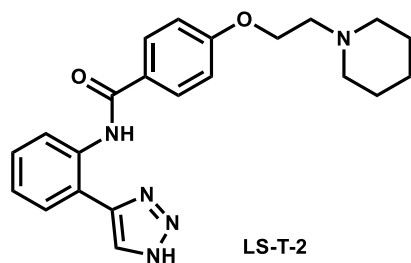


HSQC Spectrum for LS-TG-4P (CDCl_3).

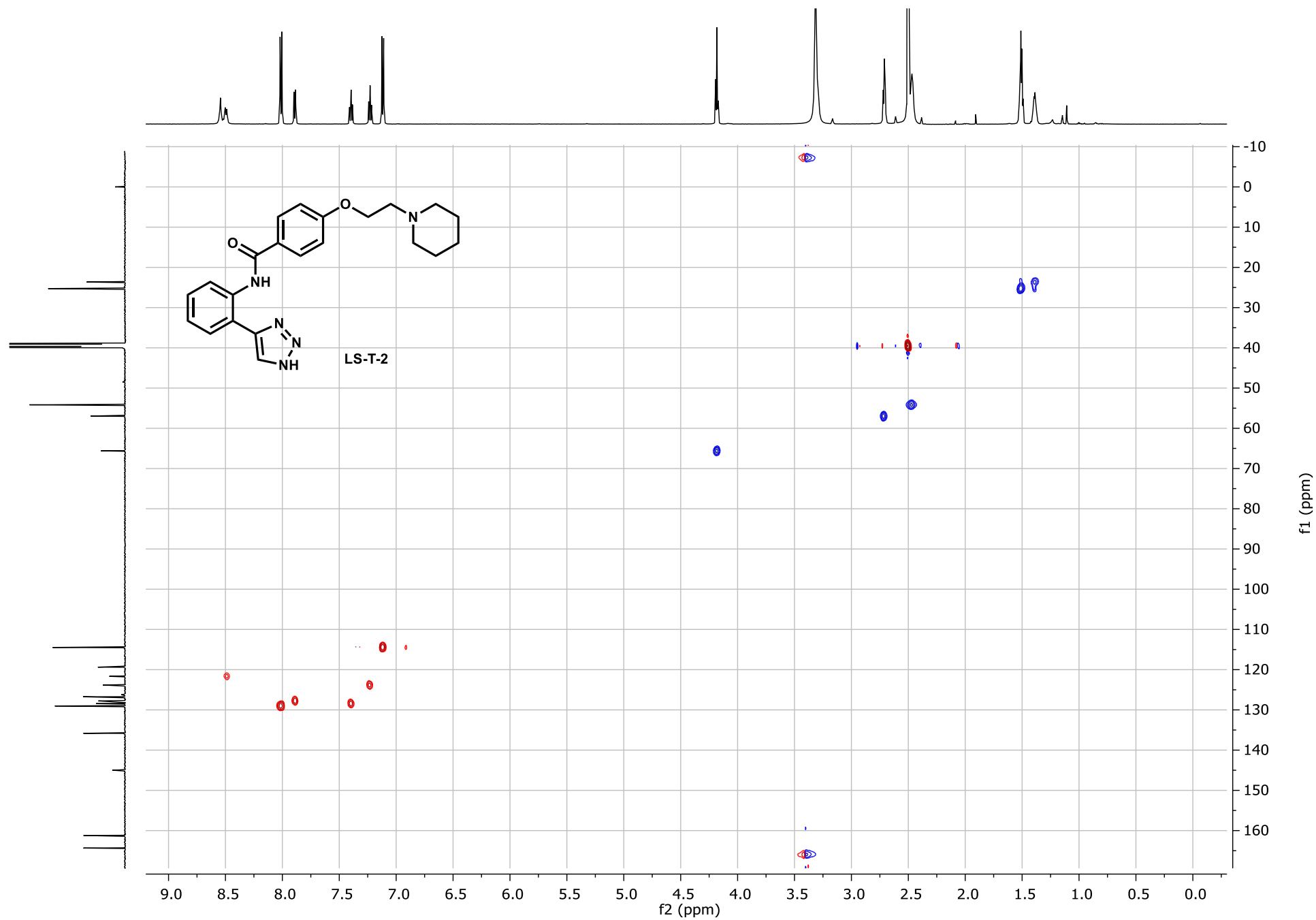




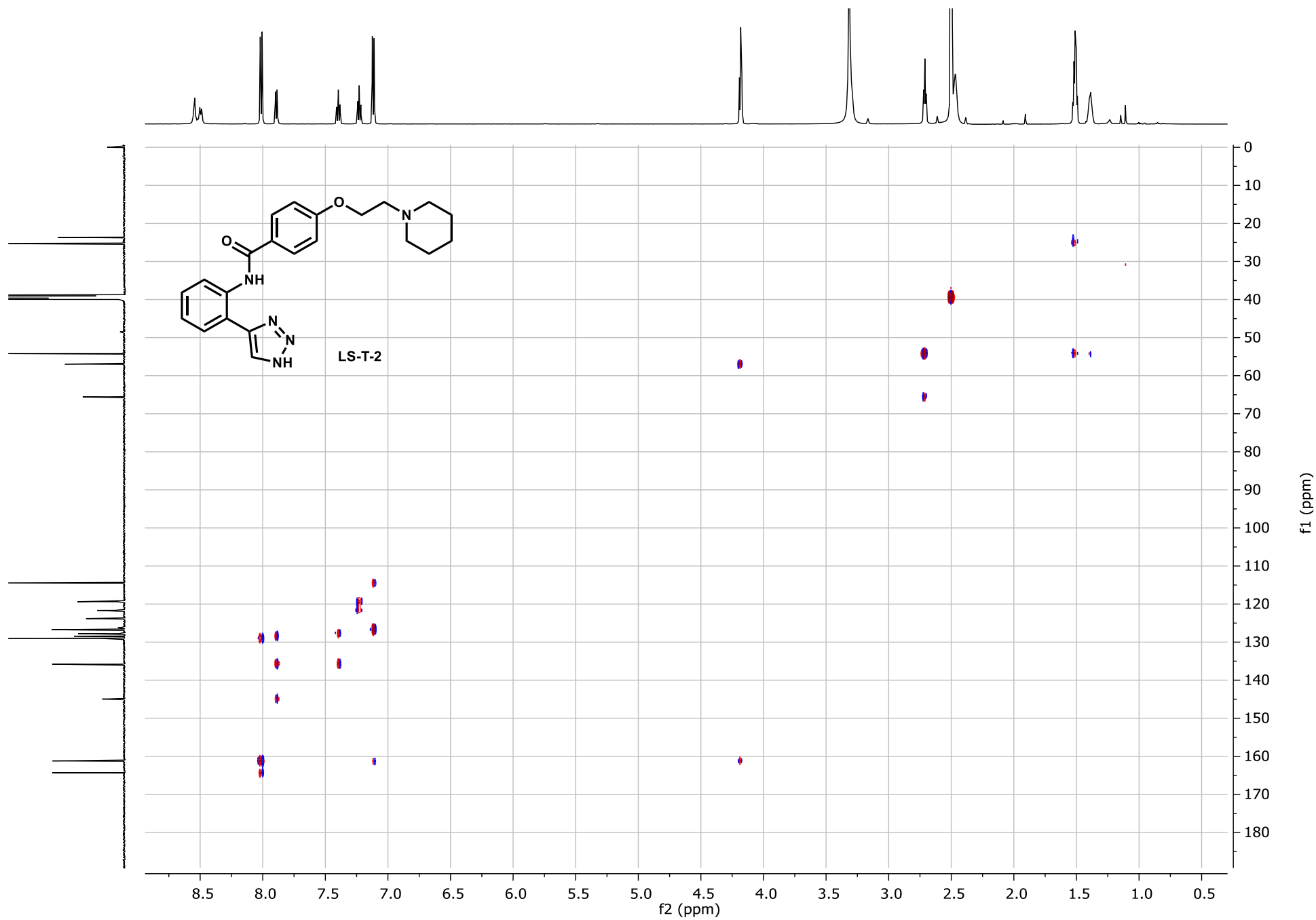
¹H NMR Spectrum for LS-T-2 (DMSO-*d*₆, 600 MHz).



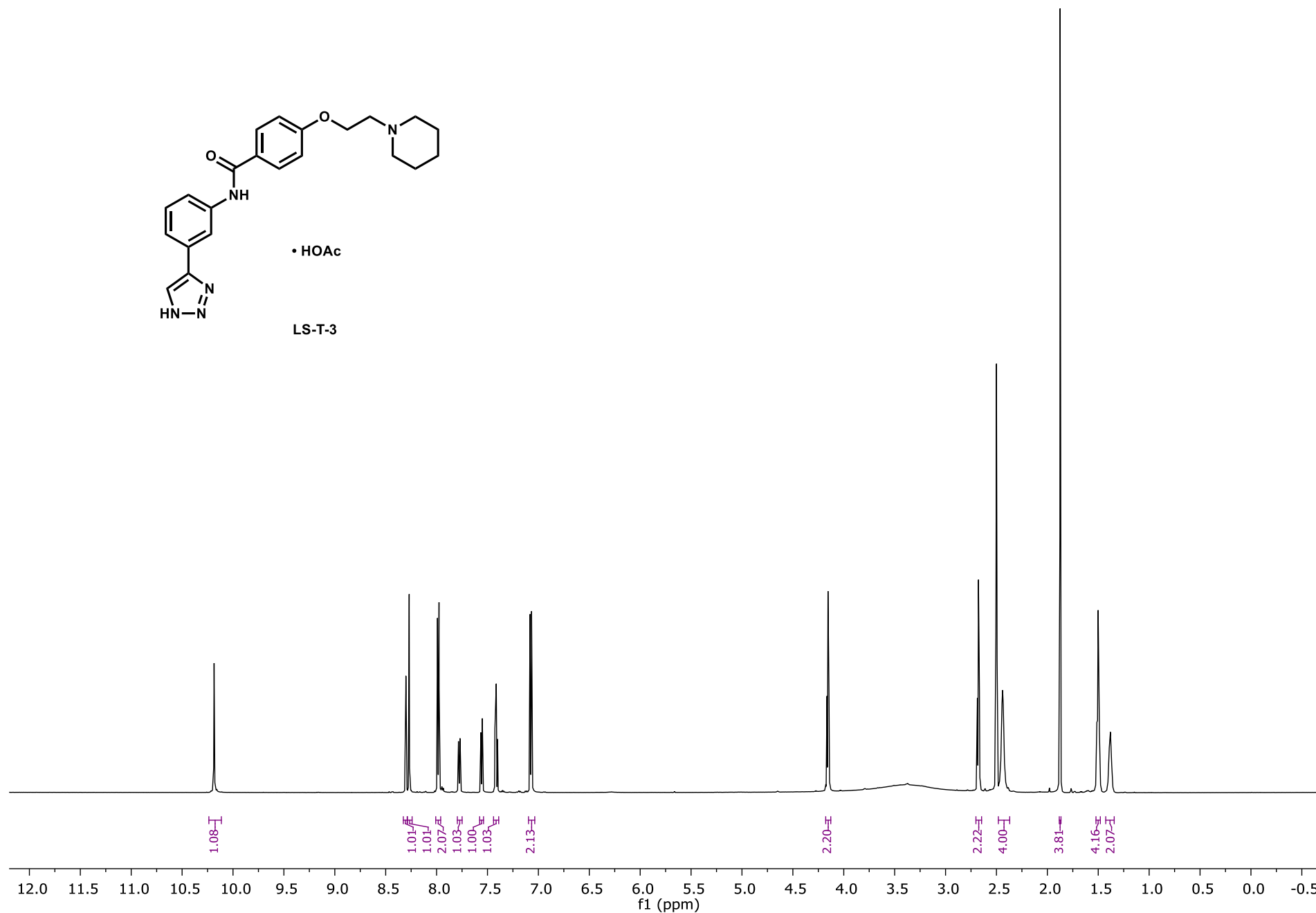
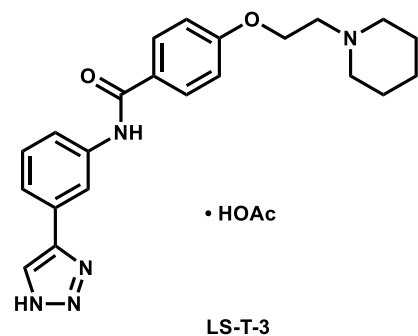
^{13}C NMR Spectrum for **LS-T-2** (DMSO- d_6 , 151 MHz).



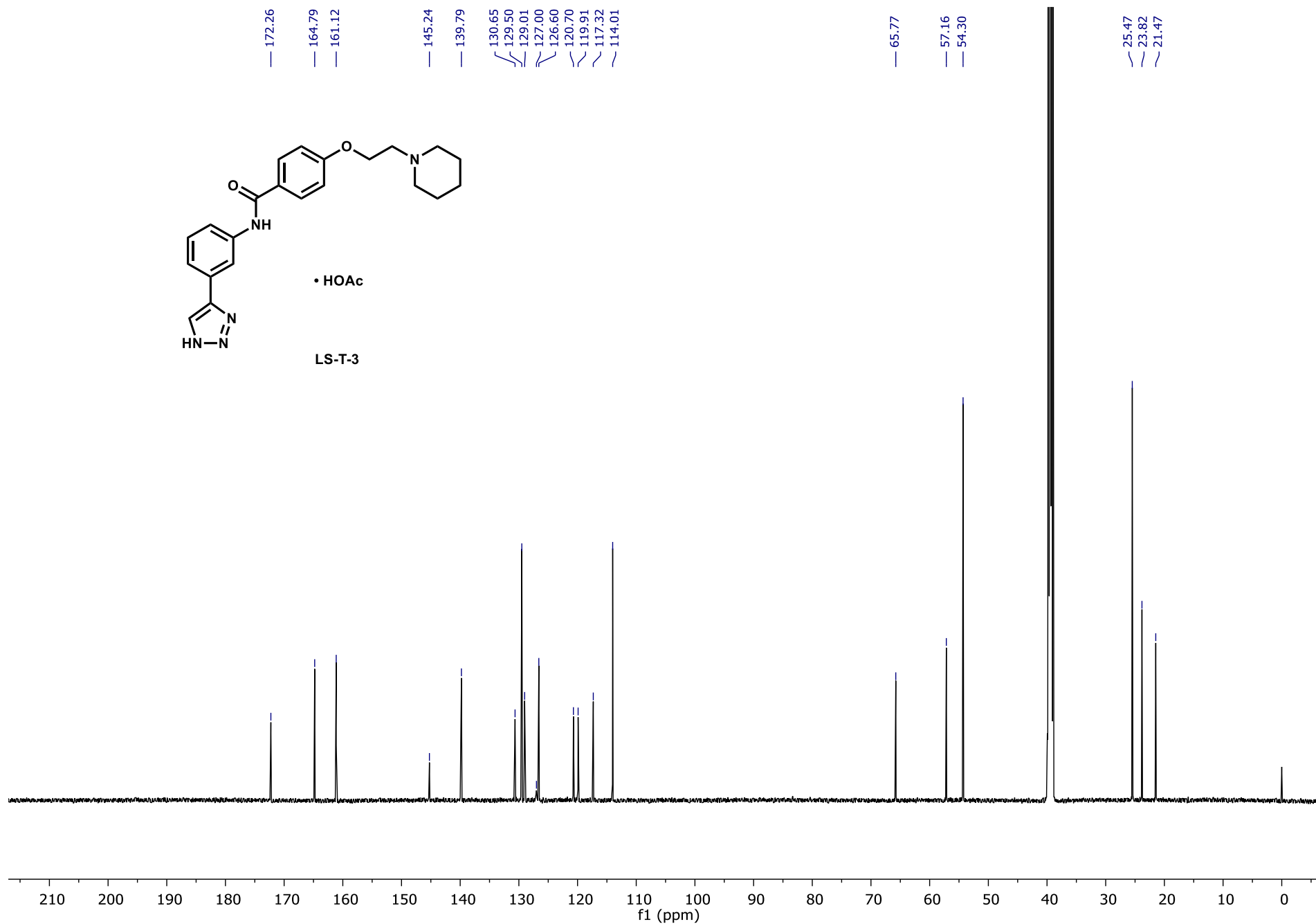
HSQC Spectrum for LS-T-2 (DMSO-*d*₆).



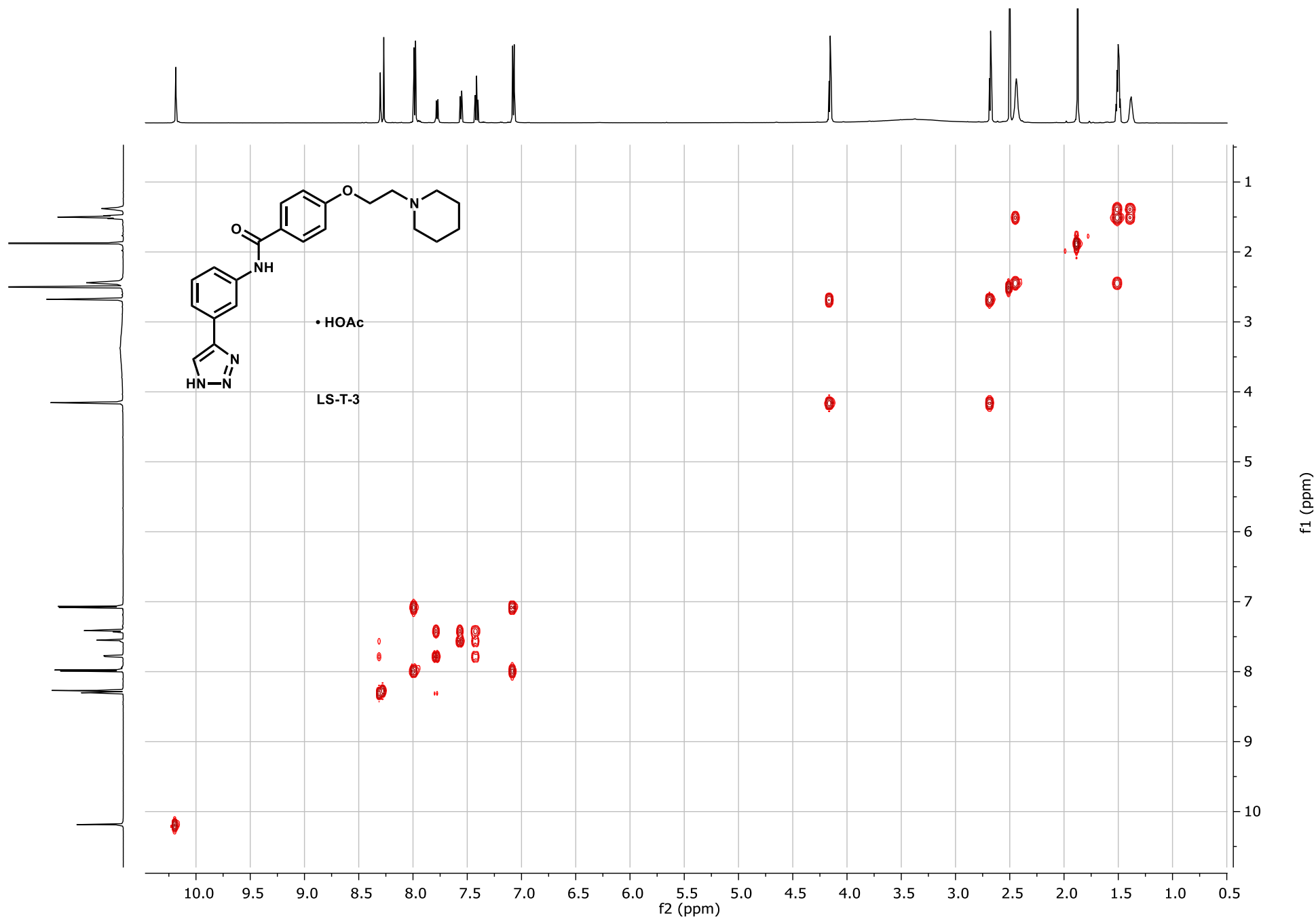
HMBC Spectrum for **LS-T-2** (DMSO-*d*₆).



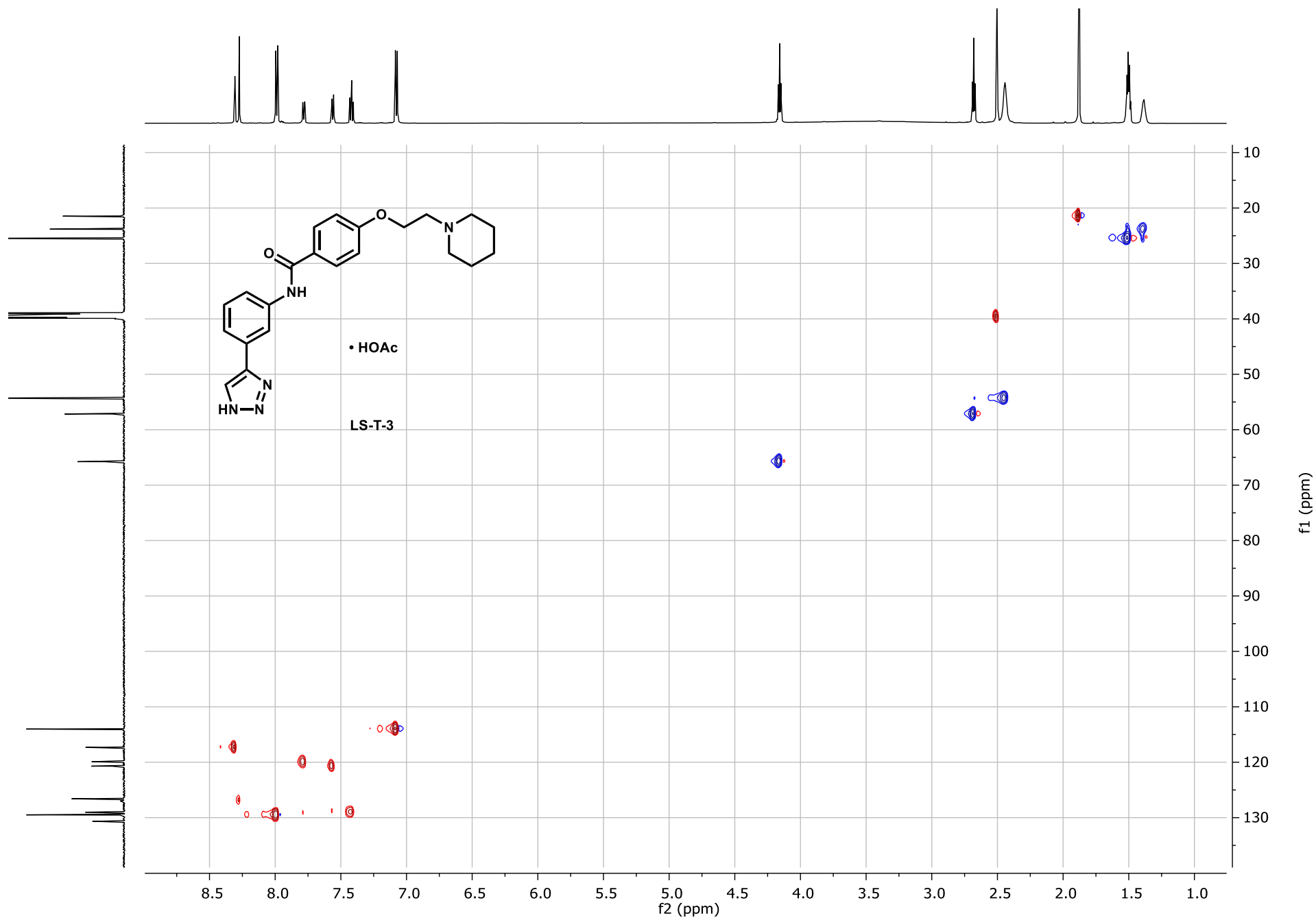
¹H NMR Spectrum for **LS-T-3** (DMSO-*d*₆, 600 MHz).

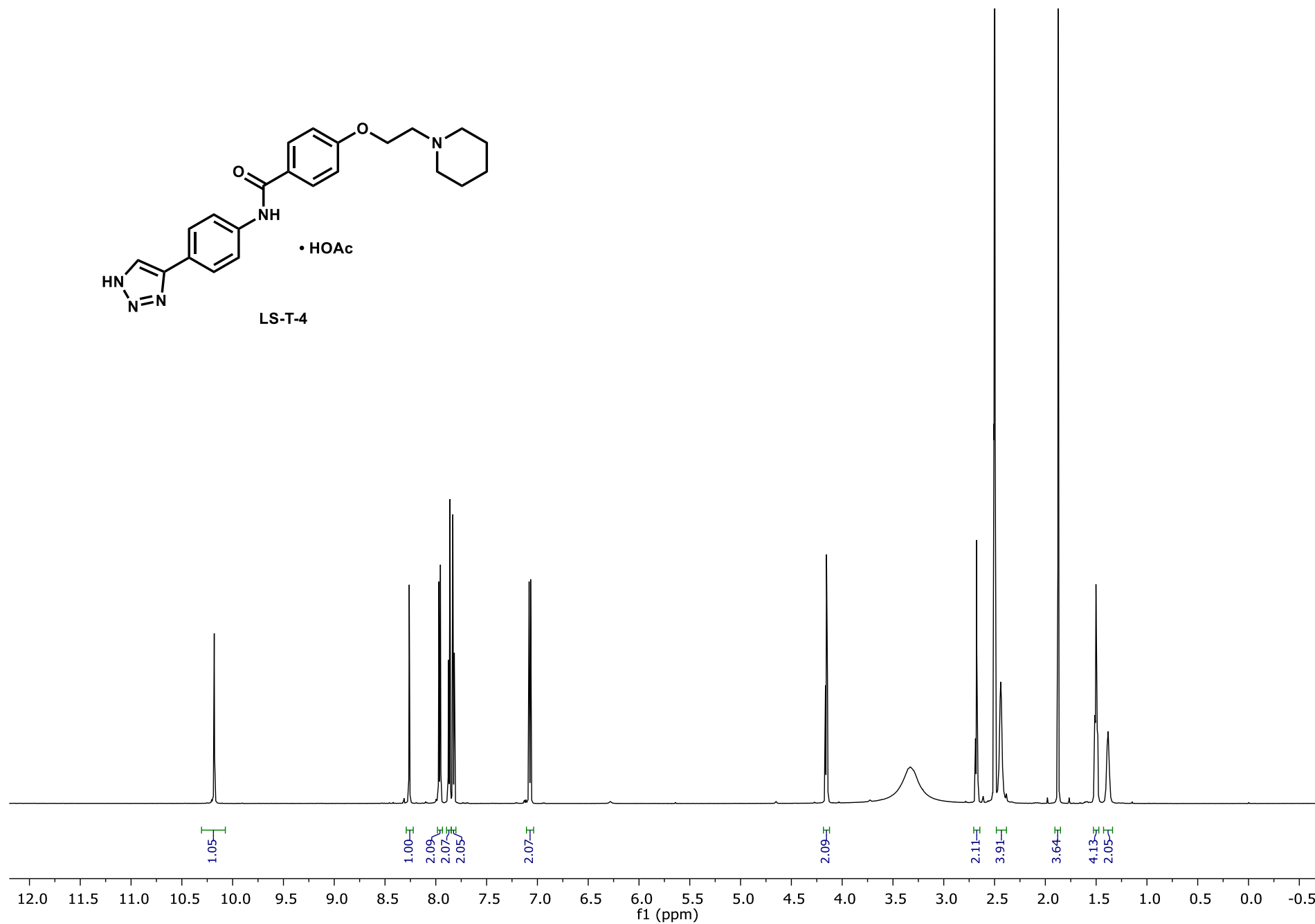
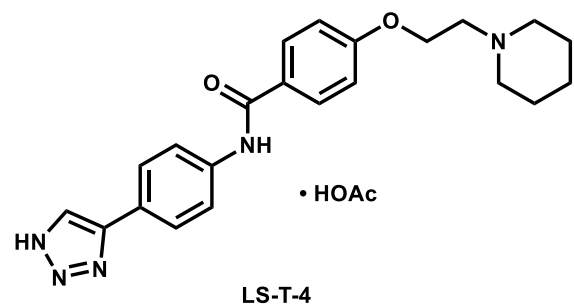


^{13}C NMR Spectrum for LS-T-3 (DMSO- d_6 , 151 MHz).

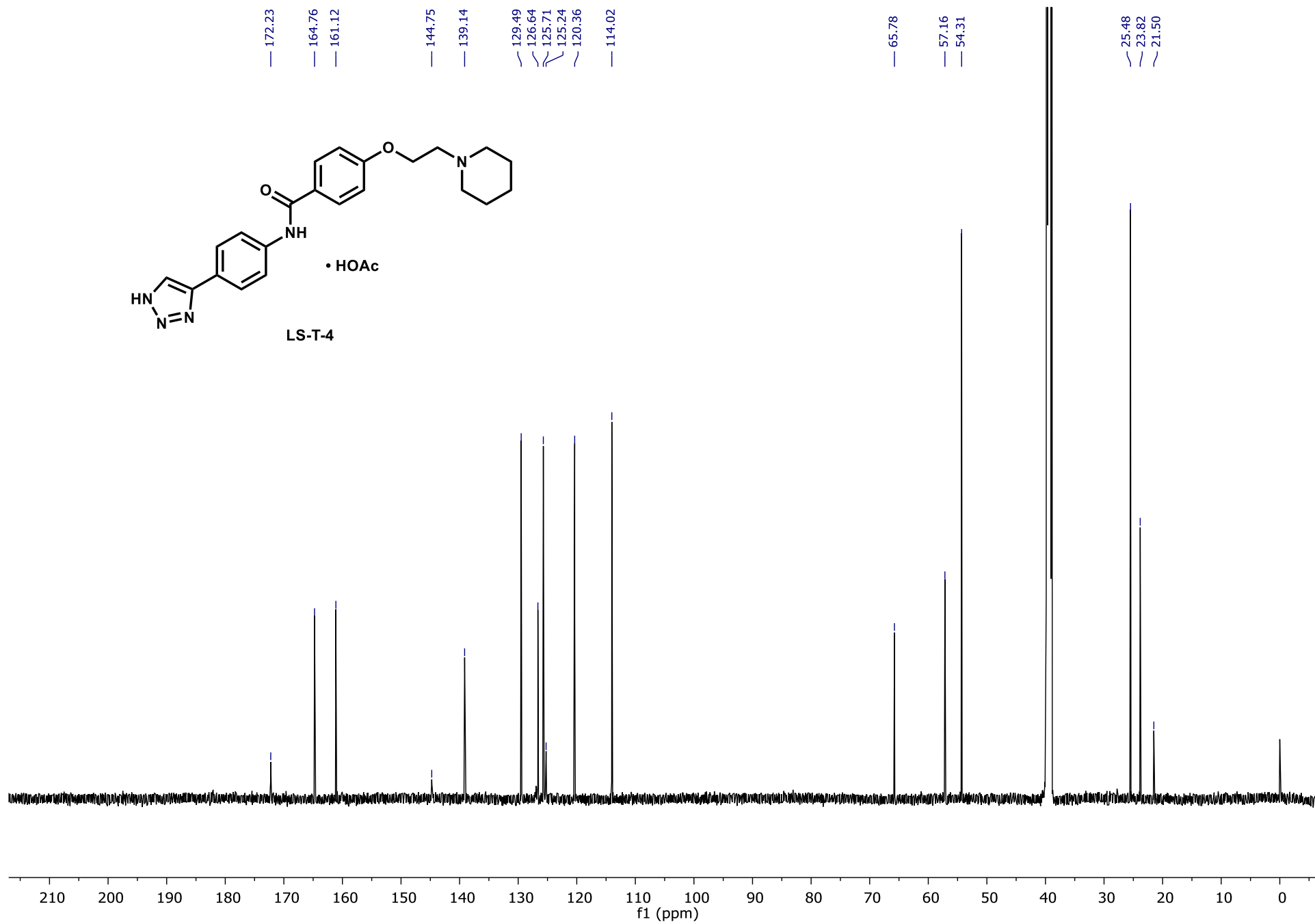
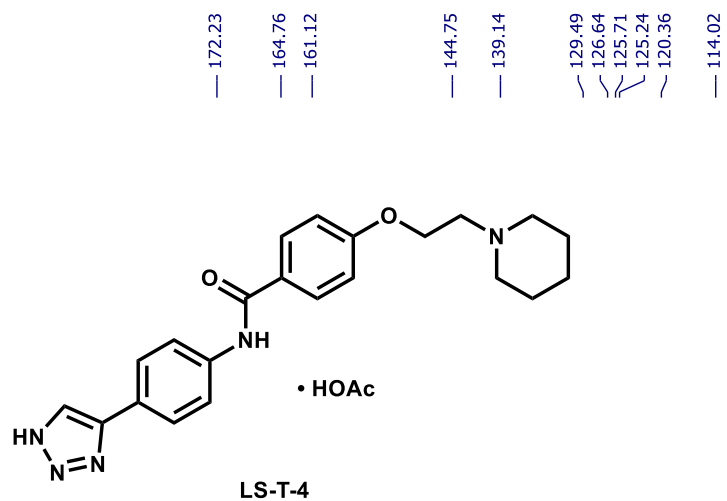


COSY Spectrum for LS-T-3 (DMSO- d_6).

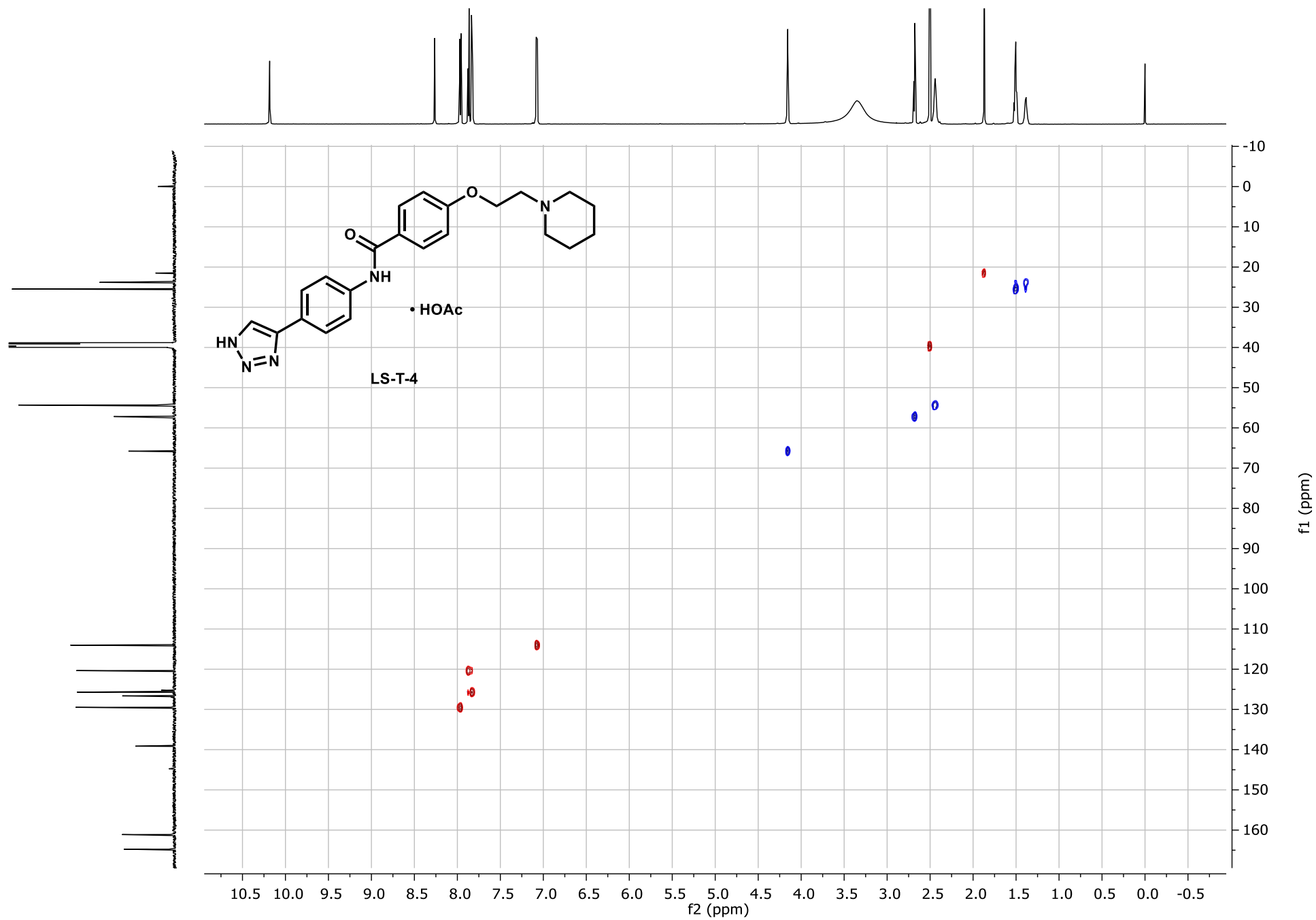




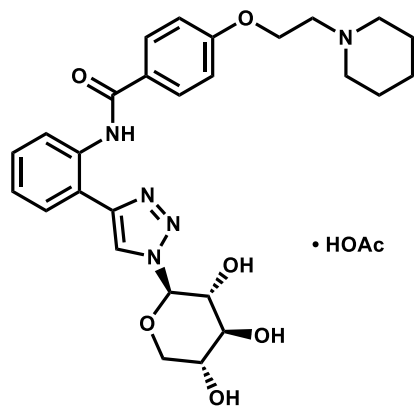
¹H NMR Spectrum for **LS-T-4** (DMSO-*d*₆, 600 MHz).



¹³C NMR Spectrum for **LS-T-4** (DMSO-*d*₆, 151 MHz).

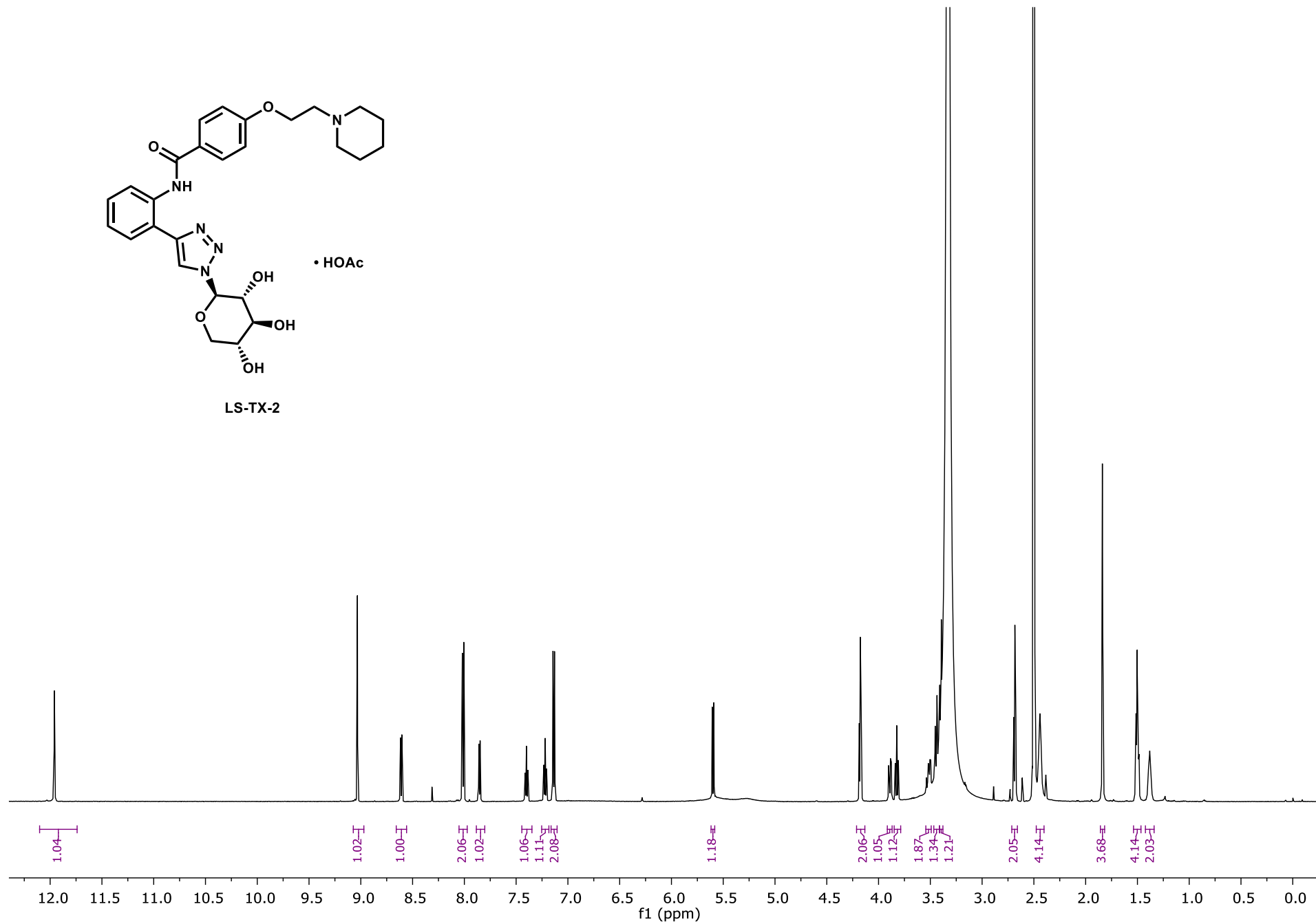


HSQC Spectrum for LS-T-4 (DMSO-*d*₆).

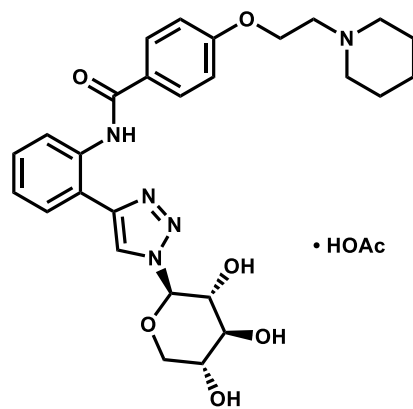


• HOAc

LS-TX-2



^1H NMR Spectrum for LS-TX-2 (DMSO- d_6 , 600 MHz).



LS-TX-2

— 164.38
— 161.47

— 146.32

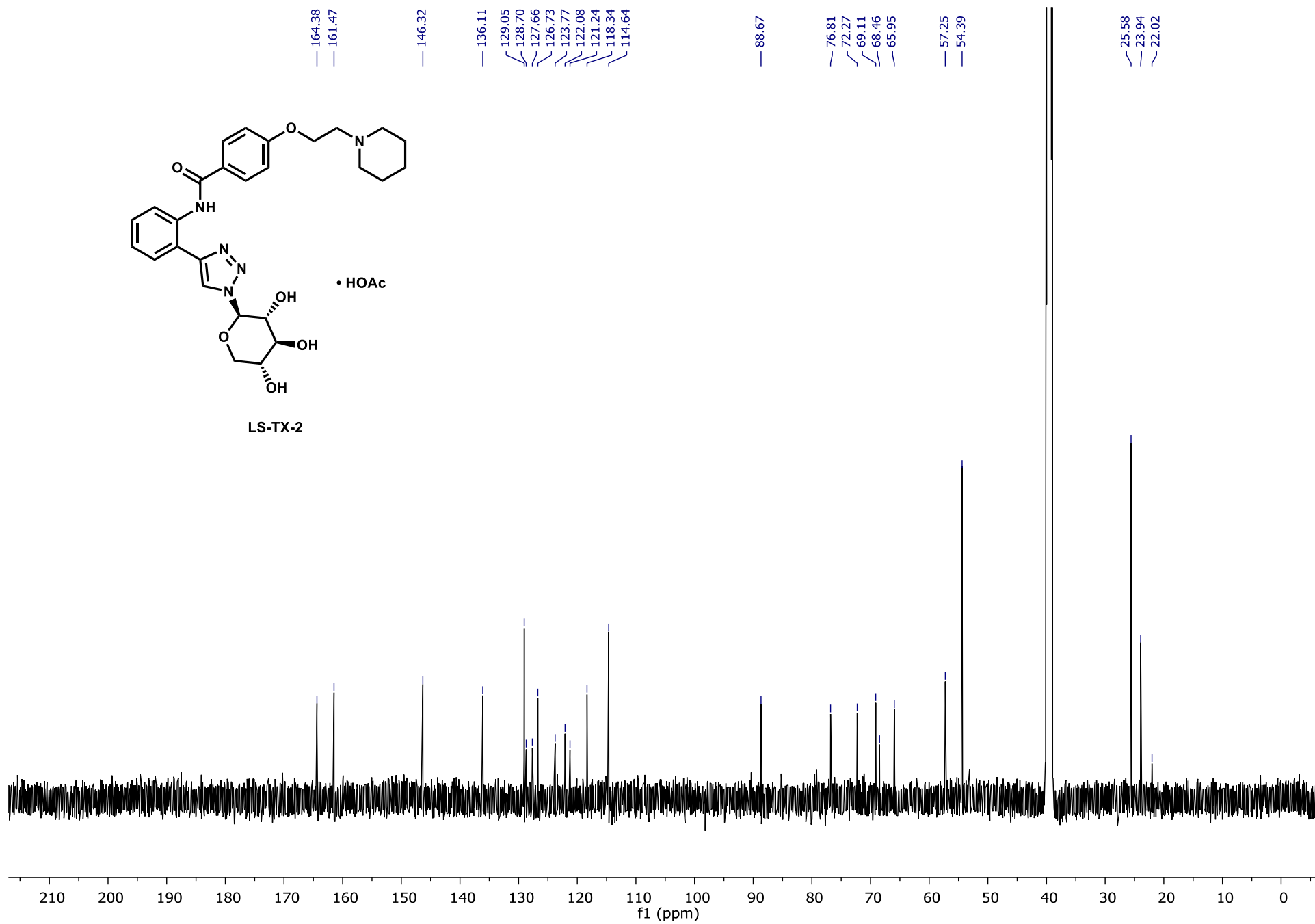
— 136.11
— 129.05
— 128.70
— 127.66
— 126.73
— 123.77
— 122.08
— 121.24
— 118.34
— 114.64

— 88.67

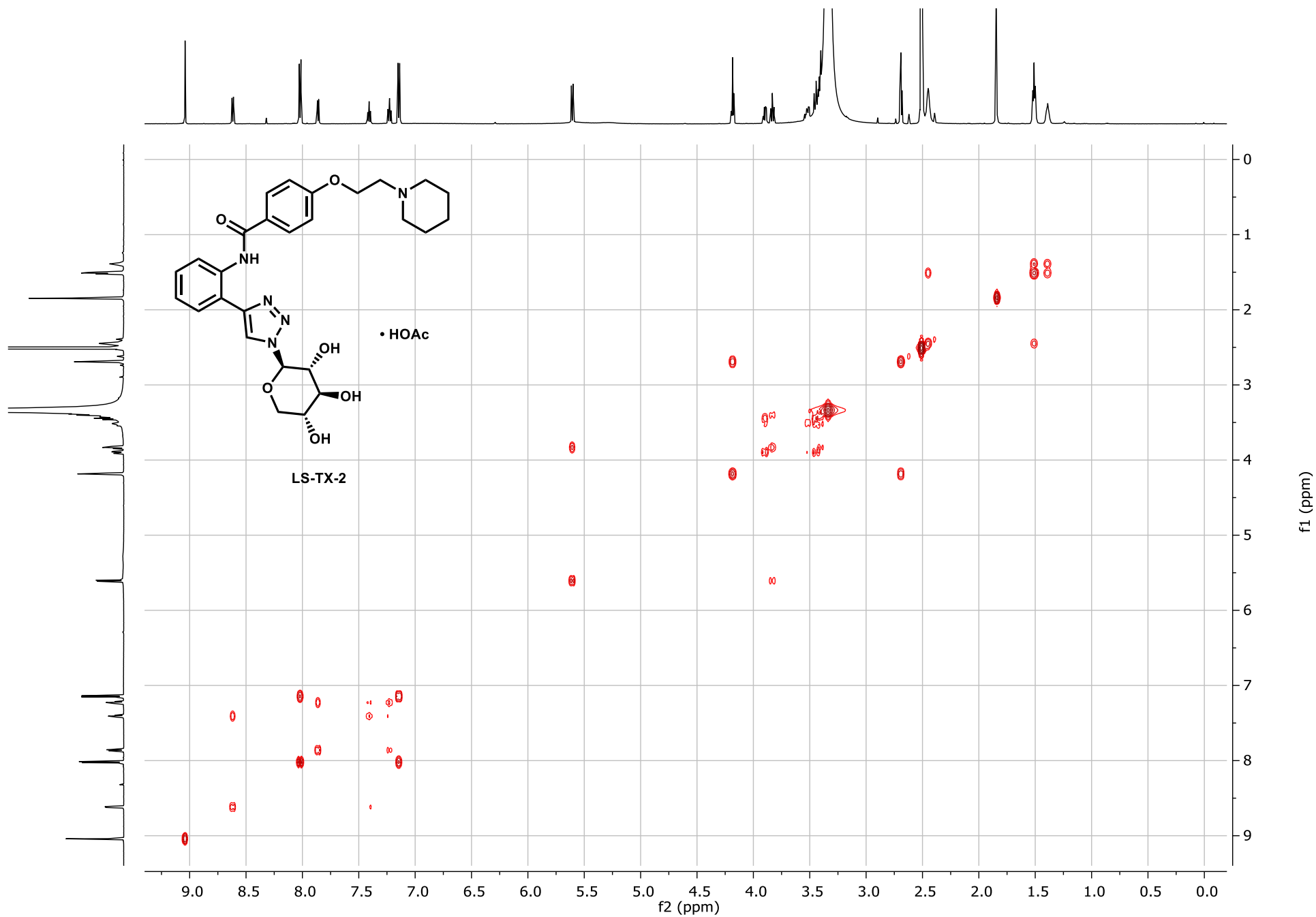
— 76.81
— 72.27
— 69.11
— 68.46
— 65.95

— 57.25
— 54.39

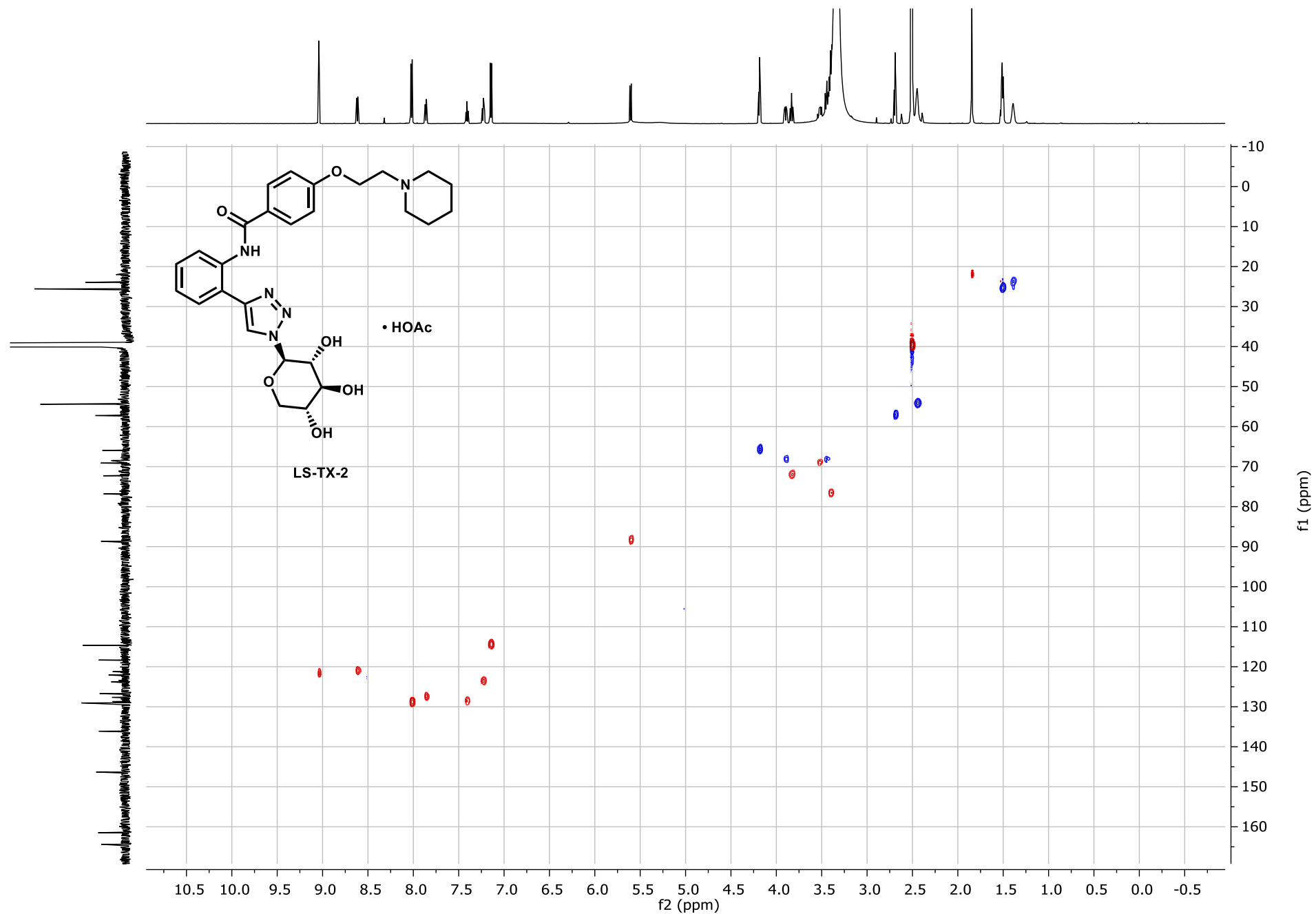
— 25.58
— 23.94
— 22.02



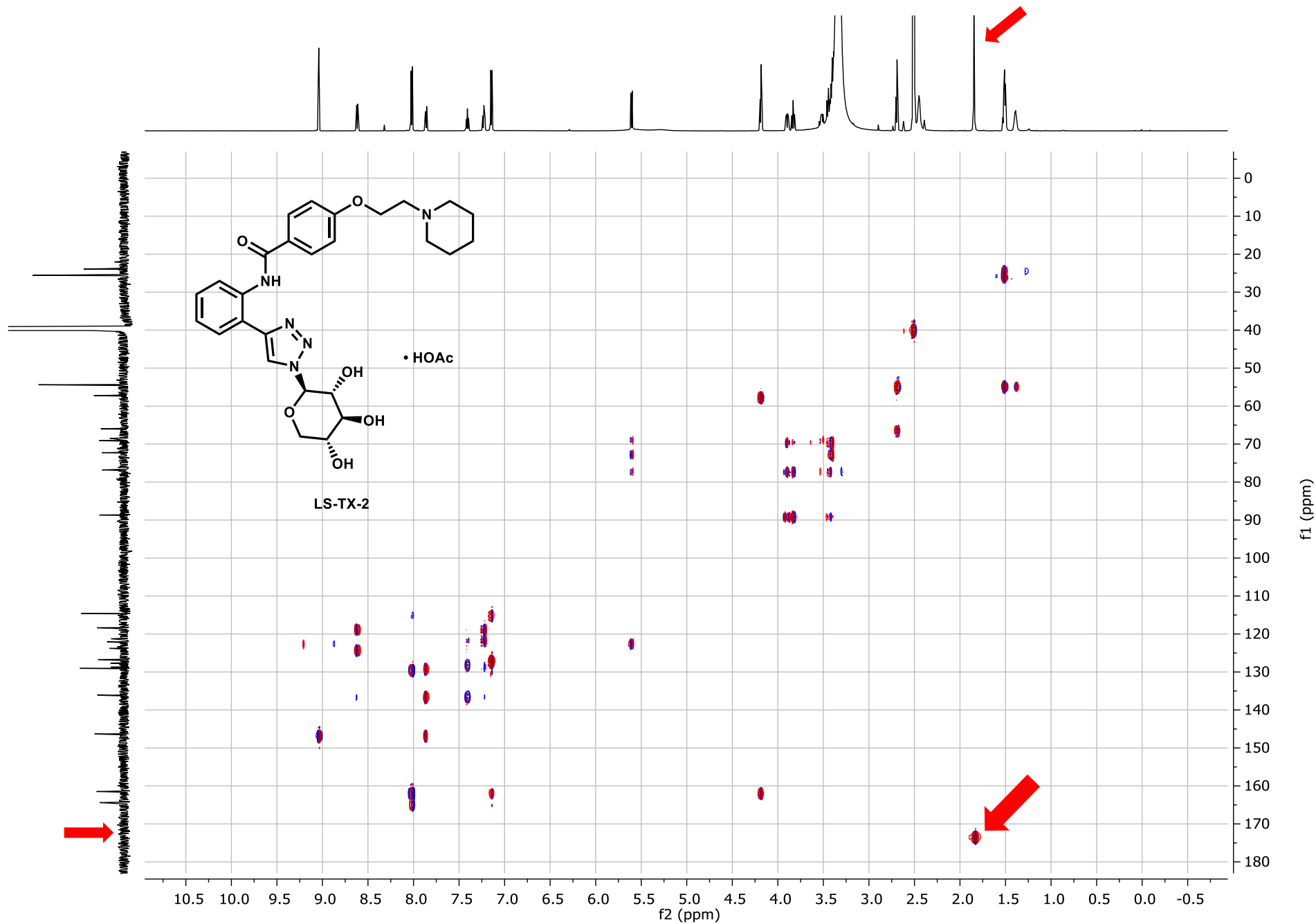
^{13}C NMR Spectrum for LS-TX-2 (DMSO- d_6 , 151 MHz).



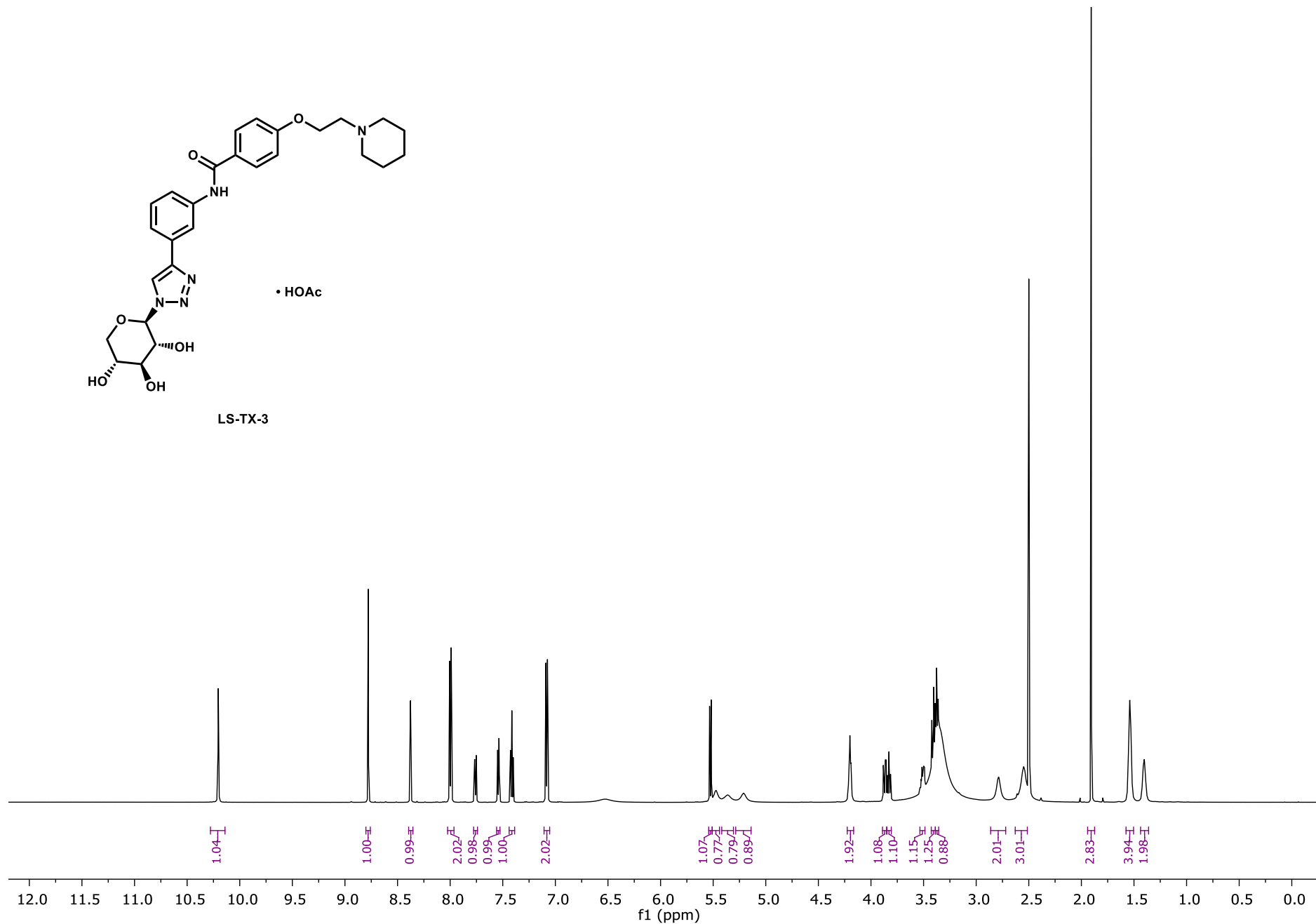
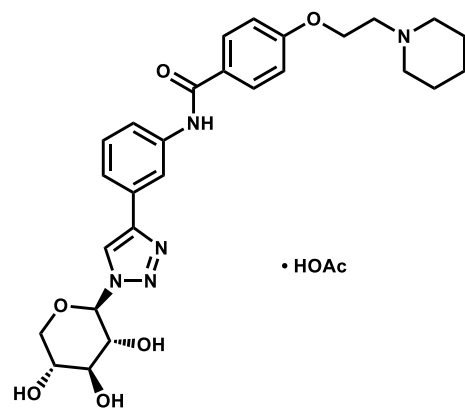
COSY Spectrum for **LS-TX-2** (DMSO-*d*₆).



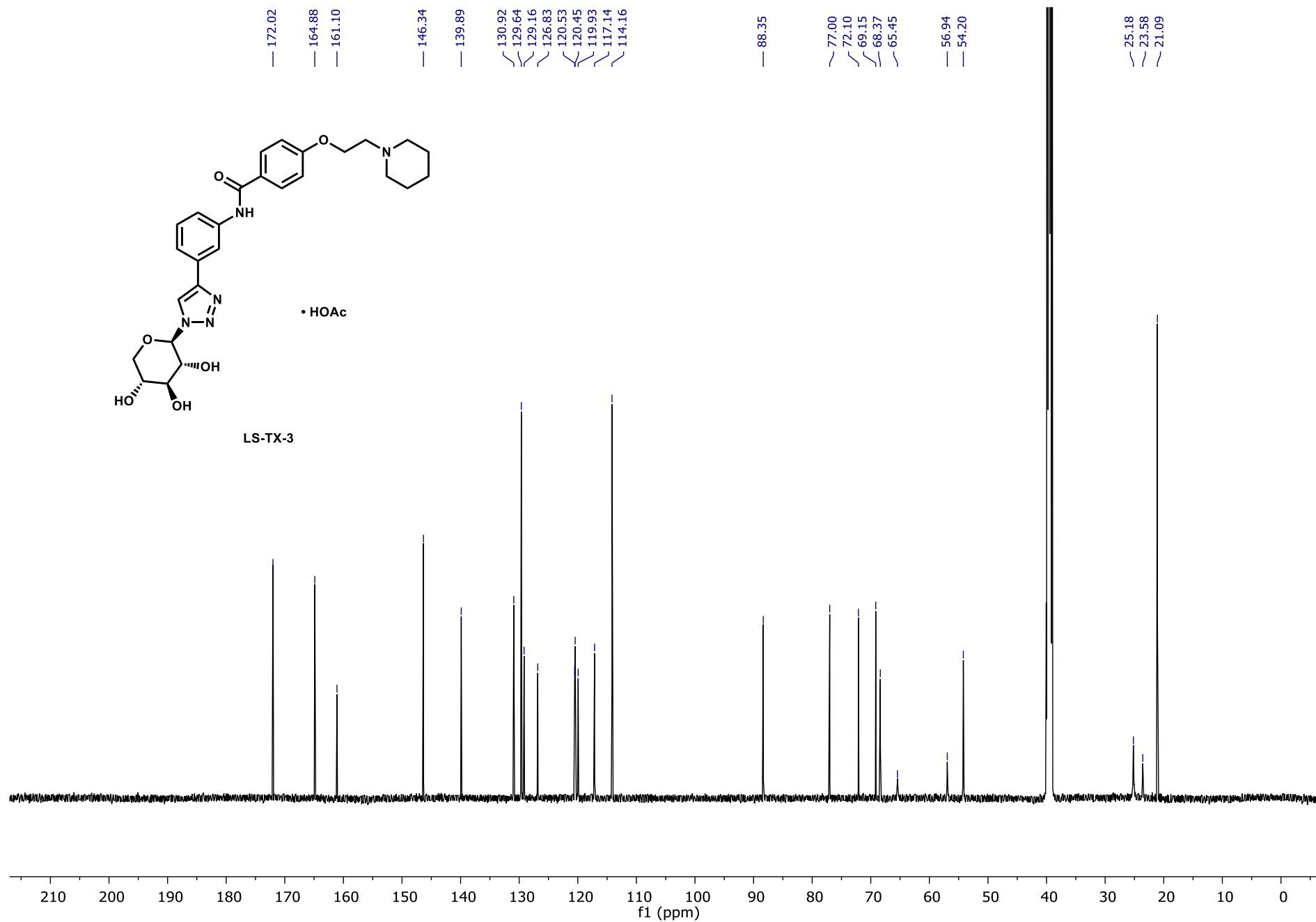
HSQC Spectrum for LS-TX-2 (DMSO-*d*₆).

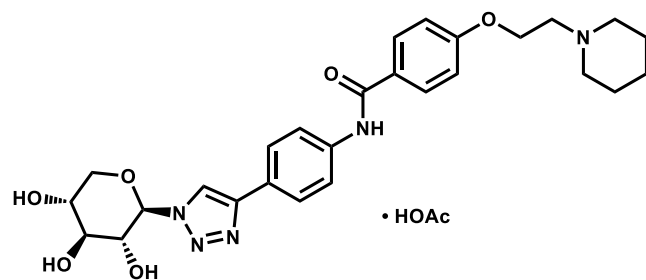


HMBC Spectrum for LS-TX-2 (DMSO- d_6). Note correlation of acetate CH_3 to the missing 172.0 ppm ^{13}C signal of the acetate carbonyl carbon.

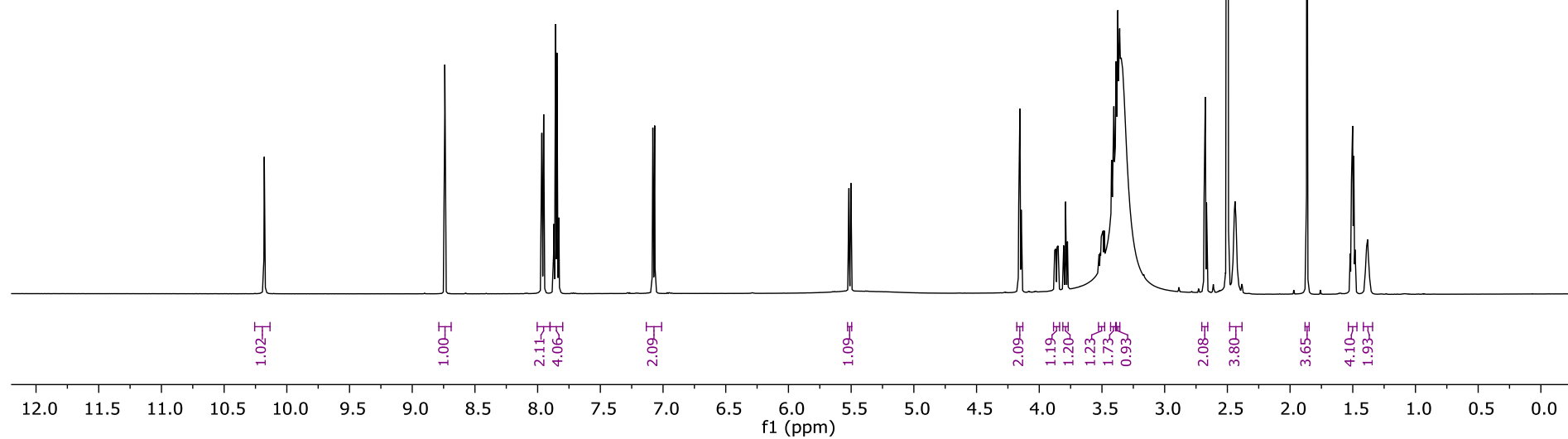


¹H NMR Spectrum for LS-TX-3 (DMSO-*d*₆, 600 MHz).

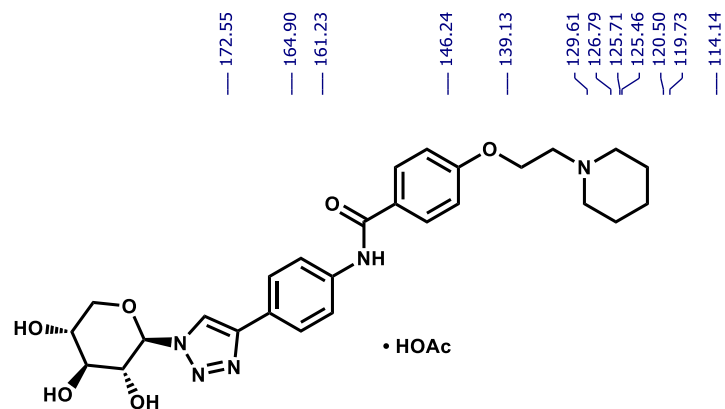




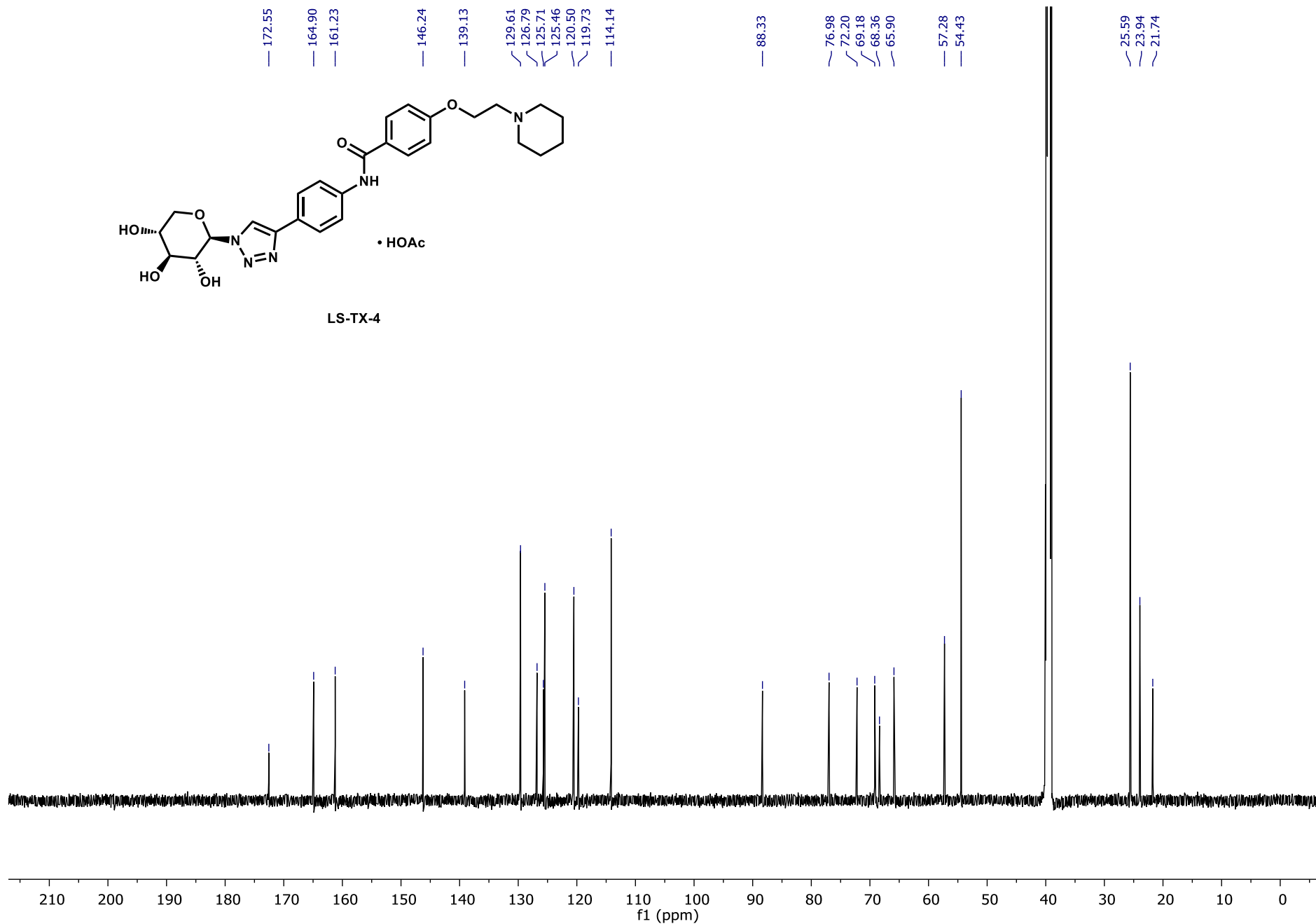
LS-TX-4



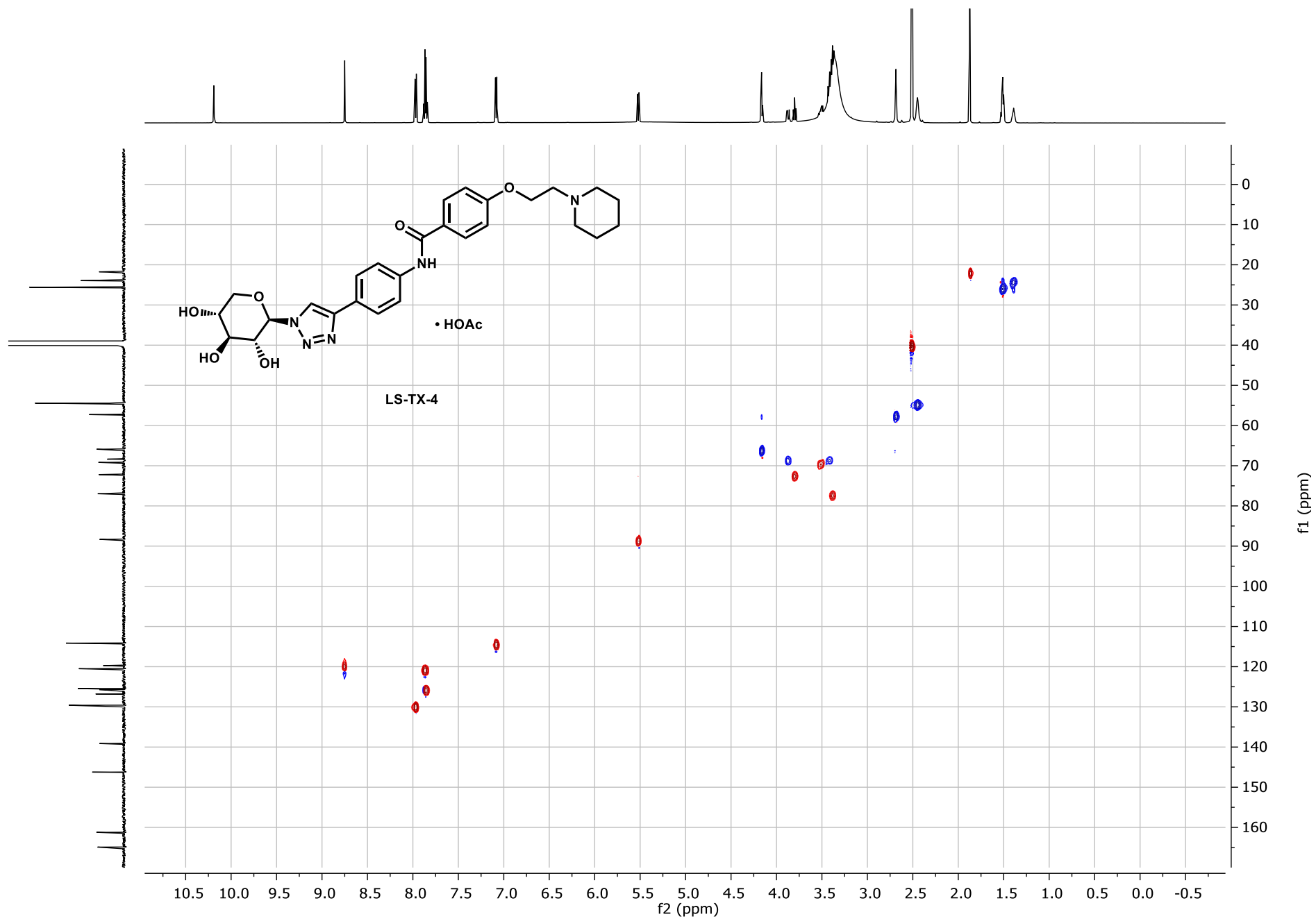
^1H NMR Spectrum for **LS-TX-4** (DMSO- d_6 , 600 MHz).



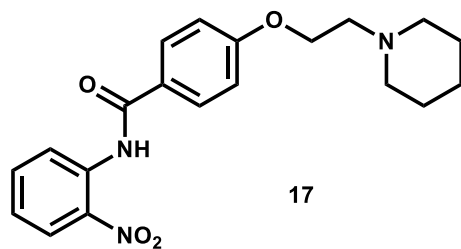
LS-TX-4



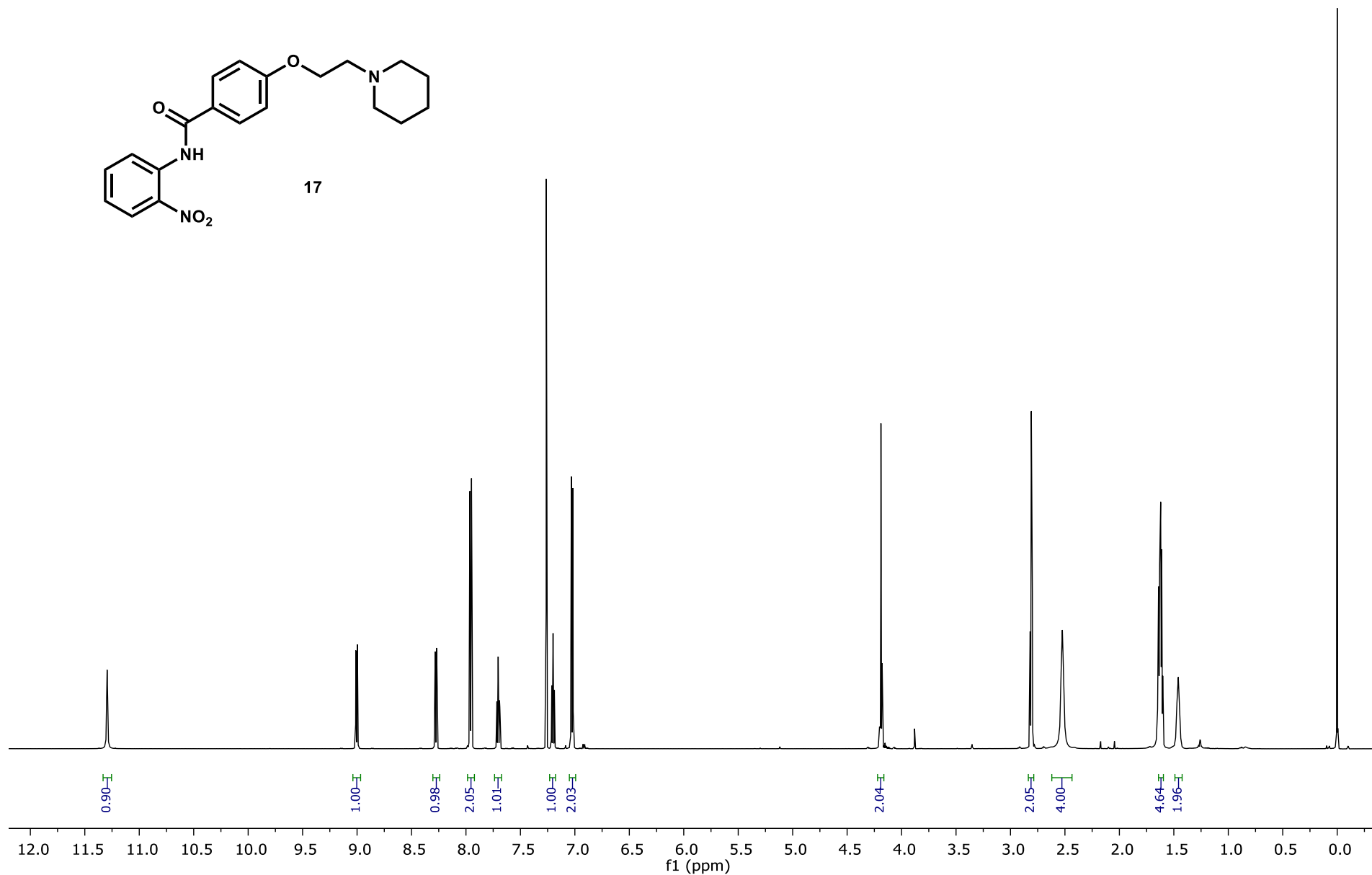
^{13}C NMR Spectrum for LS-TX-4 (DMSO- d_6 , 151 MHz).



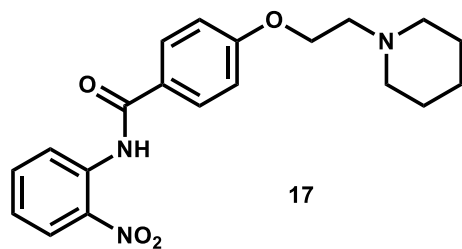
HSQC Spectrum for LS-TX-4 (DMSO- d_6).



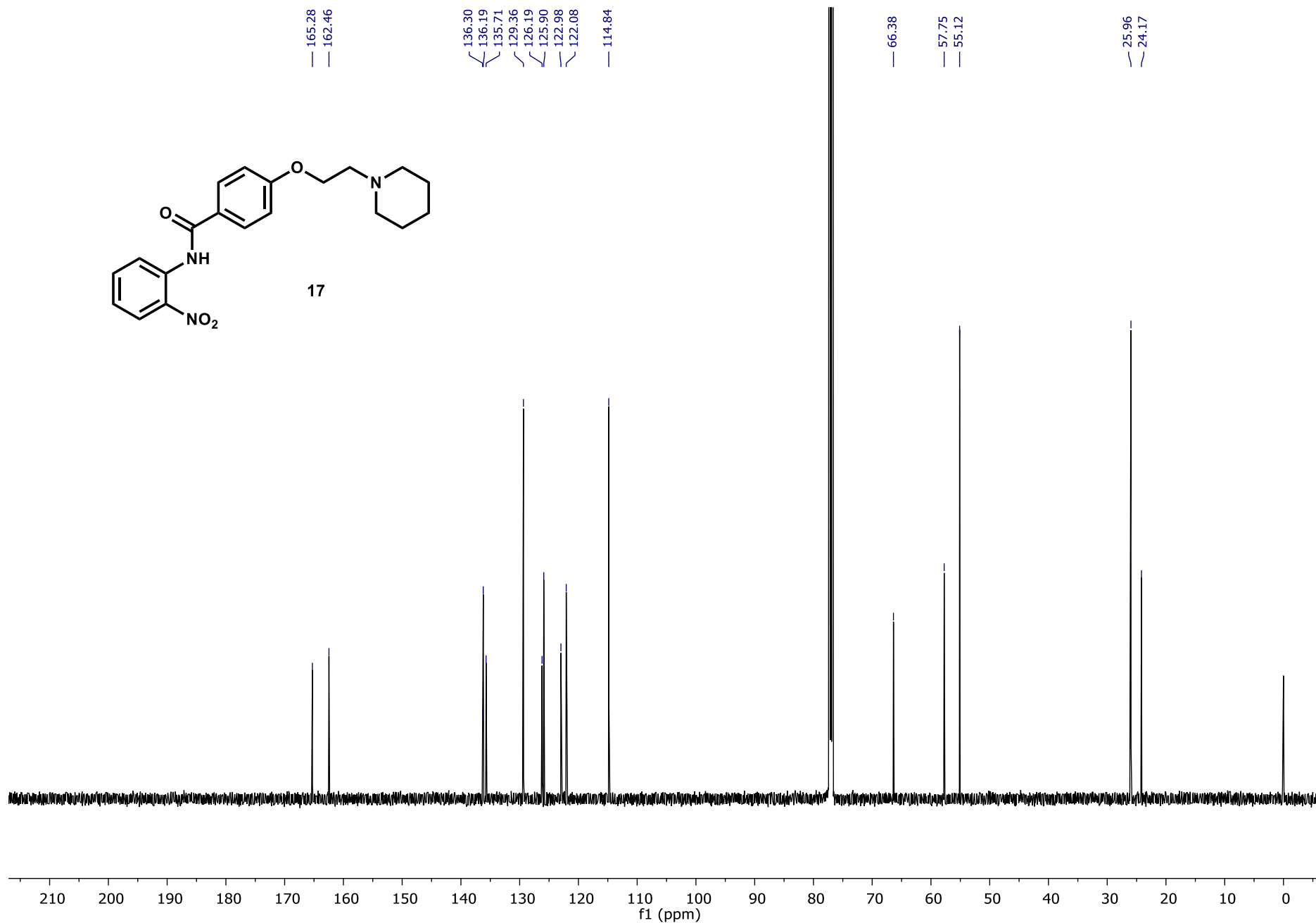
17



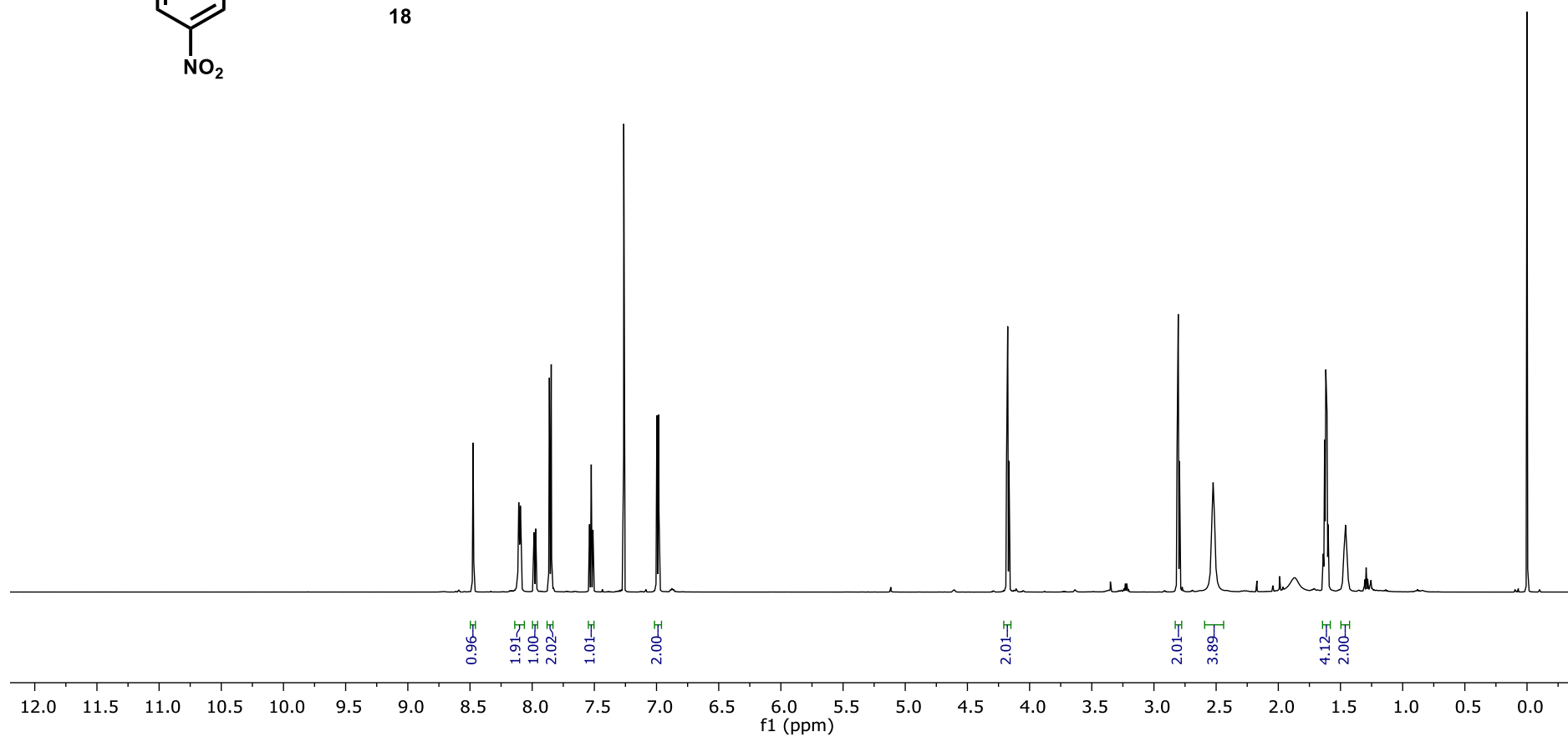
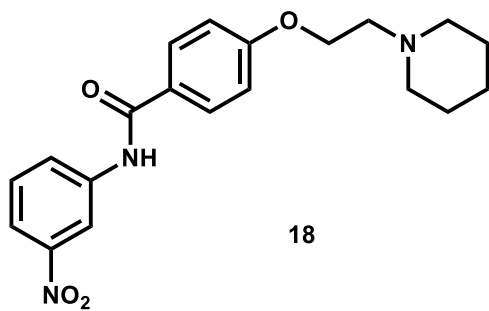
¹H NMR Spectrum for Compound 17 (CDCl₃, 600 MHz).



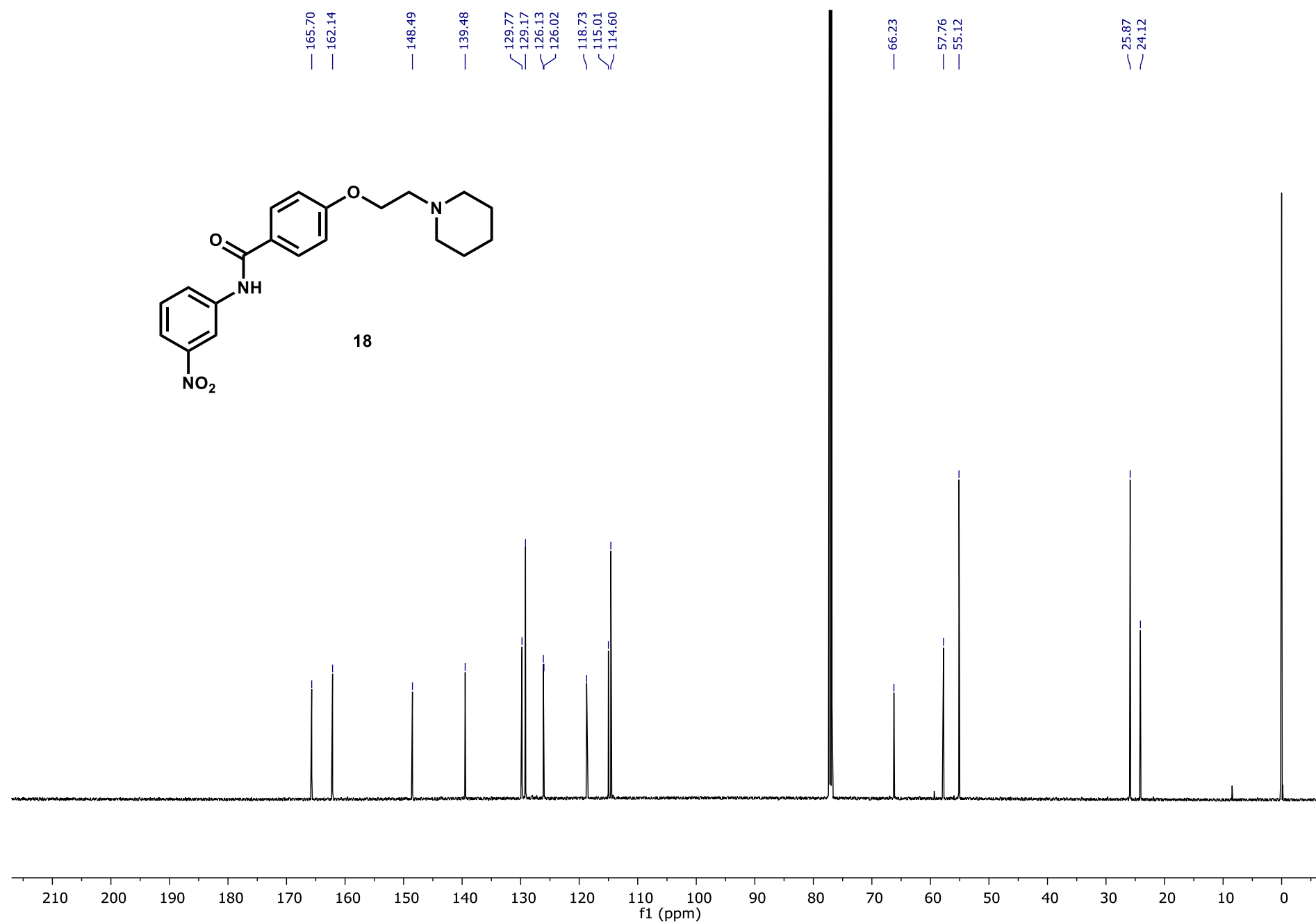
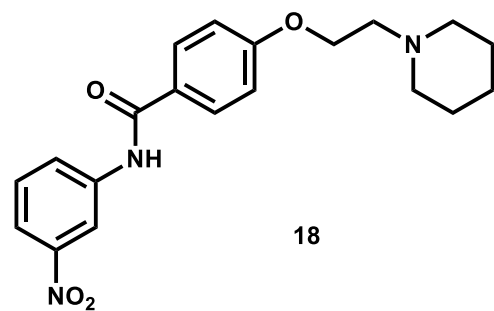
17



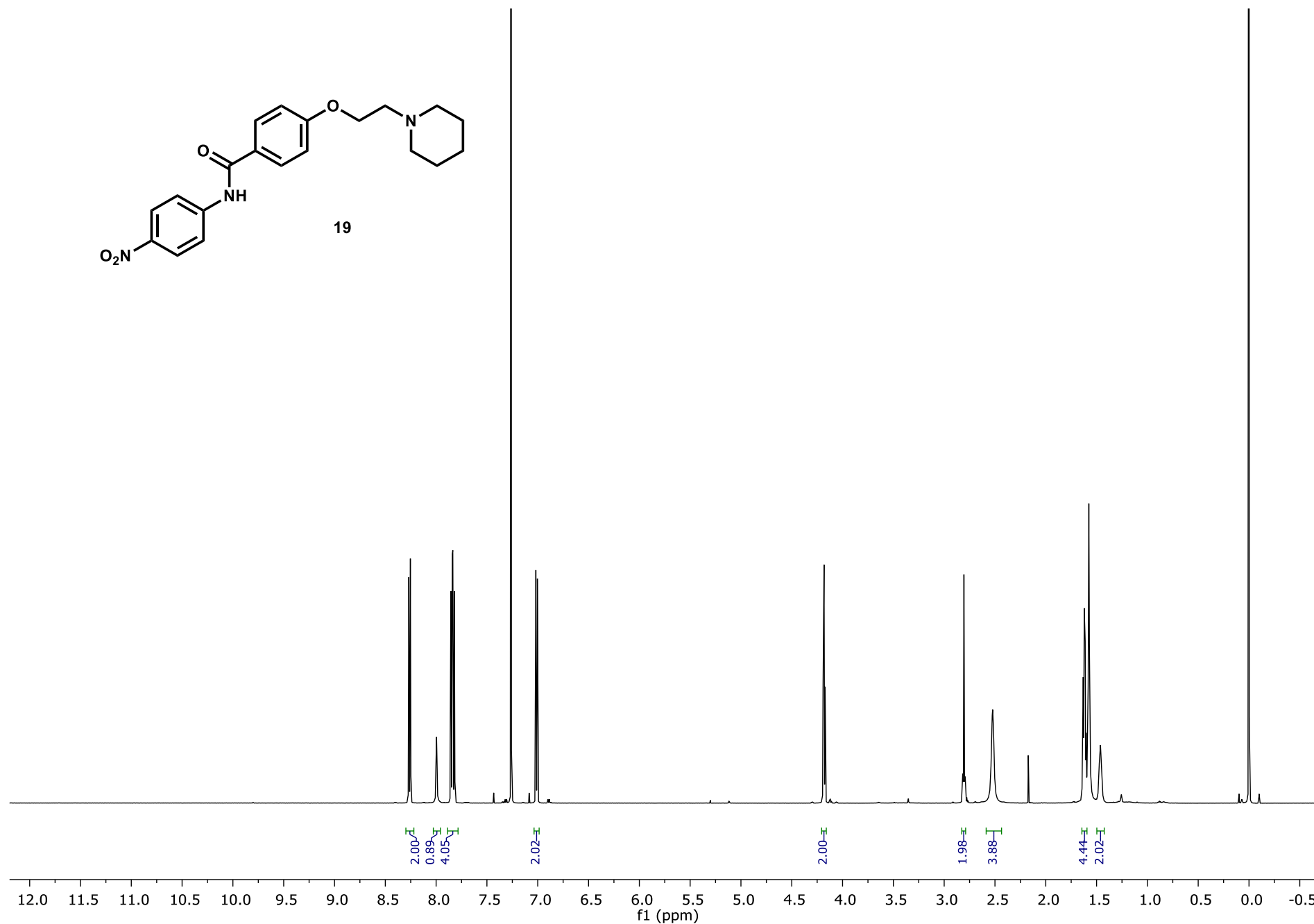
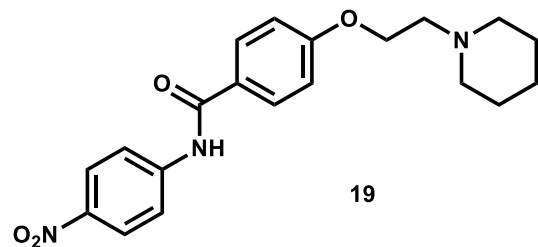
¹³C NMR Spectrum for Compound 17 (CDCl₃, 151 MHz).



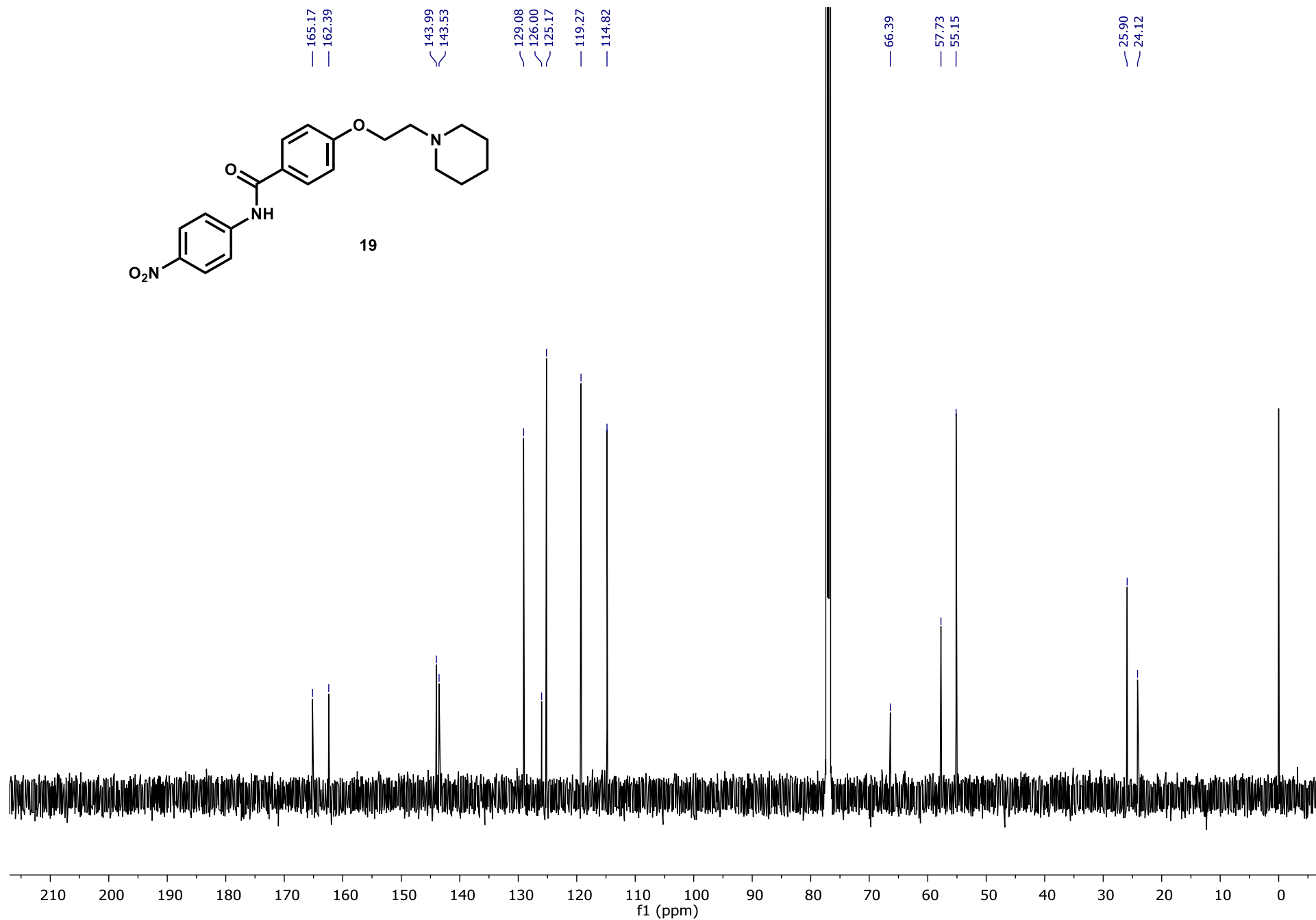
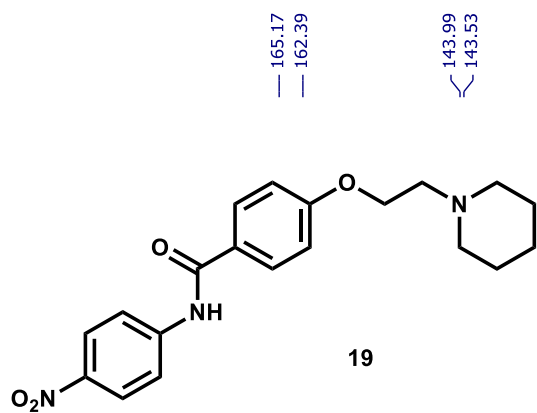
^1H NMR Spectrum for Compound **18** (CDCl_3 , 600 MHz).



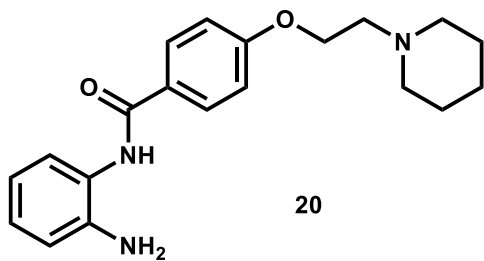
¹³C NMR Spectrum for Compound **18** (CDCl₃, 151 MHz).



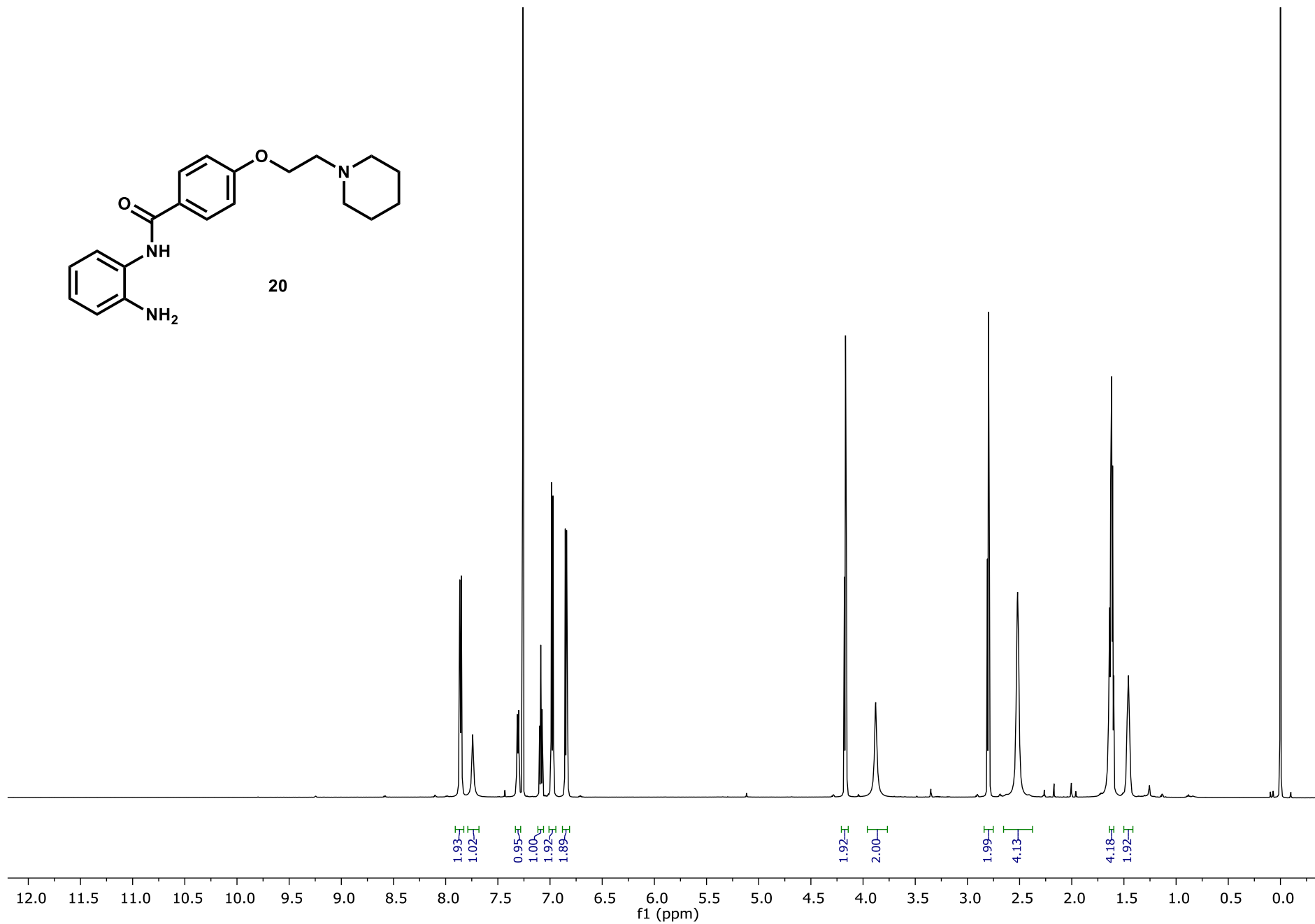
¹H NMR Spectrum for Compound **19** (CDCl₃, 600 MHz).



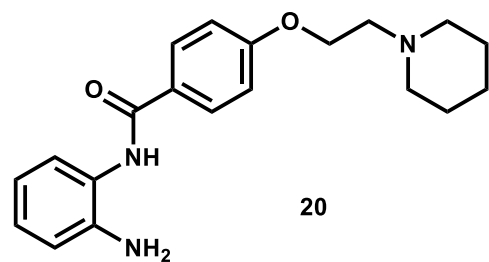
¹³C NMR Spectrum for Compound **19** (CDCl₃, 151 MHz).



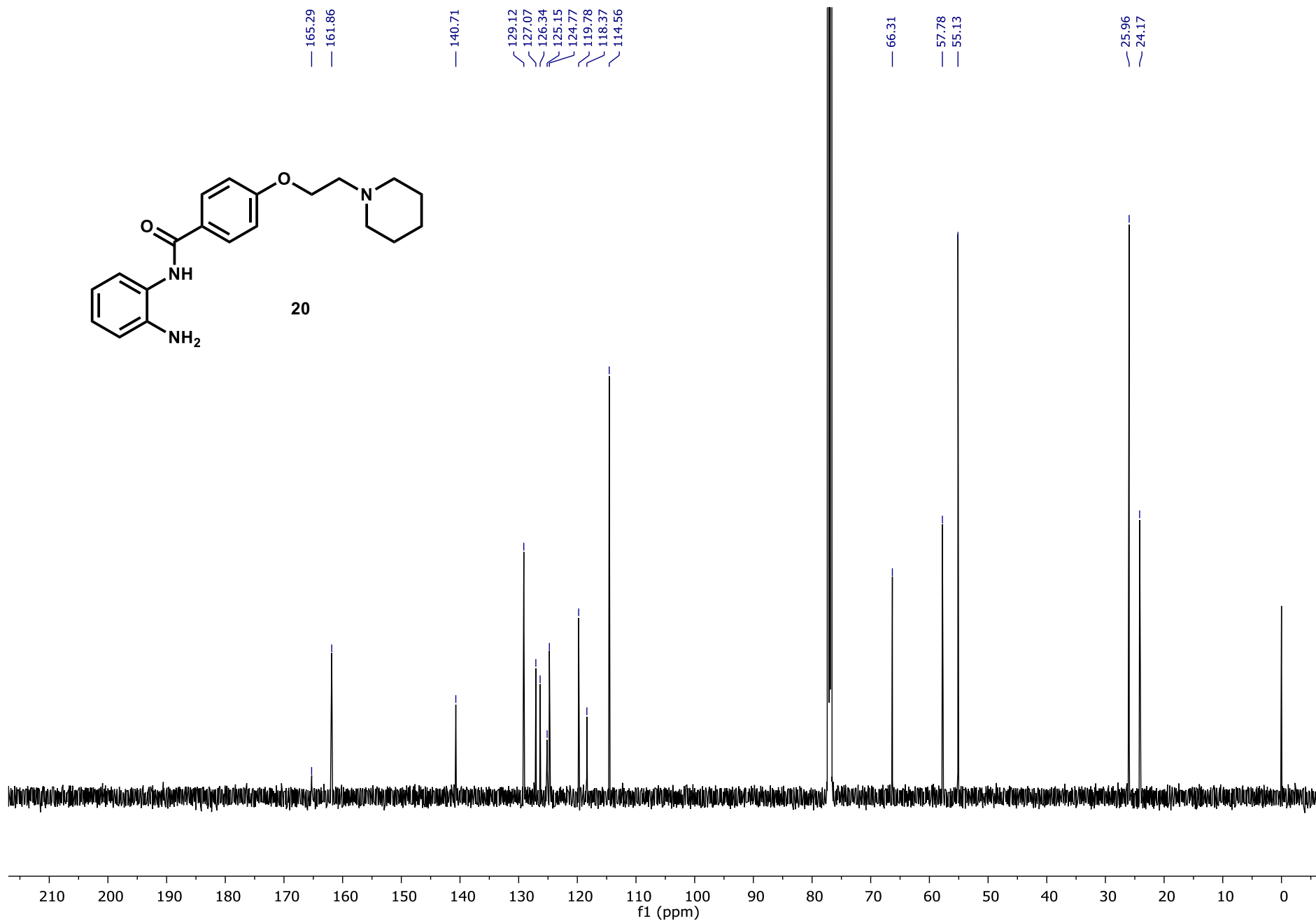
20



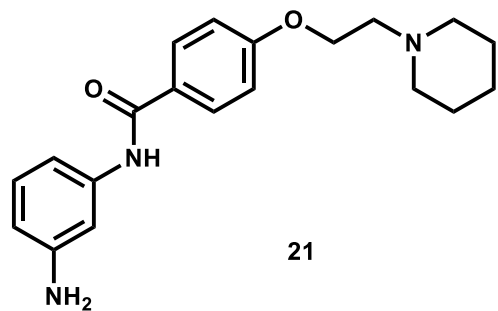
¹H NMR Spectrum for Compound **20** (CDCl₃, 600 MHz).



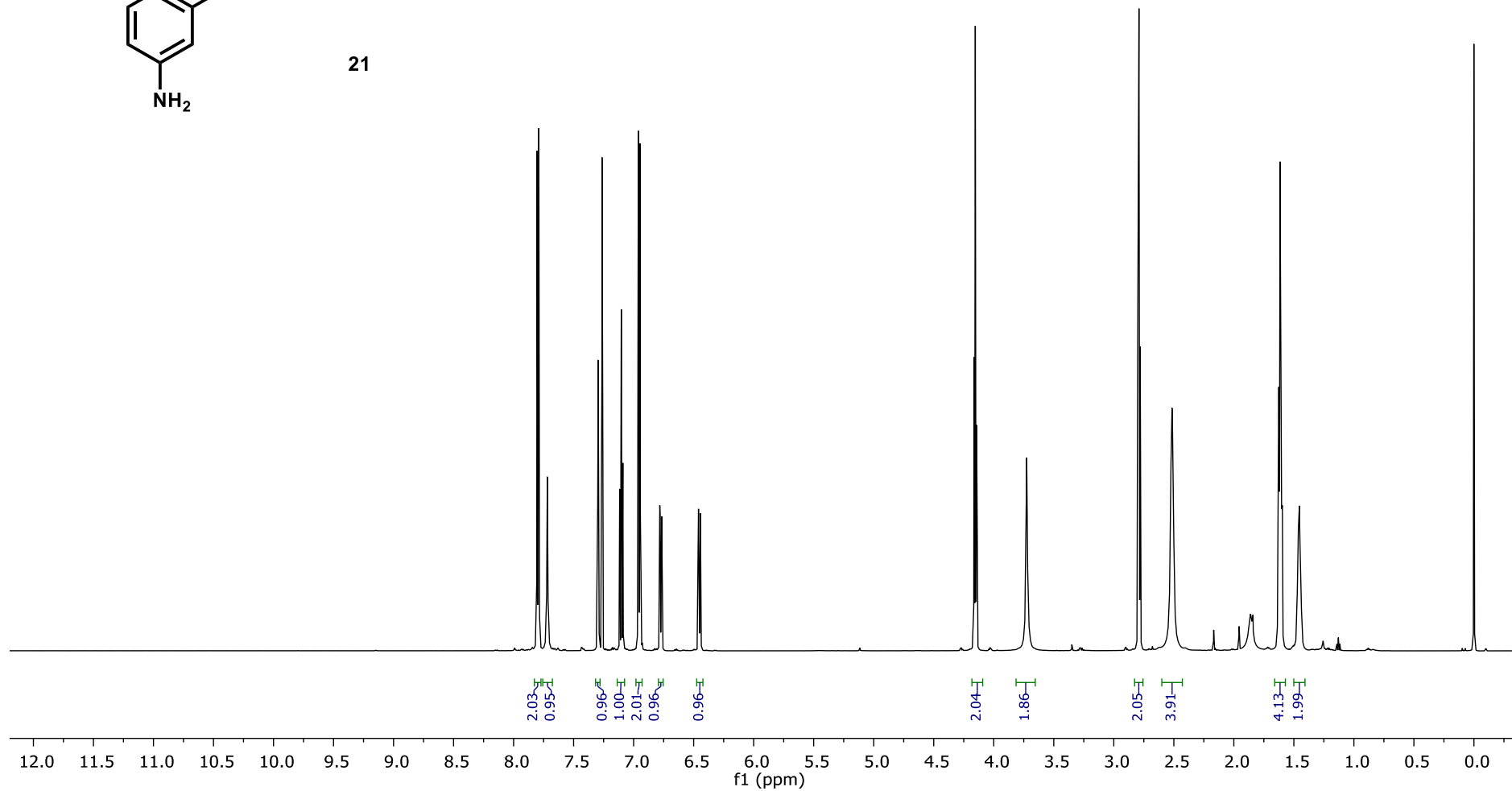
20



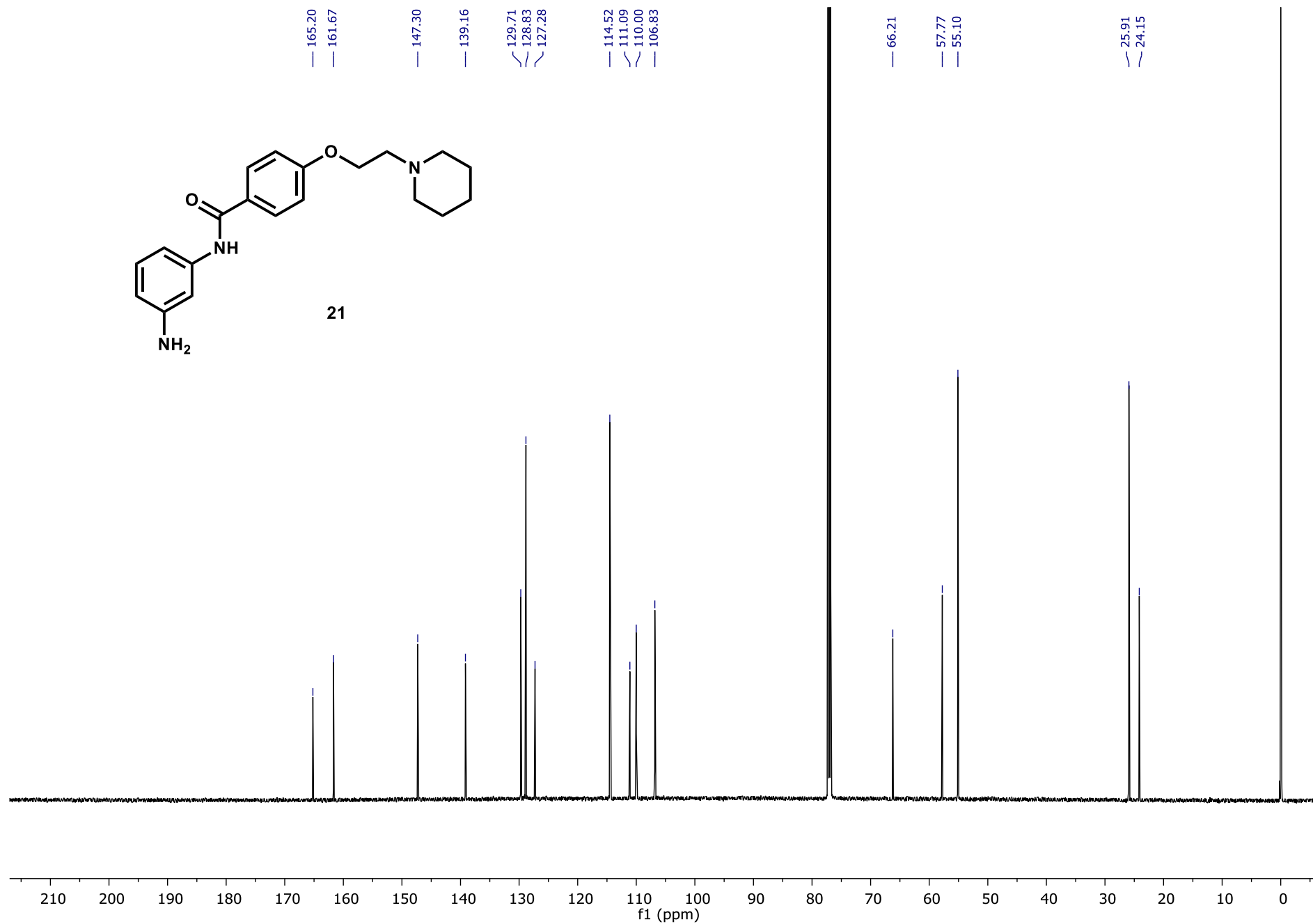
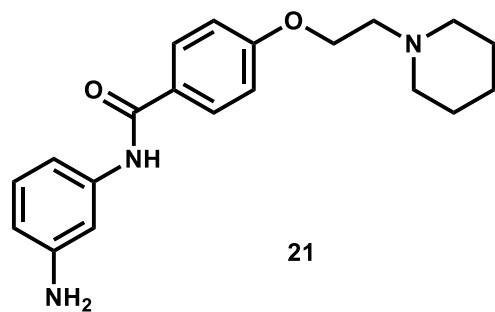
¹³C NMR Spectrum for Compound **20** (CDCl₃, 151 MHz).



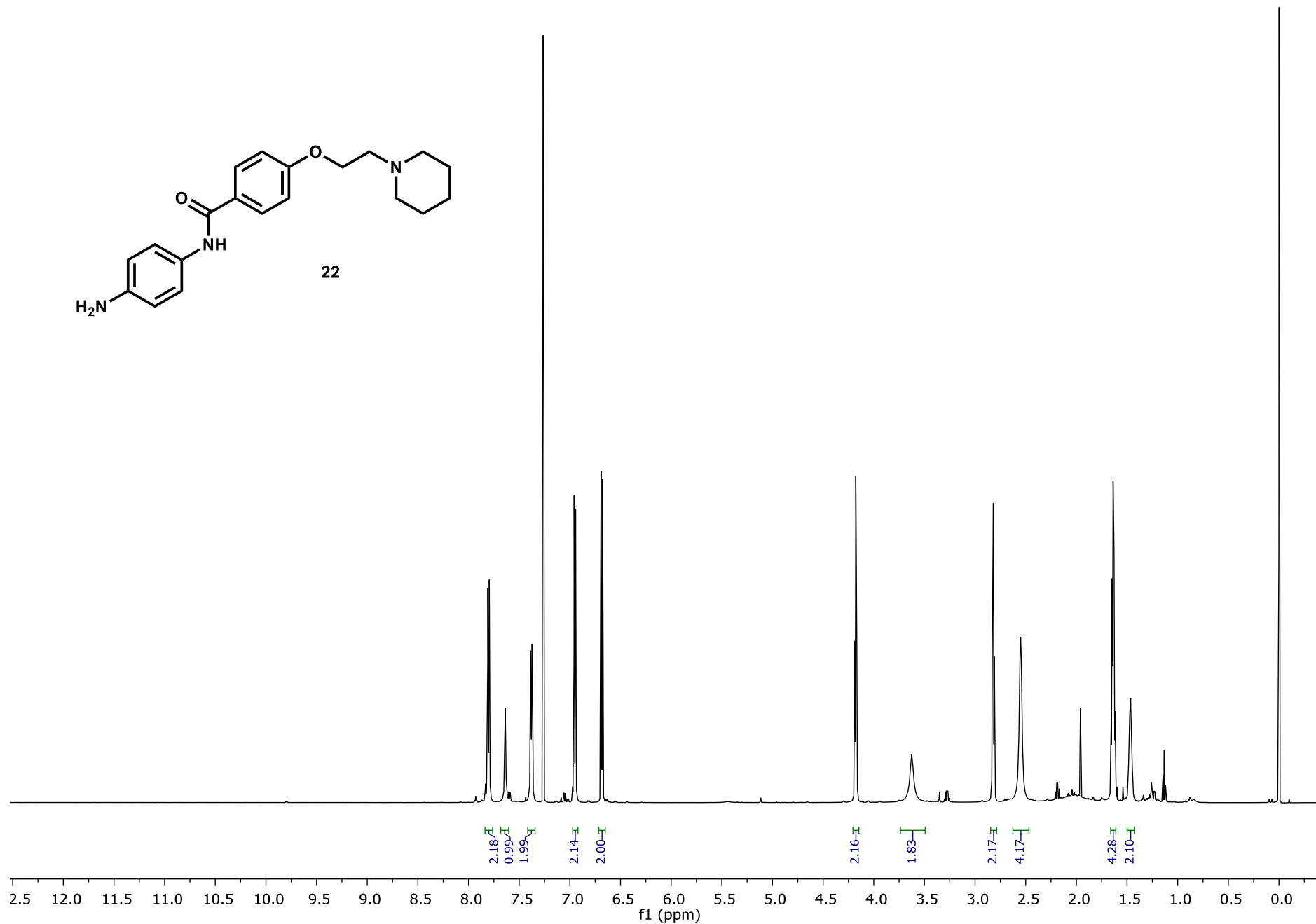
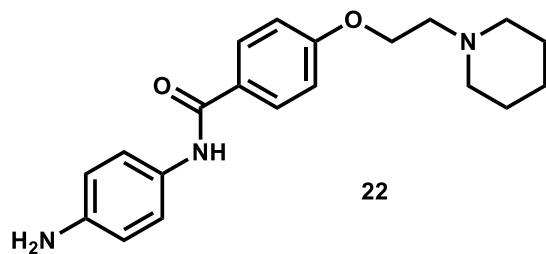
21



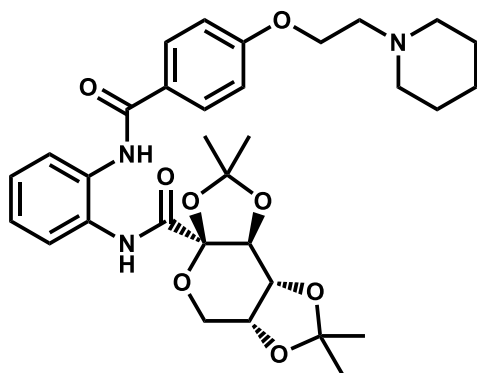
¹H NMR Spectrum for Compound **21** (CDCl₃, 600 MHz).



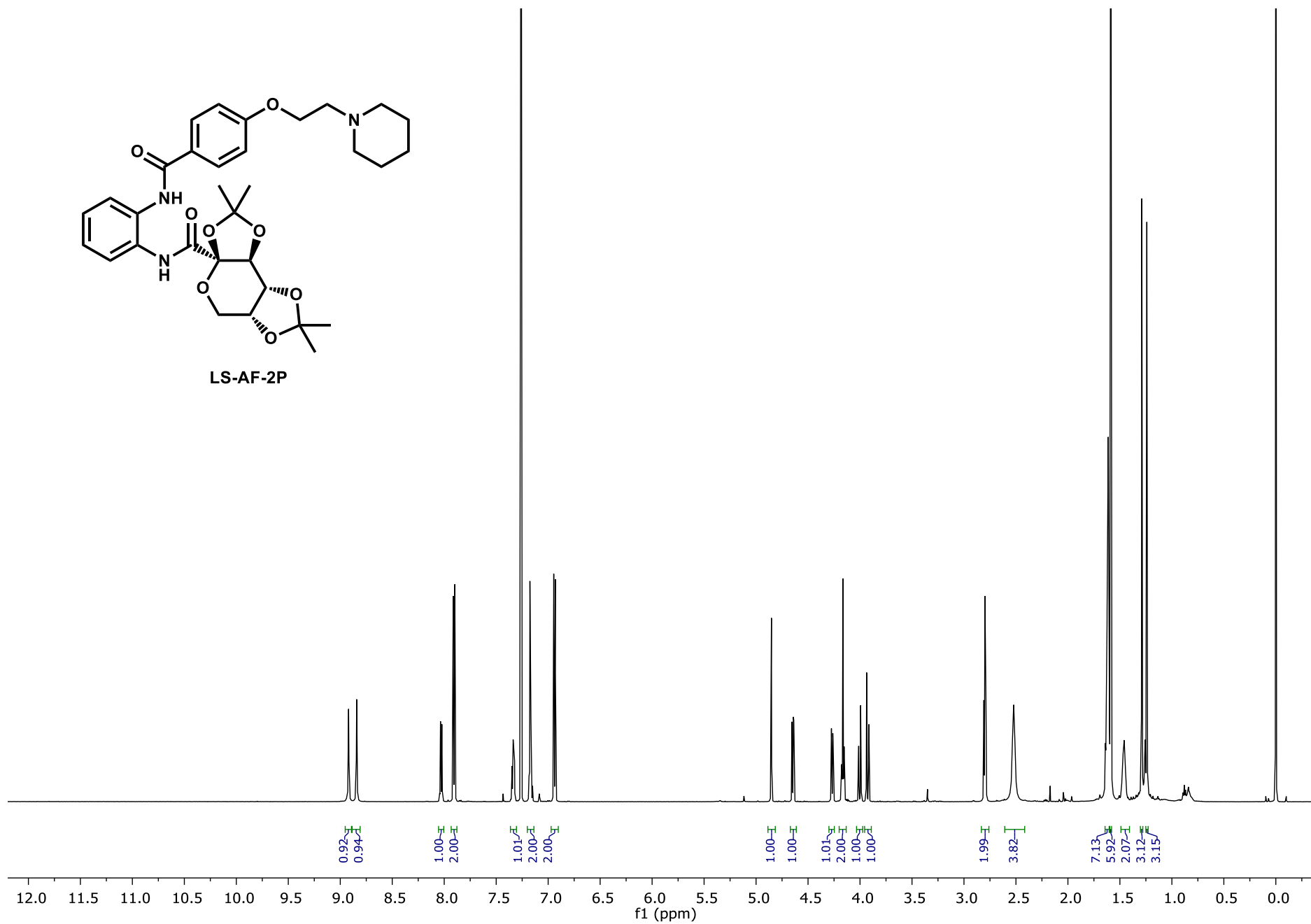
¹³C NMR Spectrum for Compound **21** (CDCl₃, 151 MHz).



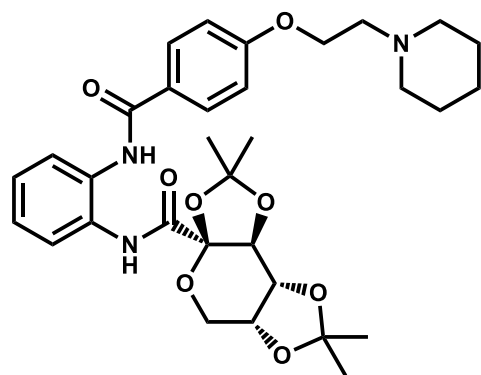
¹H NMR Spectrum for Compound **22** (CDCl₃, 600 MHz). Crude compound taken directly to next step without further purification.



LS-AF-2P



^1H NMR Spectrum for **LS-AF-2P** (CDCl_3 , 600 MHz).



LS-AF-2P

167.69
164.94
161.64

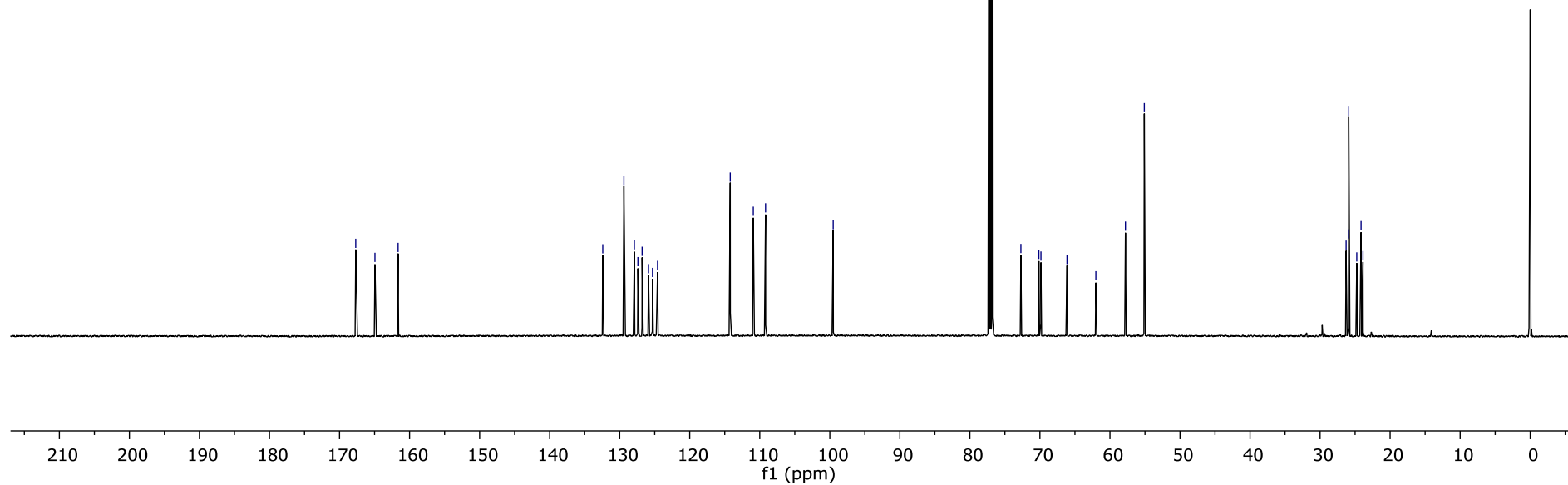
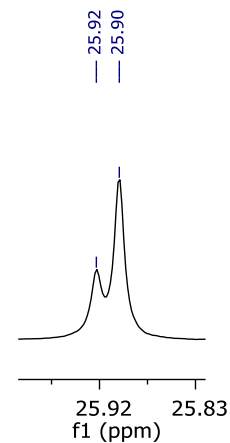
132.42
129.40
127.91
127.40
126.80
125.88
125.31
124.59

114.22
110.92
109.17

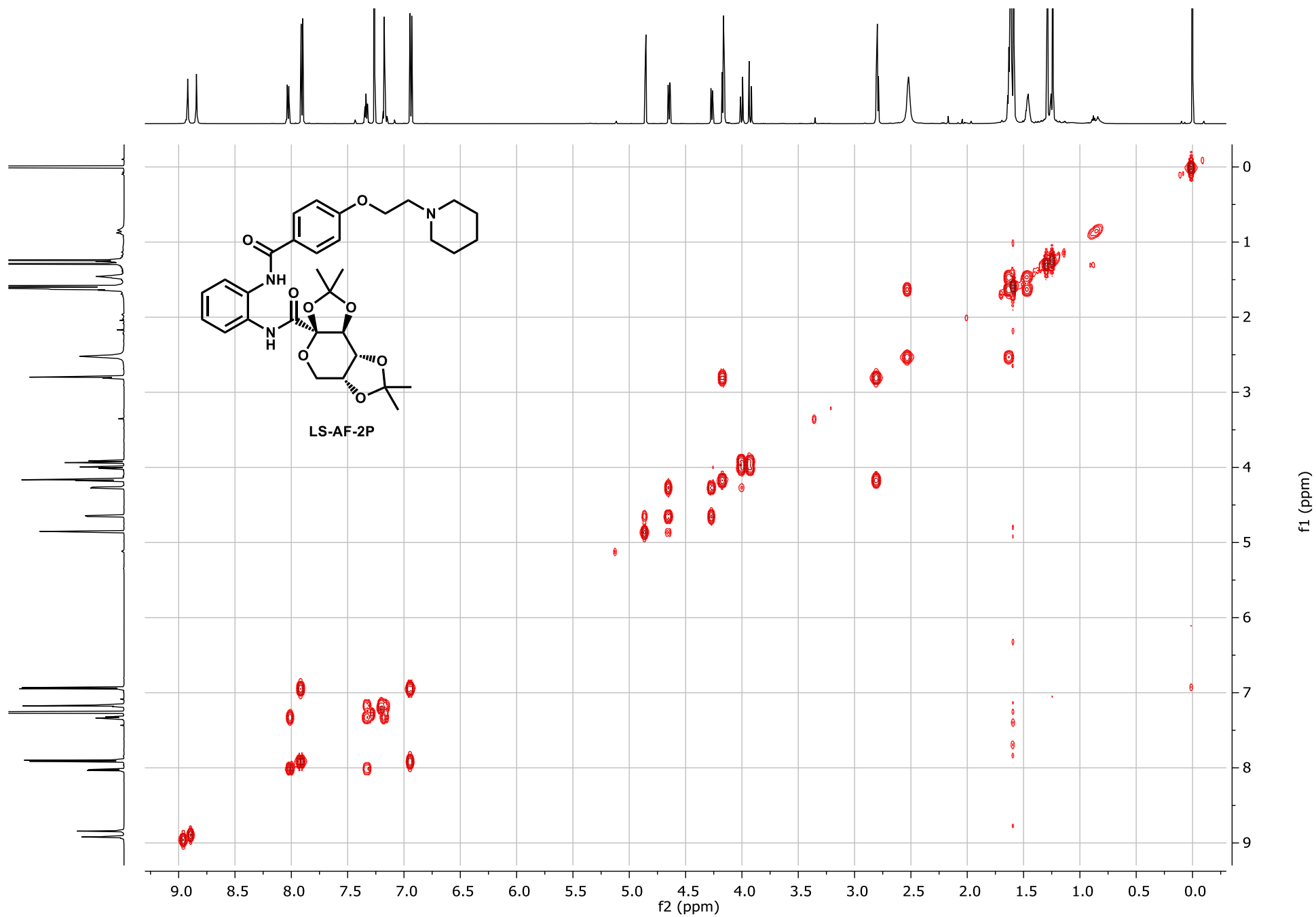
99.52

72.72
70.15
69.85
66.13
62.01
57.79
55.09

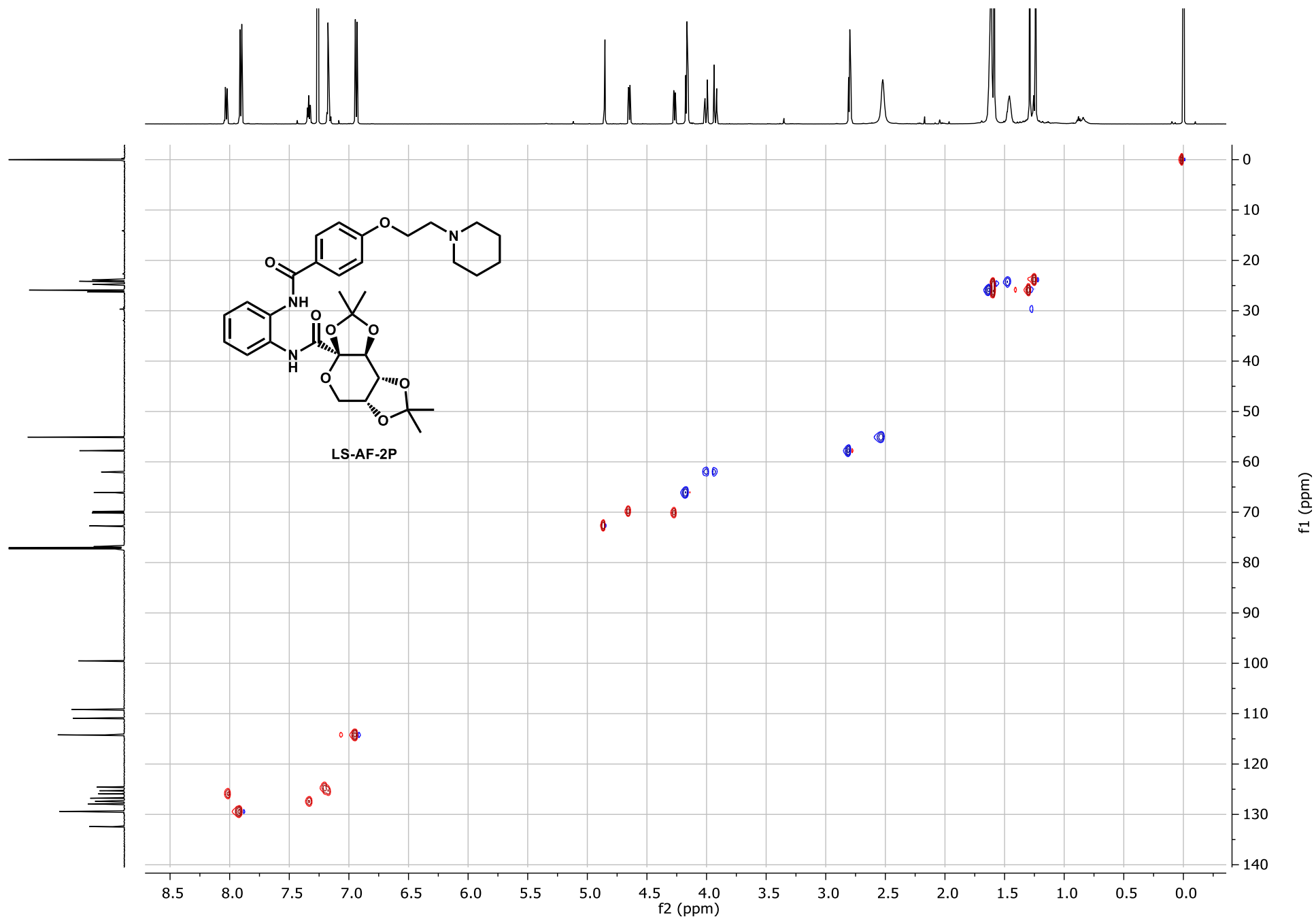
26.28
25.92
25.90
24.76
24.15
23.87

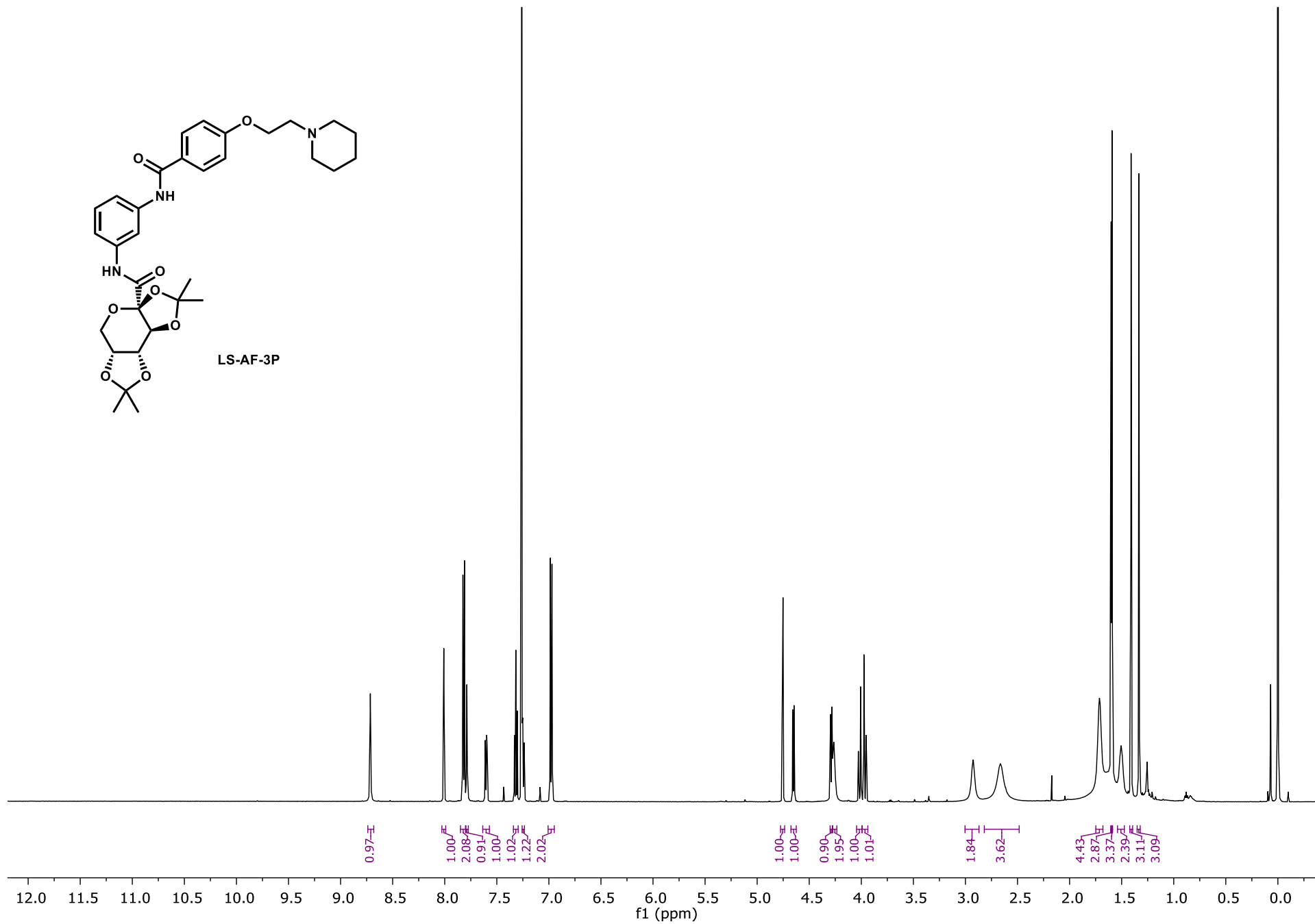
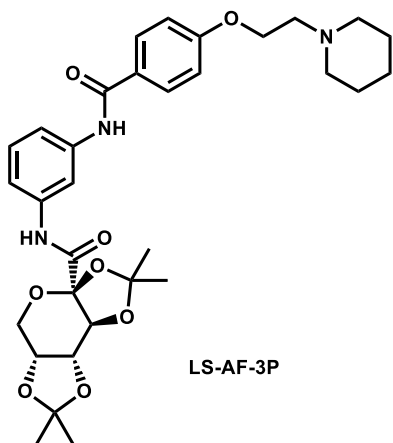


^{13}C NMR Spectrum for LS-AF-2P (CDCl_3 , 151 MHz).

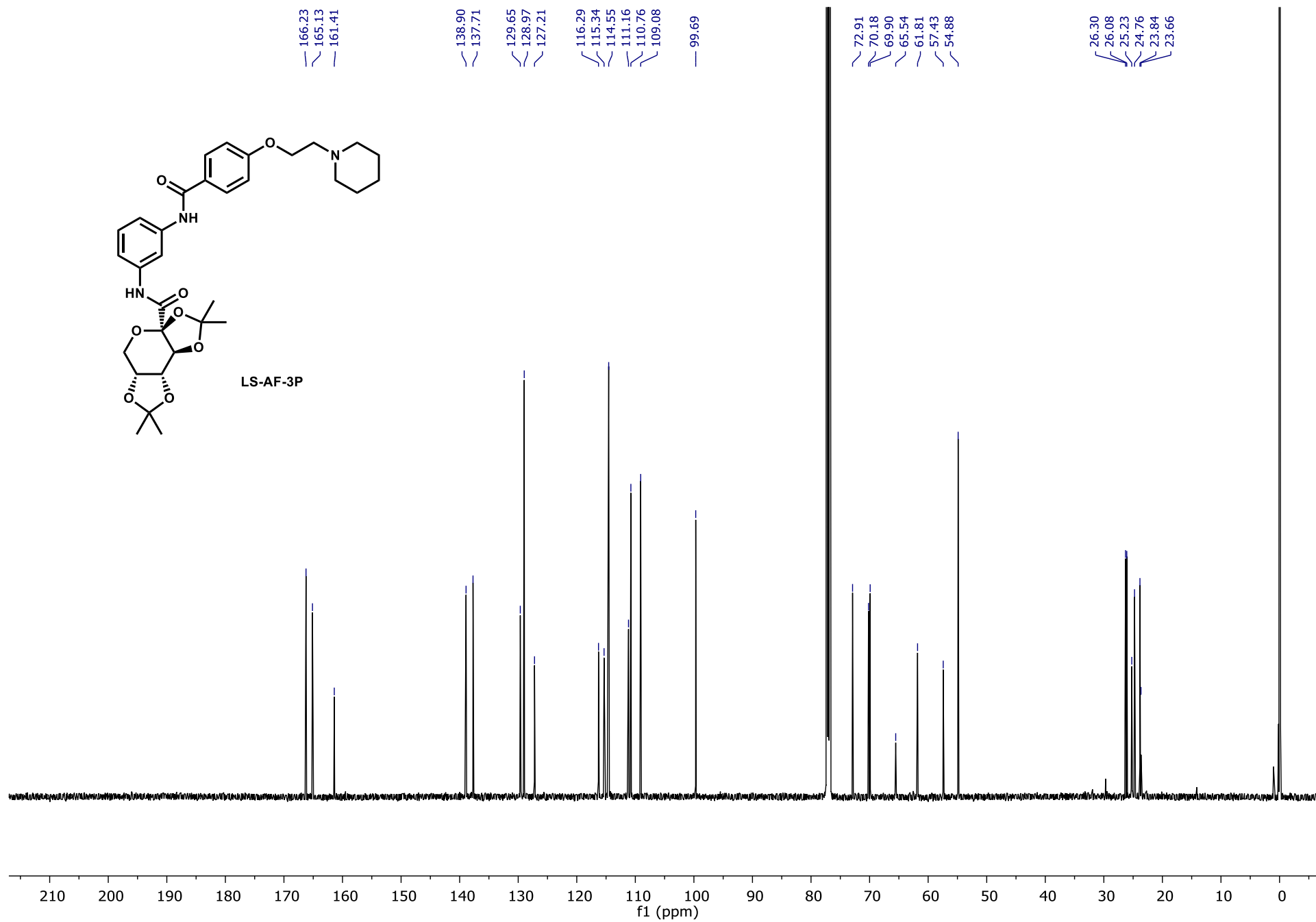
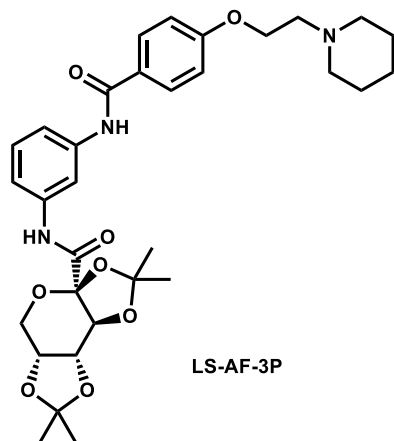


COSY Spectrum for **LS-AF-2P** (CDCl₃).

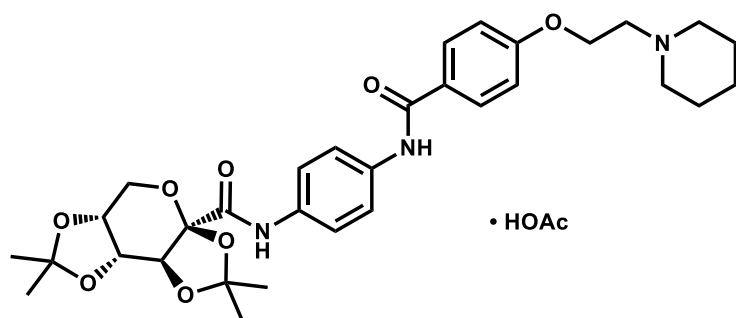




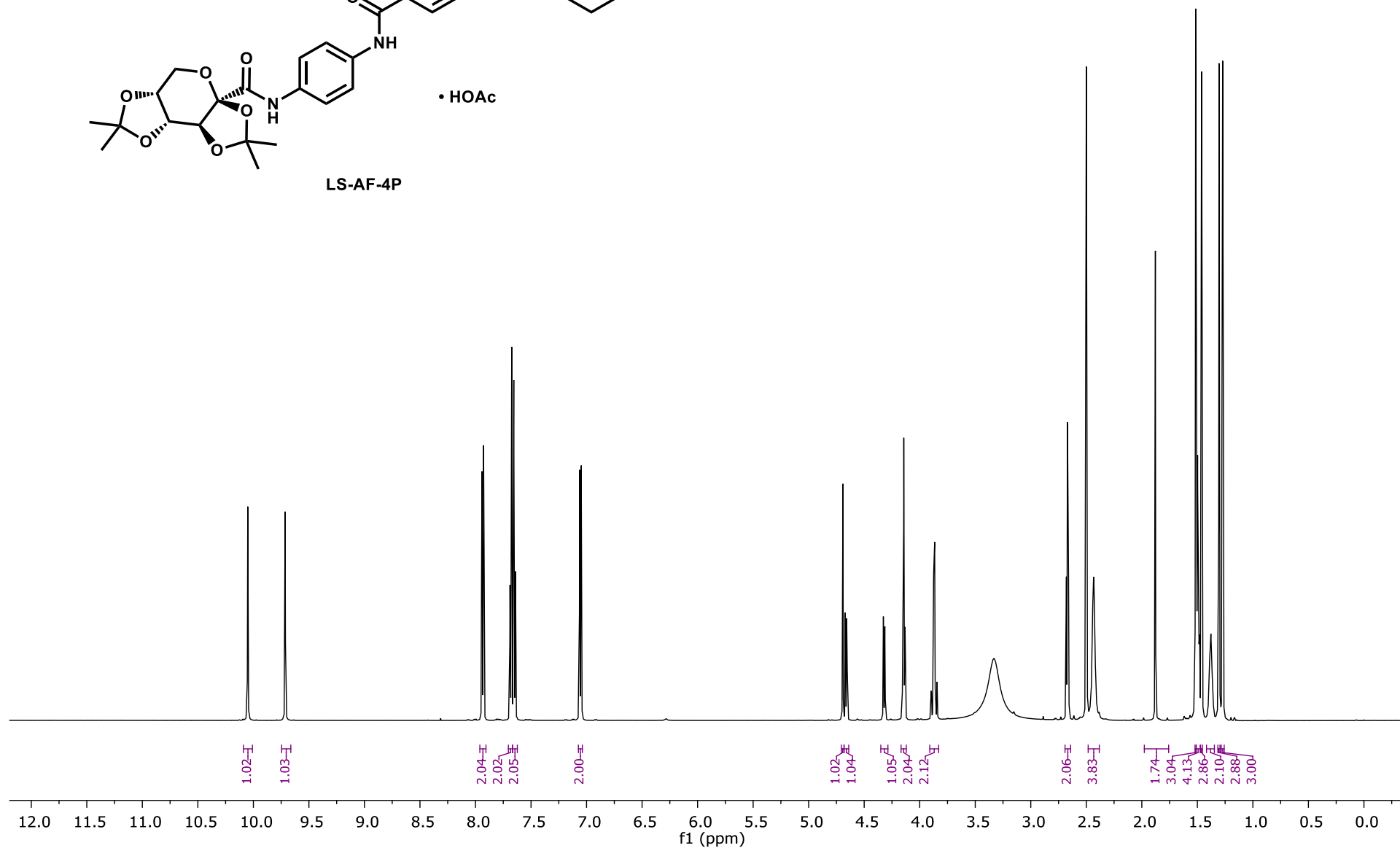
^1H NMR Spectrum for **LS-AF-3P** (CDCl_3 , 600 MHz).



^{13}C NMR Spectrum for LS-AF-3P (CDCl_3 , 151 MHz).



LS-AF-4P



¹H NMR Spectrum for LS-AF-4P (DMSO-*d*₆, 600 MHz).

