

Synthesis and Preliminary Anti-inflammatory Activity

Exploration of Novel Derivatives of Kirenol

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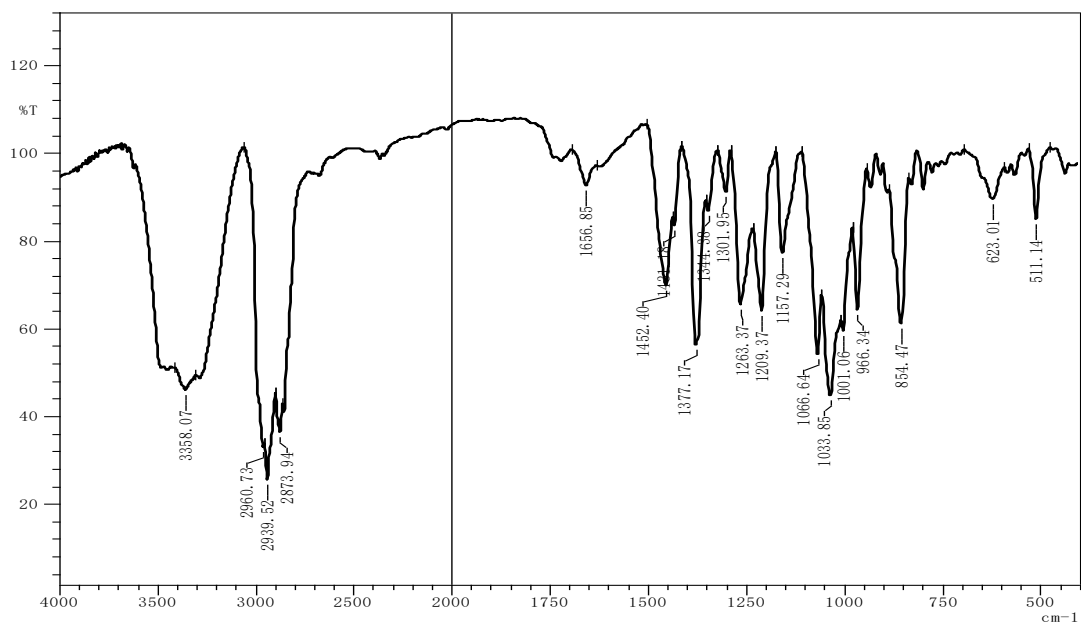
Supporting Information

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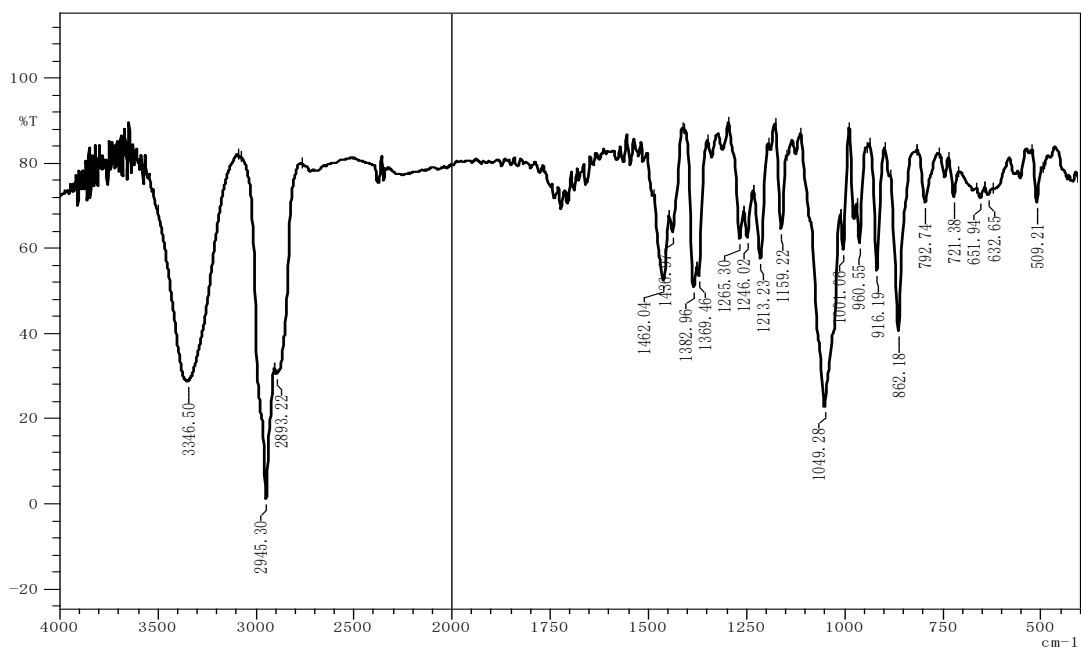
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IR(KBr) of compounds 2-20d

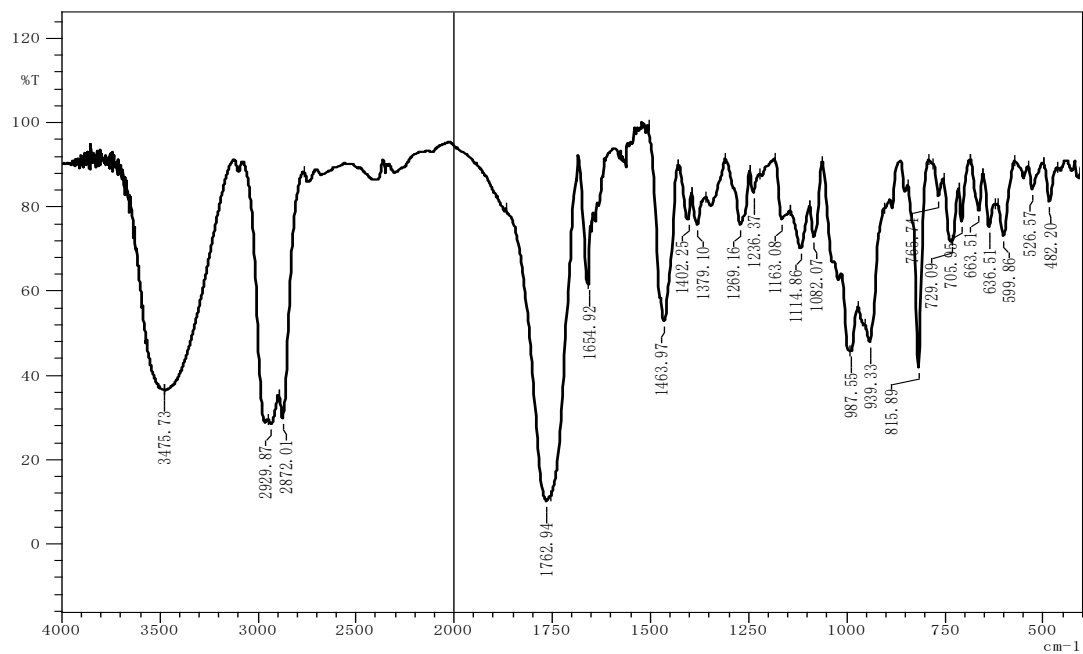
For compound **2**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



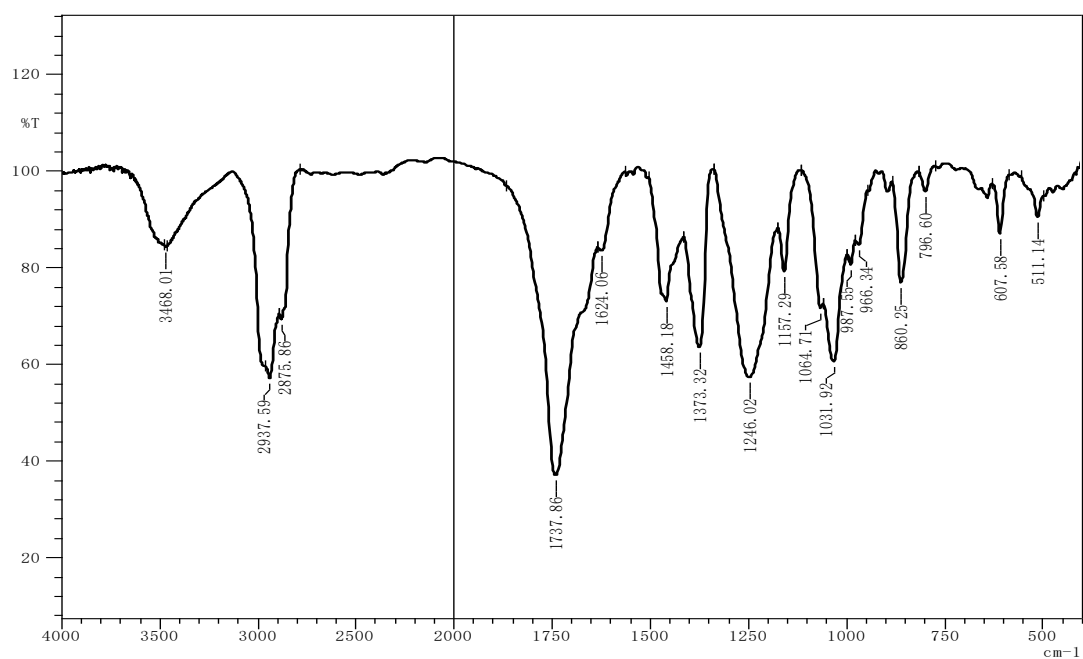
For compound **3**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



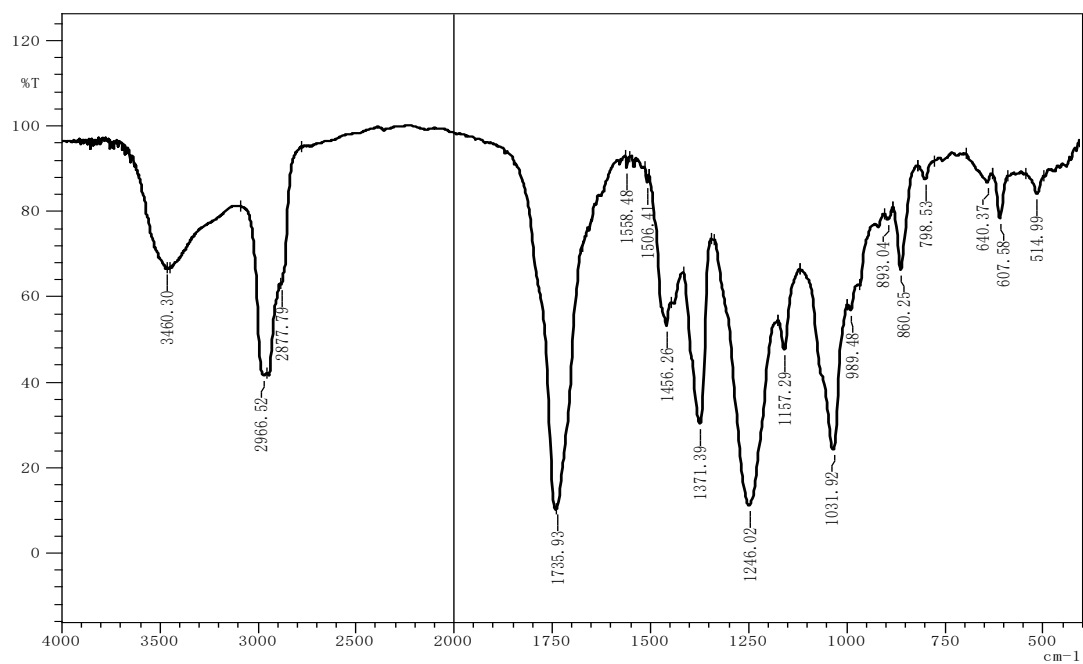
For compound **4**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



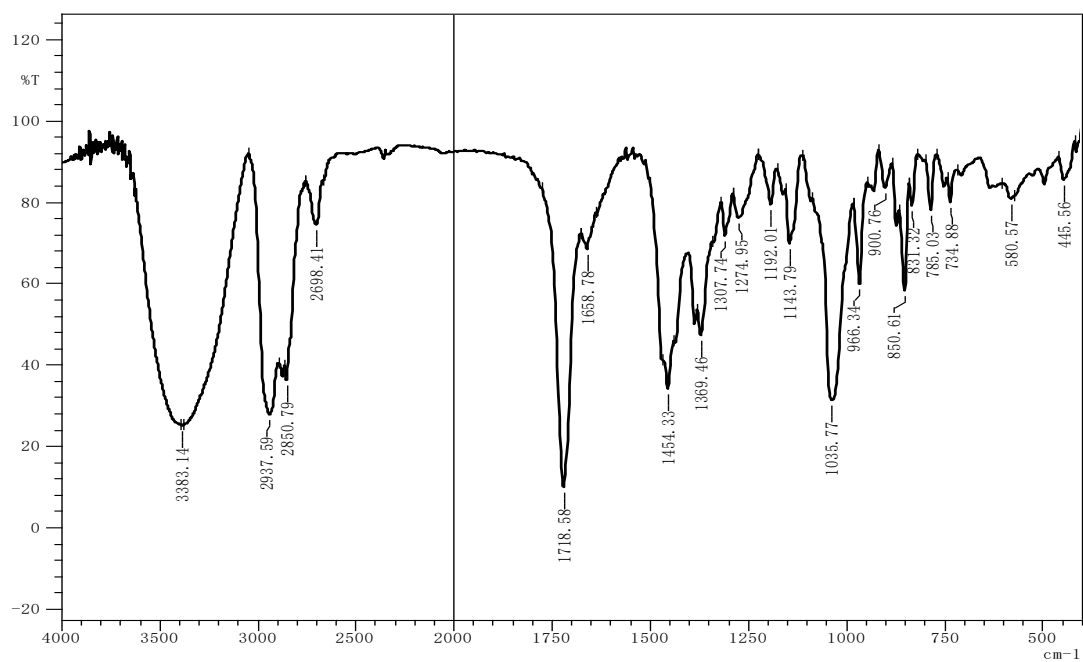
For compound 5, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



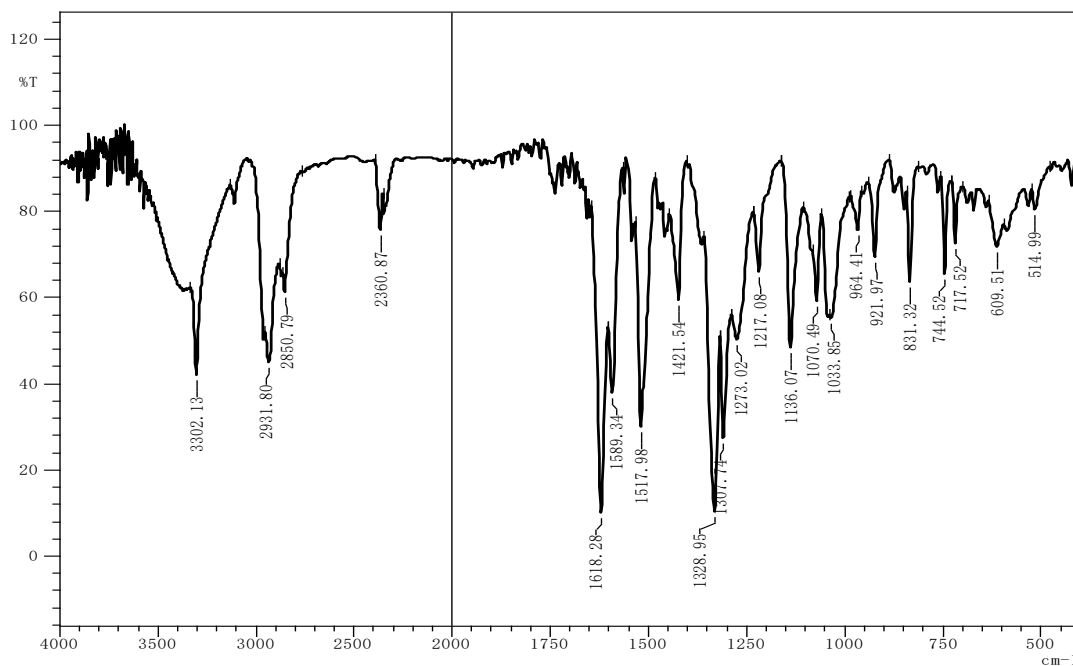
For compound 6, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



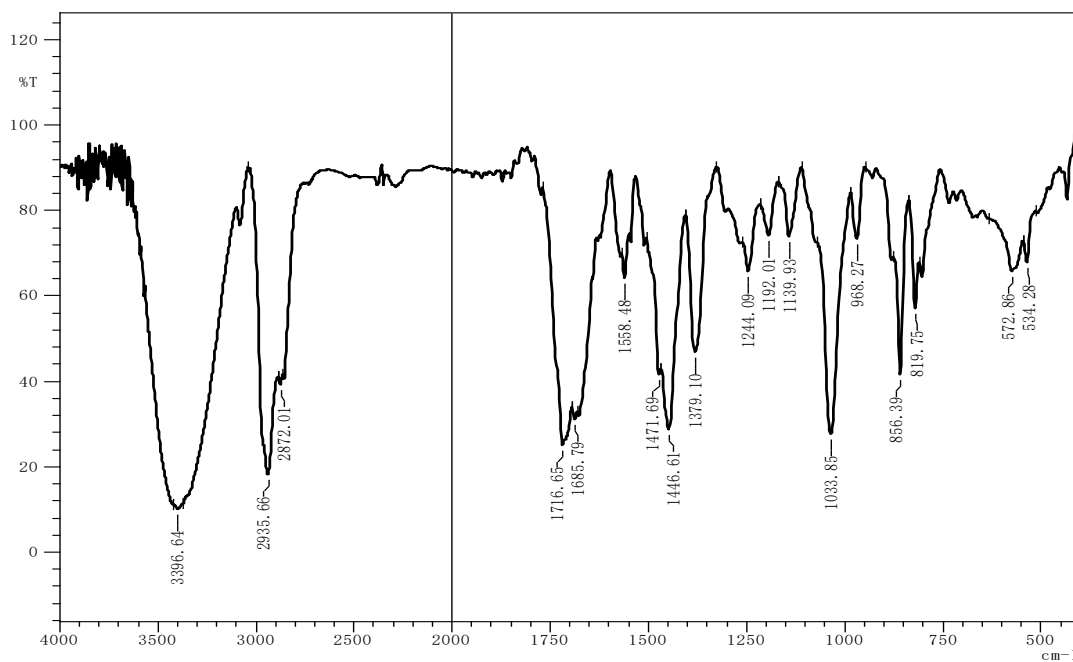
For compound 7, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



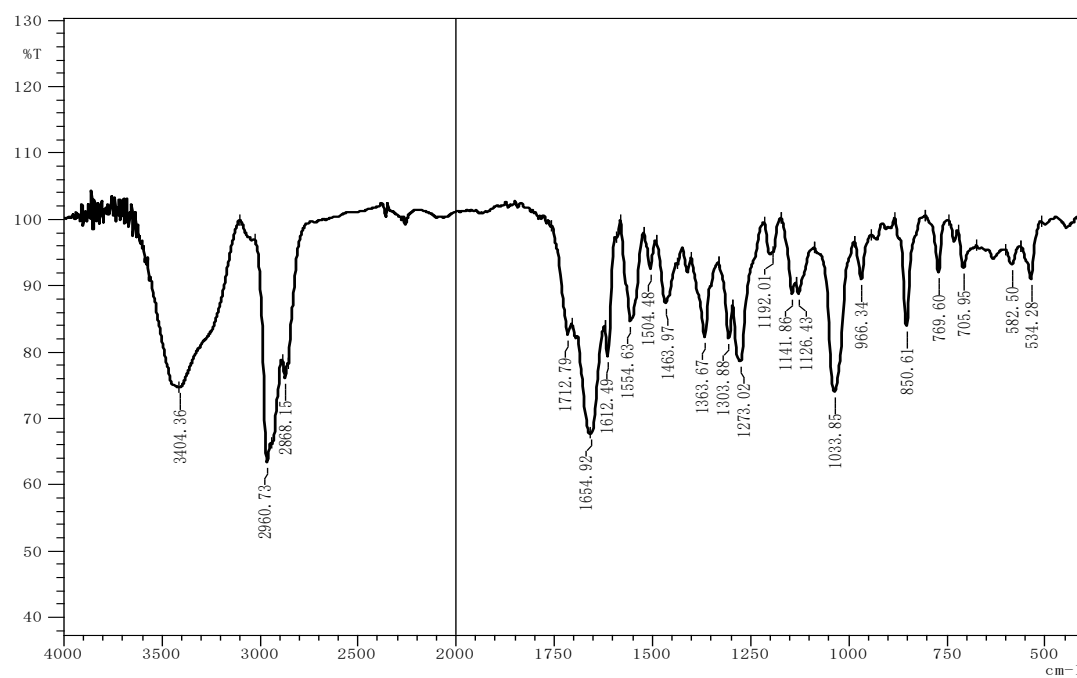
For compound 8a, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



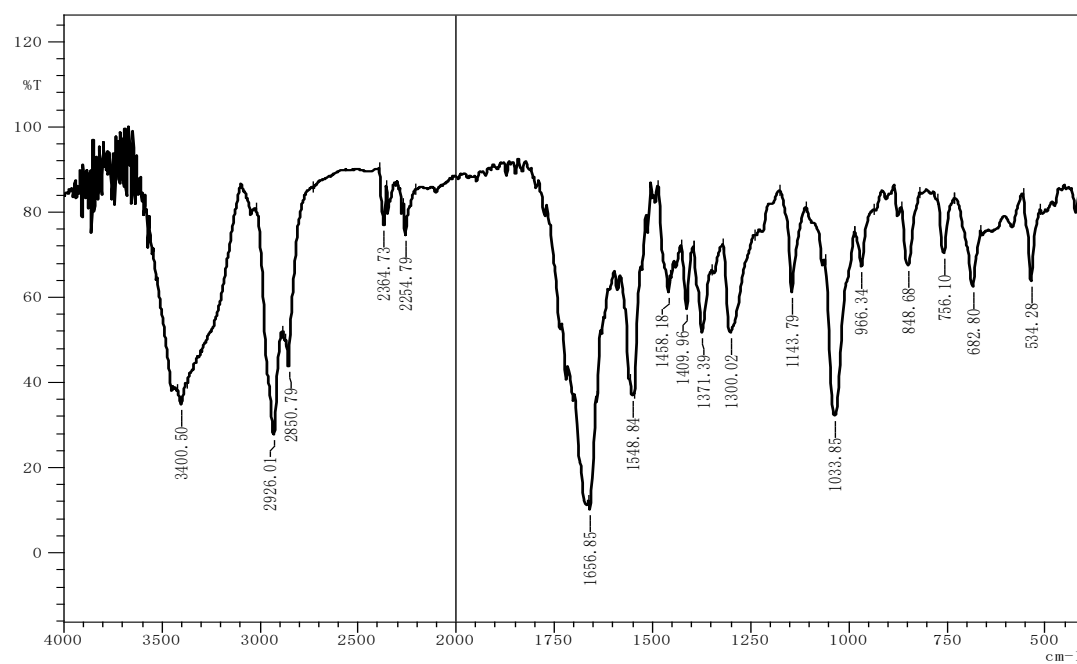
For compound **8b**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



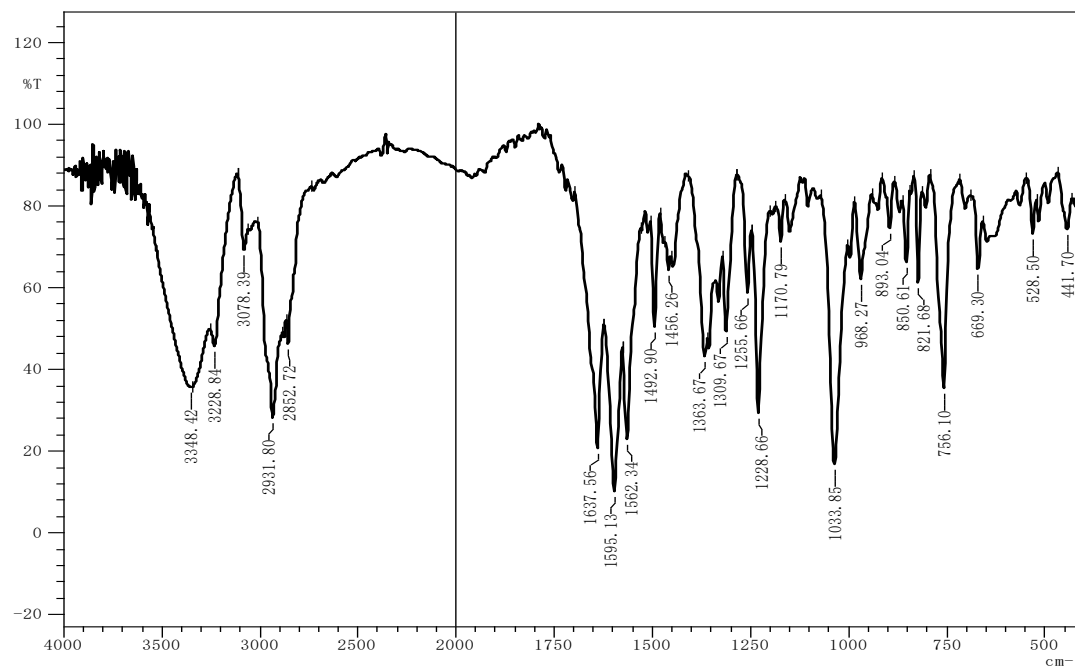
For compound **8c**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



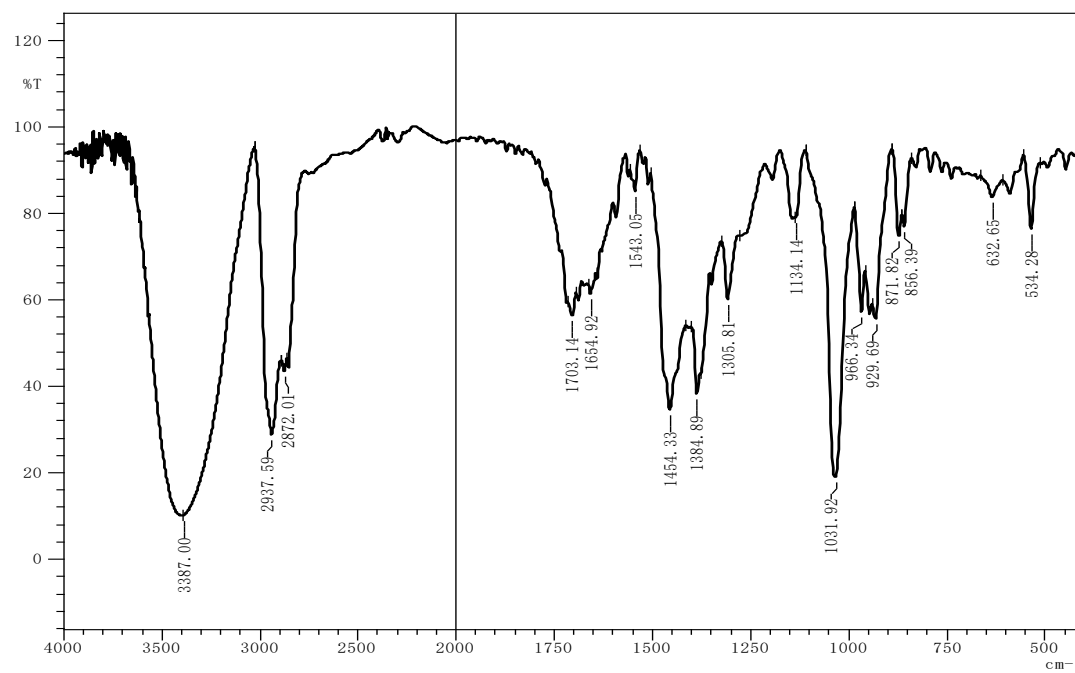
For compound **8d**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



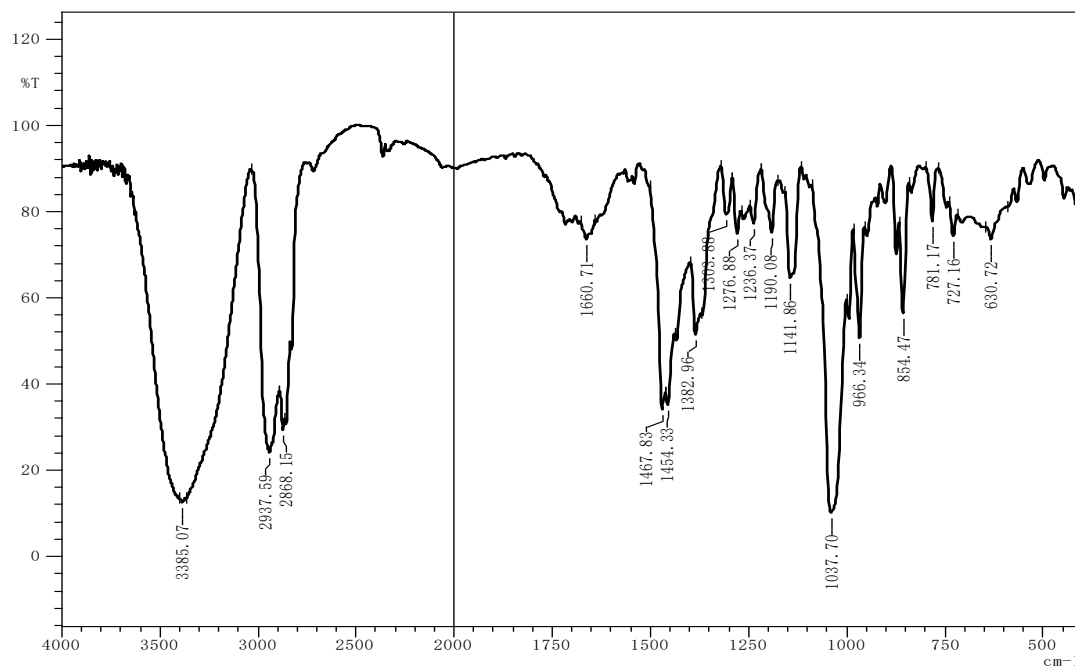
For compound **8e**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



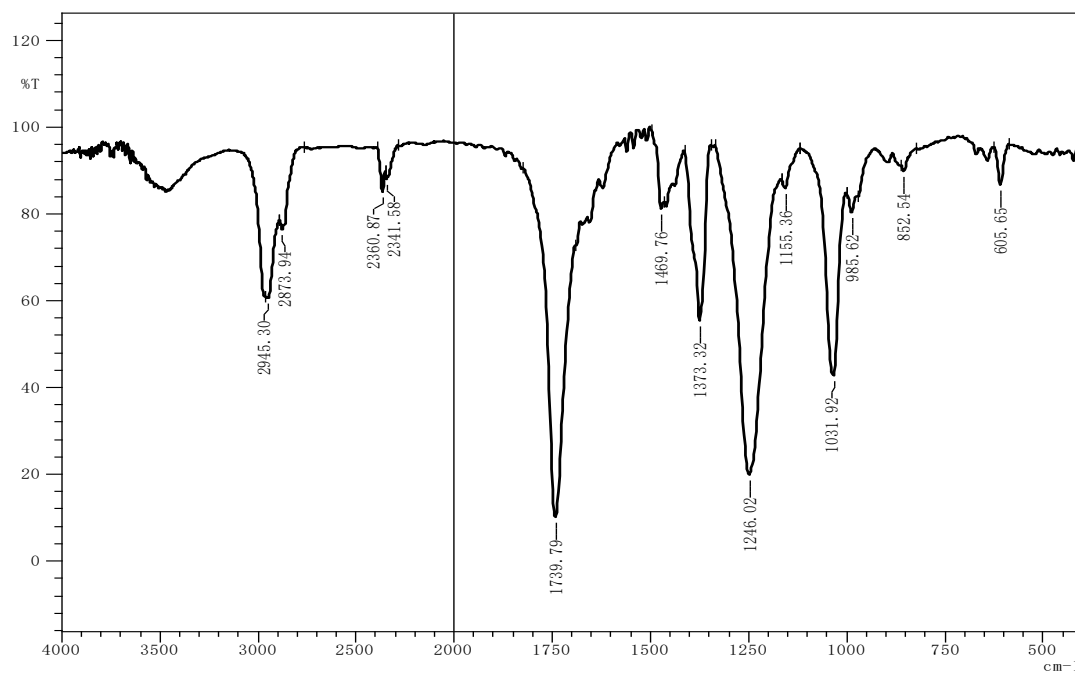
For compound **9**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



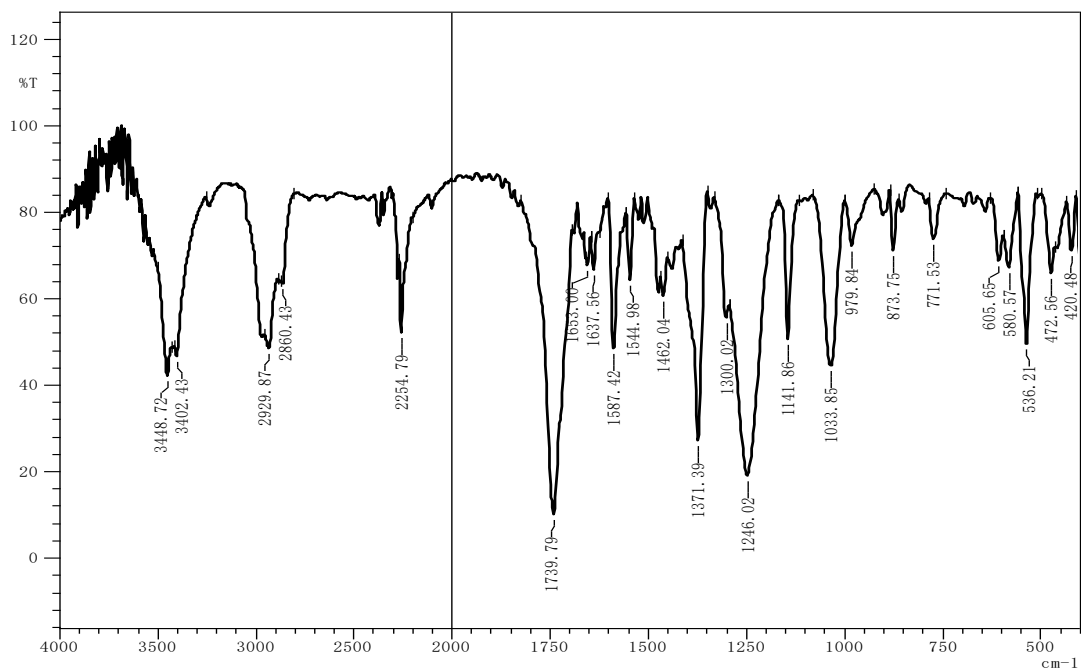
For compound **10**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



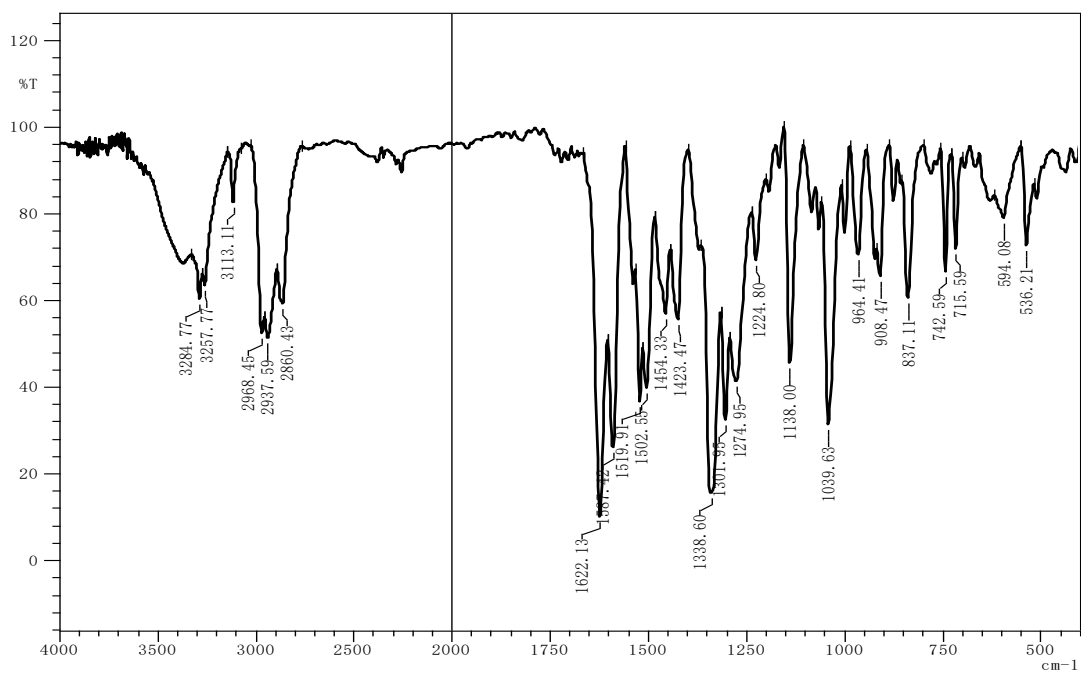
For compound **11**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



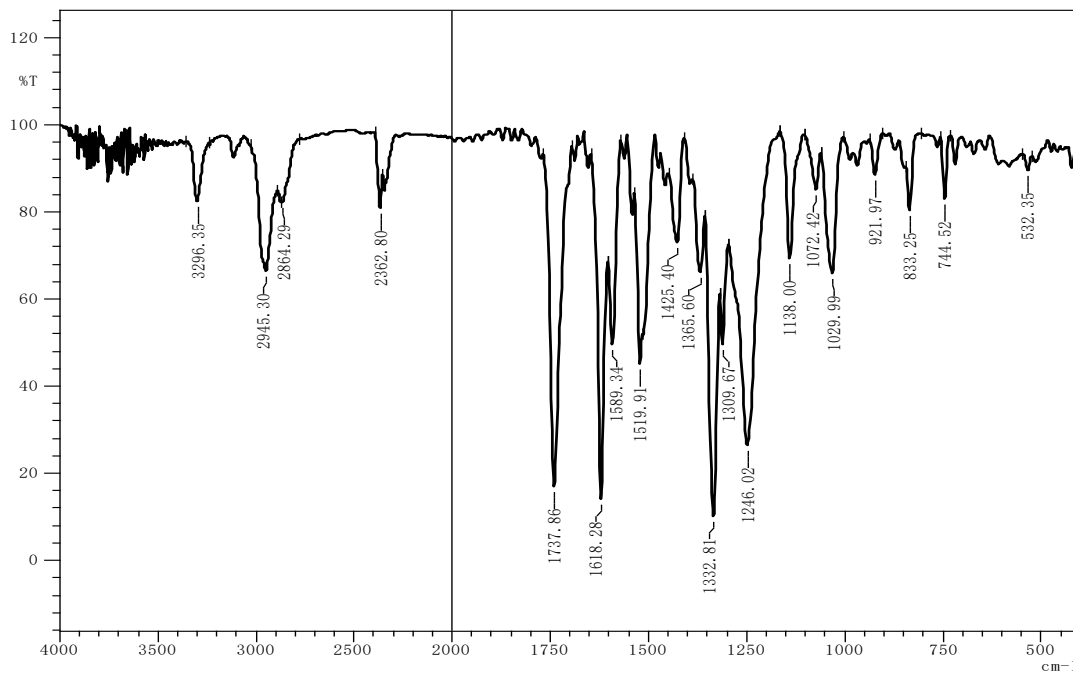
For compound **12**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



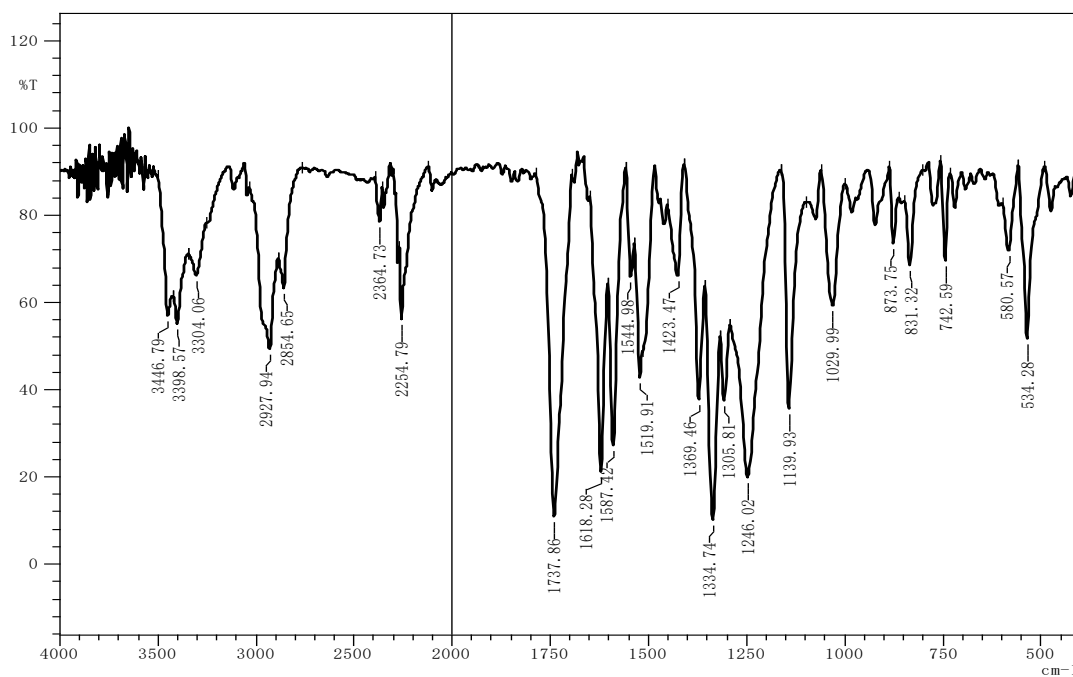
For compound **13**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



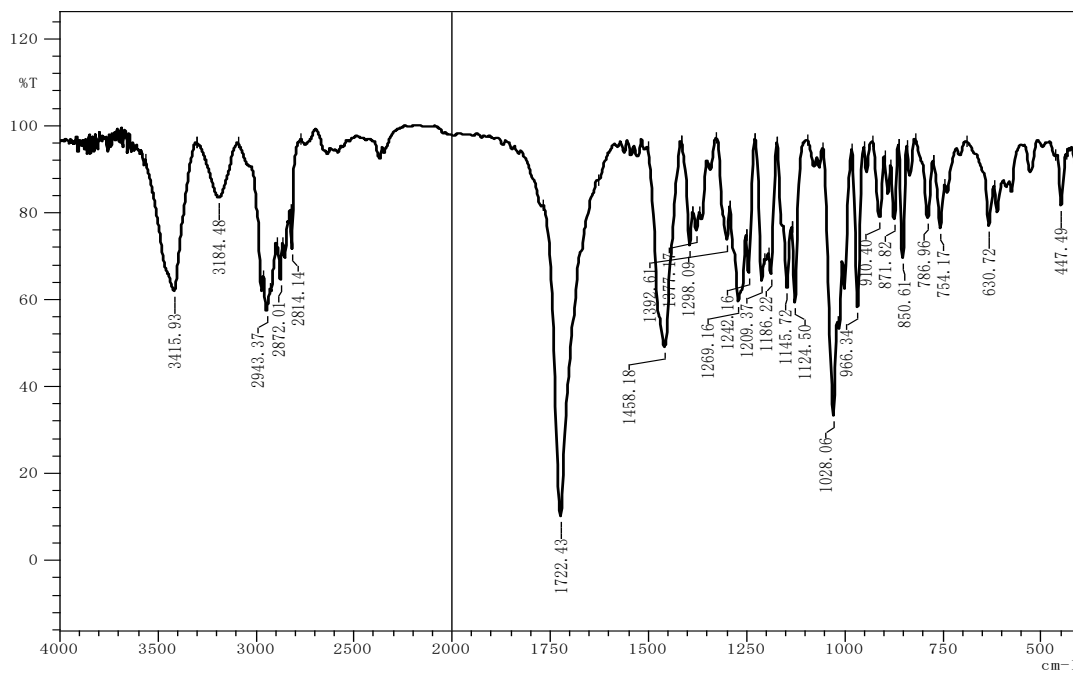
For compound **14**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



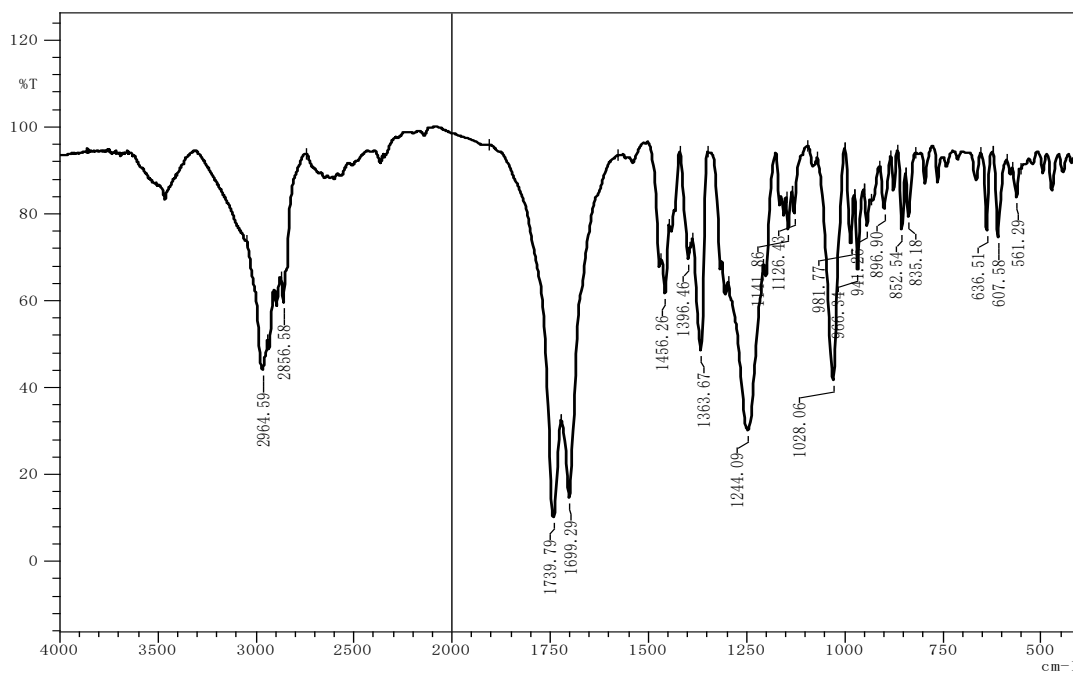
For compound **15**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



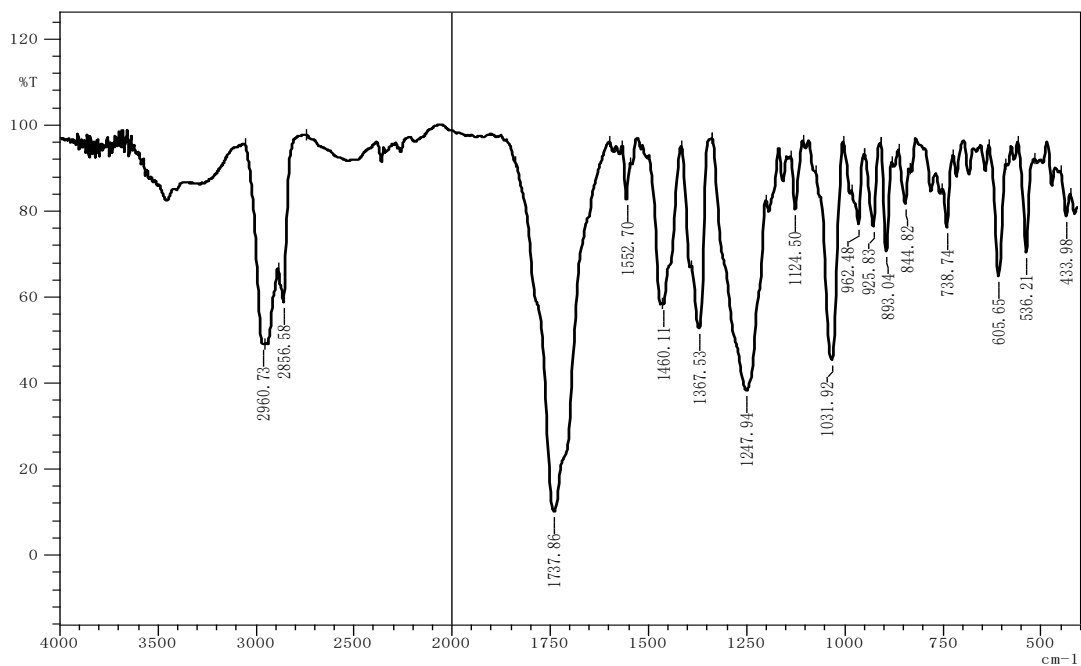
For compound **16**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



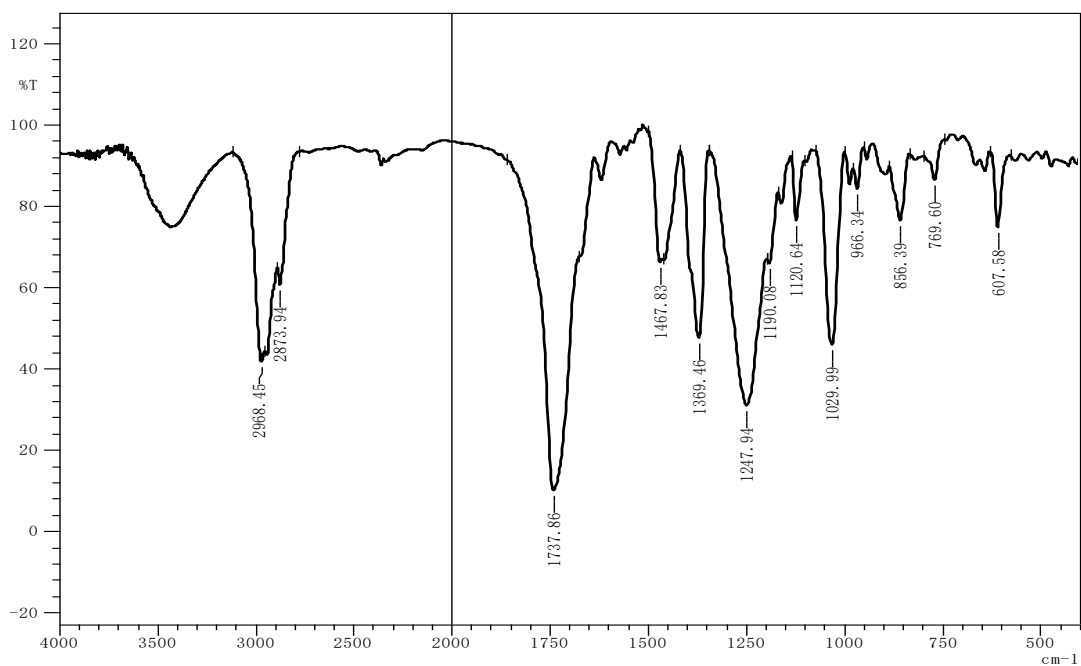
For compound **17**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



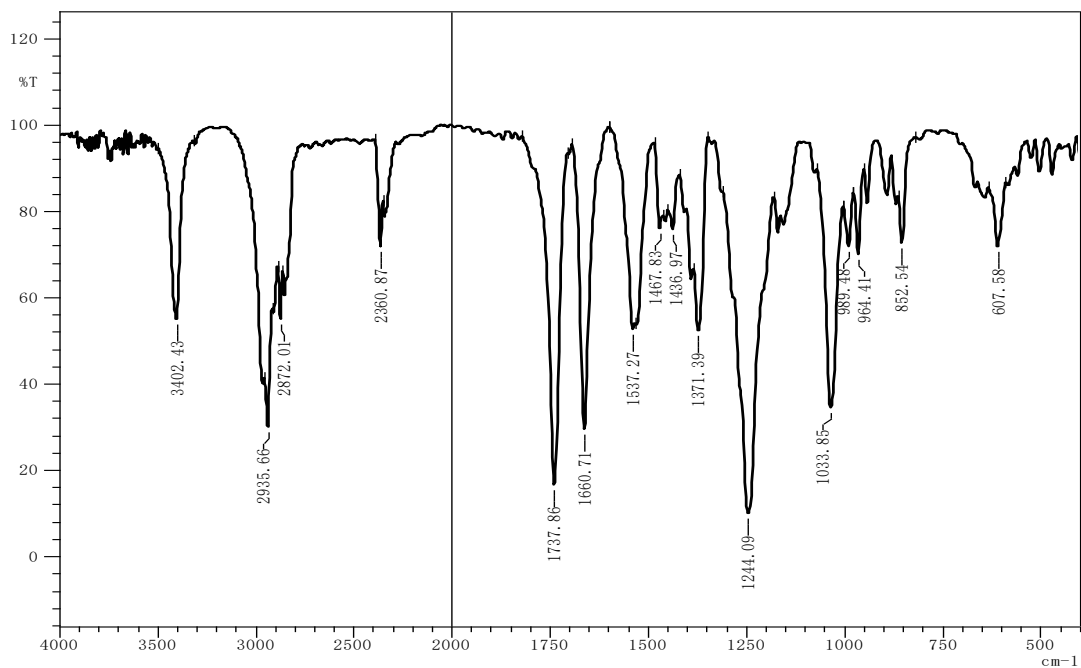
For compound **18**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



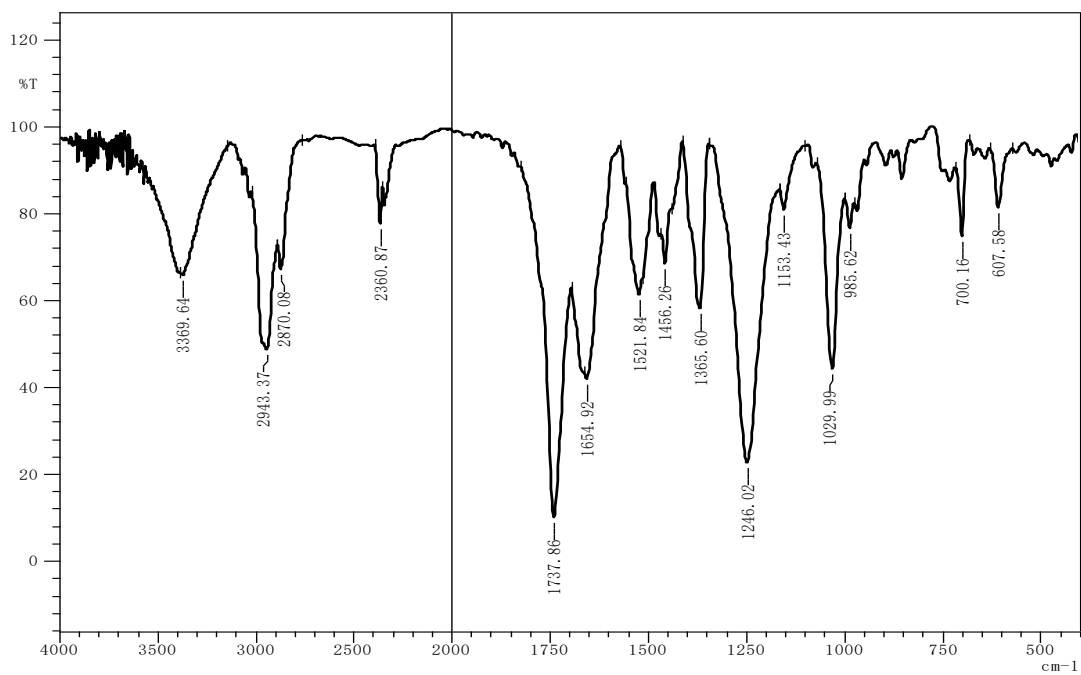
For compound **19a**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



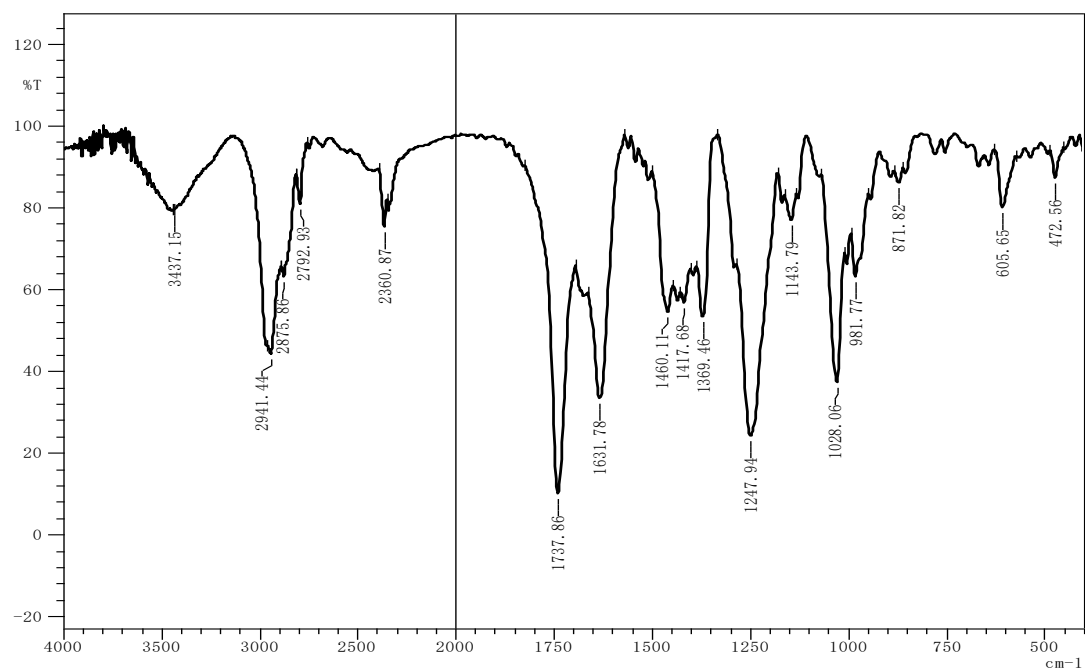
For compound **19b**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



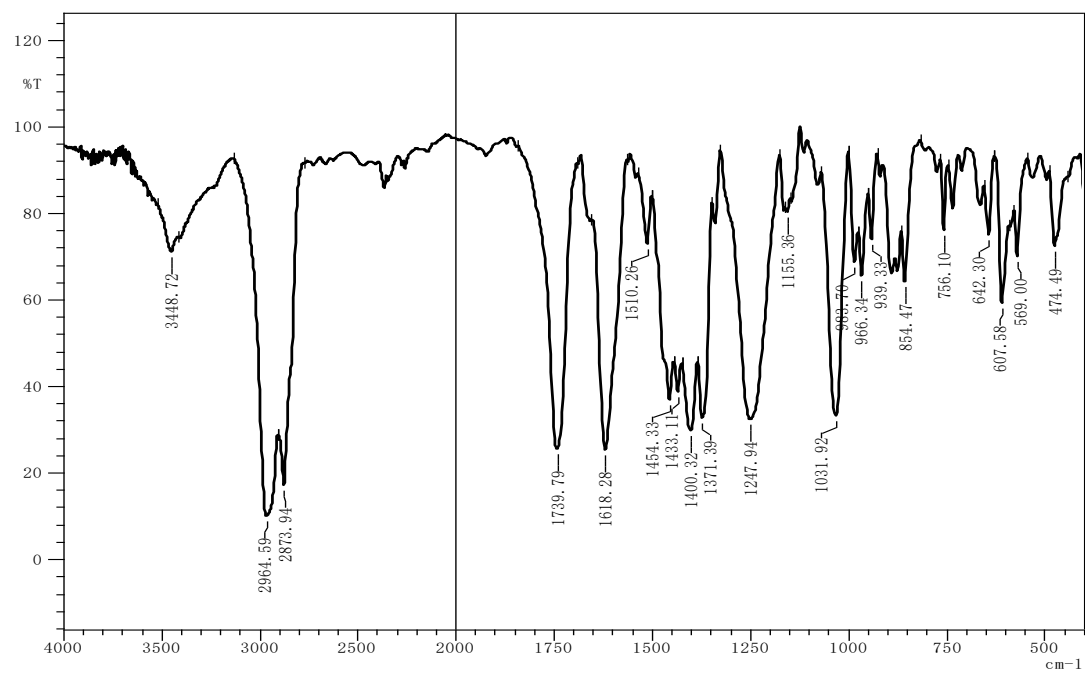
For compound **19c**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



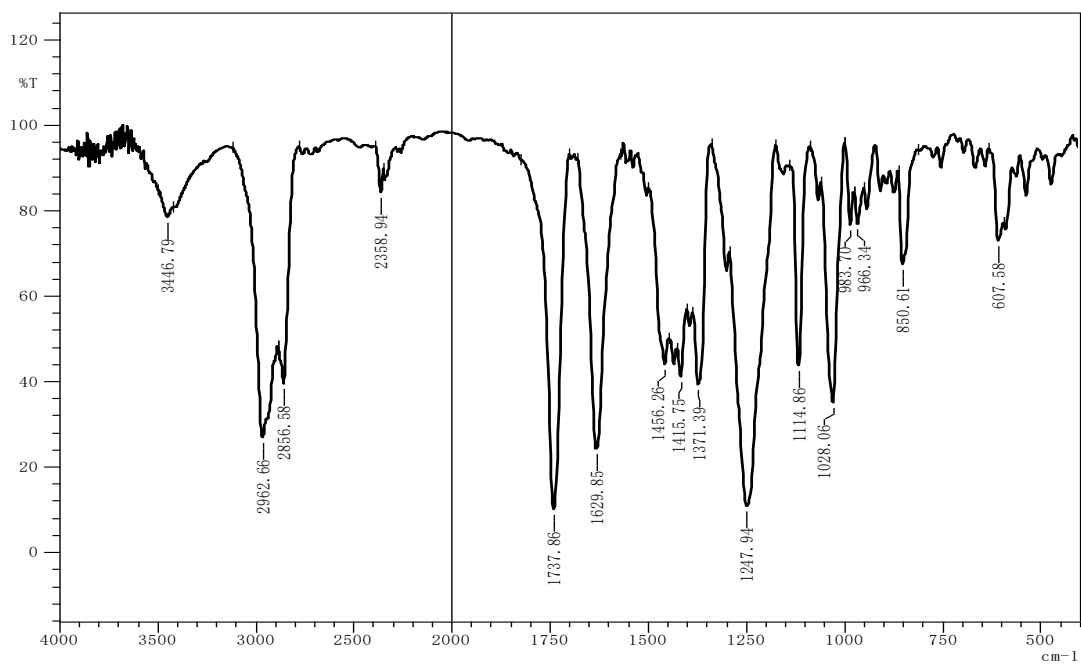
For compound **19d**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



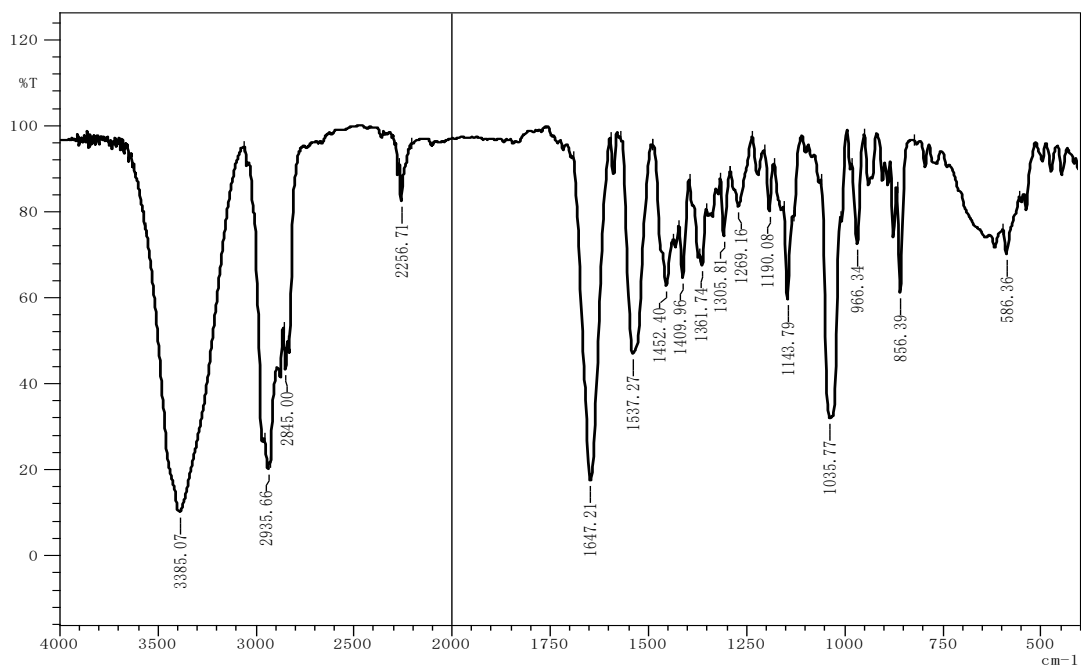
For compound **19e**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



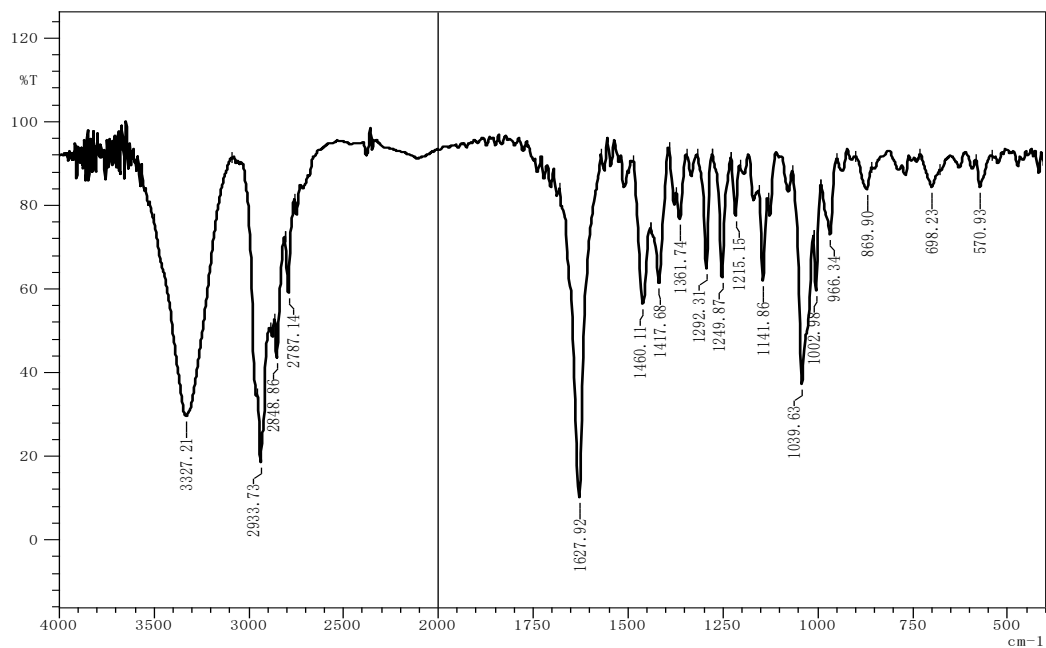
For compound **19f**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



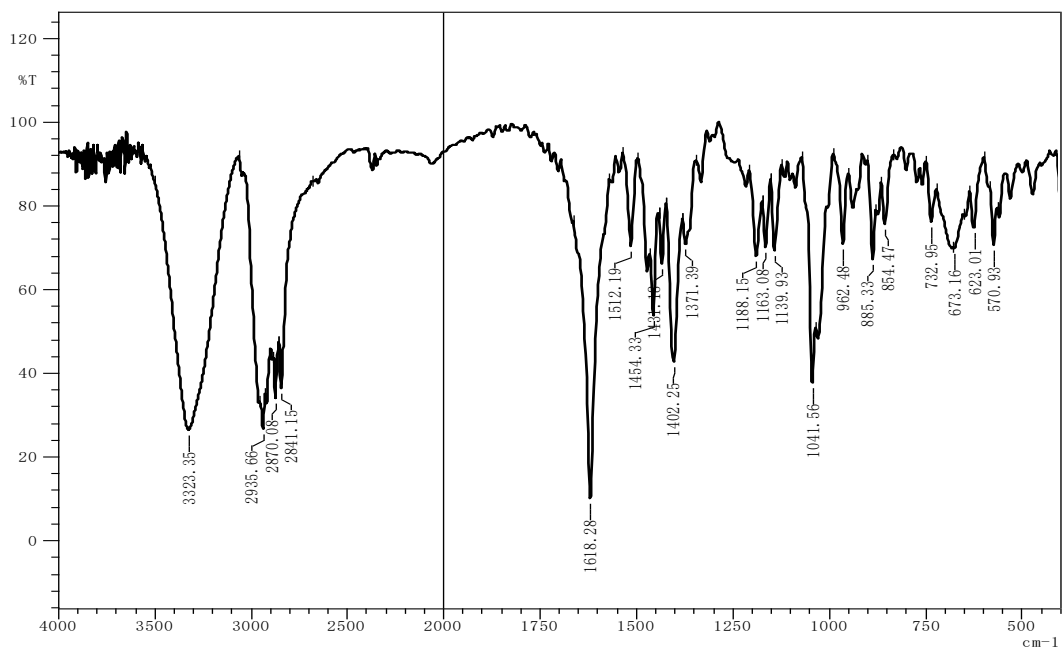
For compound **20a**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



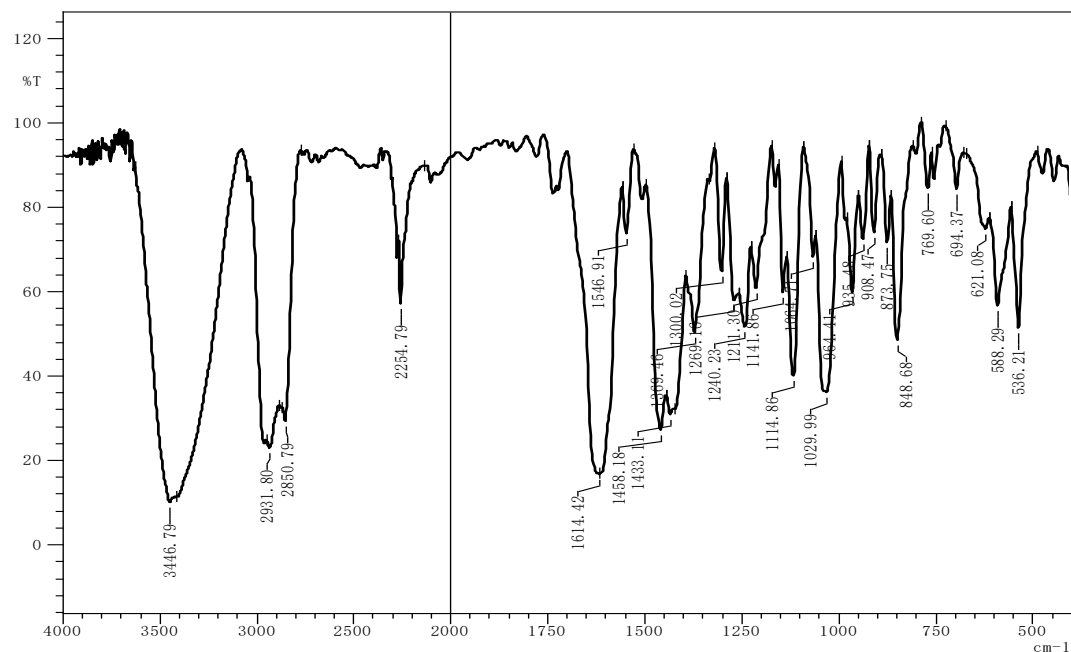
For compound **20b**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



For compound **20c**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:

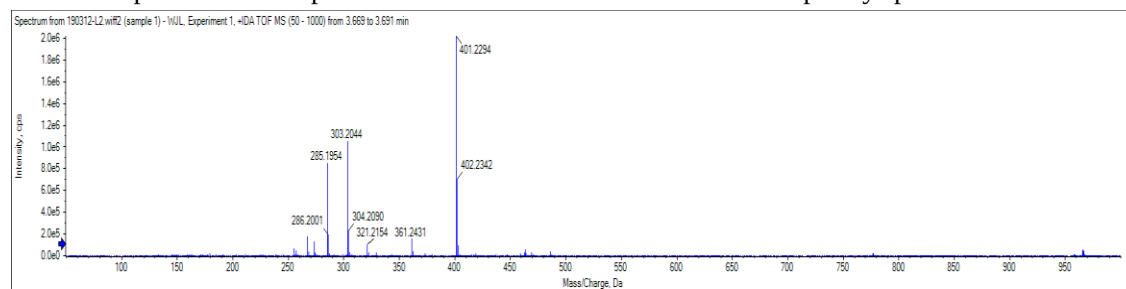


For compound **20d**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:

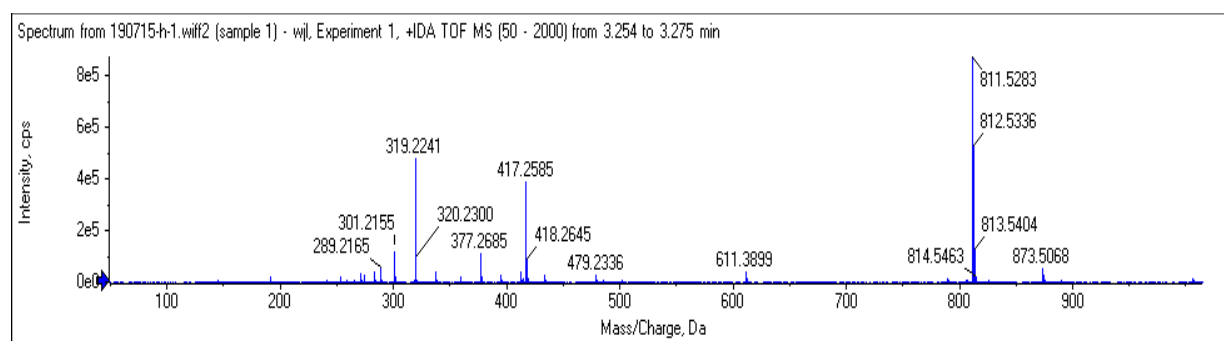


Mass spectra of compounds 2-20d

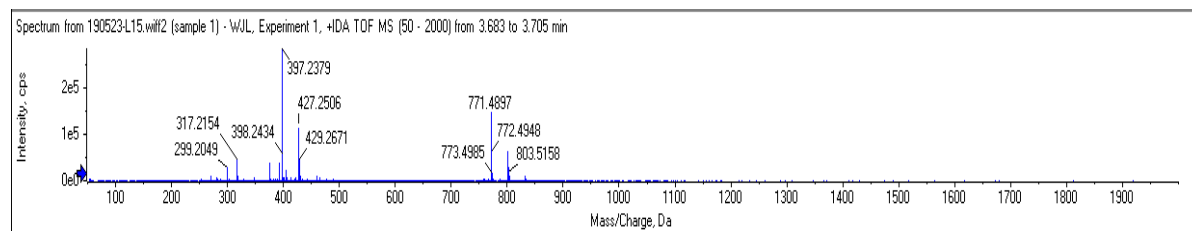
ESI mass spectrum of compound **2** recorded on an AGILENT 1200 Capillary spectrometer:



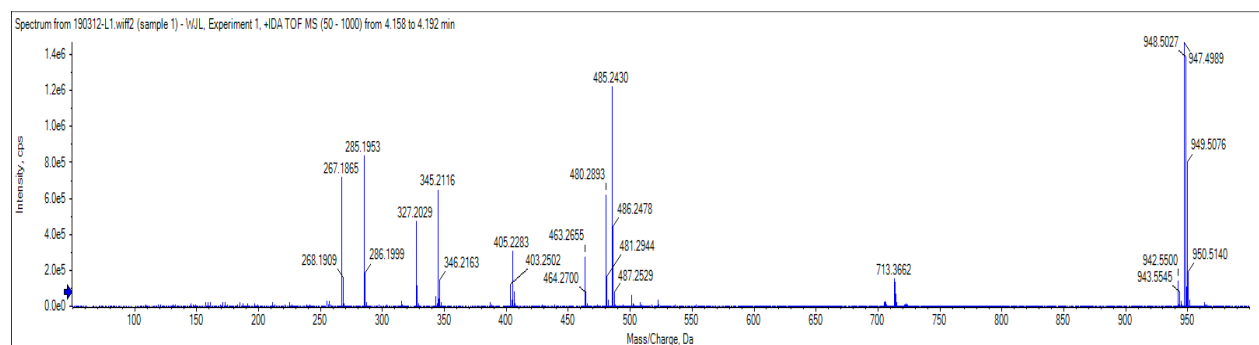
ESI mass spectrum of compound **3** recorded on an AGILENT 1200 Capillary spectrometer:



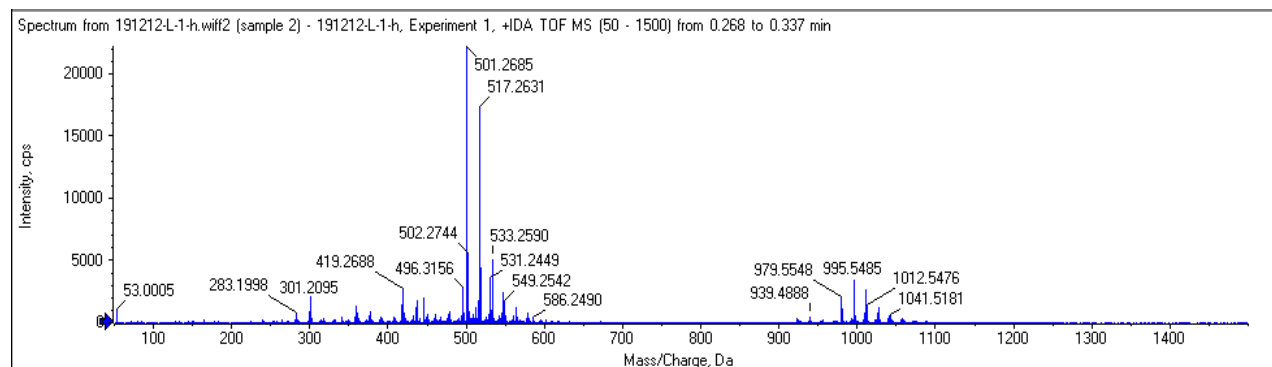
ESI mass spectrum of compound **4** recorded on an AGILENT 1200 Capillary spectrometer:



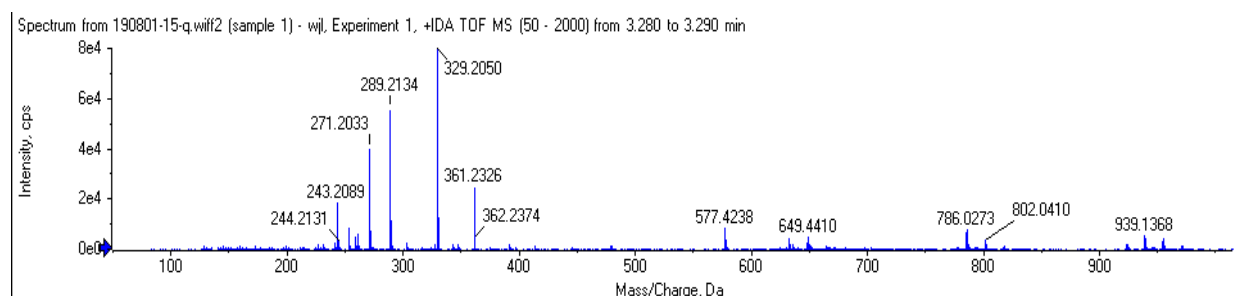
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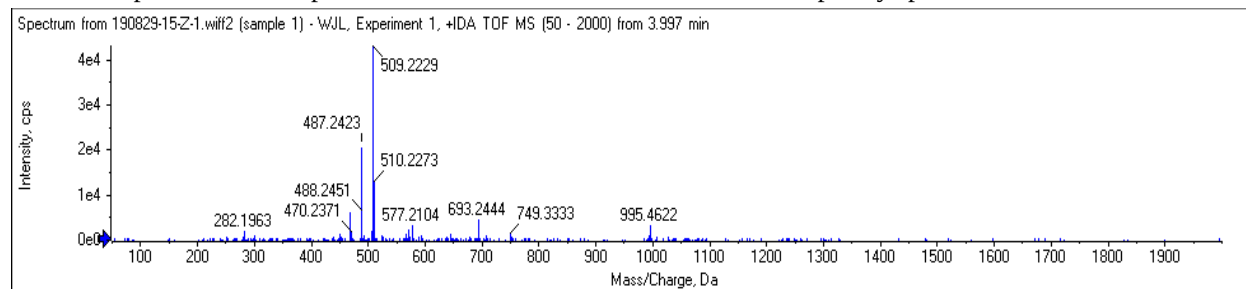
ESI mass spectrum of compound **6** recorded on an AGILENT 1200 Capillary spectrometer:



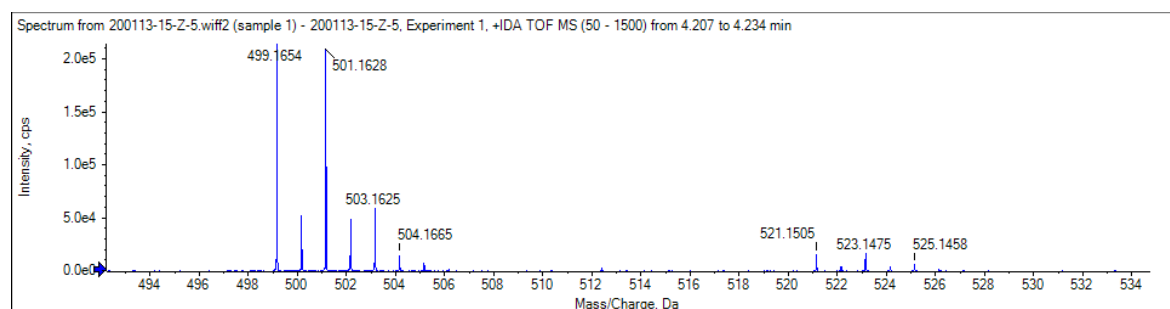
ESI mass spectrum of compound **7** recorded on an AGILENT 1200 Capillary spectrometer:



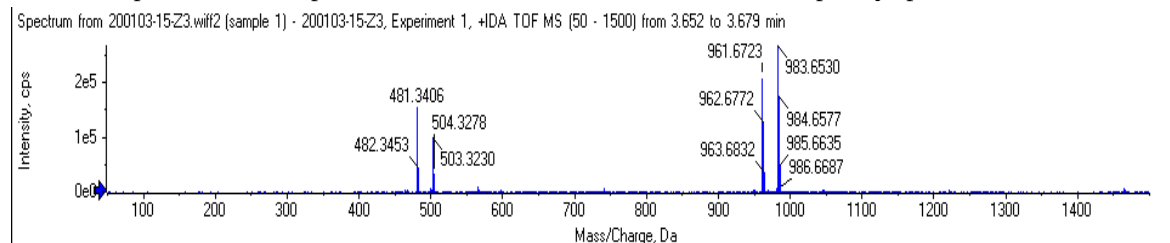
ESI mass spectrum of compound **8a** recorded on an AGILENT 1200 Capillary spectrometer:



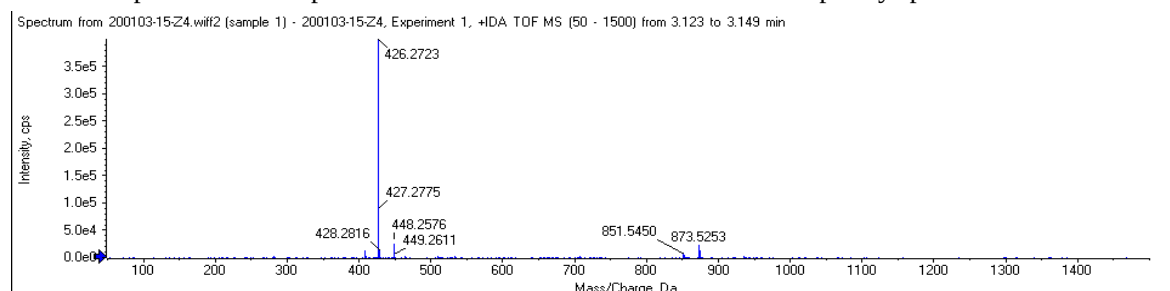
ESI mass spectrum of compound **8b** recorded on an AGILENT 1200 Capillary spectrometer:



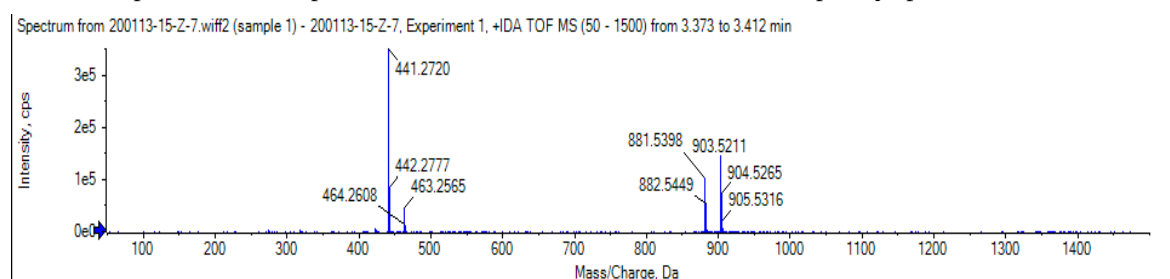
ESI mass spectrum of compound **8c** recorded on an AGILENT 1200 Capillary spectrometer:



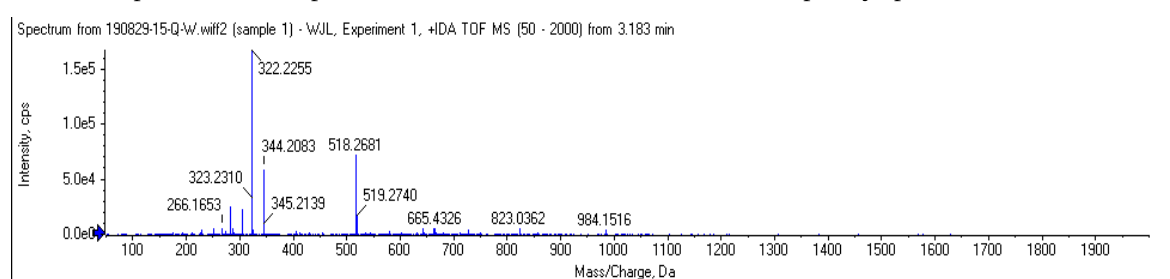
ESI mass spectrum of compound **8d** recorded on an AGILENT 1200 Capillary spectrometer:



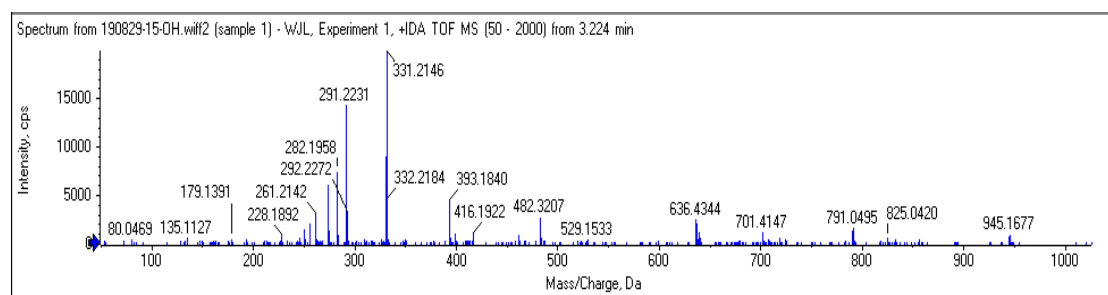
ESI mass spectrum of compound **8e** recorded on an AGILENT 1200 Capillary spectrometer:



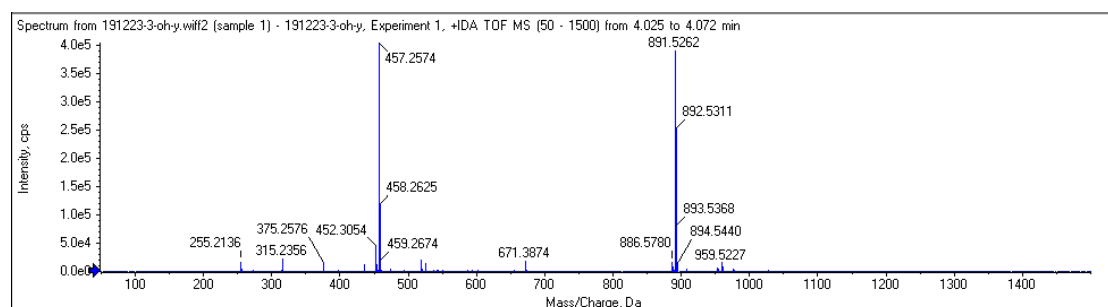
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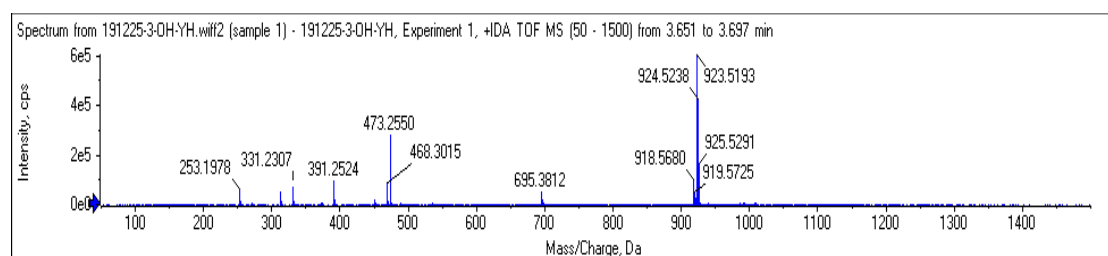
ESI mass spectrum of compound **10** recorded on an AGILENT 1200 Capillary spectrometer:



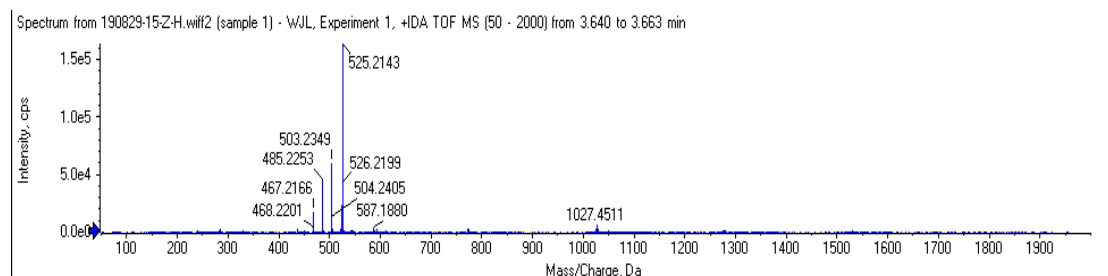
ESI mass spectrum of compound **11** recorded on an AGILENT 1200 Capillary spectrometer:



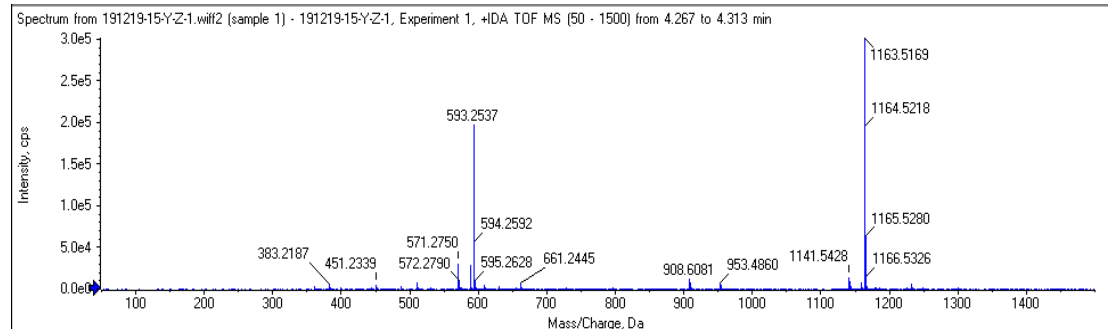
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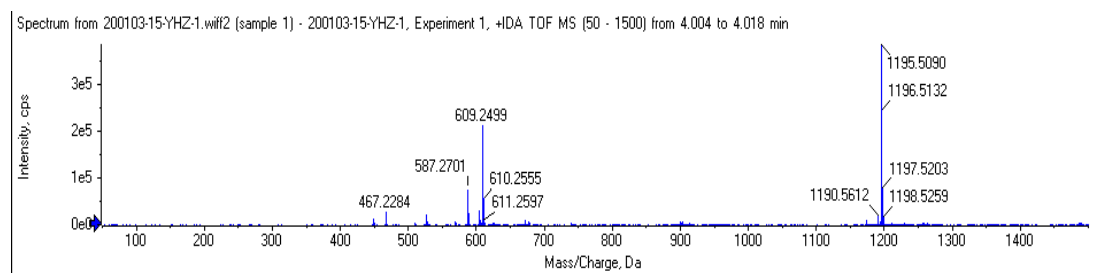
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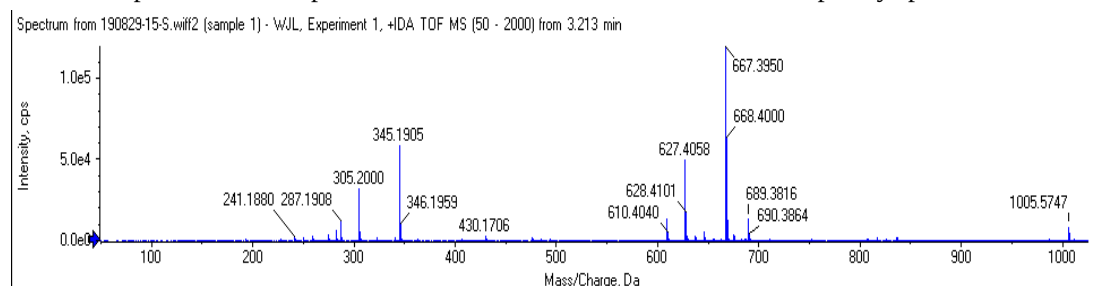
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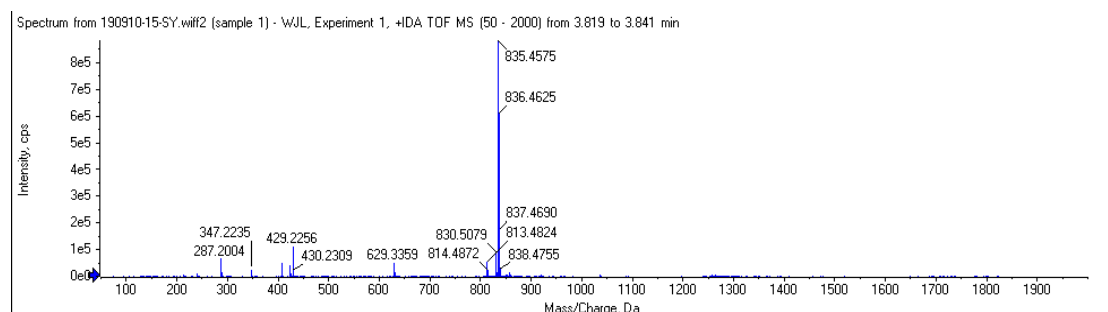
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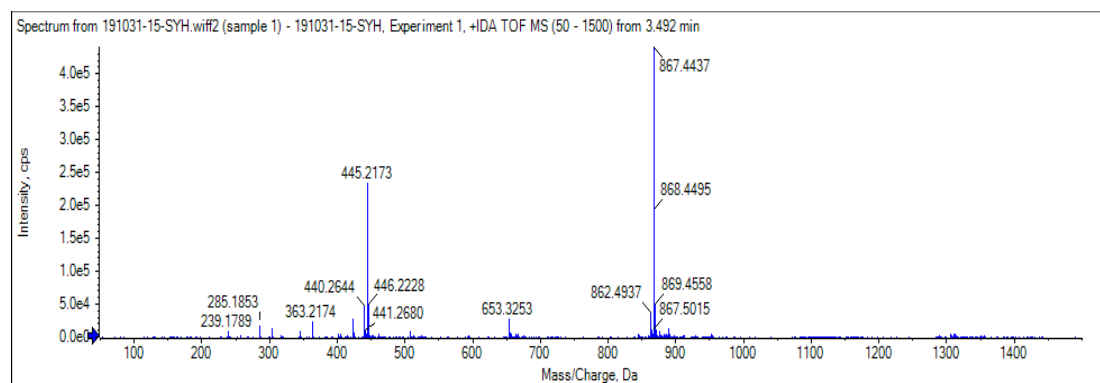
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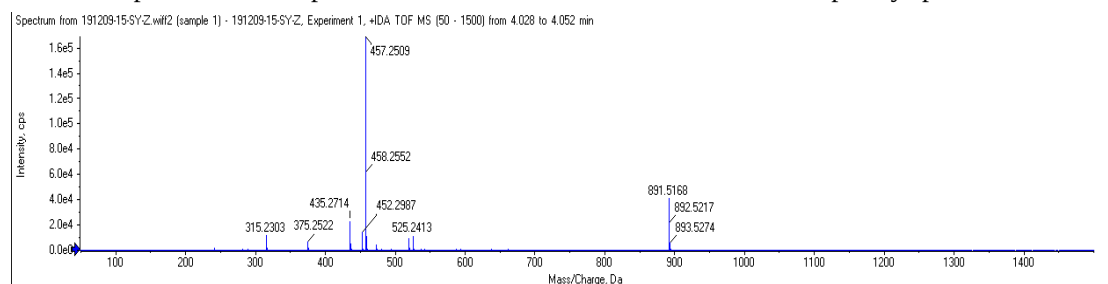
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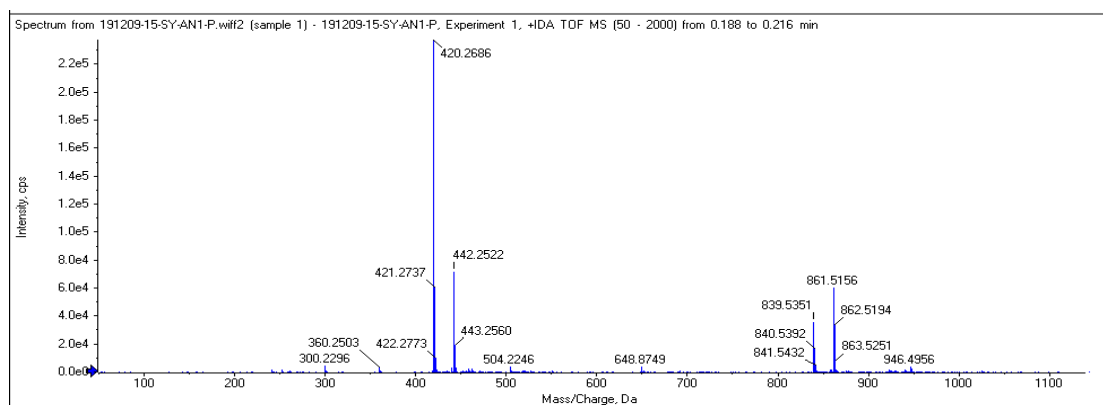
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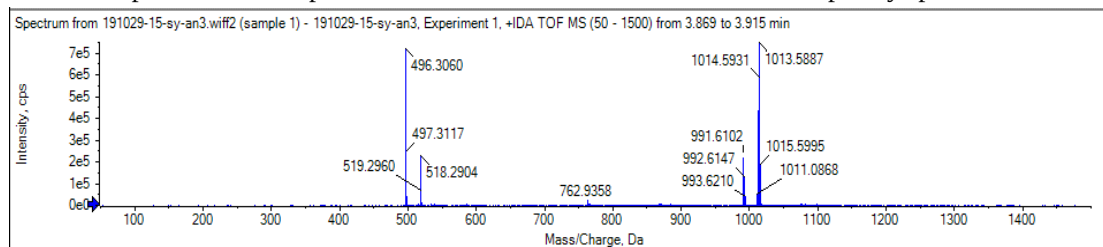
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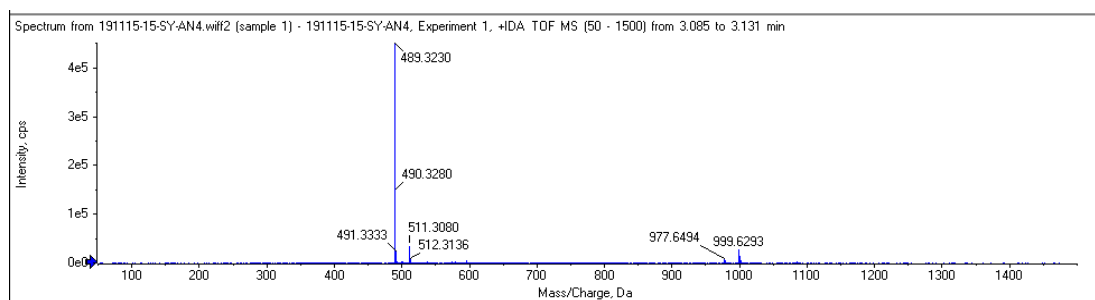
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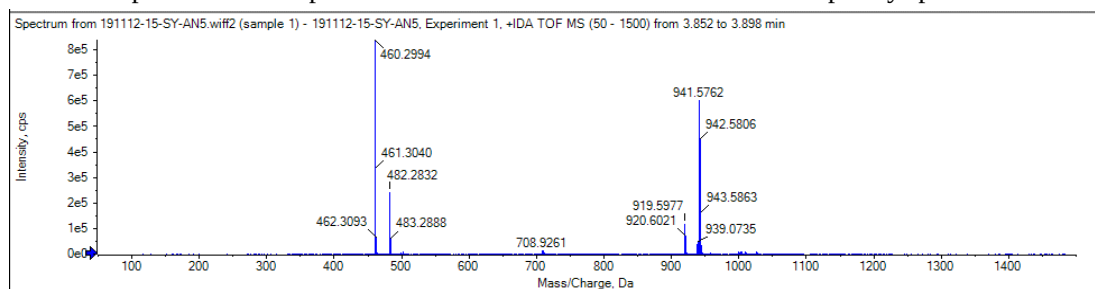
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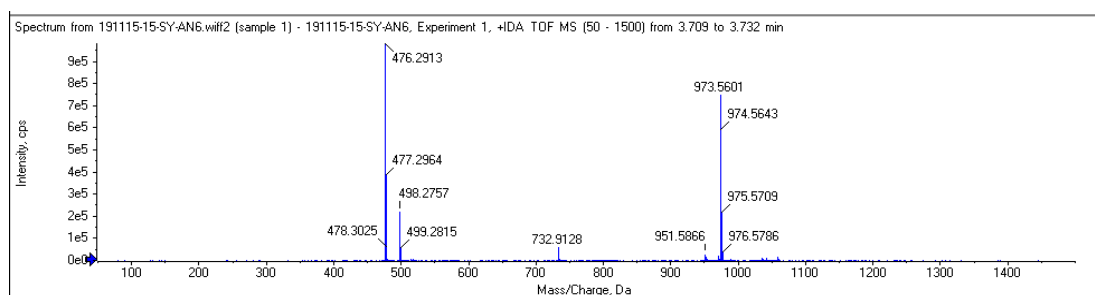
ESI mass spectrum of compound **19d** recorded on an AGILENT 1200 Capillary spectrometer:



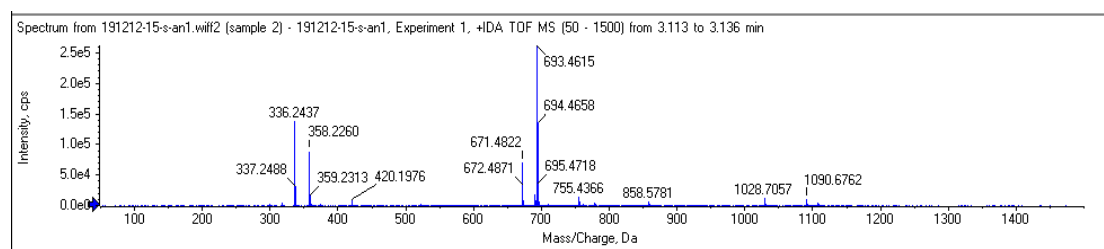
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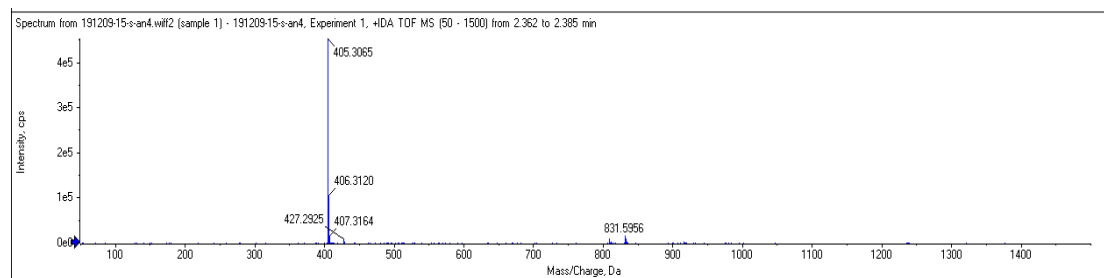
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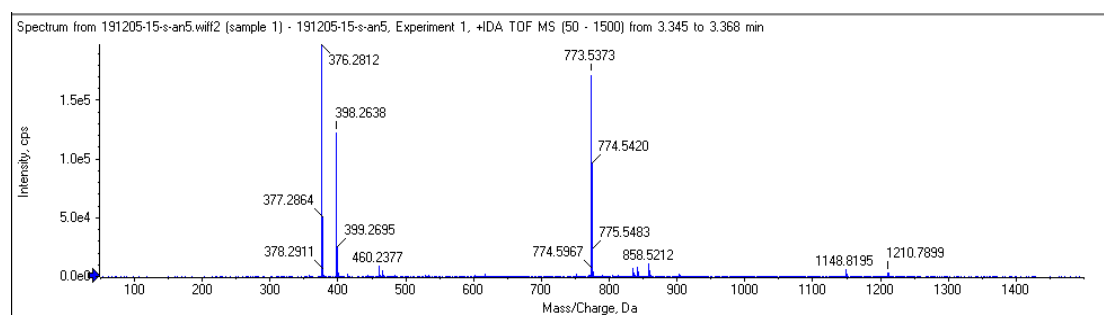
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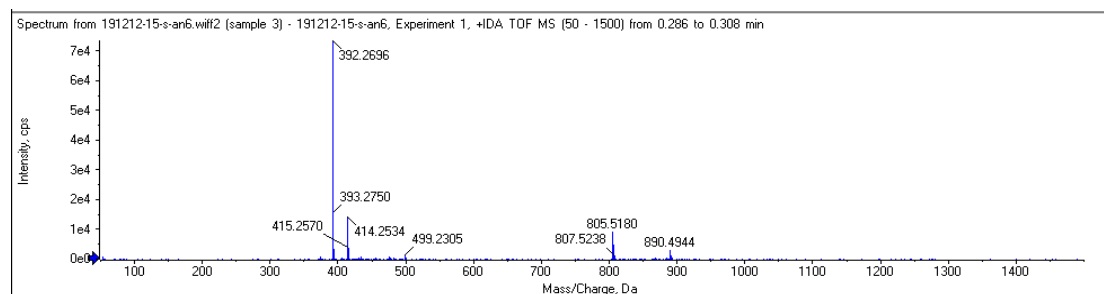
ESI mass spectrum of compound **20b** recorded on an AGILENT 1200 Capillary spectrometer:



ESI mass spectrum of compound **20c** recorded on an AGILENT 1200 Capillary spectrometer:

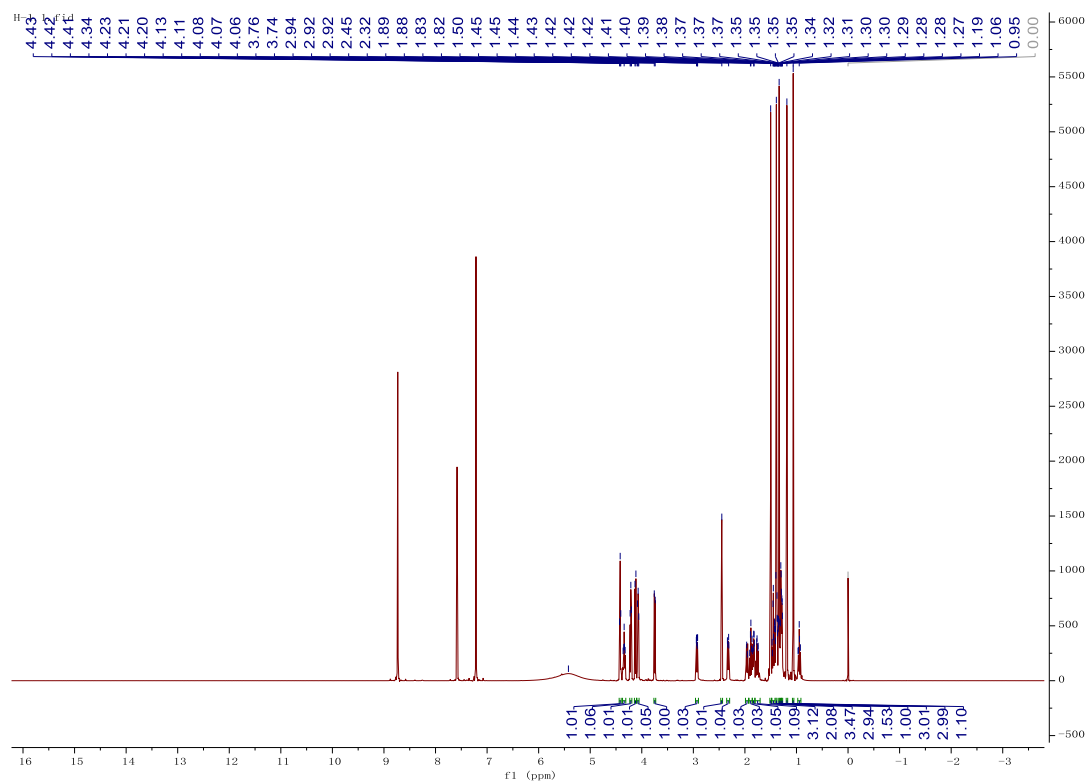
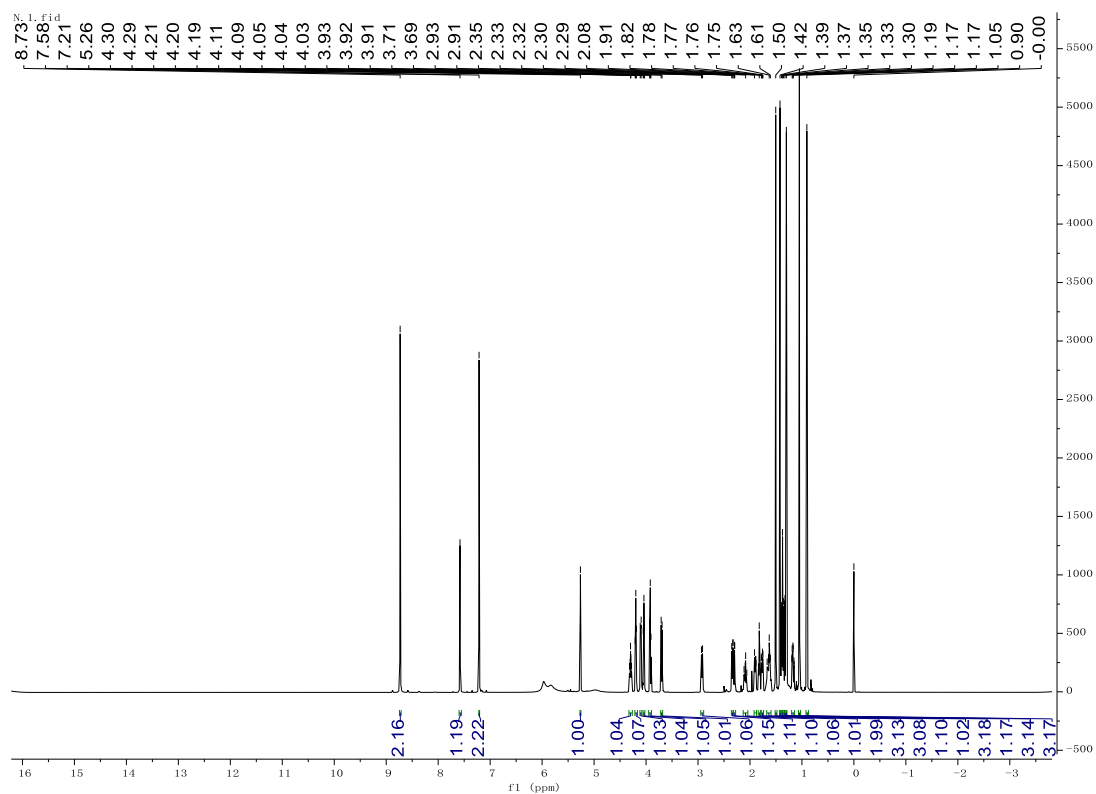


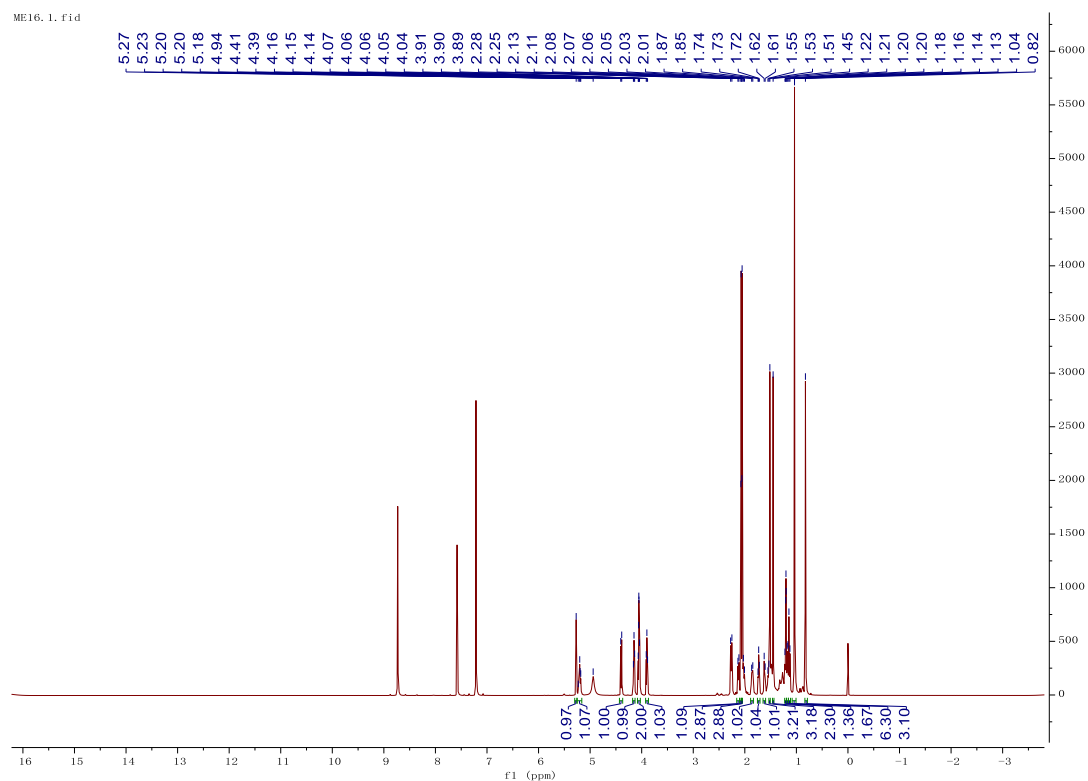
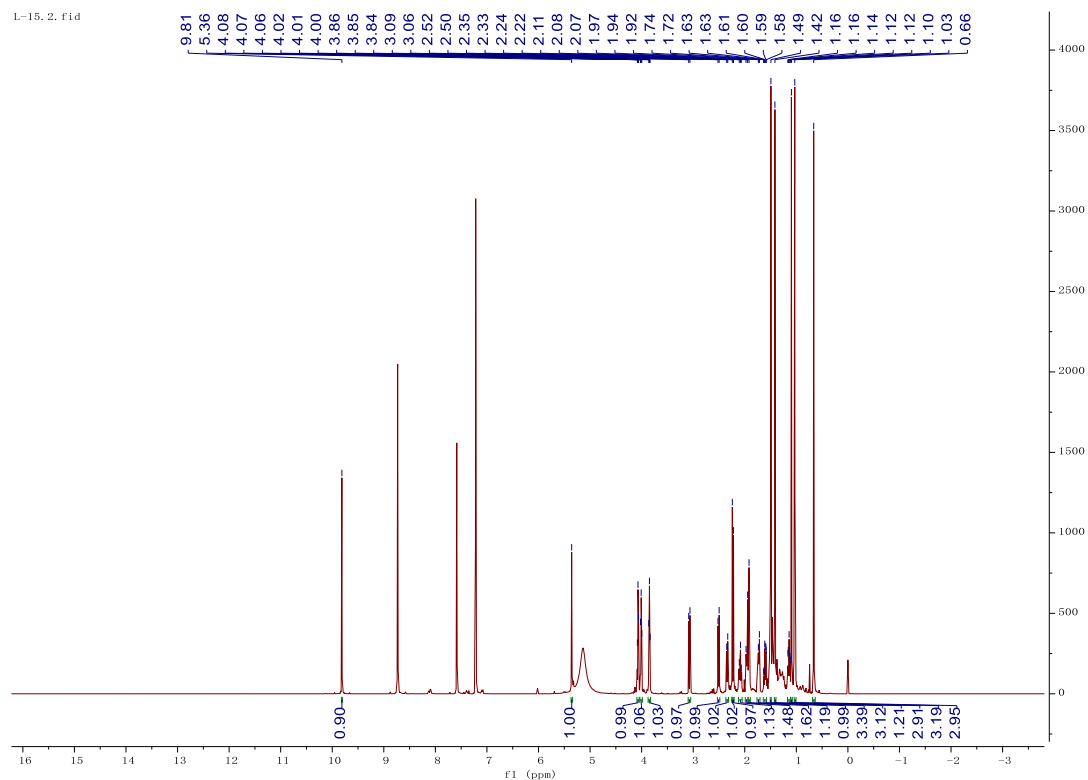
ESI mass spectrum of compound **20d** recorded on an AGILENT 1200 Capillary spectrometer:

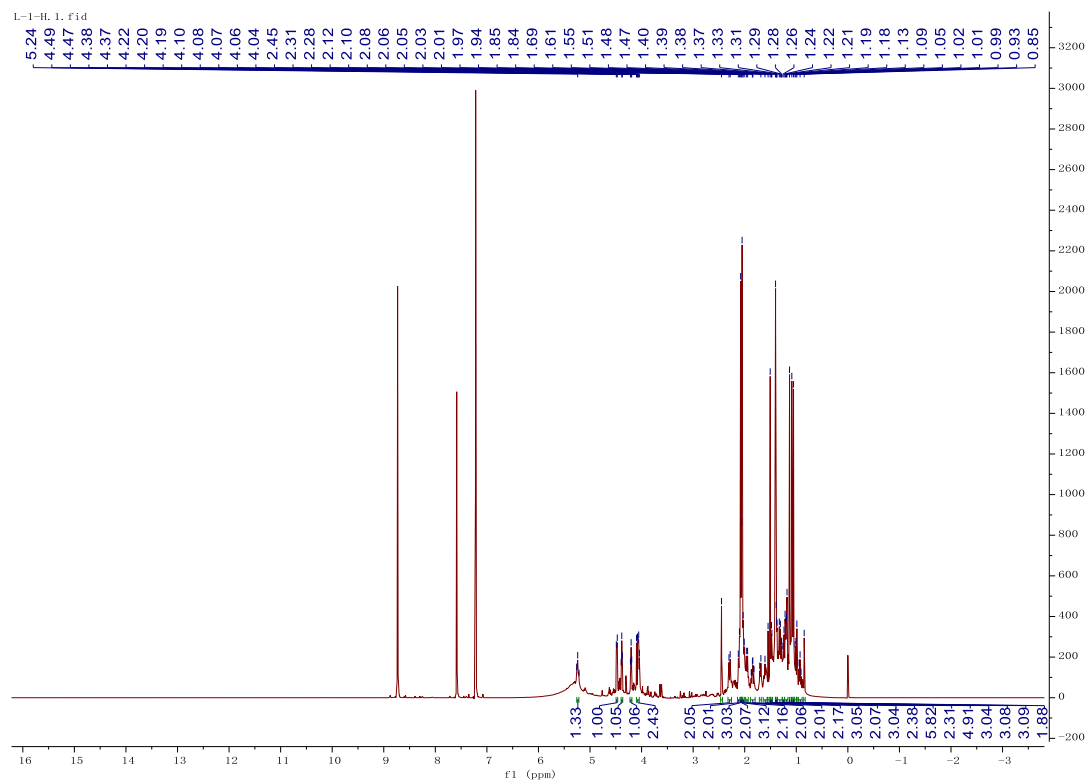


¹H NMR (600MHz) of compounds 2-20d

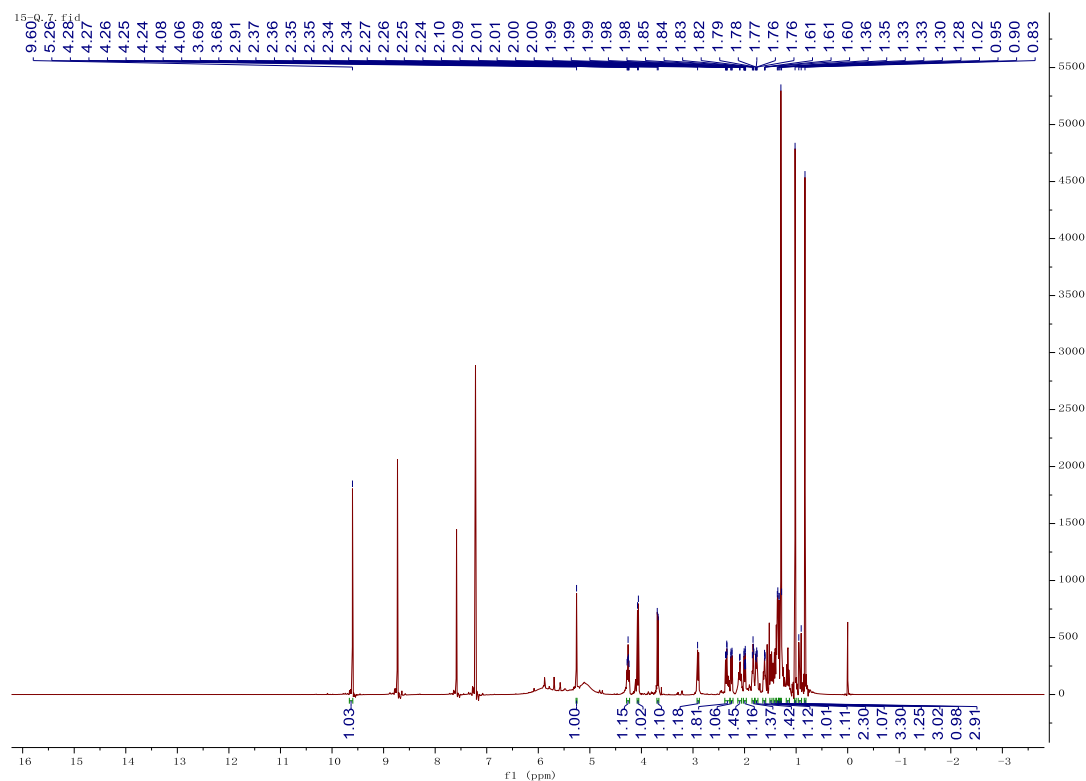
¹H NMR (600MHz) of compound **2** recorded on a Bruker Avance III 600 spectrometer
(600MHz,pyridine-d₅):



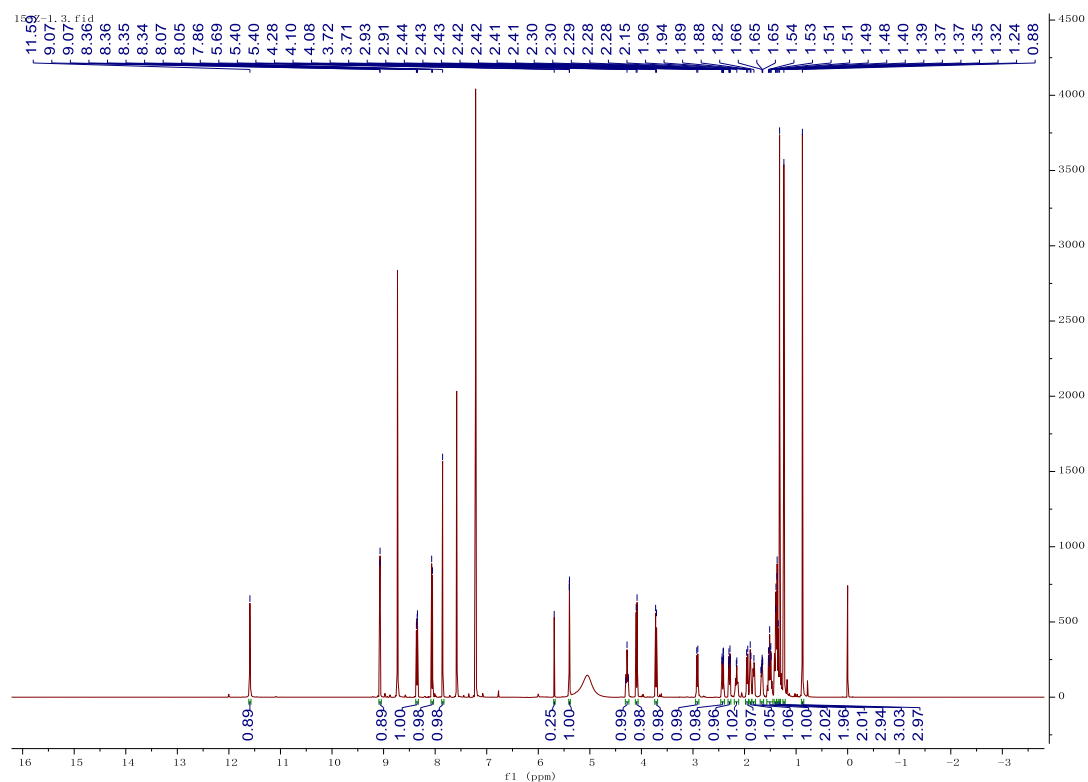




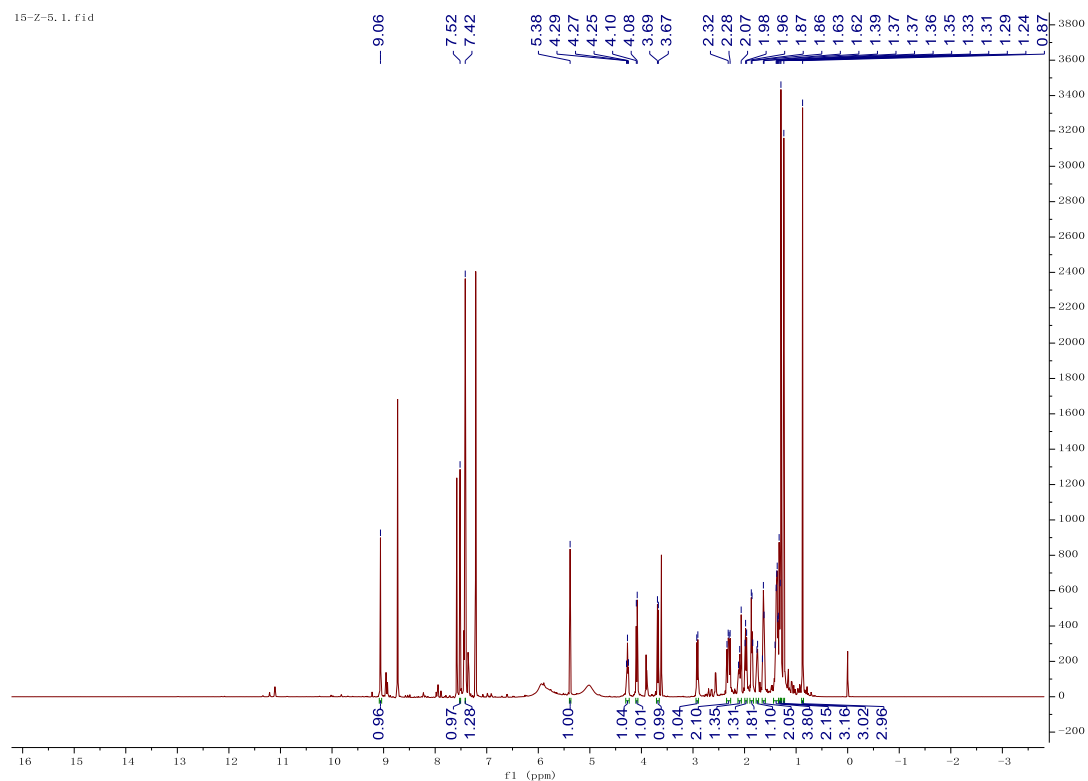
1H NMR (600MHz) of compound **7** recorded on a Bruker Avance III 600 spectrometer (600MHz,pyridine-d₅):



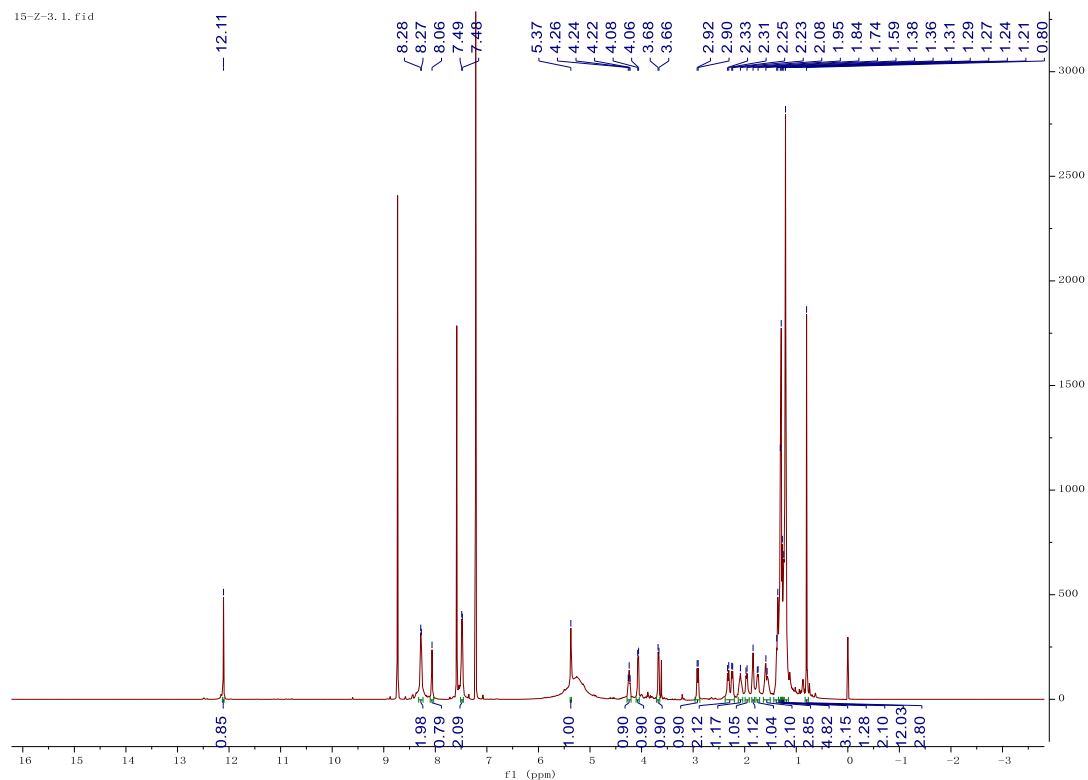
1H NMR (600MHz) of compound **8a** recorded on a Bruker Avance III 600 spectrometer (600MHz,pyridine-d₅):



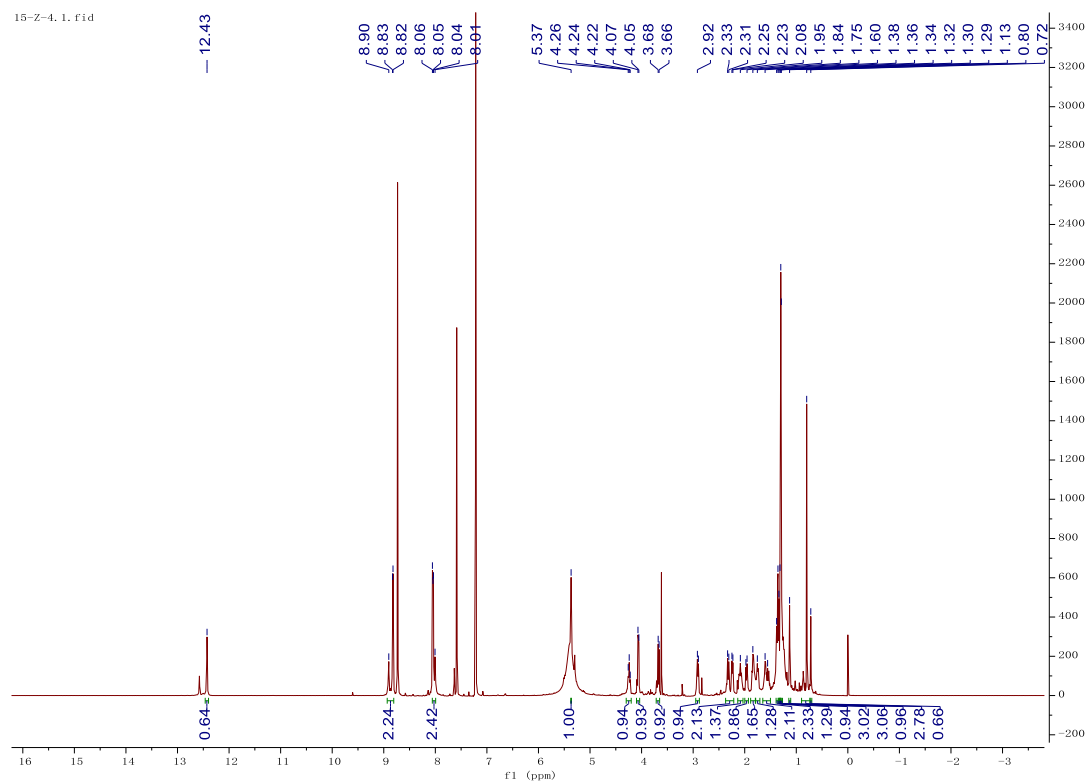
^1H NMR (600MHz) of compound **8b** recorded on a Bruker Avance III 600 spectrometer (600MHz,pyridine- d_5):



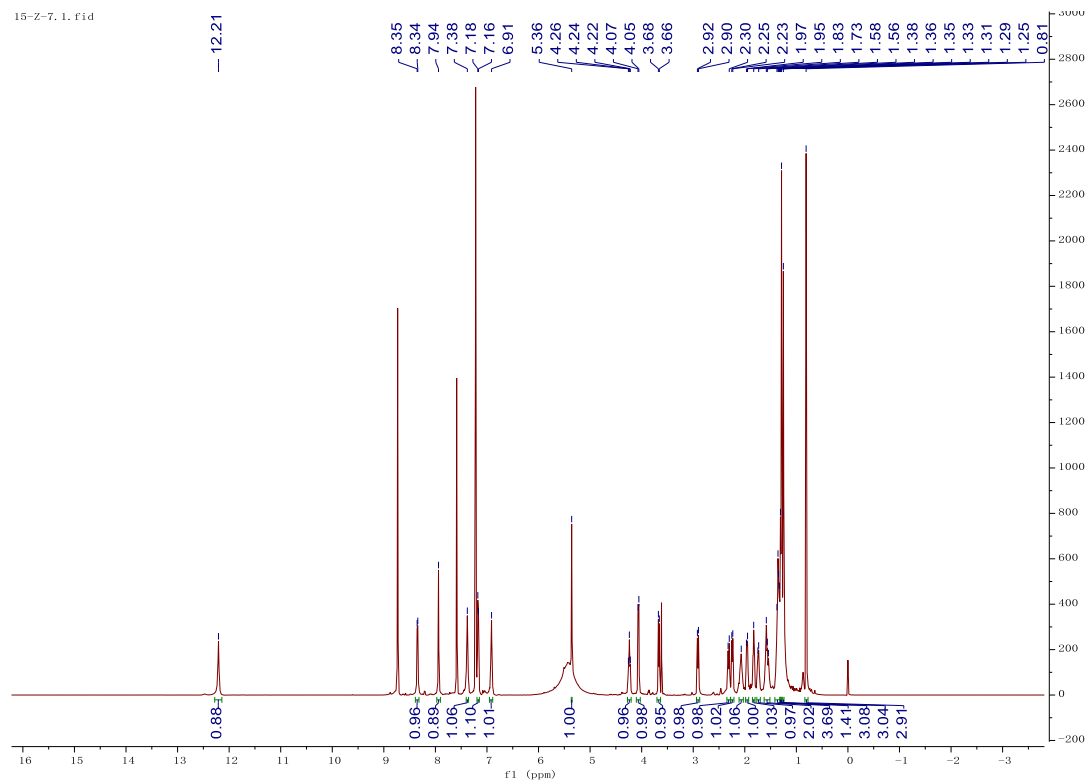
^1H NMR (600MHz) of compound **8c** recorded on a Bruker Avance III 600 spectrometer (600MHz,pyridine- d_5):



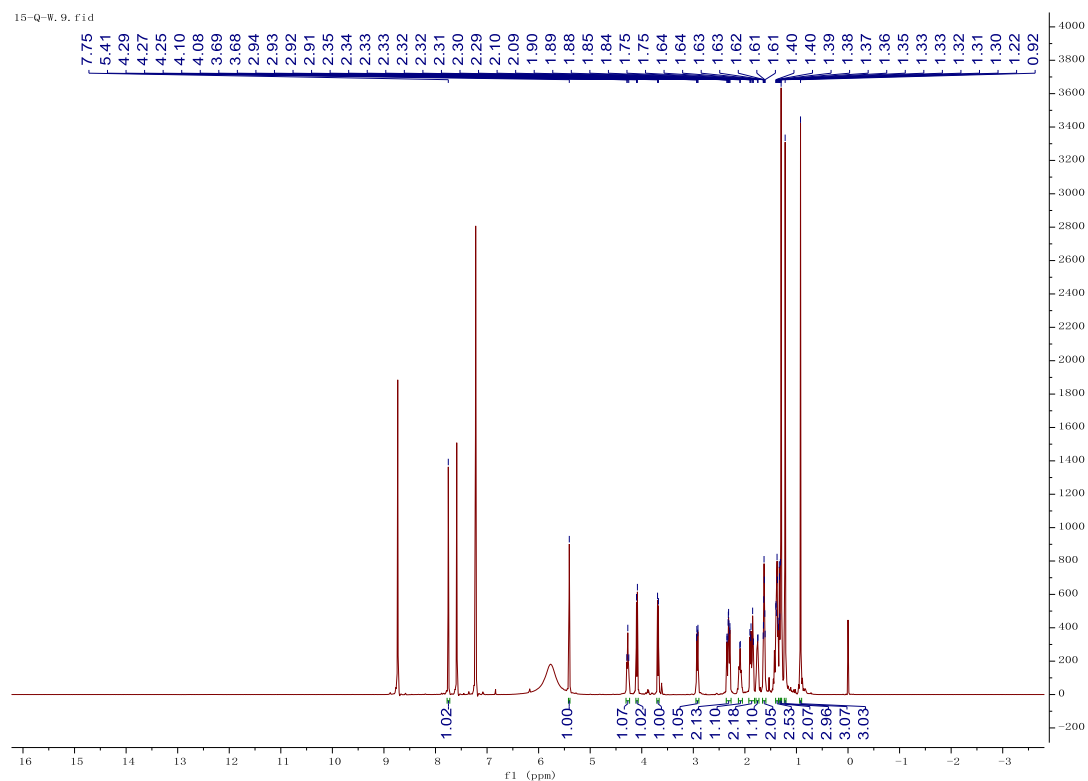
^1H NMR (600MHz) of compound **8d** recorded on a Bruker Avance III 600 spectrometer (600MHz,pyridine- d_5):



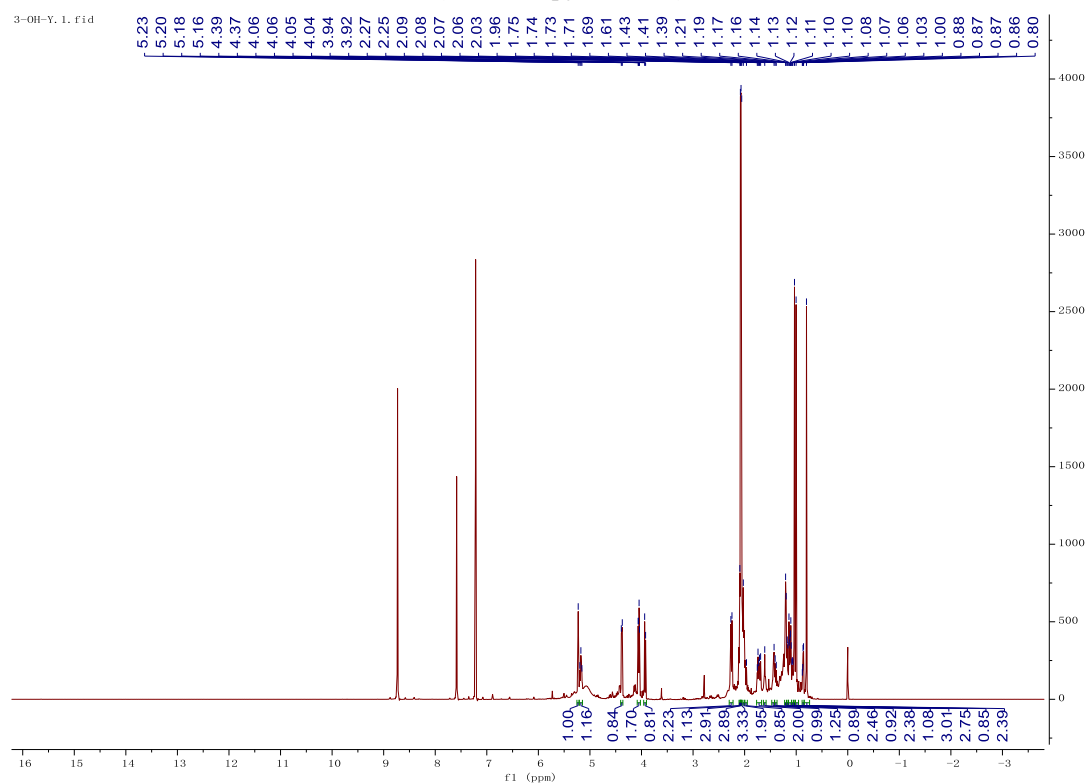
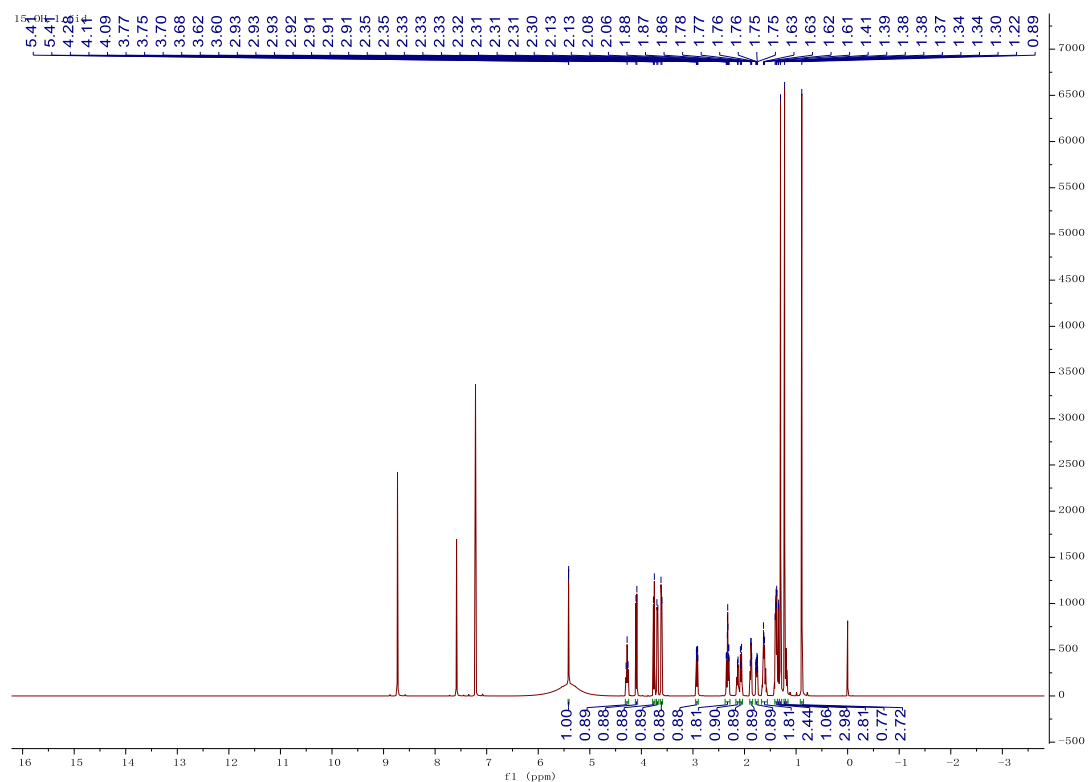
^1H NMR (600MHz) of compound **8e** recorded on a Bruker Avance III 600 spectrometer (600MHz,pyridine- d_5):

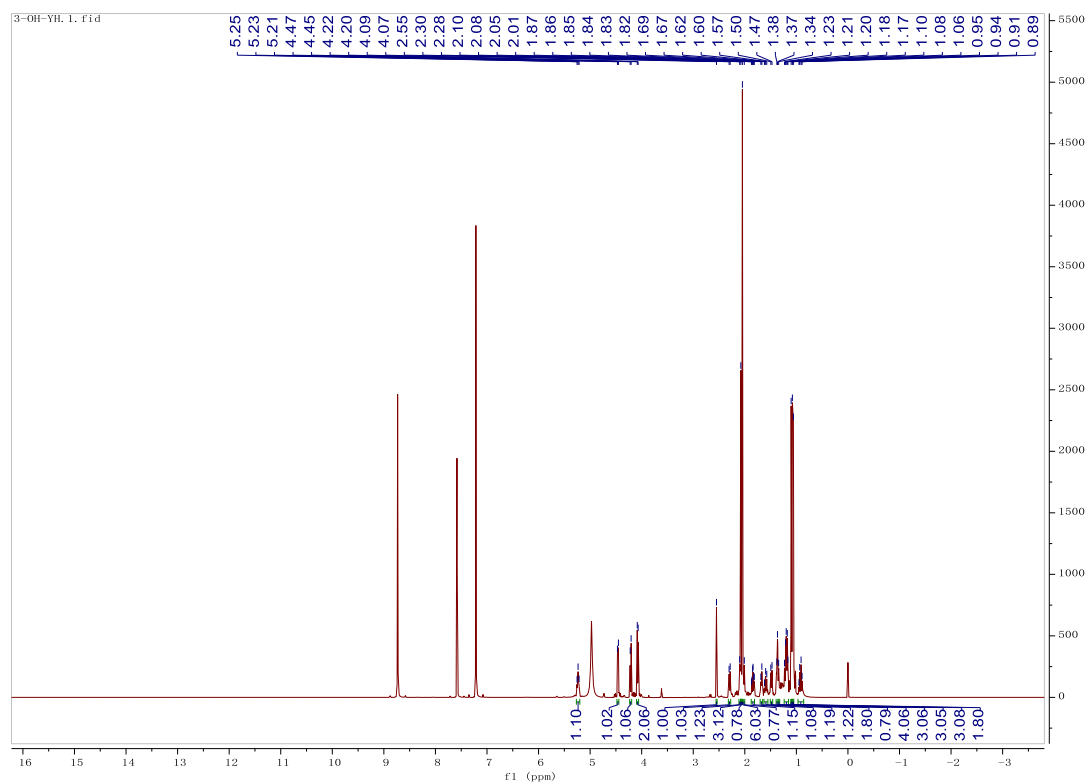


^1H NMR (600MHz) of compound **9** recorded on a Bruker Avance III 600 spectrometer (600MHz,pyridine- d_5):

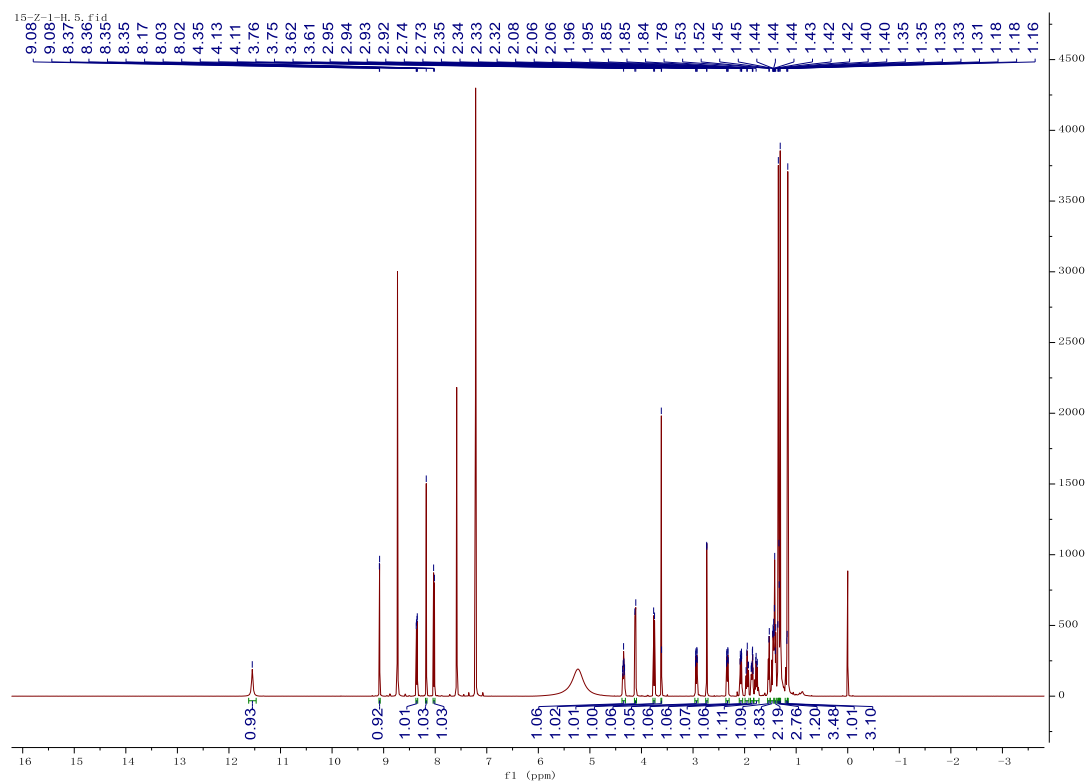


^1H NMR (600MHz) of compound **10** recorded on a Bruker Avance III 600 spectrometer (600MHz,pyridine- d_5):

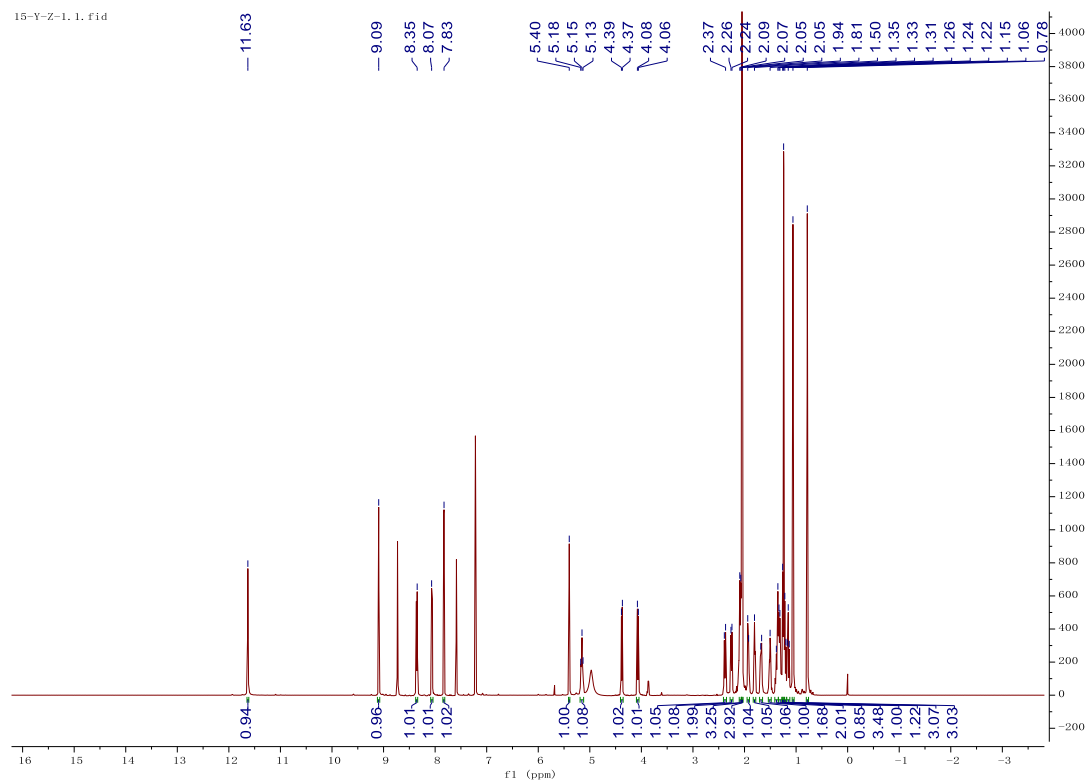




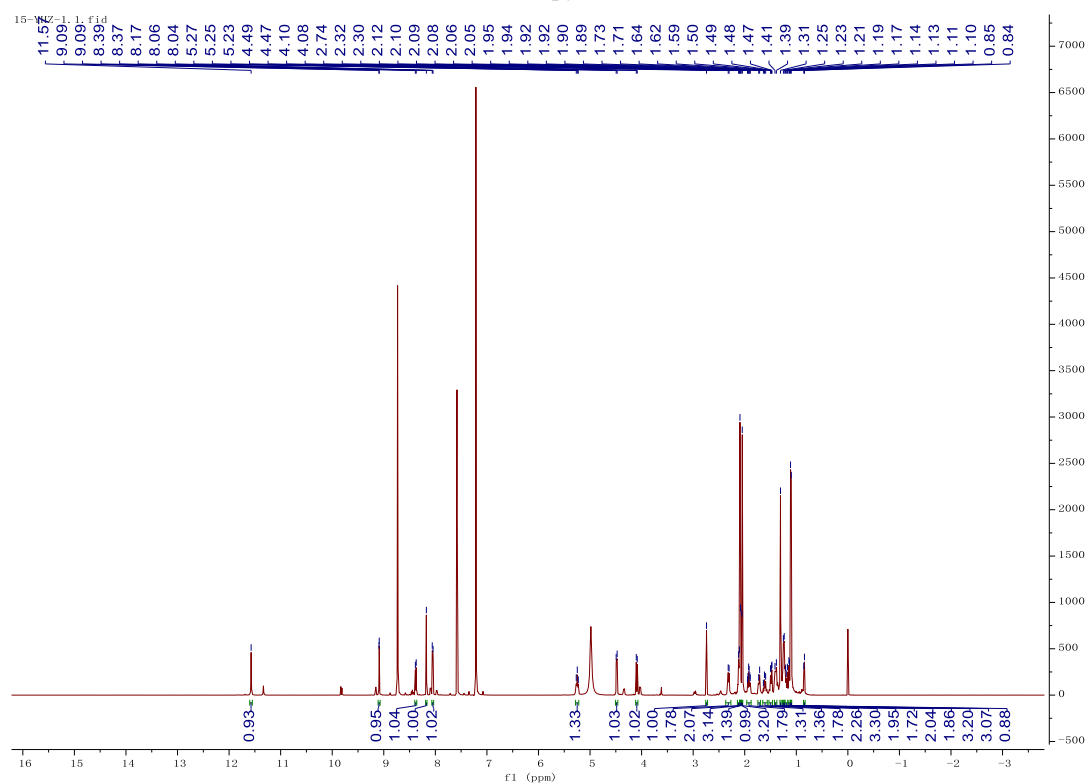
^1H NMR (600MHz) of compound **13** recorded on a Bruker Avance III 600 spectrometer (600MHz,pyridine- d_5):



^1H NMR (600MHz) of compound **14** recorded on a Bruker Avance III 600 spectrometer (600MHz,pyridine- d_5):

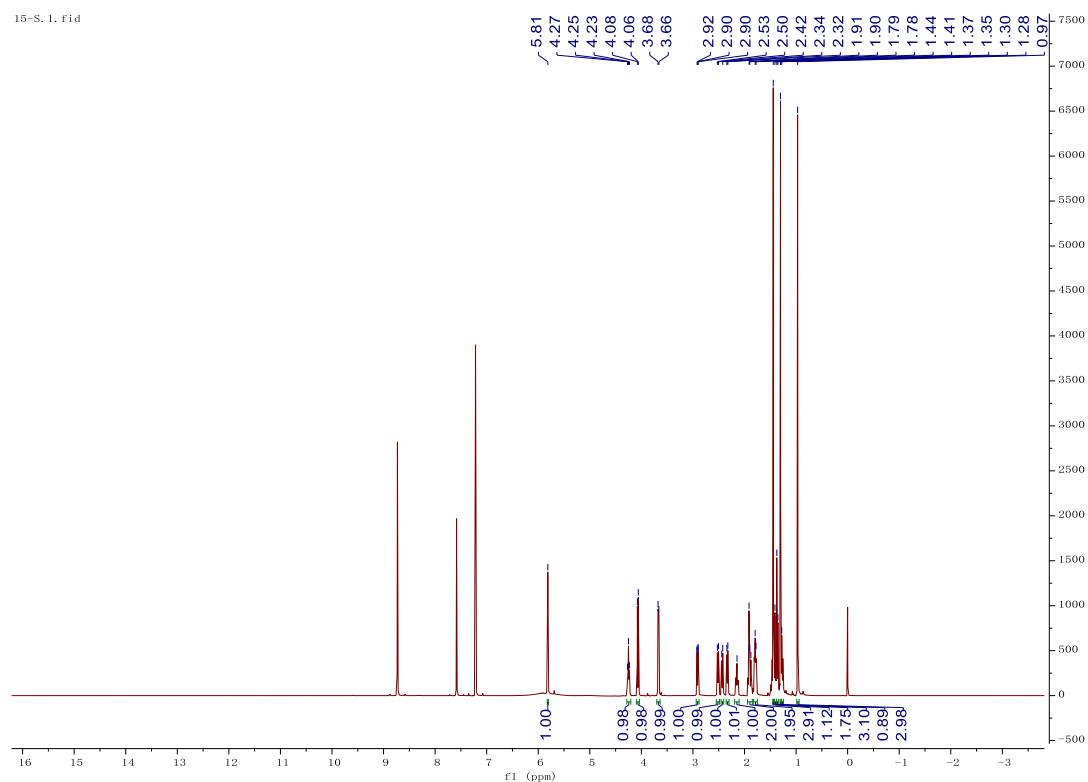


^1H NMR (600MHz) of compound **15** recorded on a Bruker Avance III 600 spectrometer
(600MHz,pyridine- d_5):



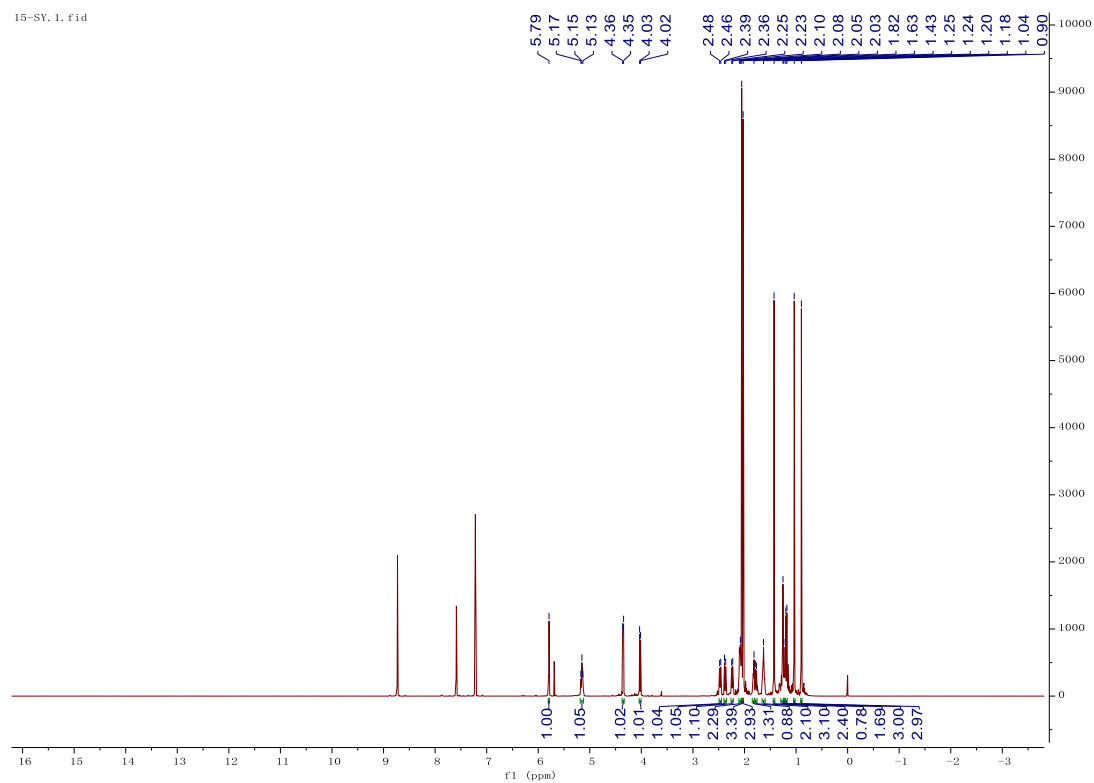
^1H NMR (600MHz) of compound **16** recorded on a Bruker Avance III 600 spectrometer
(600MHz,pyridine- d_5):

15-S, 1, f1d



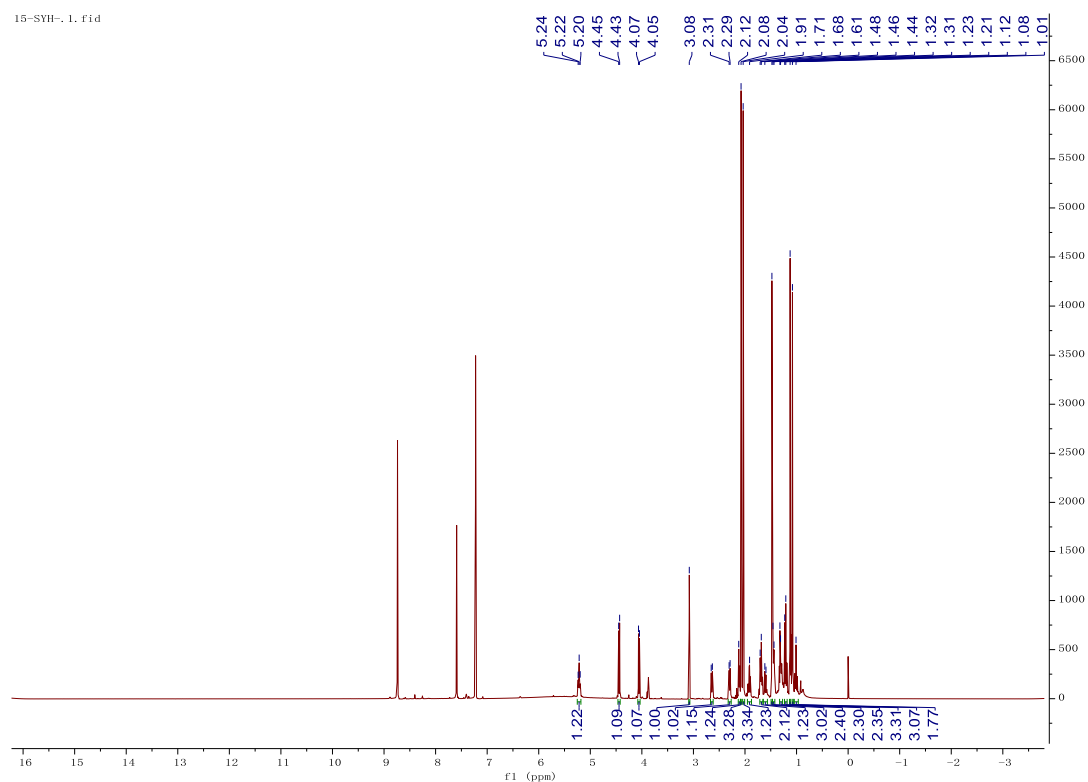
^1H NMR (600MHz) of compound **17** recorded on a Bruker Avance III 600 spectrometer (600MHz,pyridine- d_5):

15-SY, 1, f1d



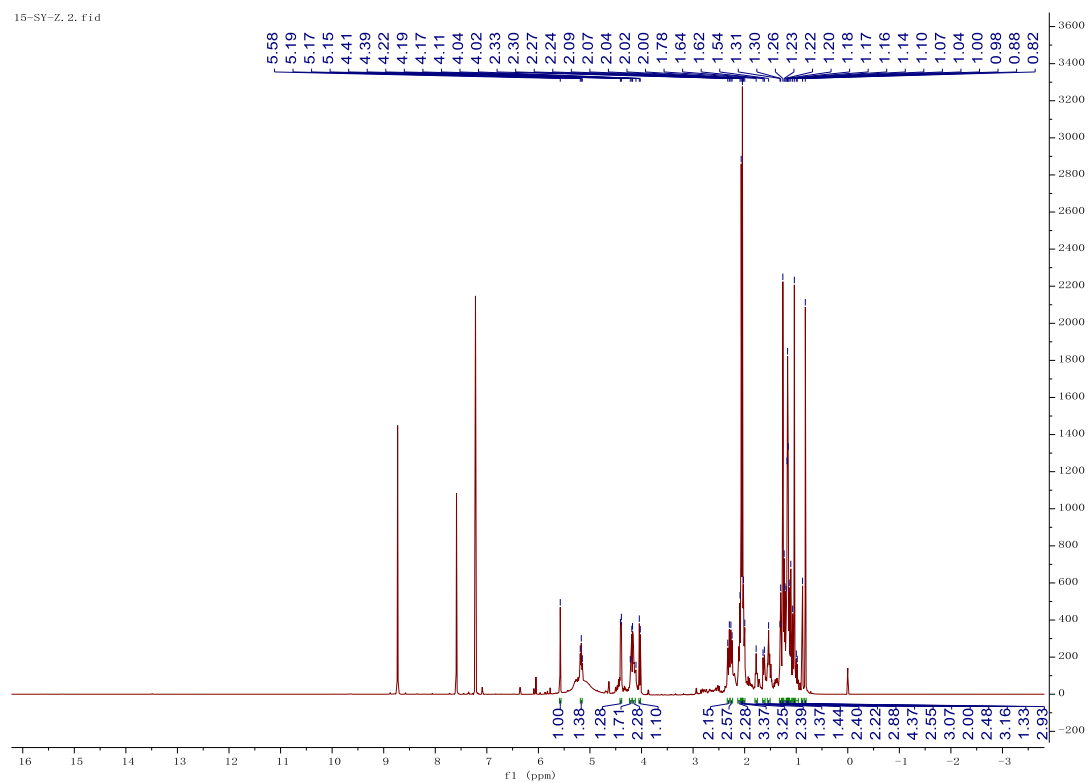
^1H NMR (600MHz) of compound **18** recorded on a Bruker Avance III 600 spectrometer (600MHz,pyridine- d_5):

15-SYH-.1.fid



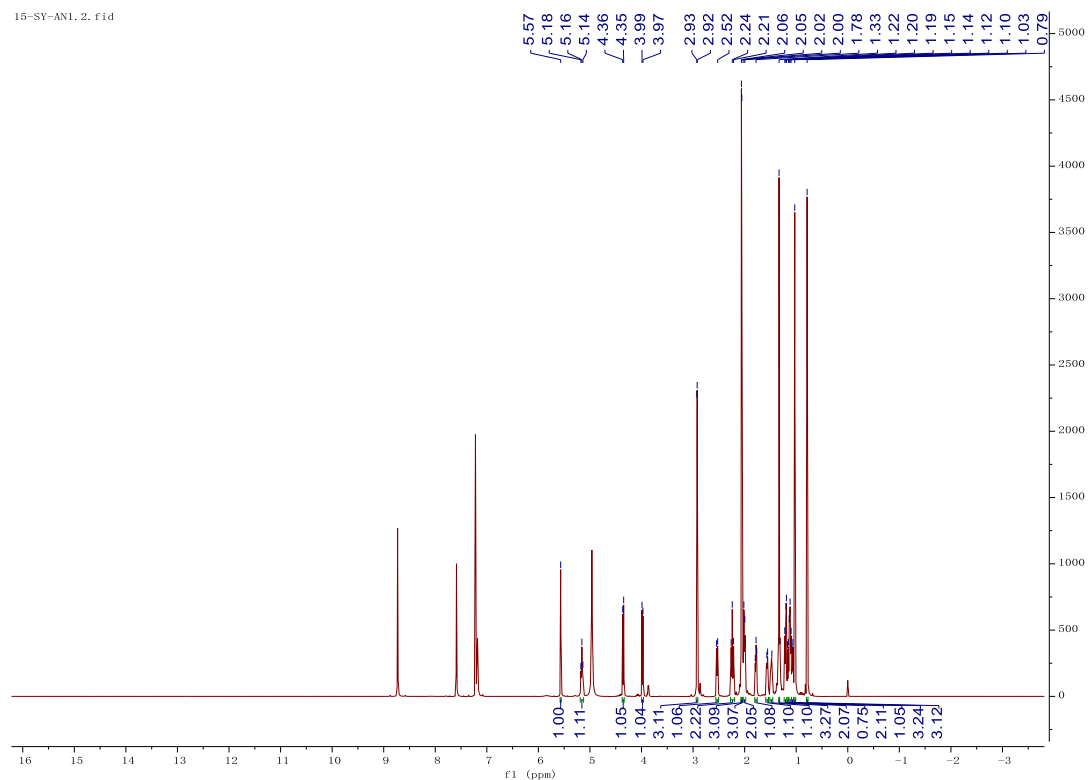
^1H NMR (600MHz) of compound **19a** recorded on a Bruker Avance III 600 spectrometer (600MHz,pyridine- d_5):

15-SY-Z.2.fid



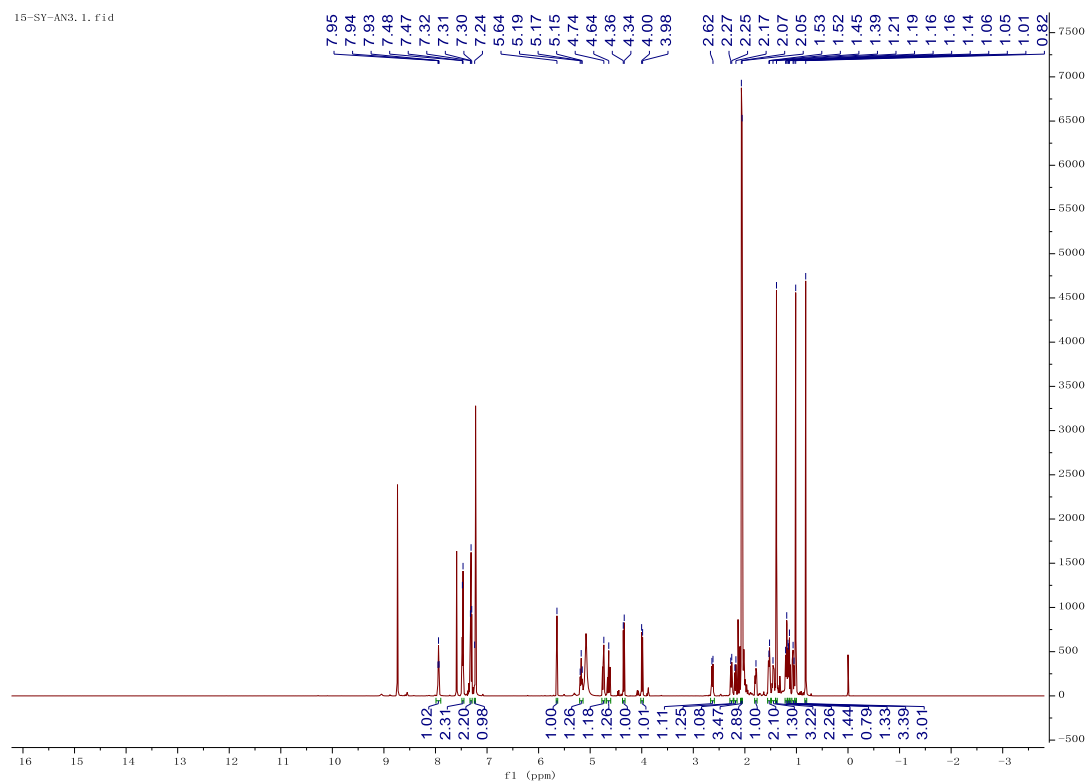
^1H NMR (600MHz) of compound **19b** recorded on a Bruker Avance III 600 spectrometer (600MHz,pyridine- d_5):

15-SY-AN1.2.fid



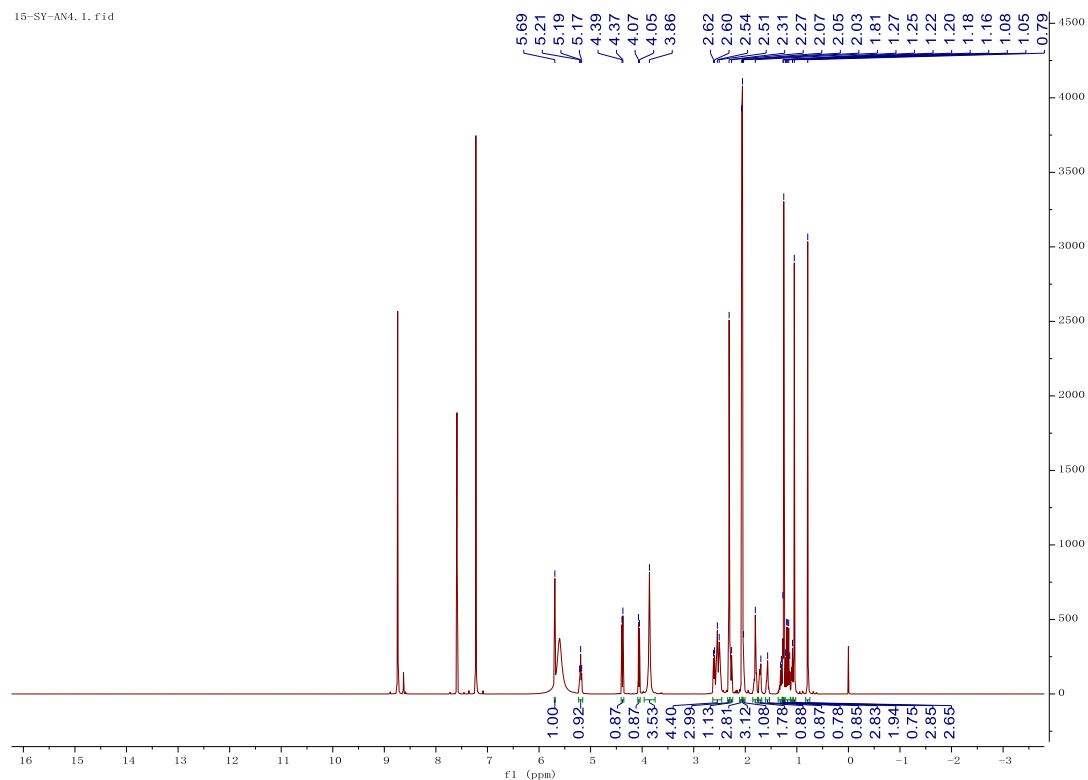
^1H NMR (600MHz) of compound **19c** recorded on a Bruker Avance III 600 spectrometer (600MHz,pyridine- d_5):

15-SY-AN3.1.fid



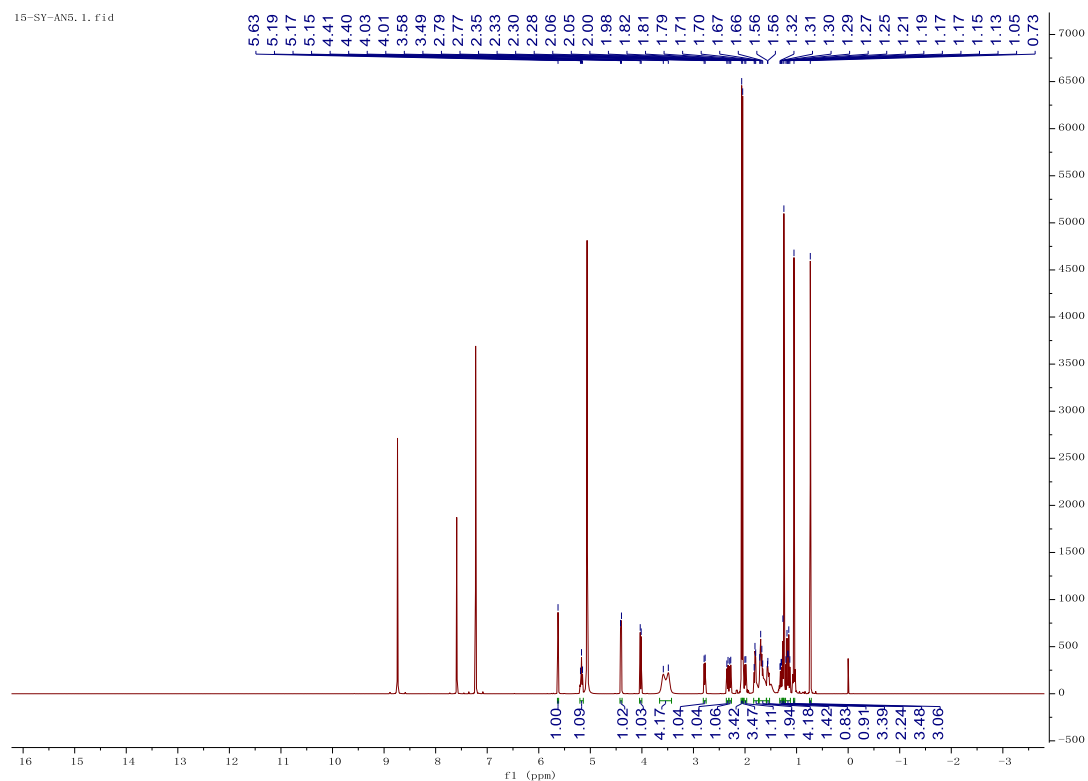
^1H NMR (600MHz) of compound **19d** recorded on a Bruker Avance III 600 spectrometer (600MHz,pyridine- d_5):

15-SY-AN4.1.fid



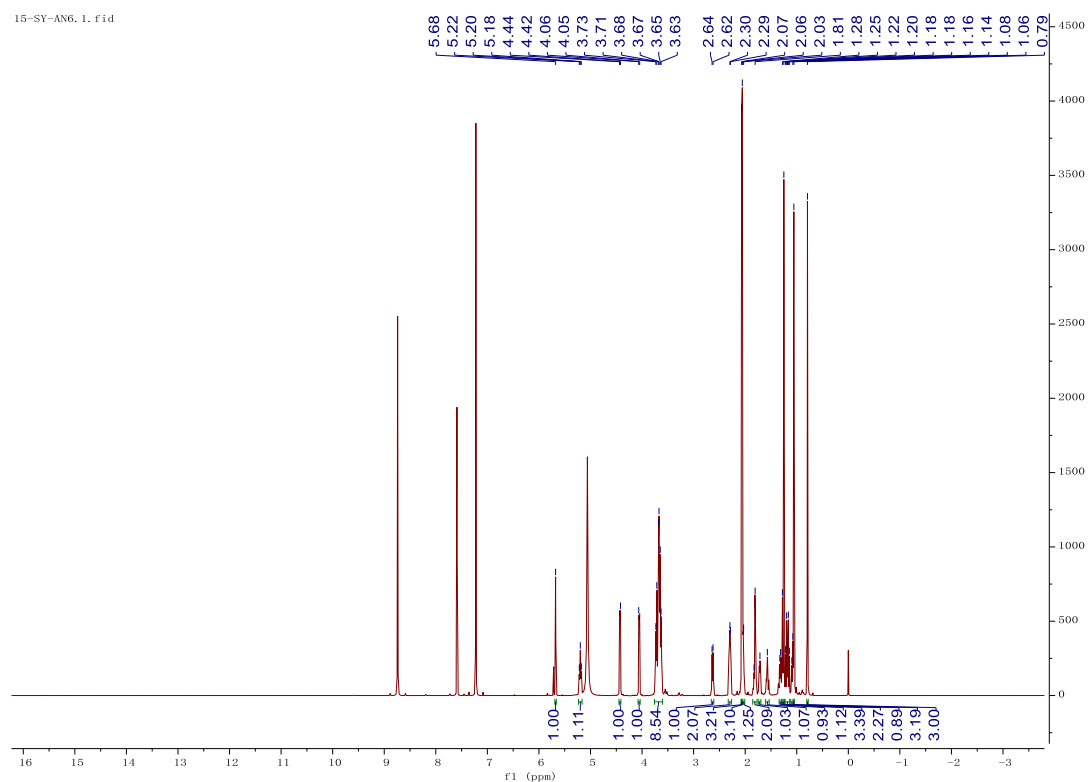
^1H NMR (600MHz) of compound **19e** recorded on a Bruker Avance III 600 spectrometer (600MHz,pyridine- d_5):

15-SY-AN5.1.fid



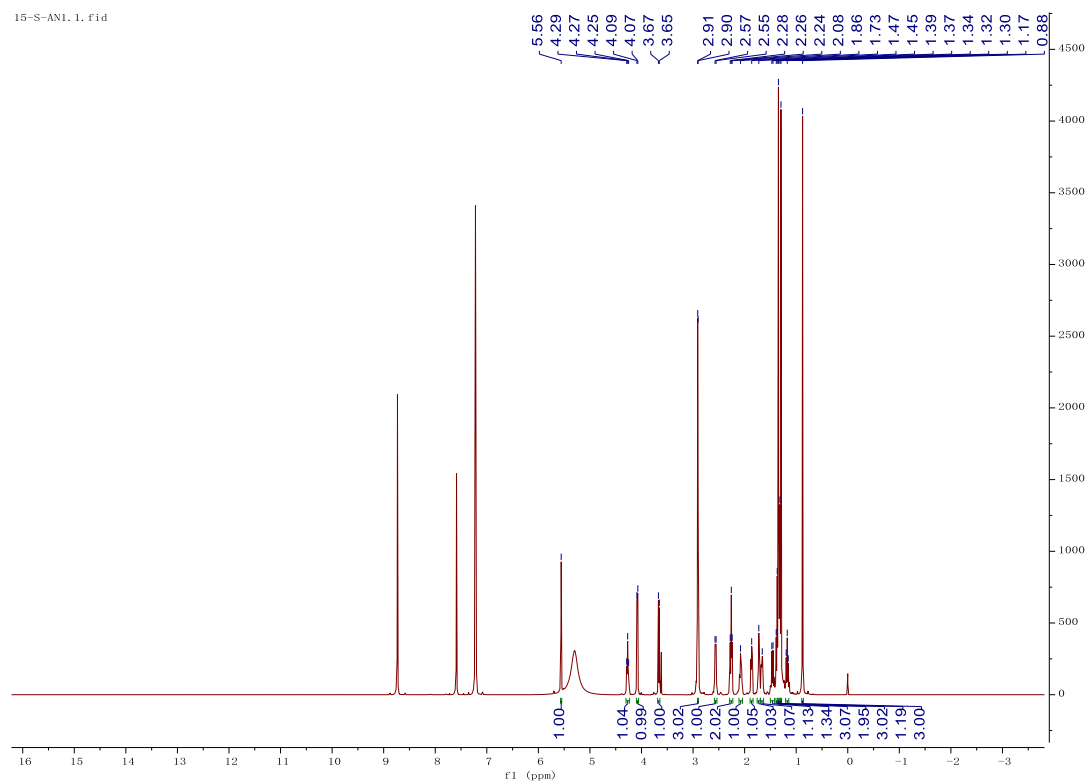
^1H NMR (600MHz) of compound **19f** recorded on a Bruker Avance III 600 spectrometer (600MHz,pyridine- d_5):

15-SY-AN6.1.fid



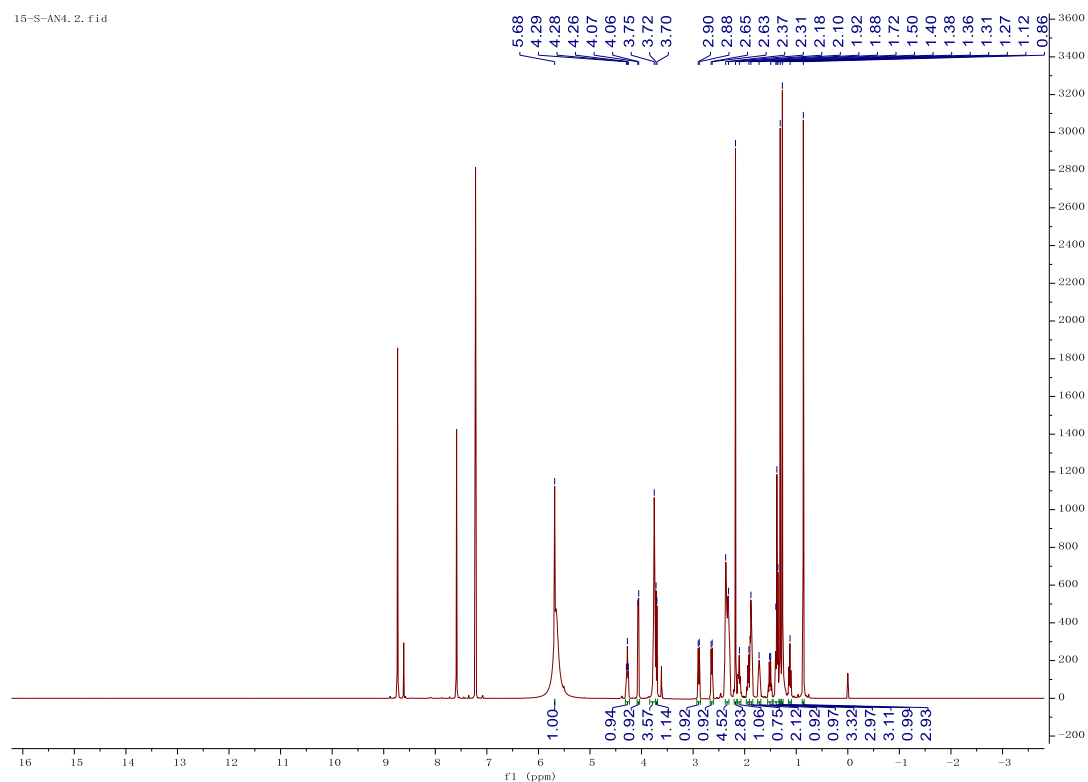
^1H NMR (600MHz) of compound **20a** recorded on a Bruker Avance III 600 spectrometer (600MHz,pyridine- d_5):

15-S-AN1.1.fid



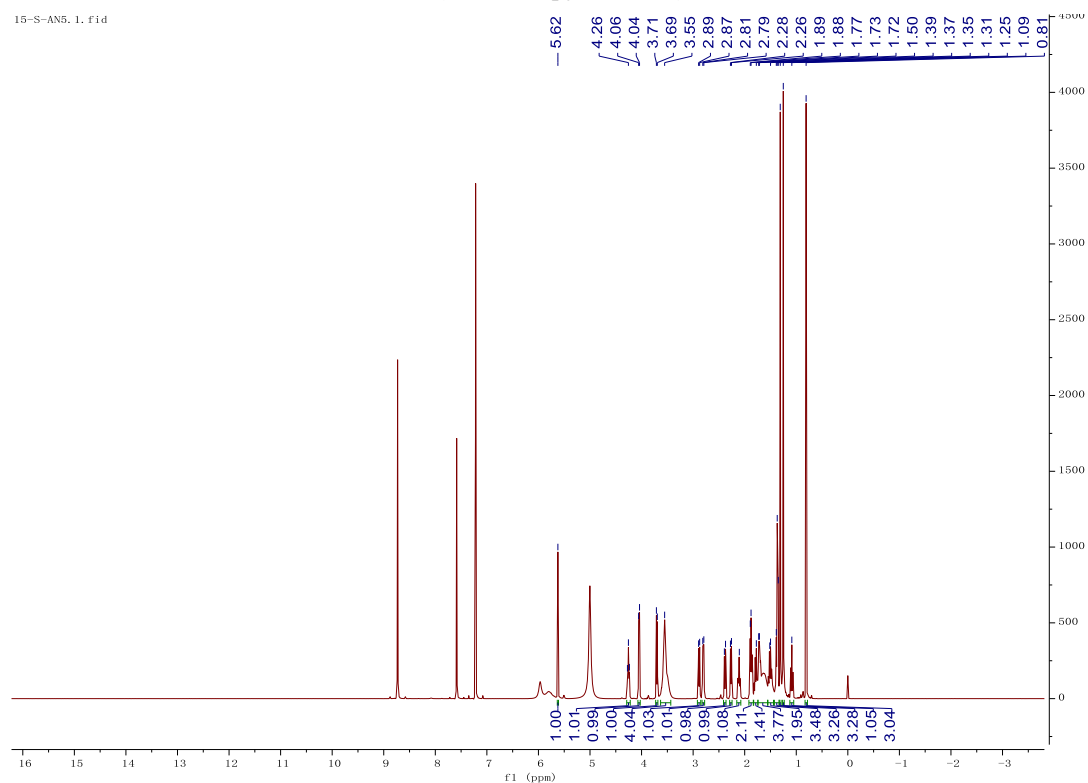
^1H NMR (600MHz) of compound **20b** recorded on a Bruker Avance III 600 spectrometer (600MHz,pyridine- d_5):

15-S-AN4. 2. f1d

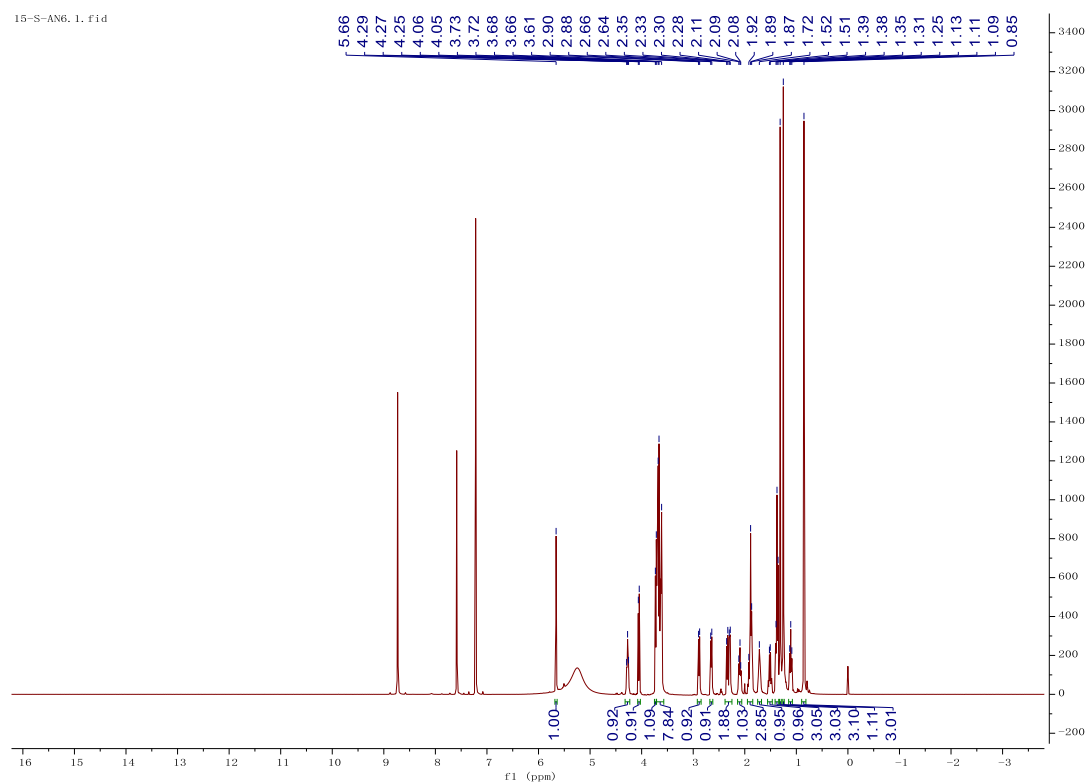


^1H NMR (600MHz) of compound **20c** recorded on a Bruker Avance III 600 spectrometer (600MHz,pyridine- d_5):

15-S-AN5. 1. f1d

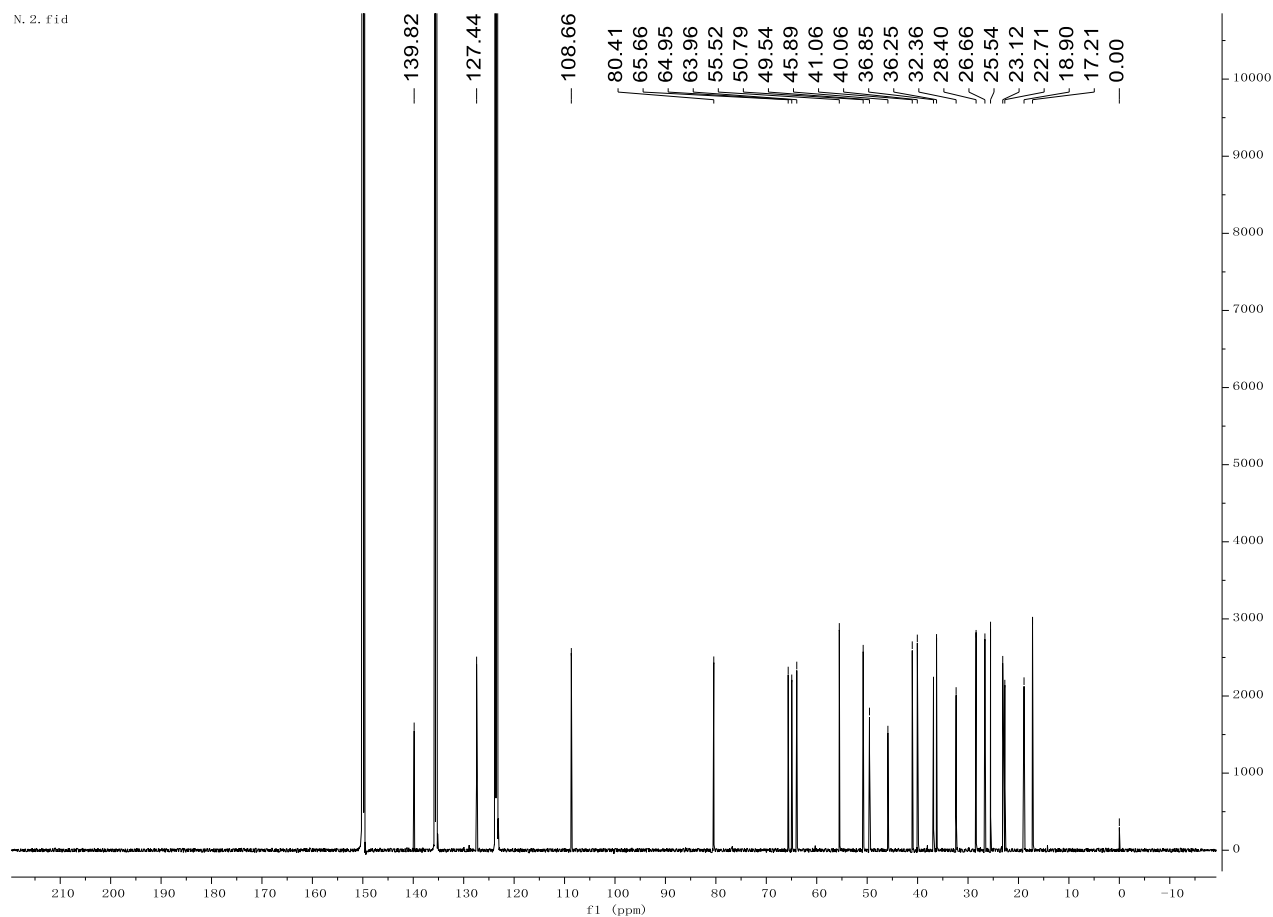


^1H NMR (600MHz) of compound **20d** recorded on a Bruker Avance III 600 spectrometer (600MHz,pyridine- d_5):

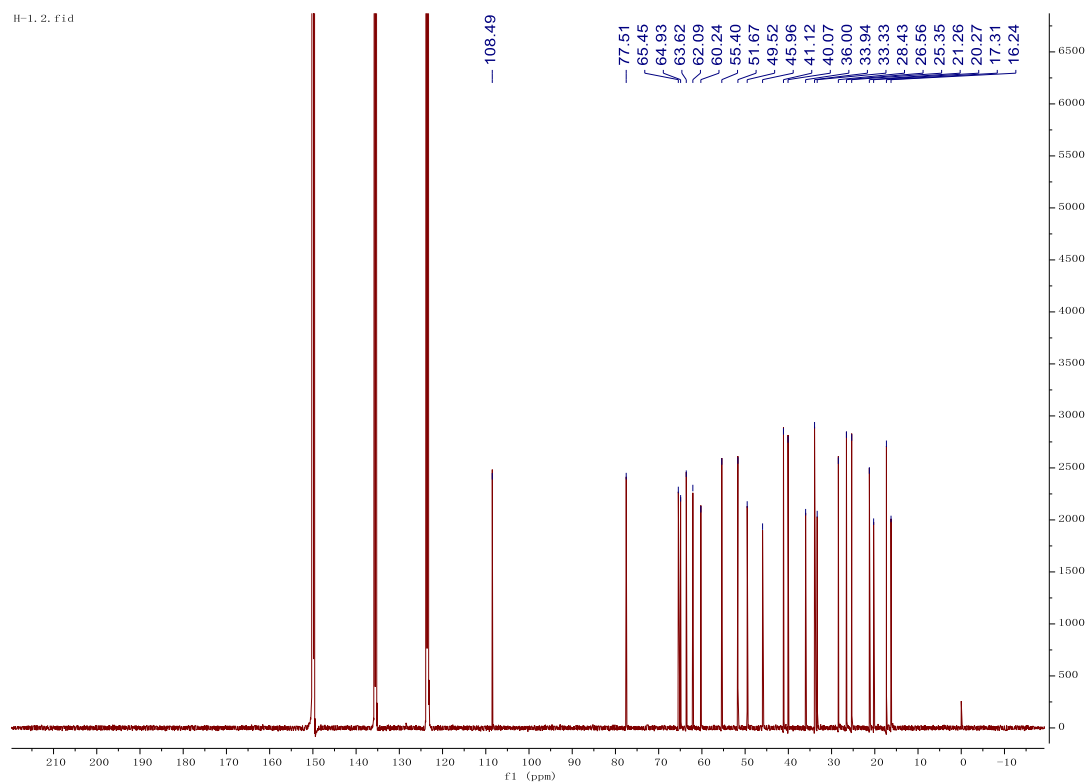


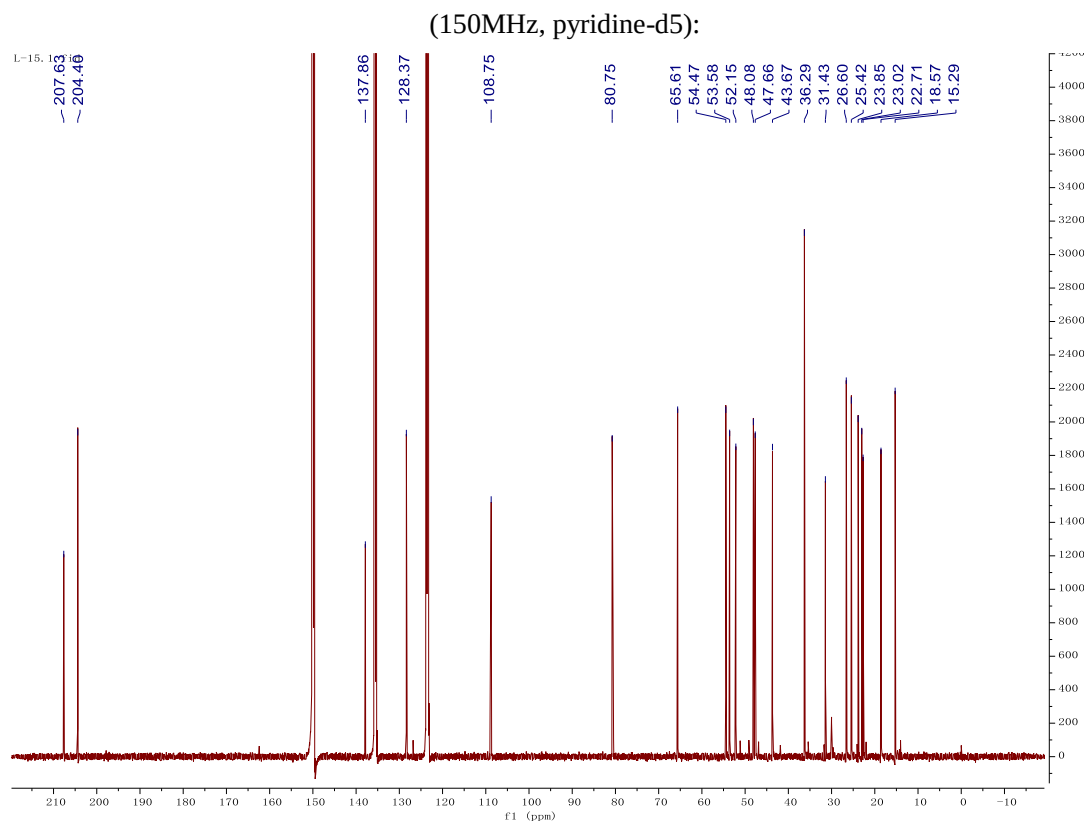
^{13}C NMR (150MHz) of compounds 2-20d

^{13}C NMR (600MHz) of compound 2 recorded on a Bruker Avance III 600 spectrometer
(150MHz, pyridine-d₅):

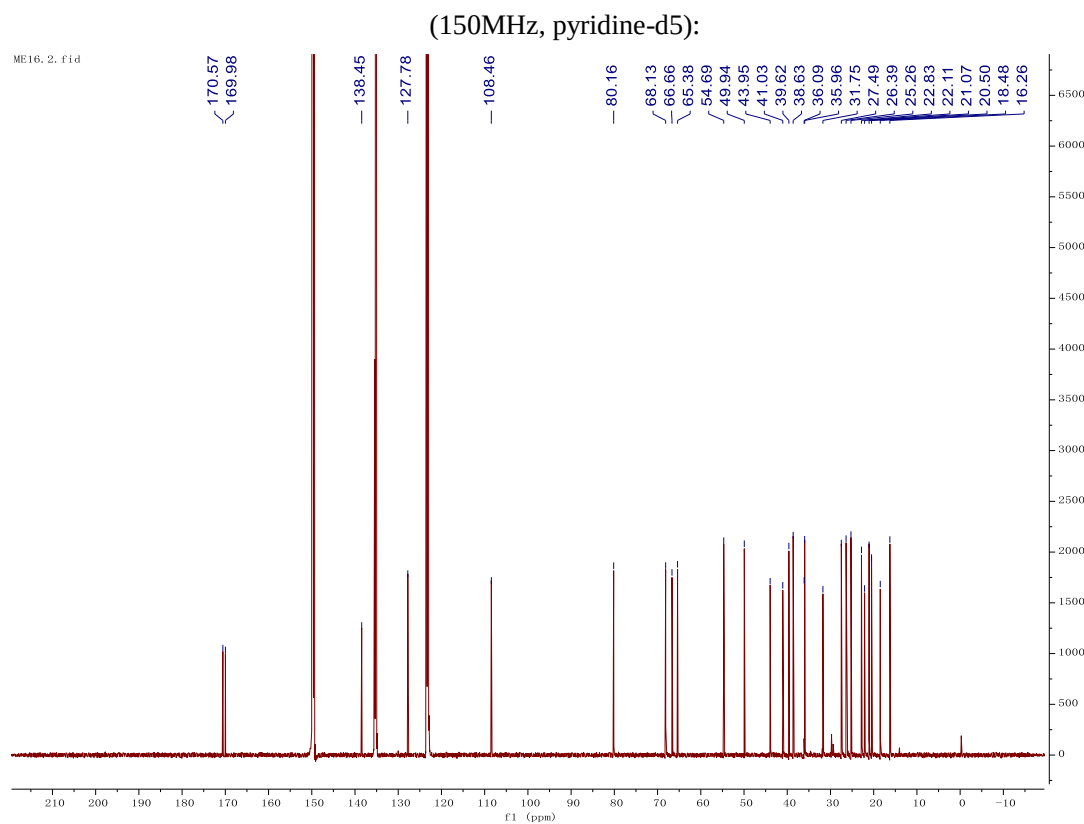


(150MHz, pyridine-d₅):

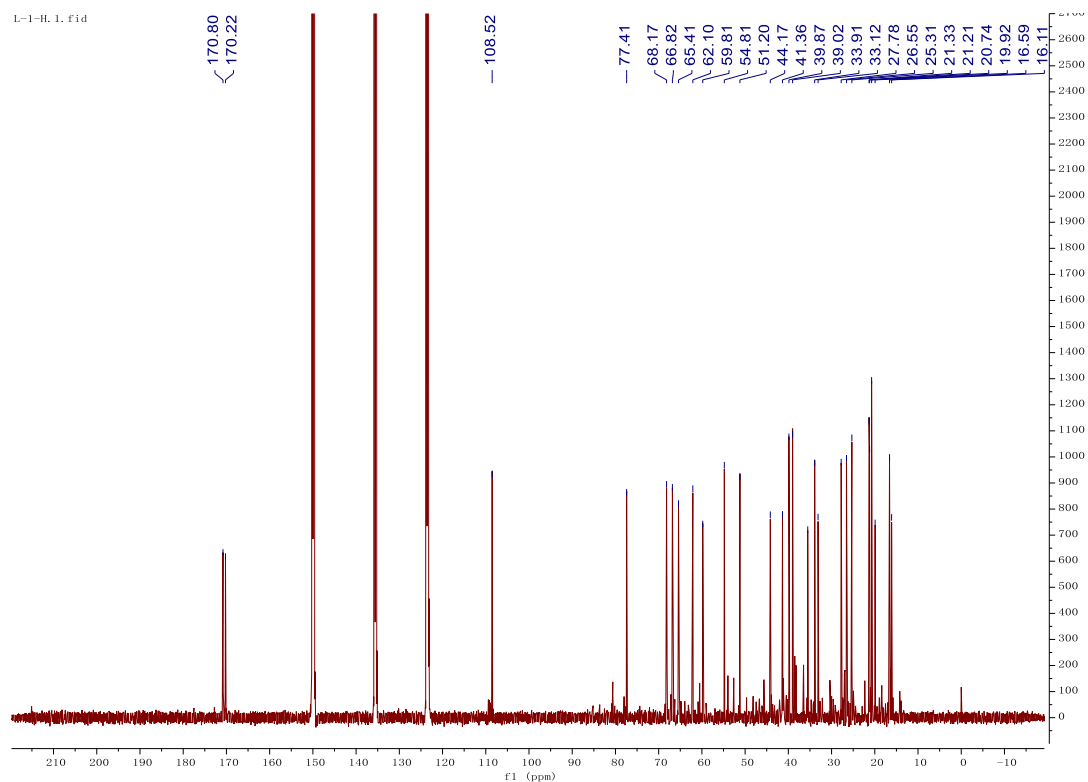




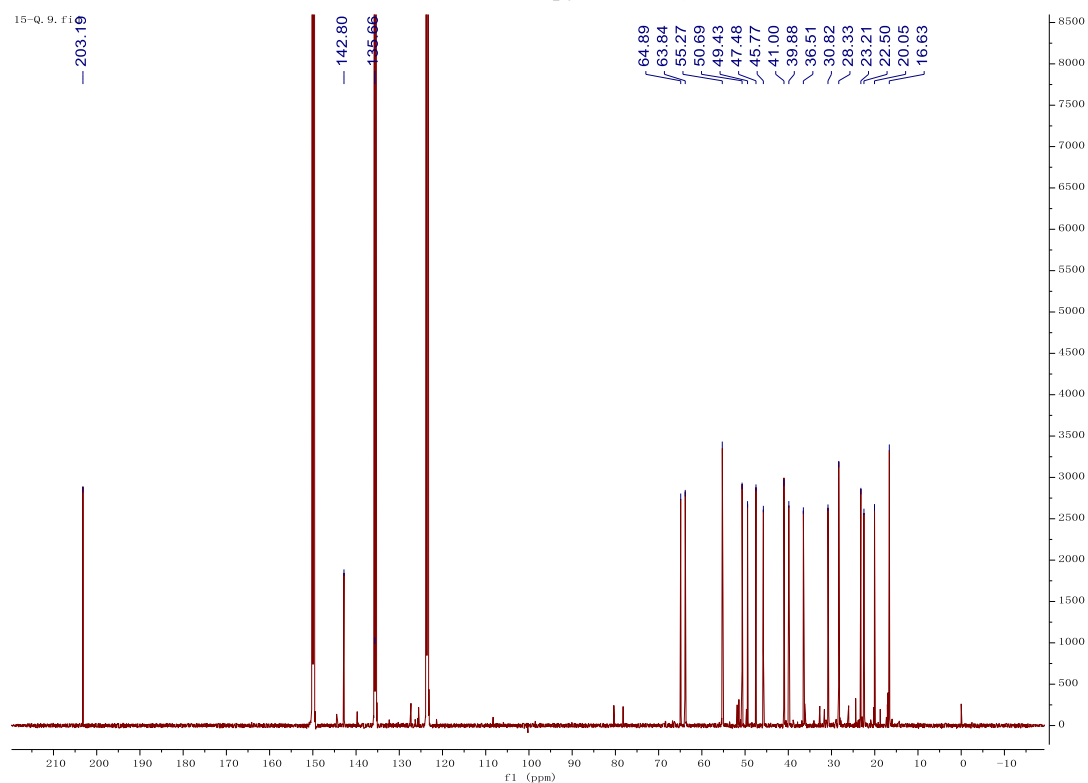
^{13}C NMR (600MHz) of compound **5** recorded on a Bruker Avance III 600 spectrometer



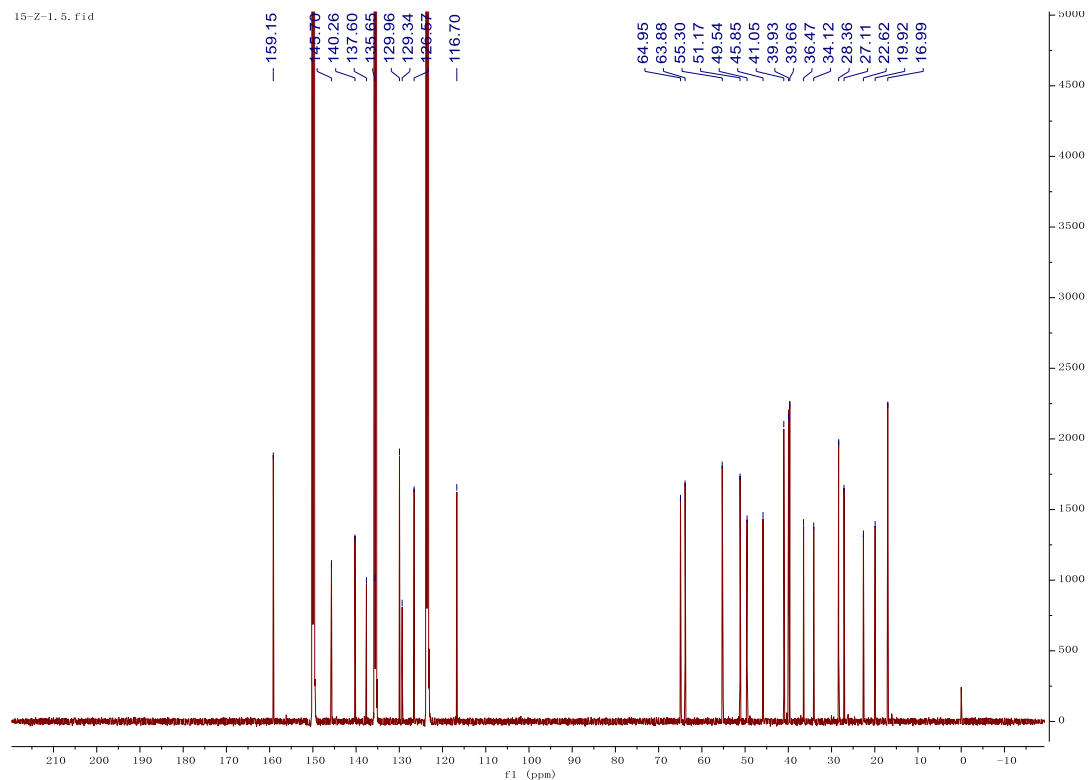
^{13}C NMR (600MHz) of compound **6** recorded on a Bruker Avance III 600 spectrometer
(150MHz, pyridine-d5):



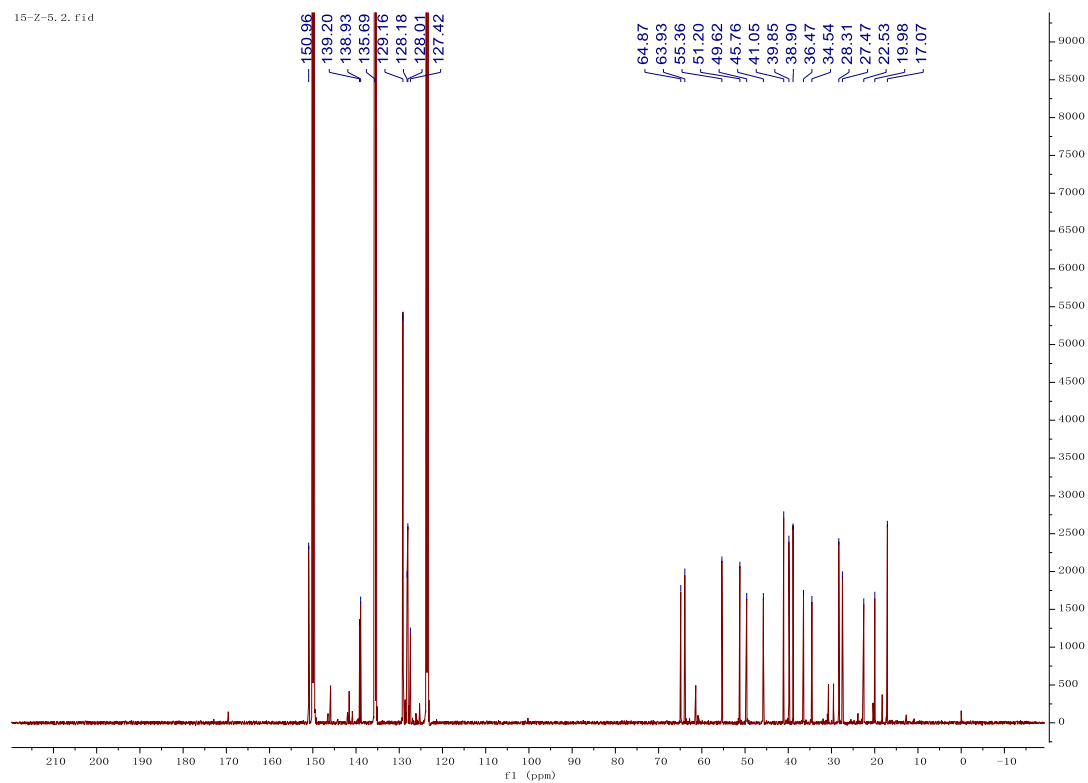
^{13}C NMR (600MHz) of compound **7** recorded on a Bruker Avance III 600 spectrometer (150MHz, pyridine-d5):



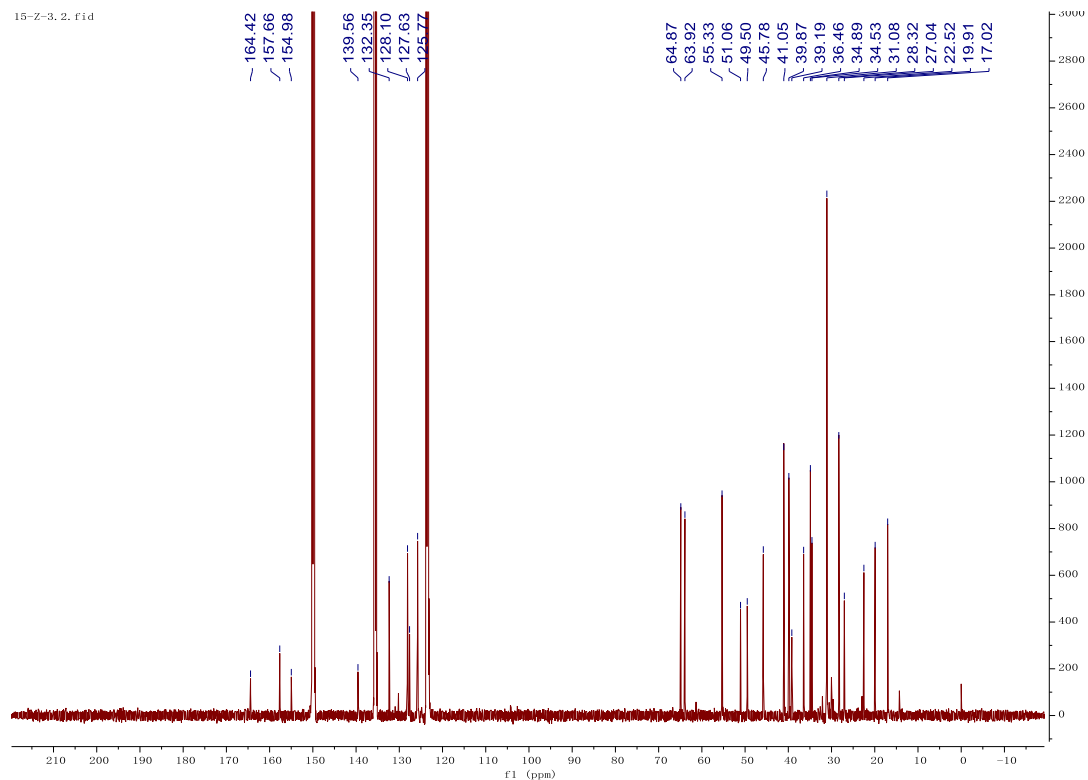
^{13}C NMR (600MHz) of compound **8a** recorded on a Bruker Avance III 600 spectrometer (150MHz, pyridine-d5):



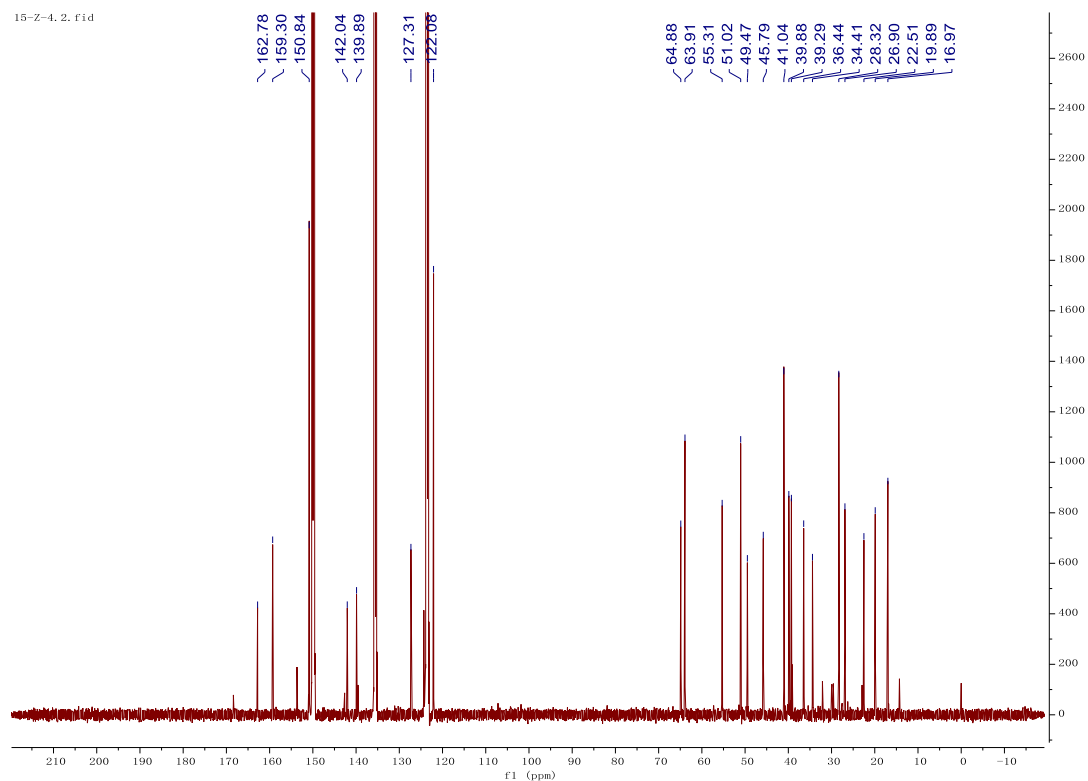
^{13}C NMR (600MHz) of compound **8b** recorded on a Bruker Avance III 600 spectrometer (150MHz, pyridine-d₅):



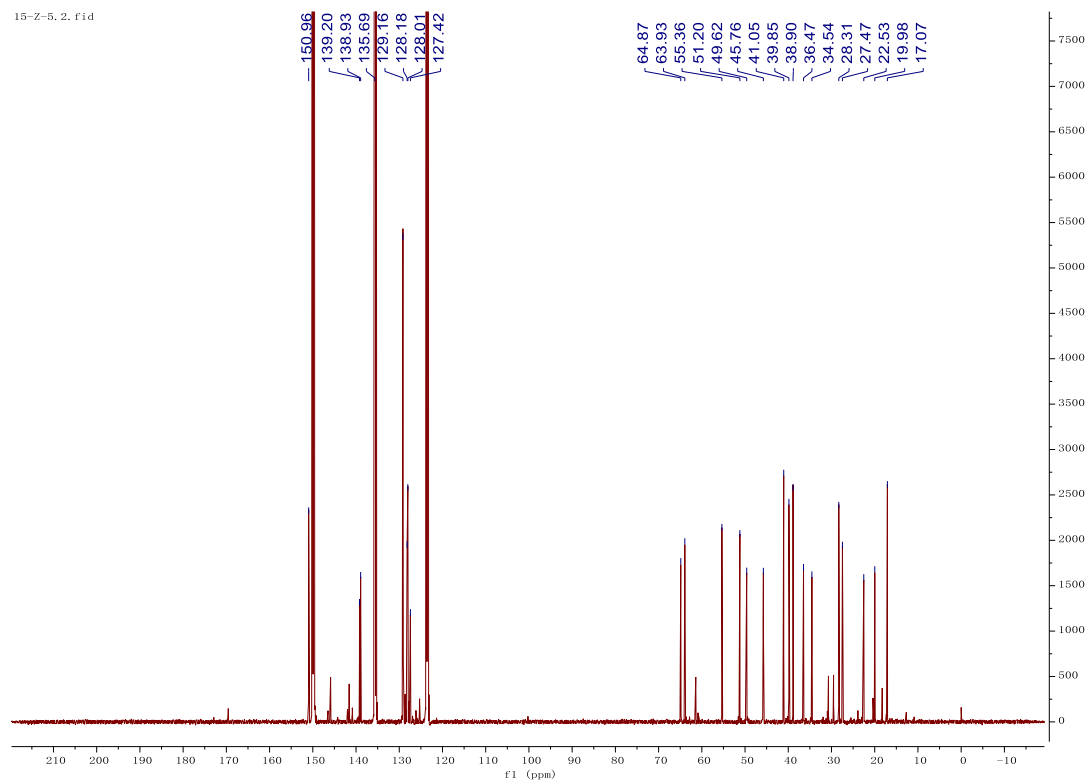
^{13}C NMR (600MHz) of compound **8c** recorded on a Bruker Avance III 600 spectrometer (150MHz, pyridine-d₅):



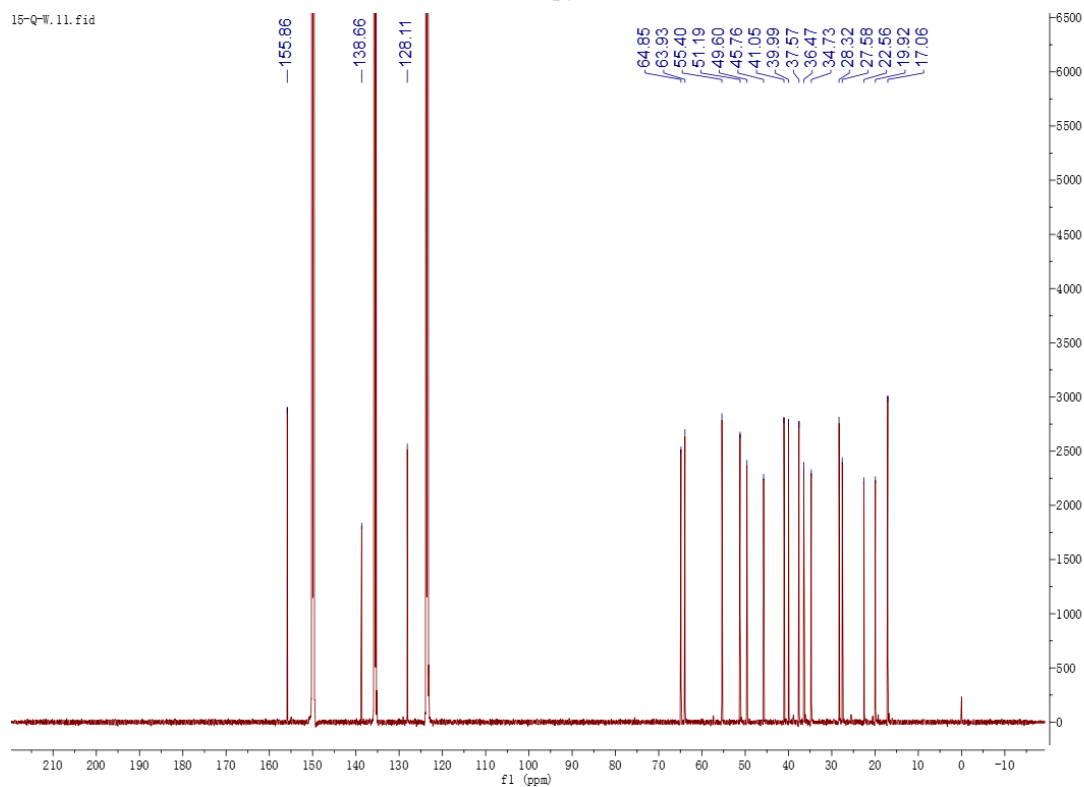
^{13}C NMR (600MHz) of compound **8d** recorded on a Bruker Avance III 600 spectrometer (150MHz, pyridine-d₅):



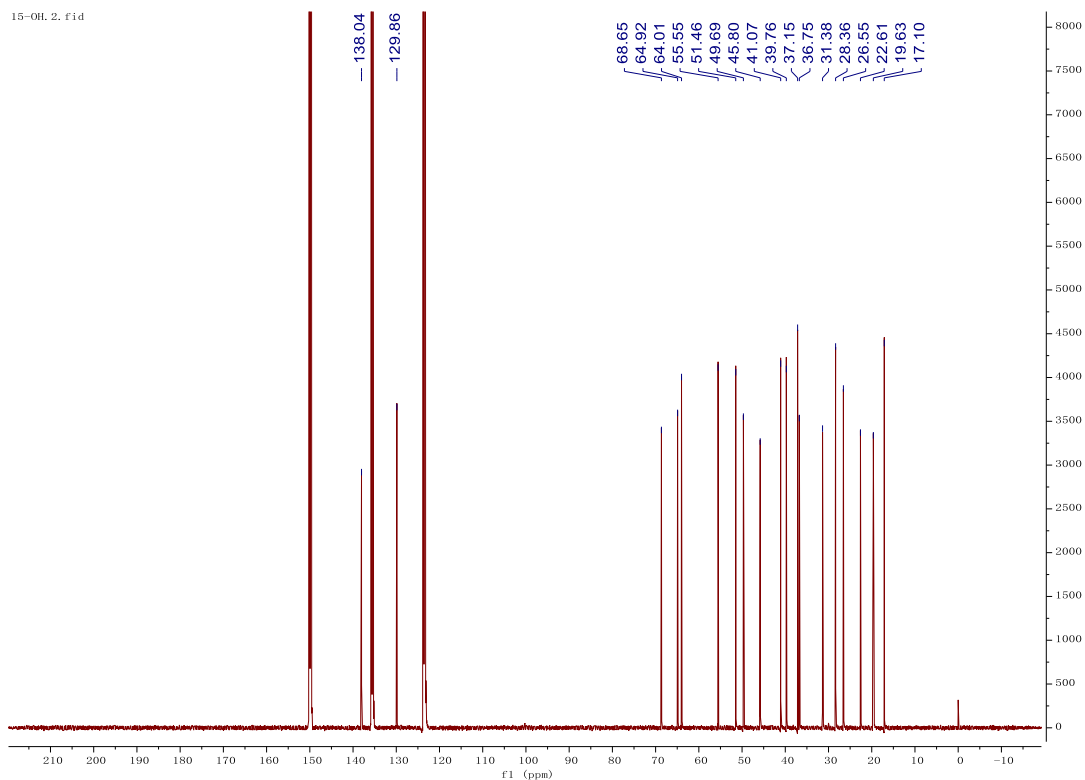
^{13}C NMR (600MHz) of compound **8e** recorded on a Bruker Avance III 600 spectrometer (150MHz, pyridine-d₅):



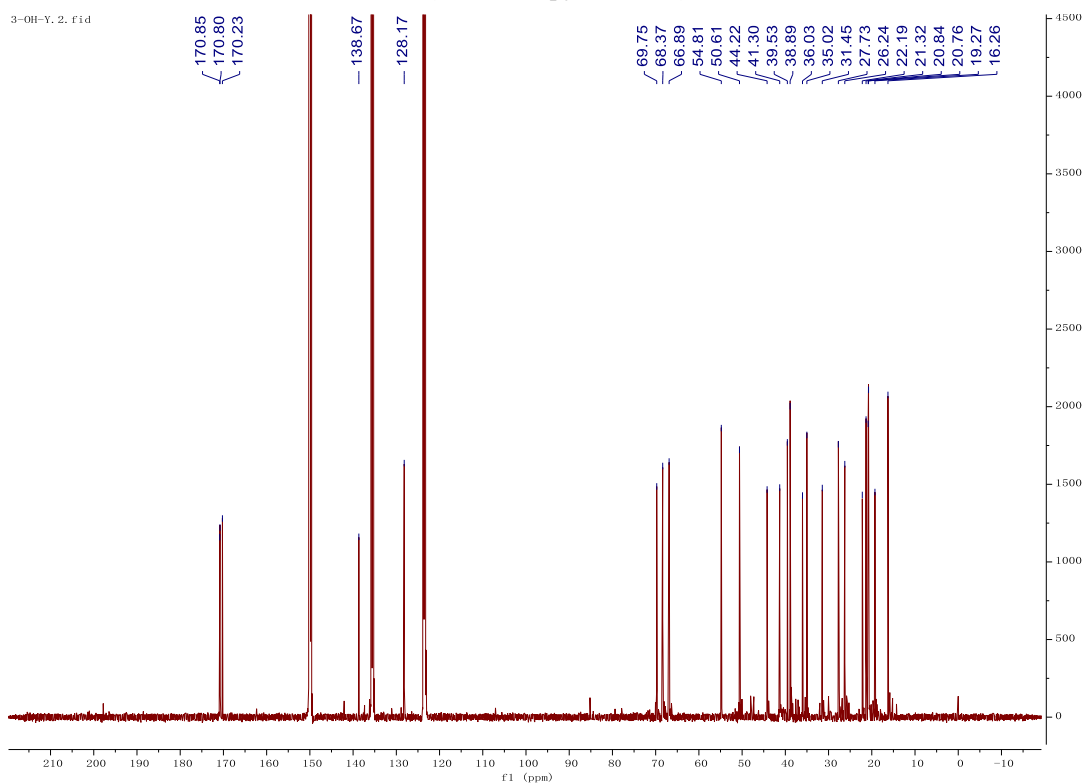
^{13}C NMR (600MHz) of compound **9** recorded on a Bruker Avance III 600 spectrometer (150MHz, pyridine-d₅):



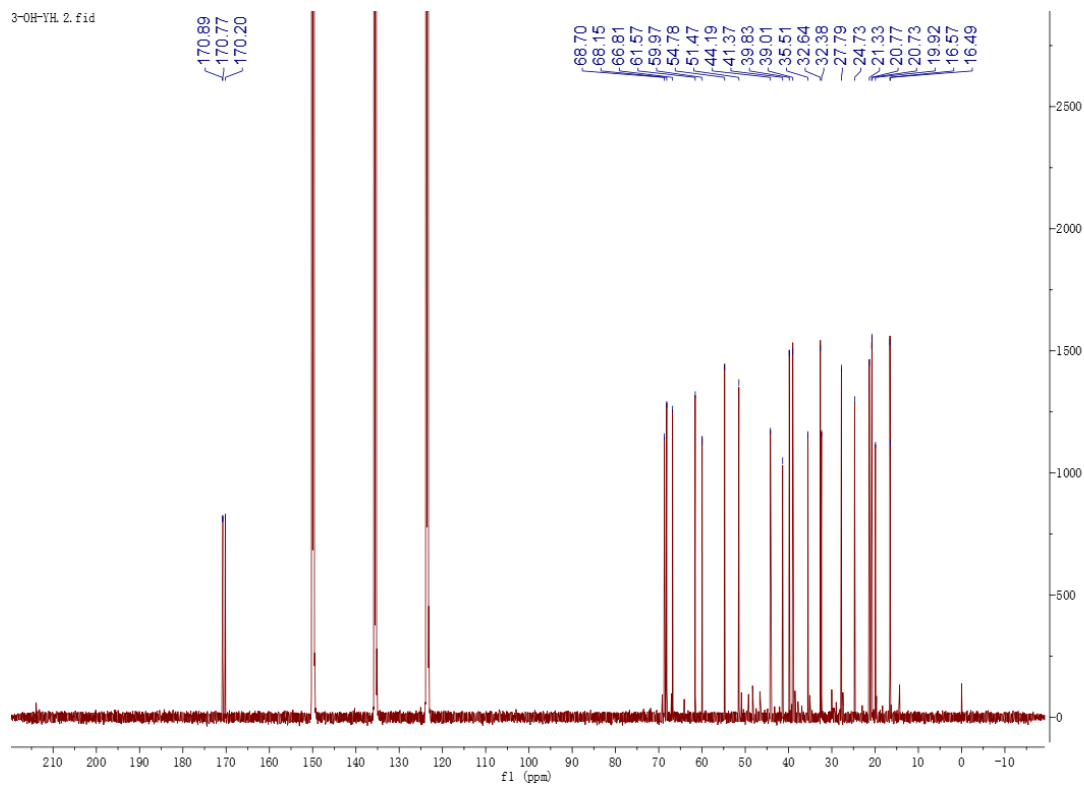
^{13}C NMR (600MHz) of compound **10** recorded on a Bruker Avance III 600 spectrometer (150MHz, pyridine-d₅):



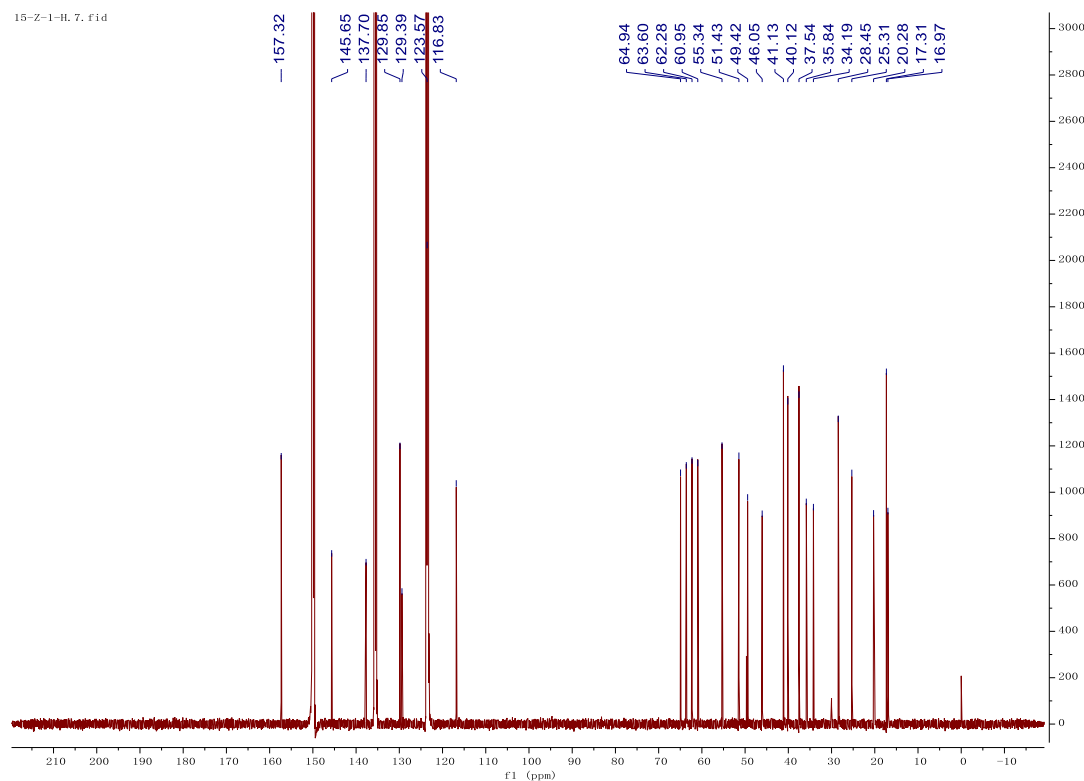
^{13}C NMR (600MHz) of compound **11** recorded on a Bruker Avance III 600 spectrometer (150MHz, pyridine-d₅):



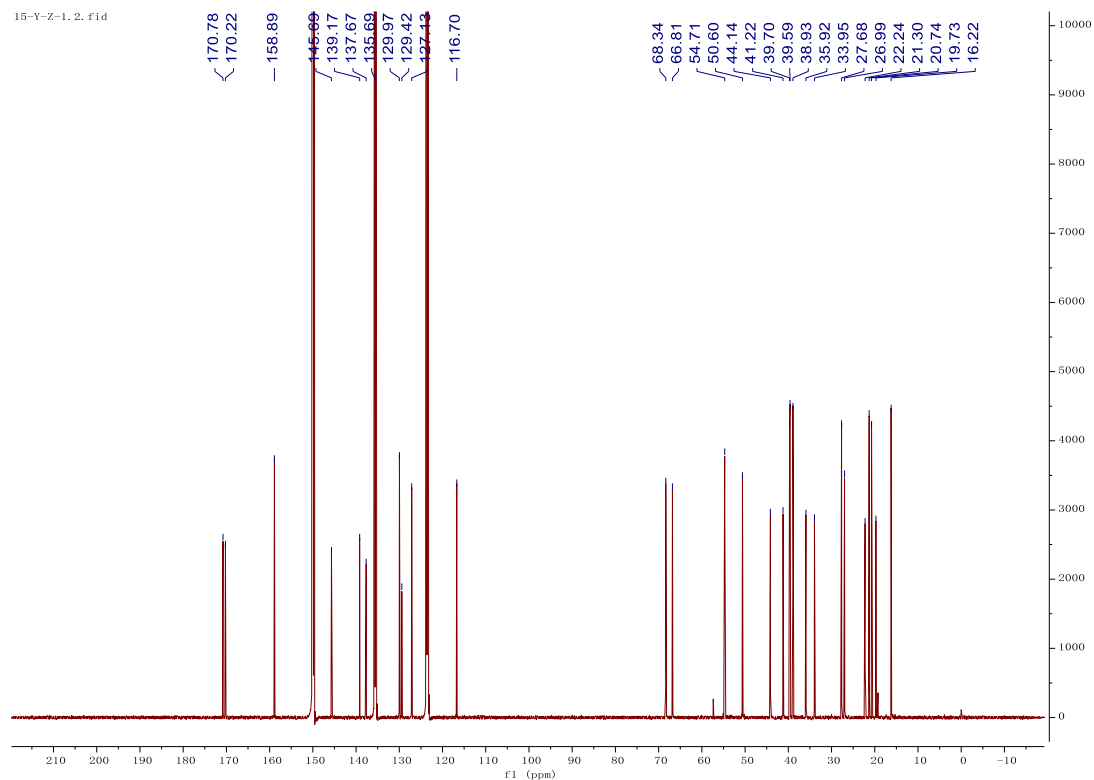
^{13}C NMR (600MHz) of compound **12** recorded on a Bruker Avance III 600 spectrometer (150MHz, pyridine-d₅):



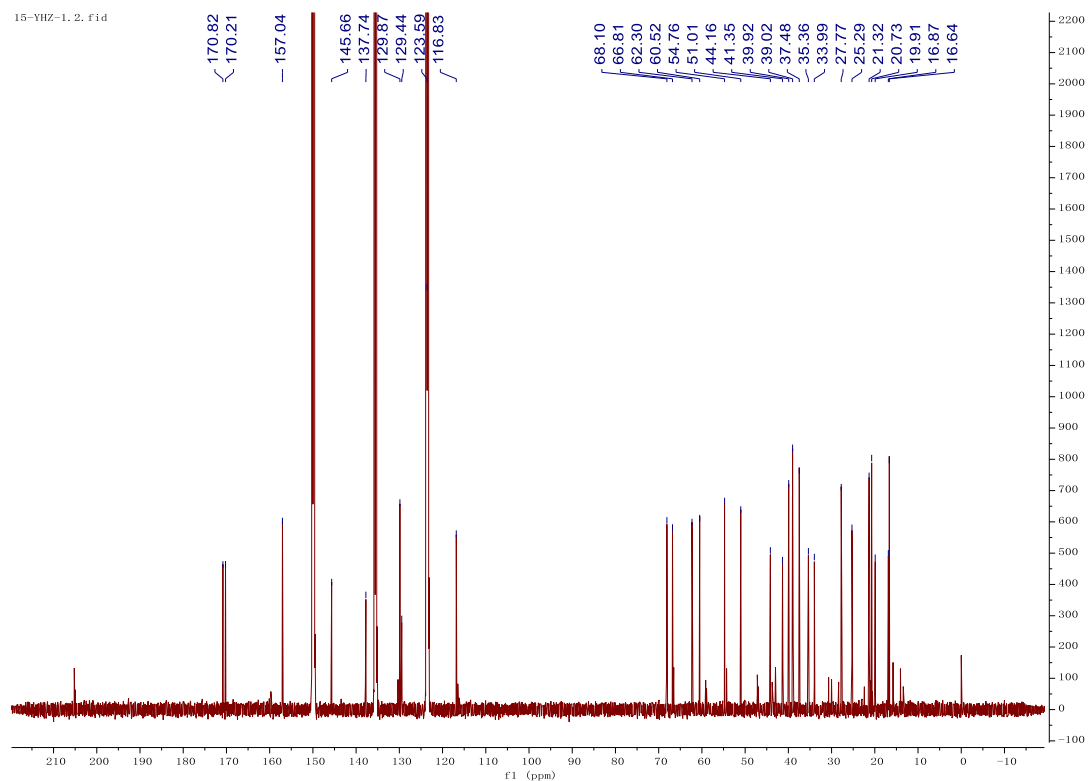
^{13}C NMR (600MHz) of compound **13** recorded on a Bruker Avance III 600 spectrometer (150MHz, pyridine-d₅):



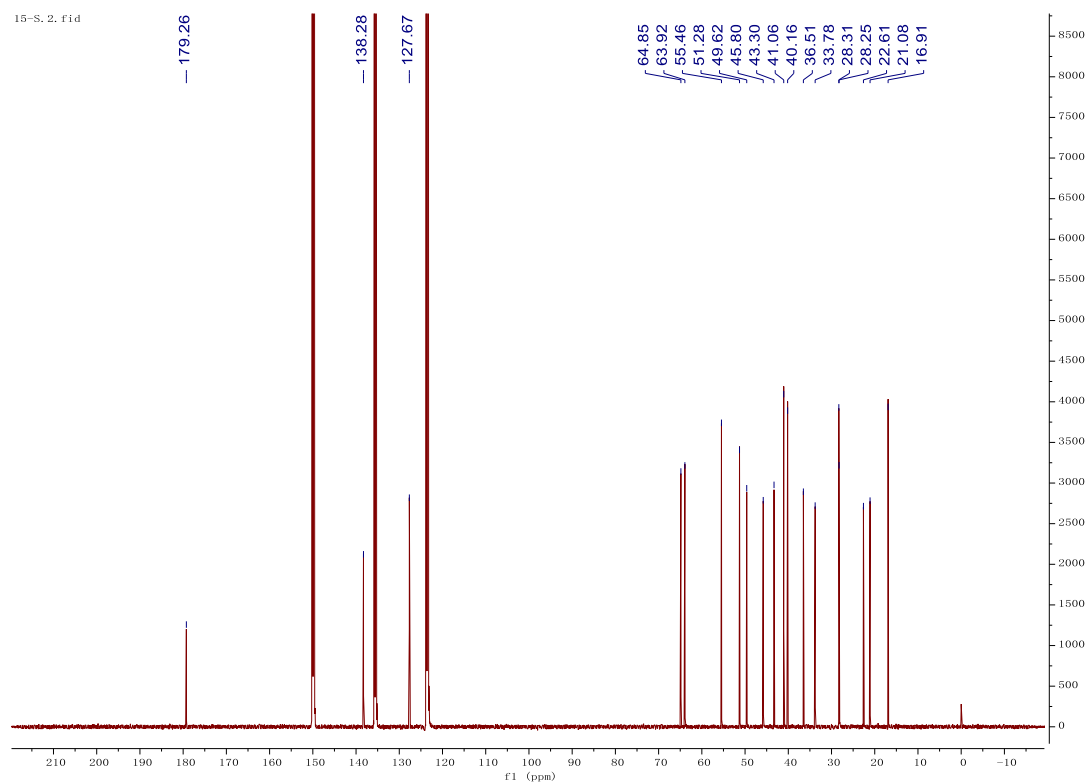
^{13}C NMR (600MHz) of compound **14** recorded on a Bruker Avance III 600 spectrometer (150MHz, pyridine-d₅):



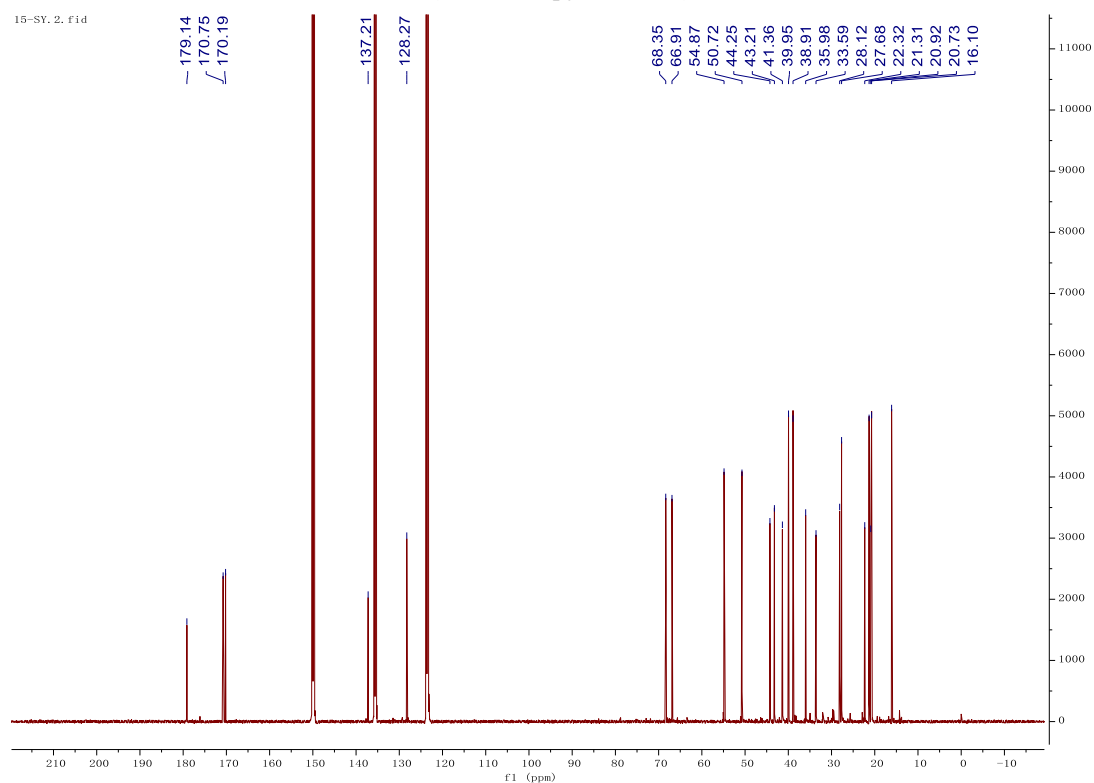
^{13}C NMR (600MHz) of compound **15** recorded on a Bruker Avance III 600 spectrometer (150MHz, pyridine-d₅):



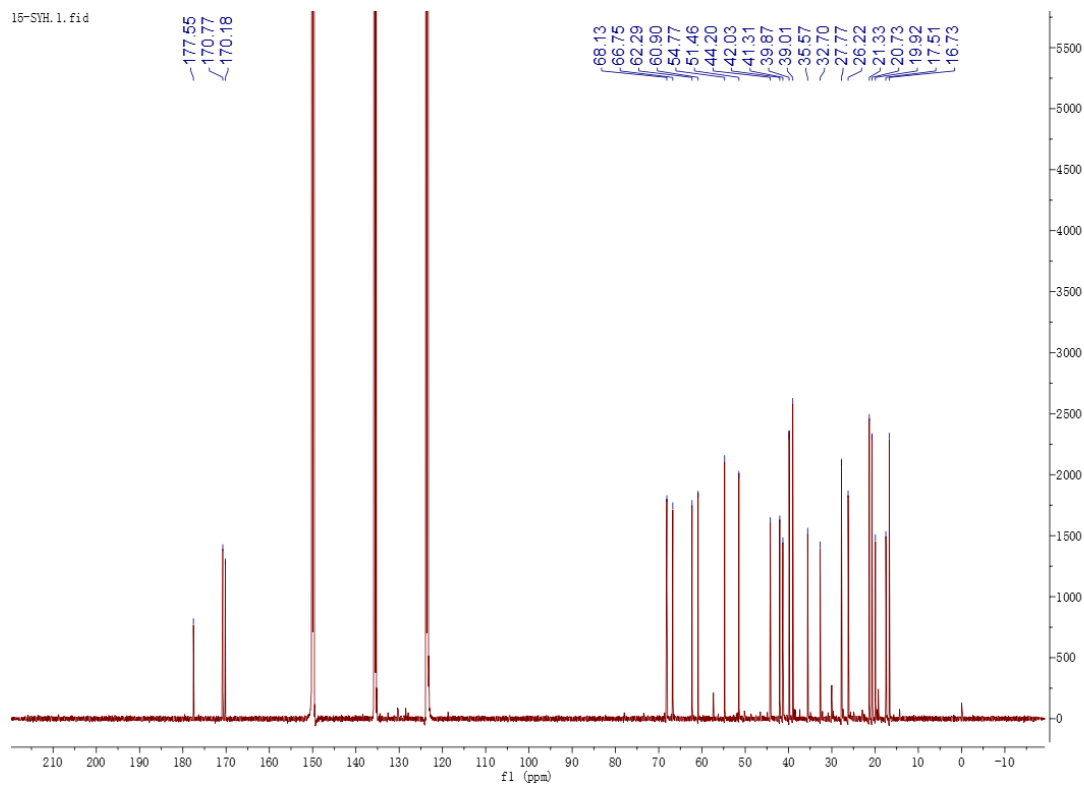
^{13}C NMR (600MHz) of compound **16** recorded on a Bruker Avance III 600 spectrometer (150MHz, pyridine-d₅):



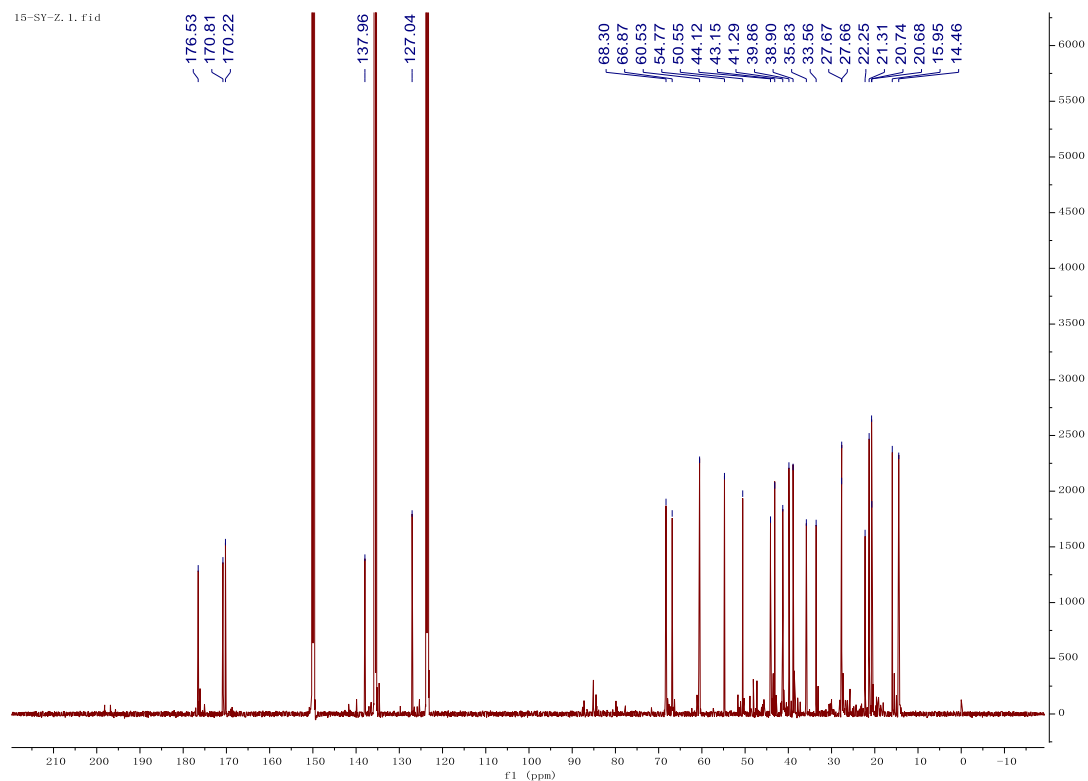
^{13}C NMR (600MHz) of compound **17** recorded on a Bruker Avance III 600 spectrometer (150MHz, pyridine-d₅):



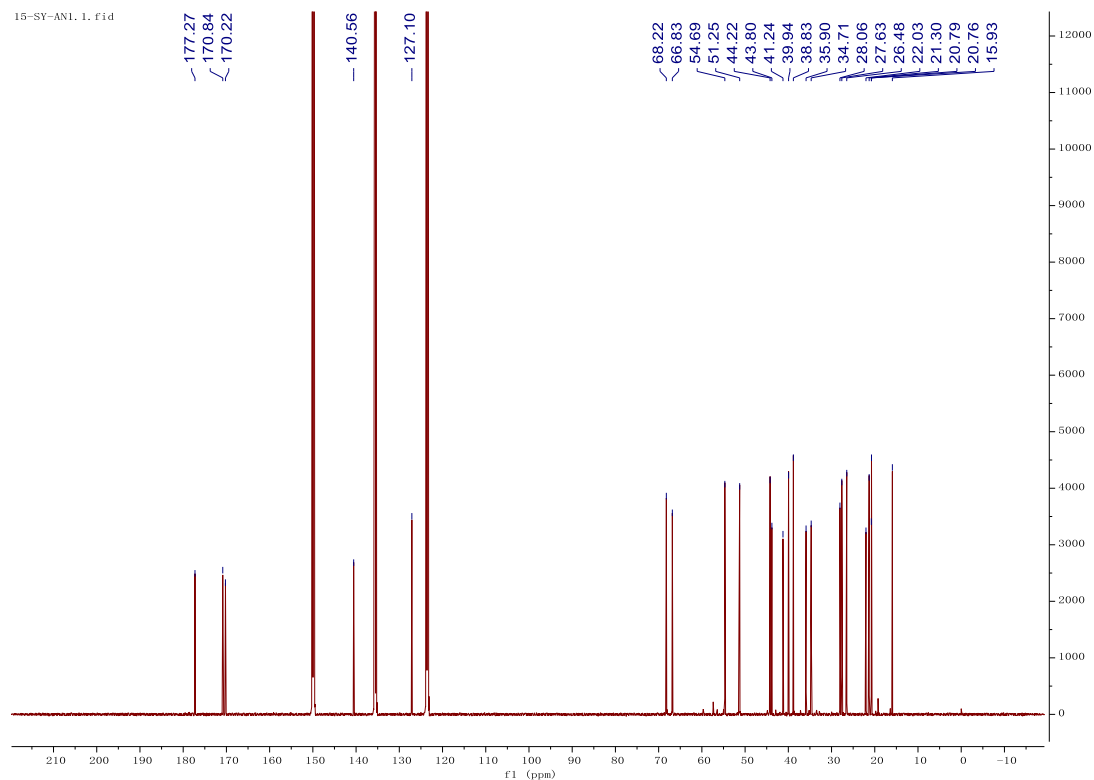
^{13}C NMR (600MHz) of compound **18** recorded on a Bruker Avance III 600 spectrometer (150MHz, pyridine-d₅):



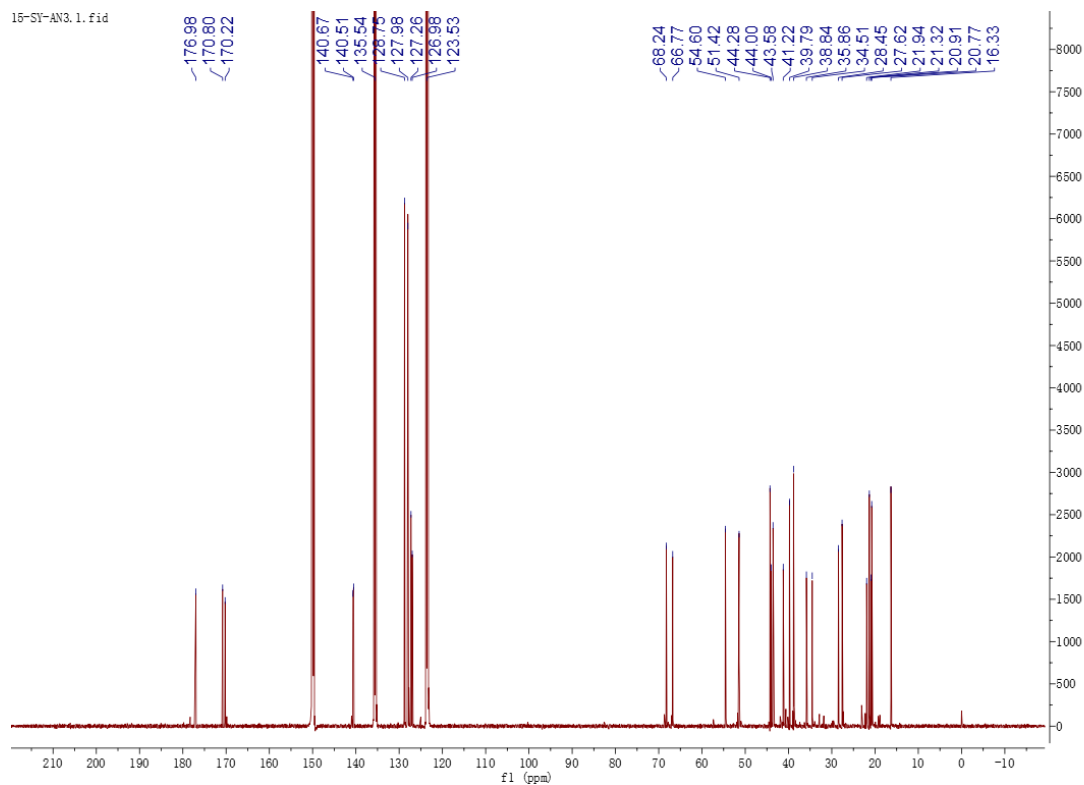
^{13}C NMR (600MHz) of compound **19a** recorded on a Bruker Avance III 600 spectrometer (150MHz, pyridine-d₅):



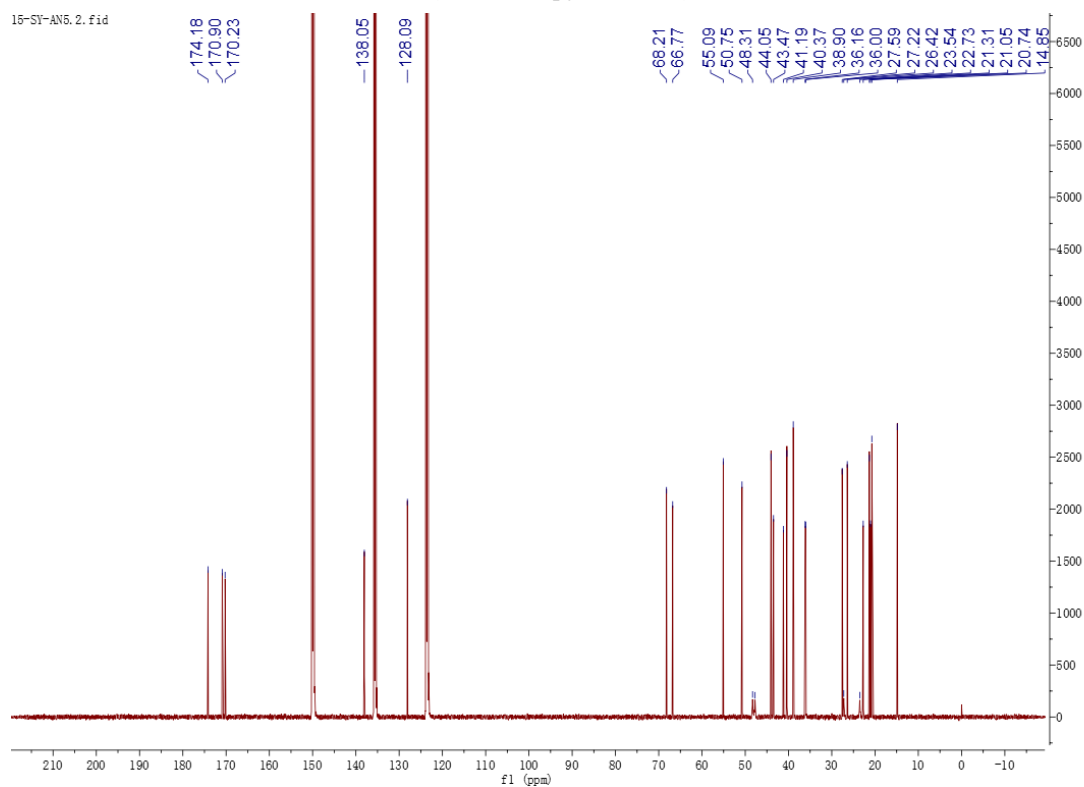
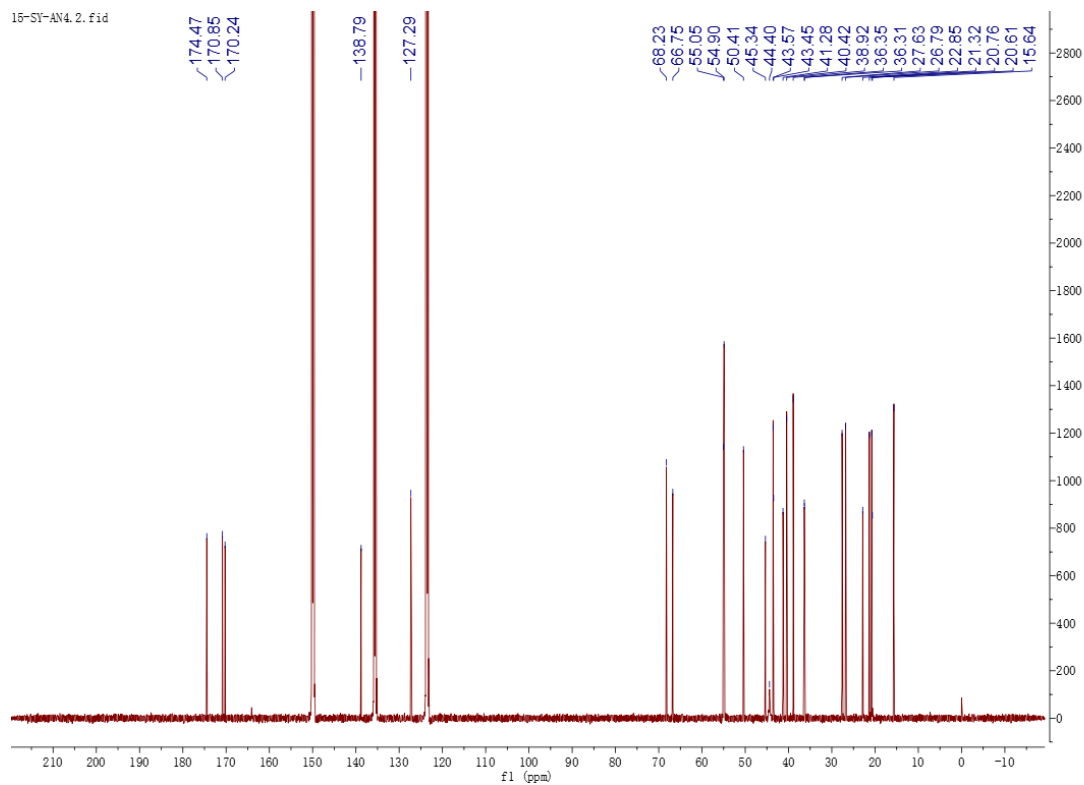
^{13}C NMR (600MHz) of compound **19b** recorded on a Bruker Avance III 600 spectrometer (150MHz, pyridine-d₅):

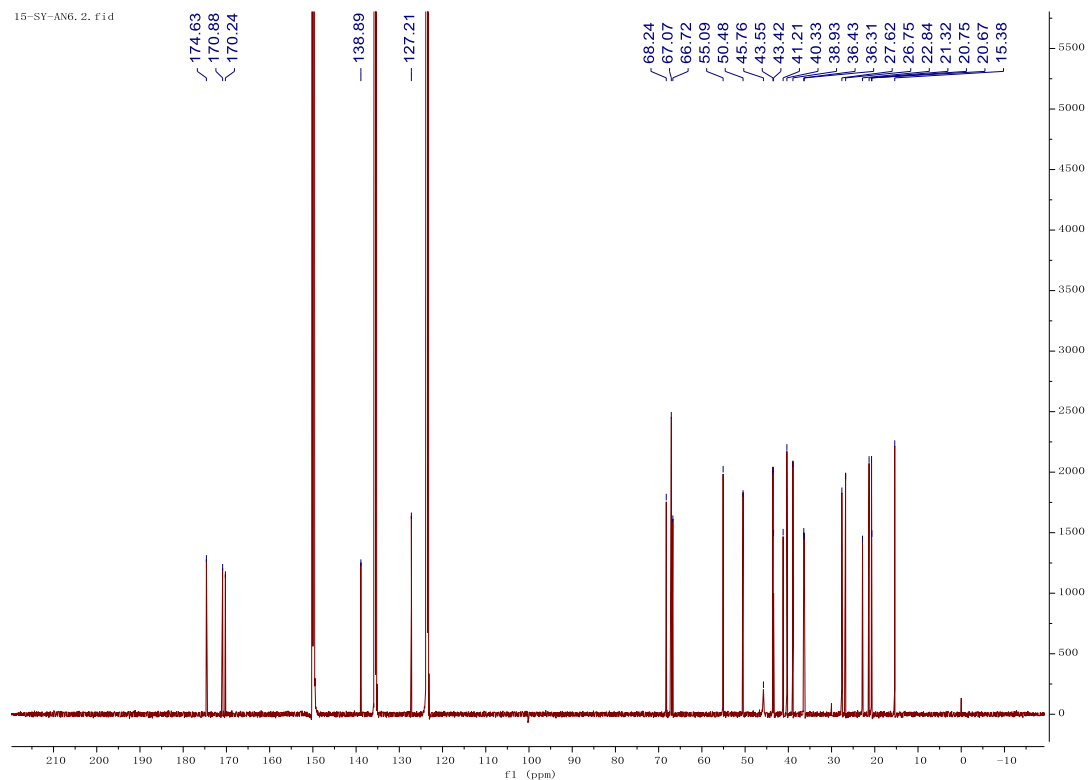


^{13}C NMR (600MHz) of compound **19c** recorded on a Bruker Avance III 600 spectrometer (150MHz, pyridine-d₅):

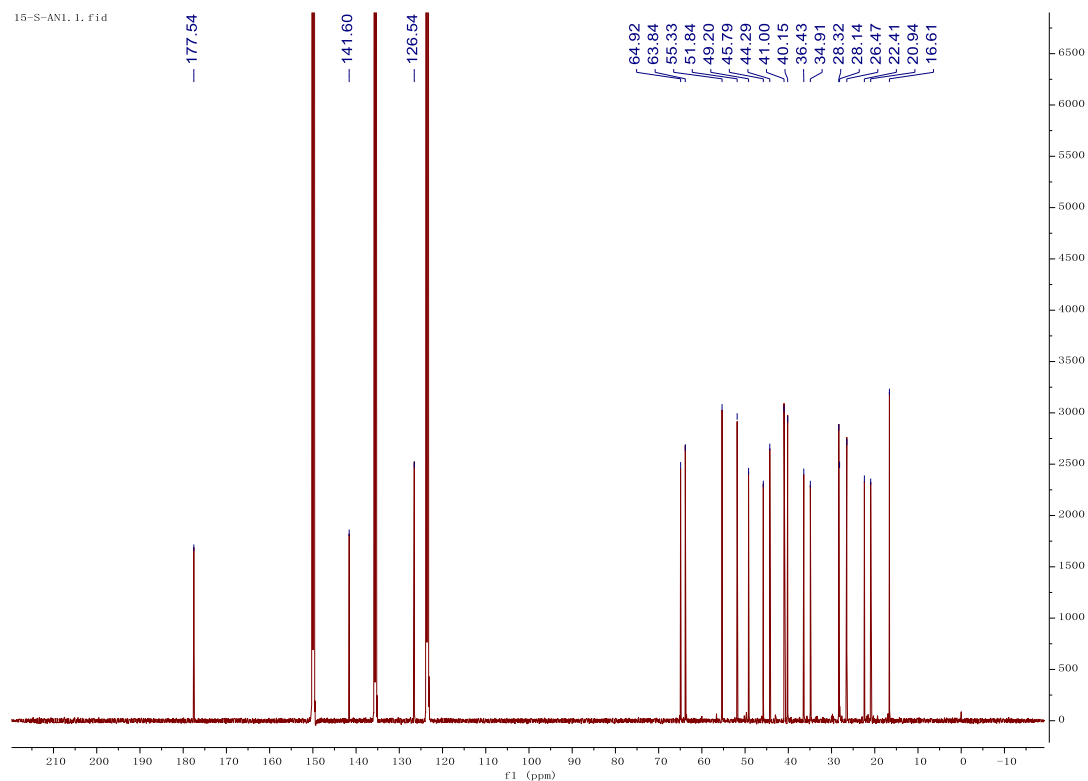


^{13}C NMR (600MHz) of compound **19d** recorded on a Bruker Avance III 600 spectrometer (150MHz, pyridine-d₅):

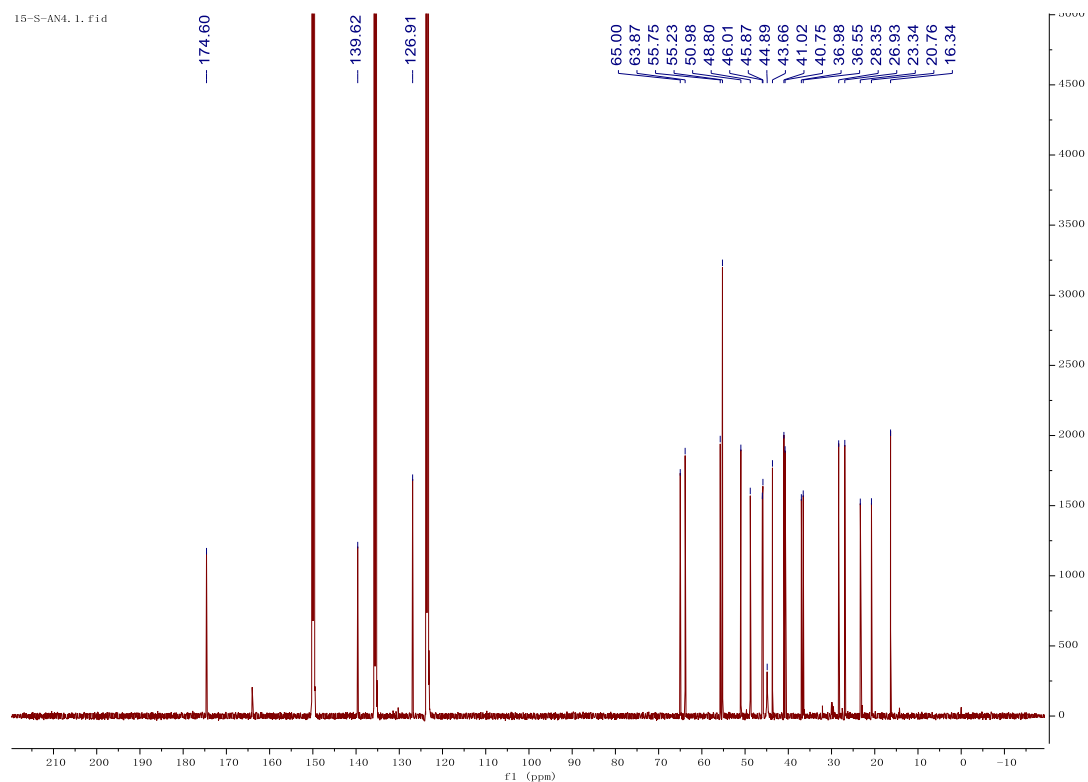




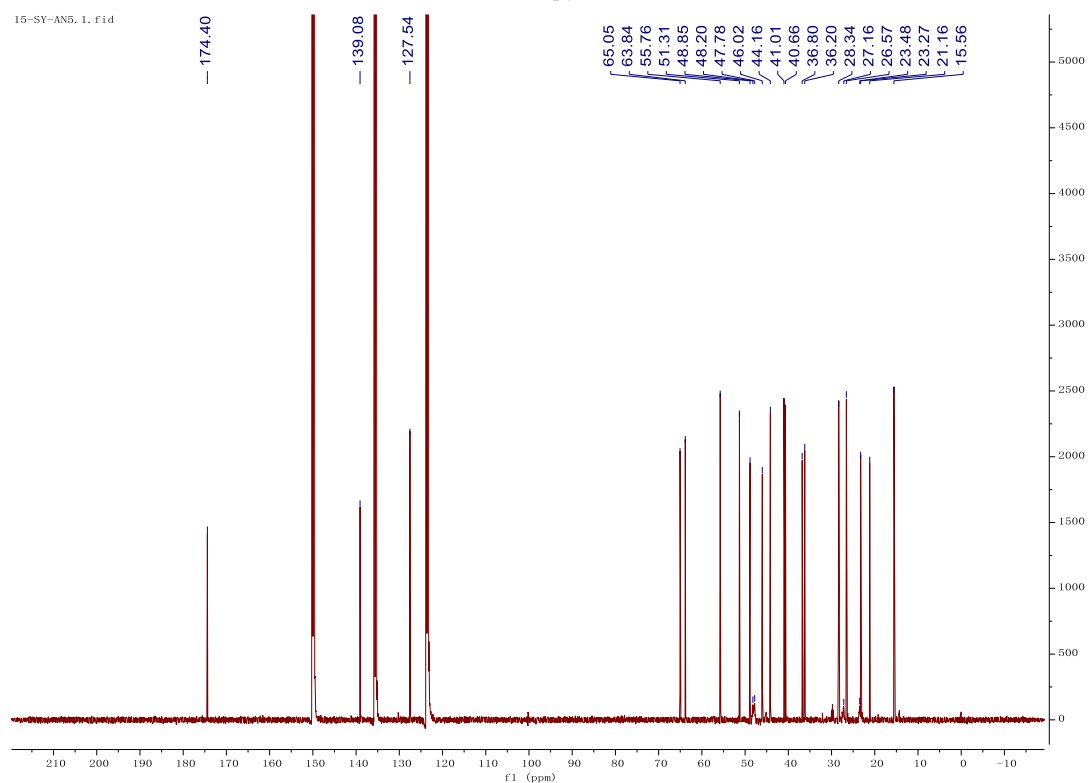
^{13}C NMR (600MHz) of compound **20a** recorded on a Bruker Avance III 600 spectrometer (150MHz, pyridine-d₅):



^{13}C NMR (600MHz) of compound **20b** recorded on a Bruker Avance III 600 spectrometer (150MHz, pyridine-d₅):



^{13}C NMR (600MHz) of compound **20c** recorded on a Bruker Avance III 600 spectrometer (150MHz, pyridine-d₅):



^{13}C NMR (600MHz) of compound **20d** recorded on a Bruker Avance III 600 spectrometer (150MHz, pyridine-d₅):

