

DESIGN, SYNTHESIS AND BIOACTIVITY EVALUATION OF NOVEL QUINAZOLINE BASED KRAS^{G12C} INHIBITORS

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^c Key Laboratory for Rare & Uncommon Diseases of Shandong Province, Jinan 250117, China;

* Corresponding author. E-mail address: sunjingyong08@hotmail.com (Jingyong Sun)

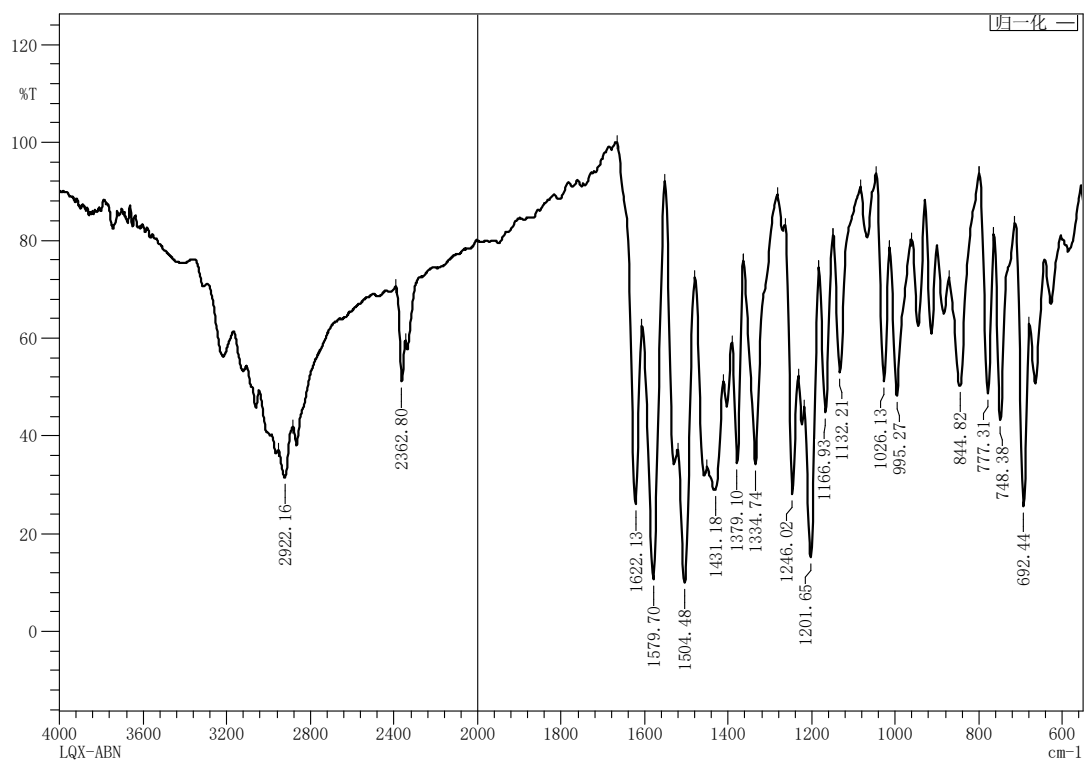
Supporting Information

Contents

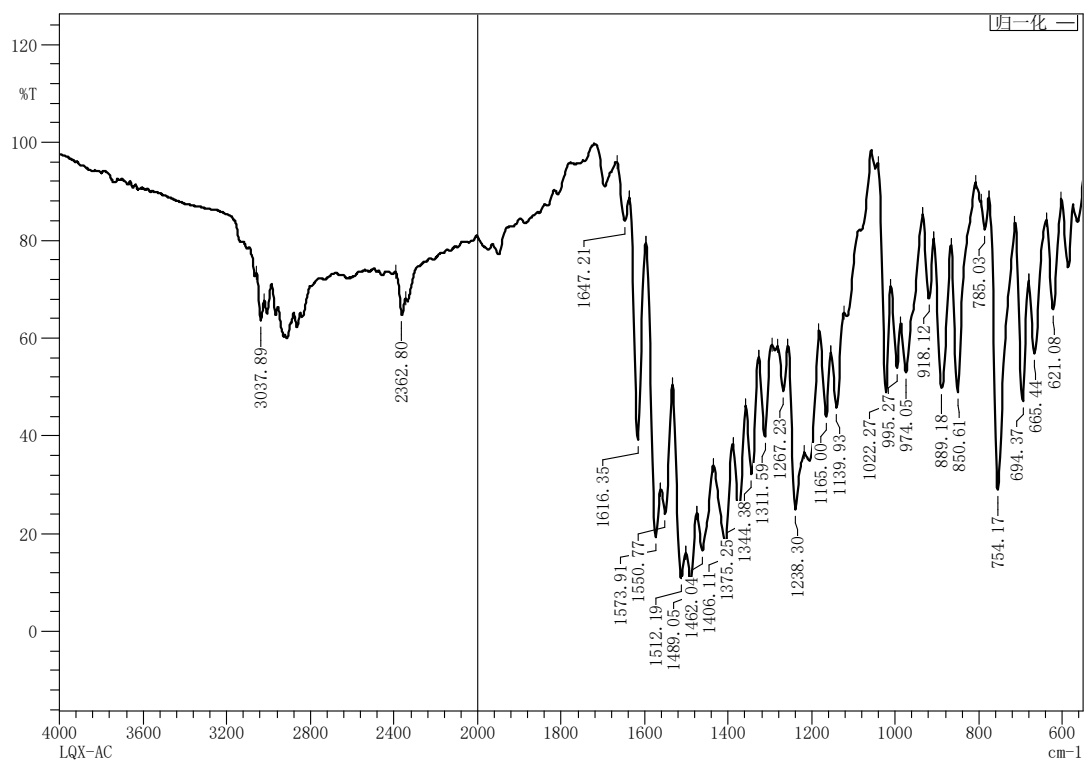
IR(KBr) of compounds 7a-8q	2
Mass spectra of compounds 7a-8q	11
¹H NMR(600 MHz) of compounds 7a-8q	16
¹³C NMR(150 MHz) of compounds 7a-8q	30

IR(KBr) of compounds

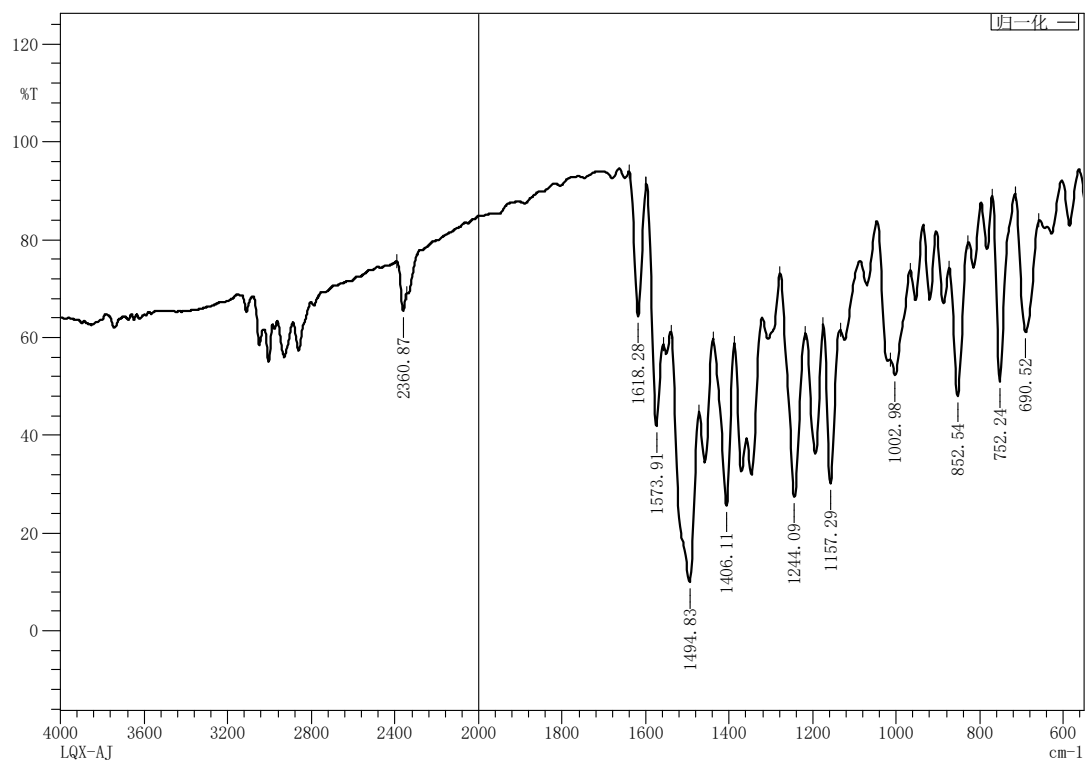
For compound **7a**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



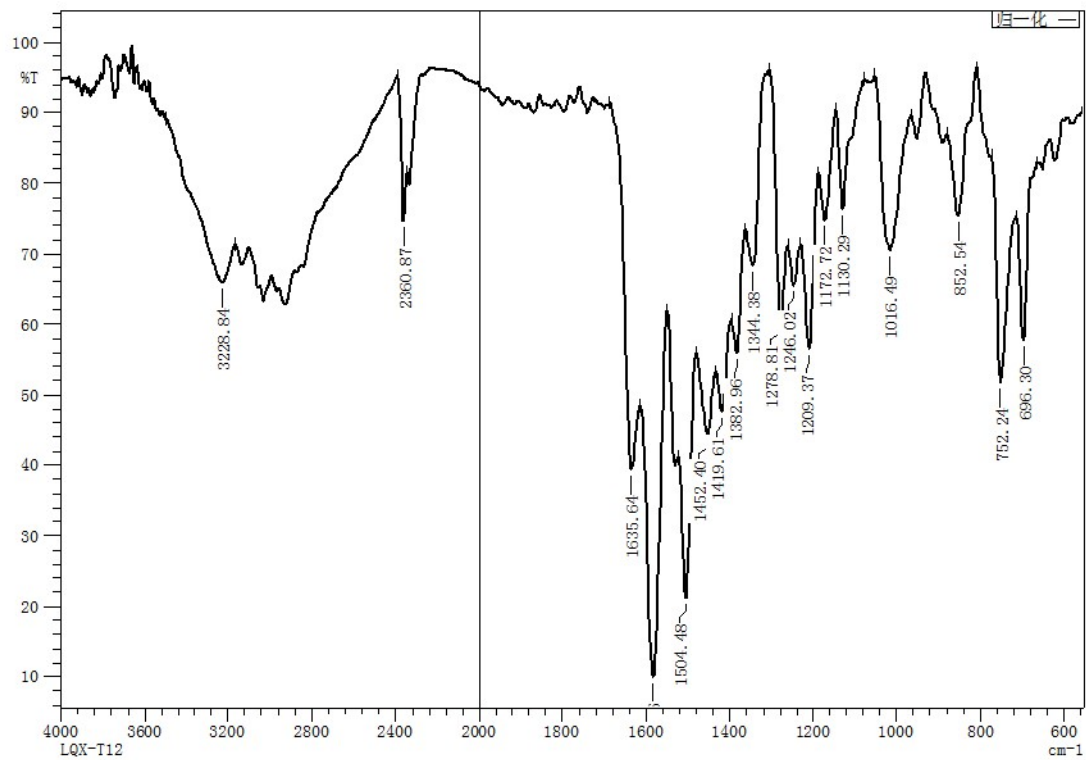
For compound **7b**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



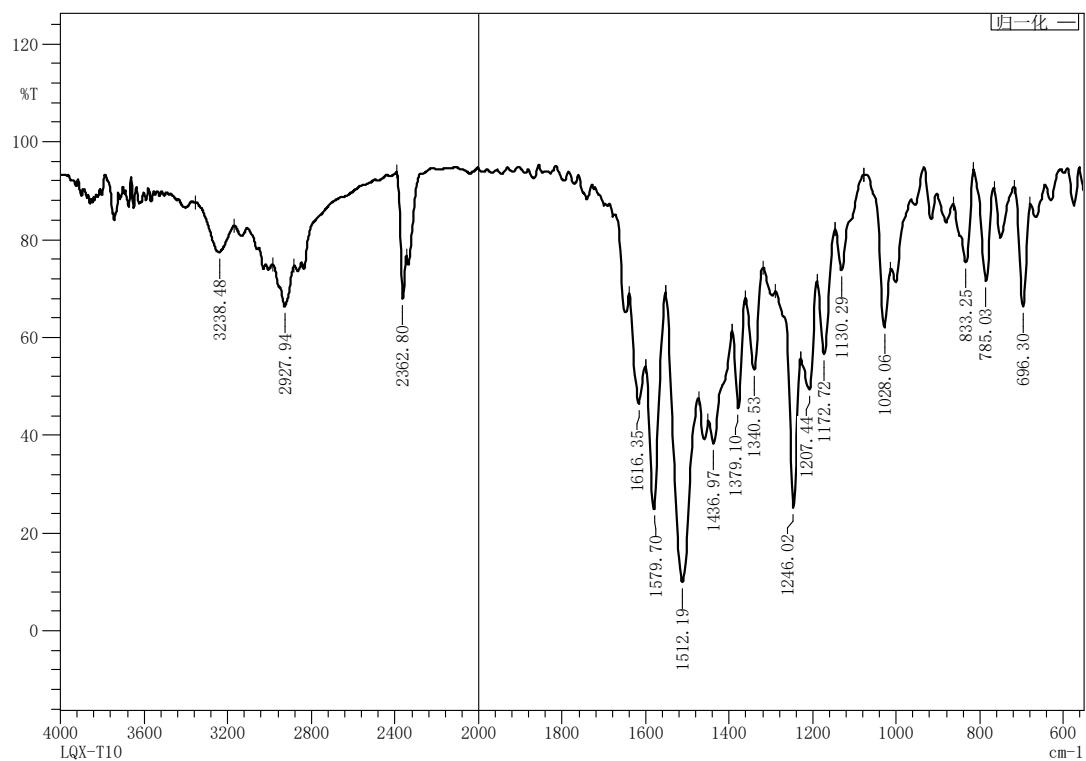
For compound **7c**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



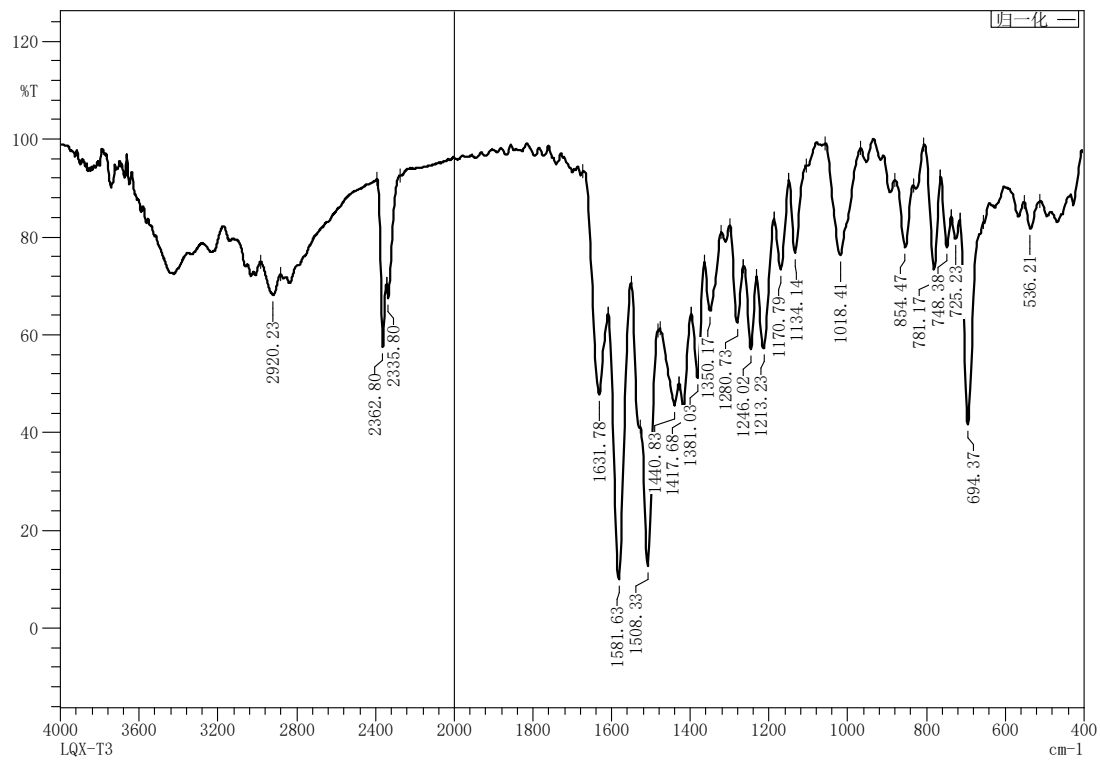
For compound **8a**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



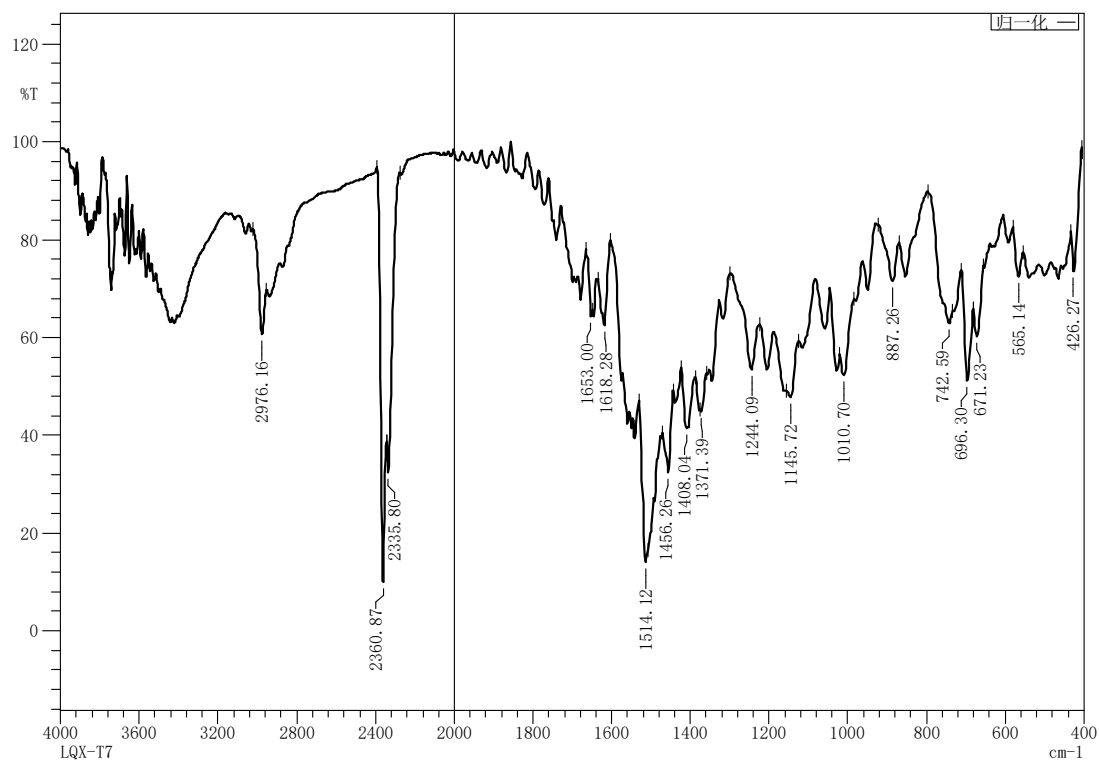
For compound **8b**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



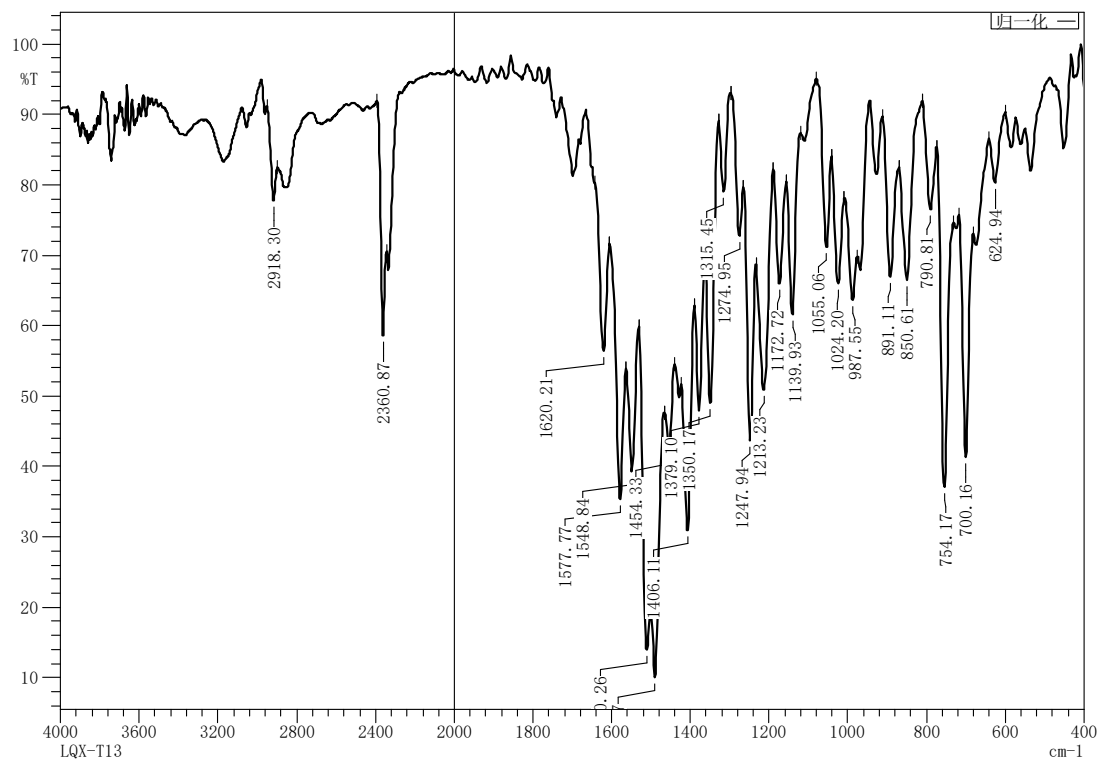
For compound **8c**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



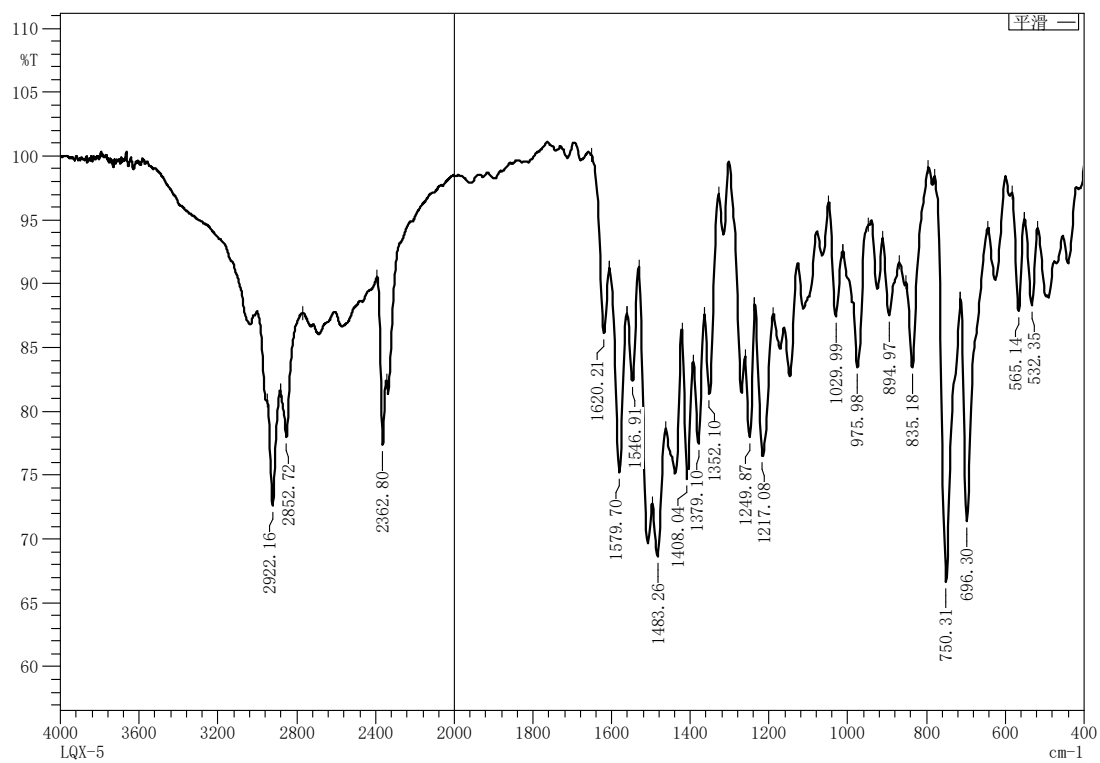
For compound **8d**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



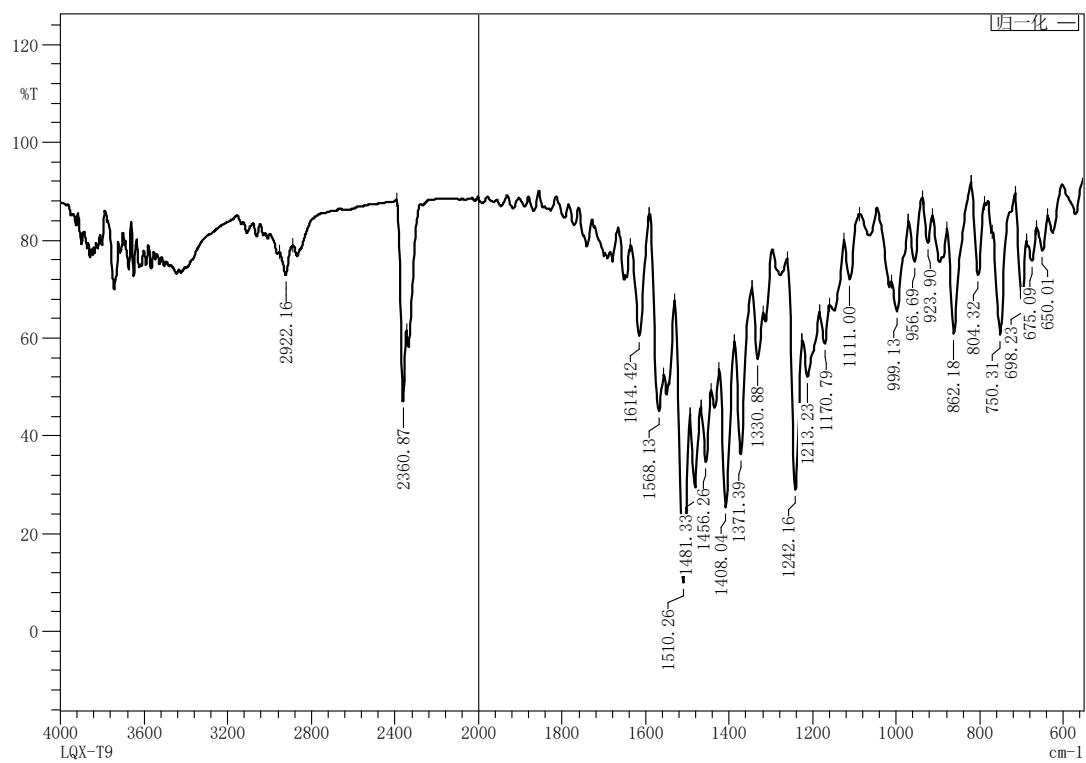
For compound **8e**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



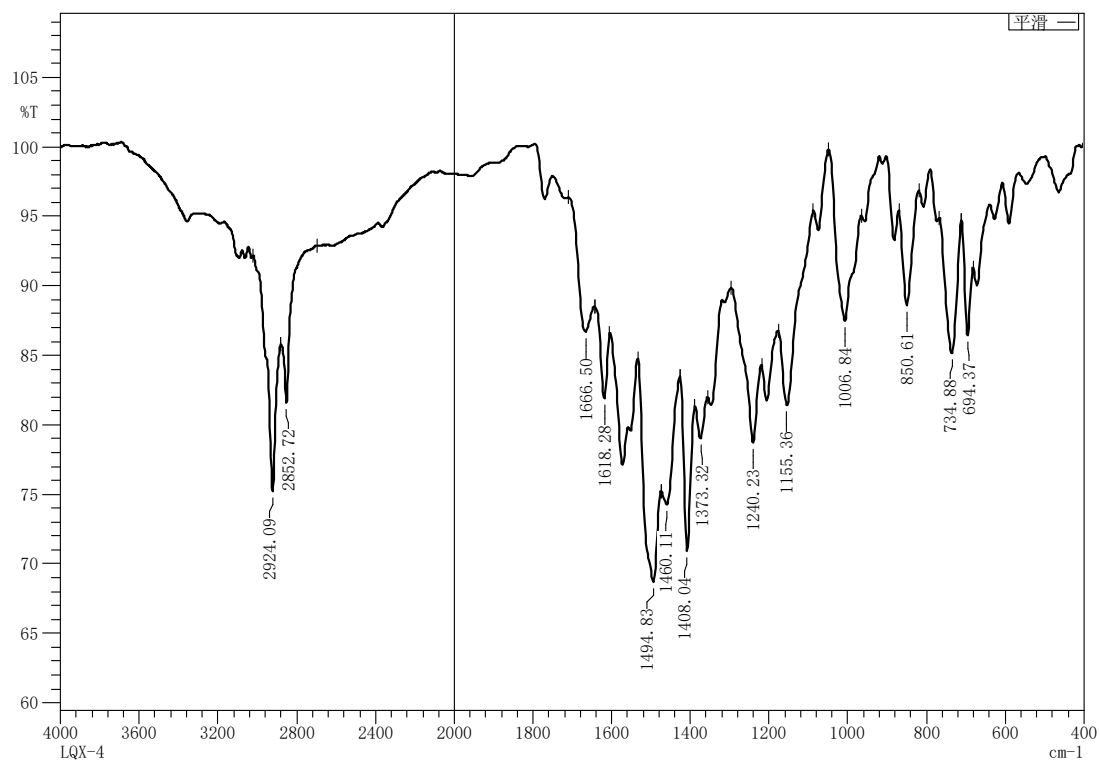
For compound **8f**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



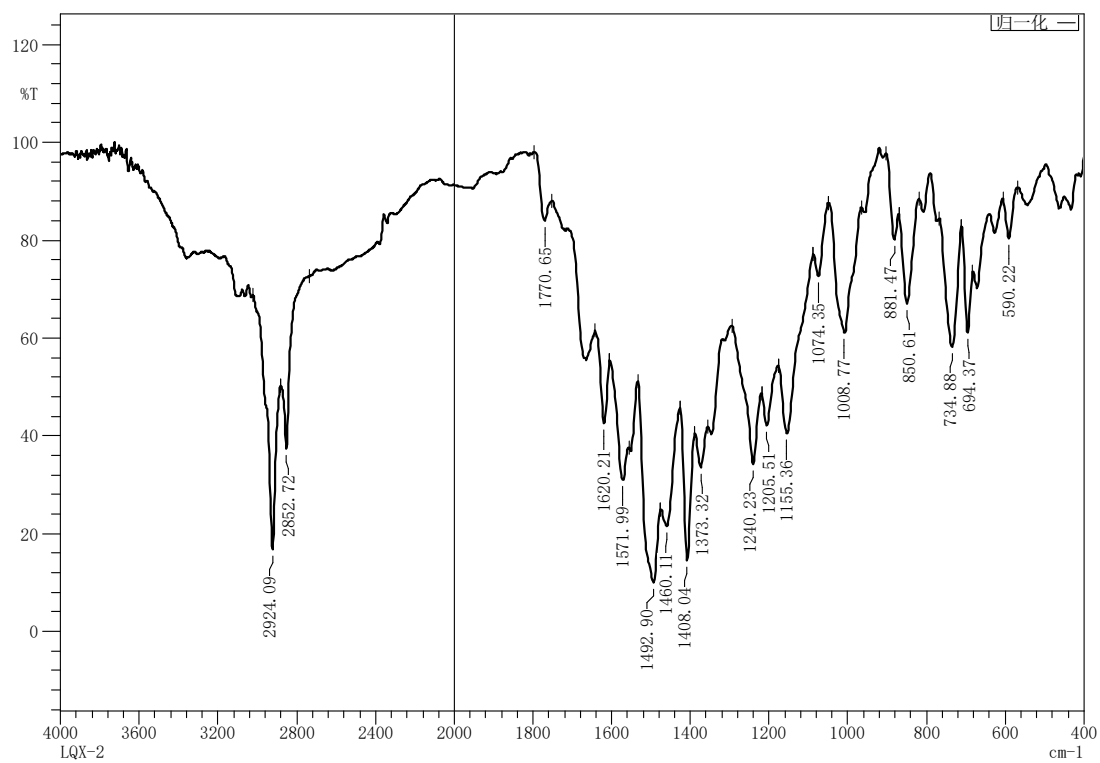
For compound **8g**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



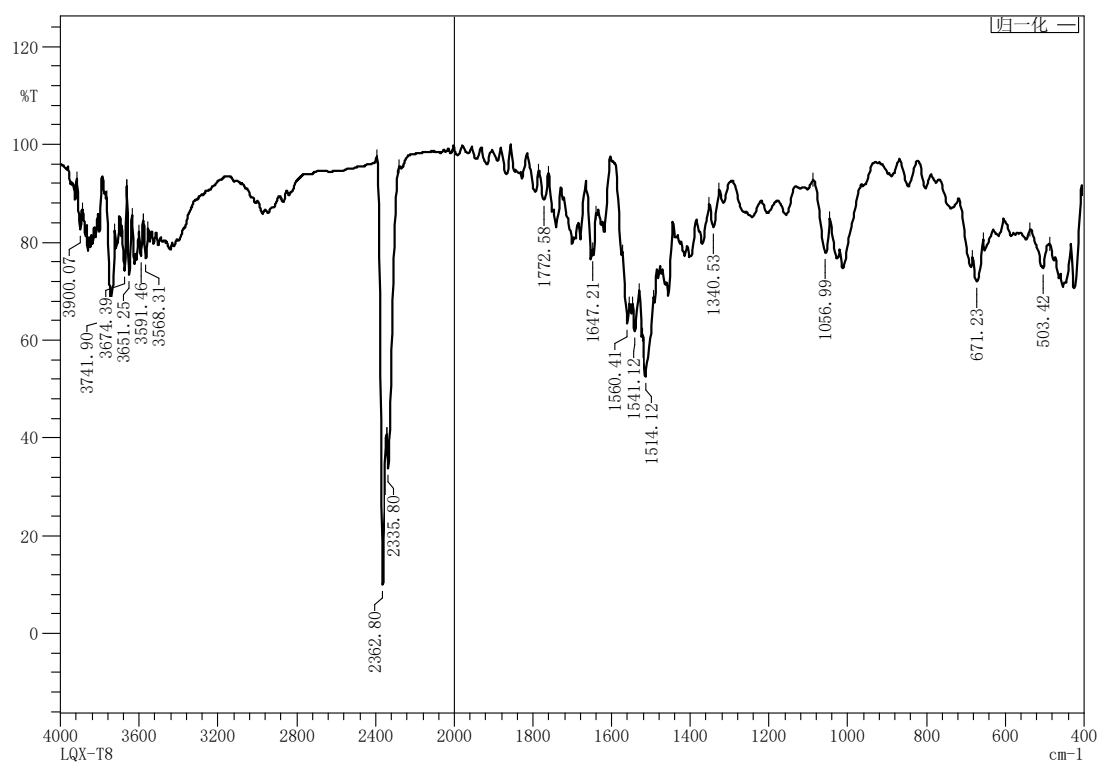
For compound **8h**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



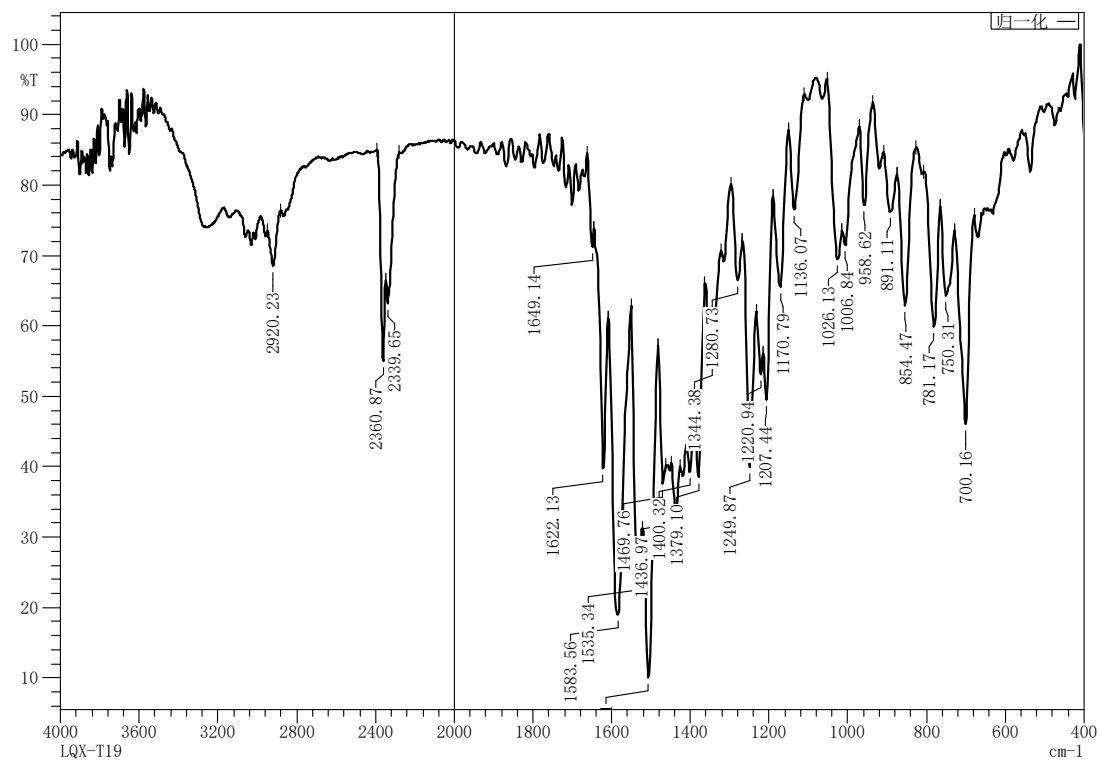
For compound **8i**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



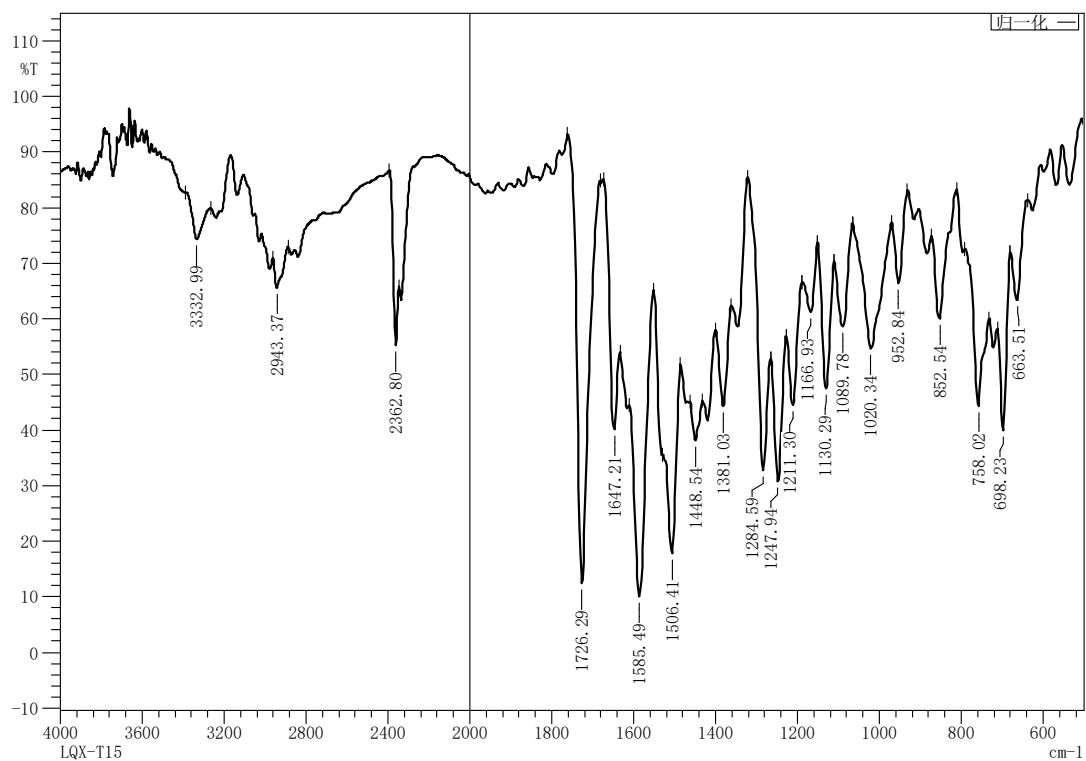
For compound **8j**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



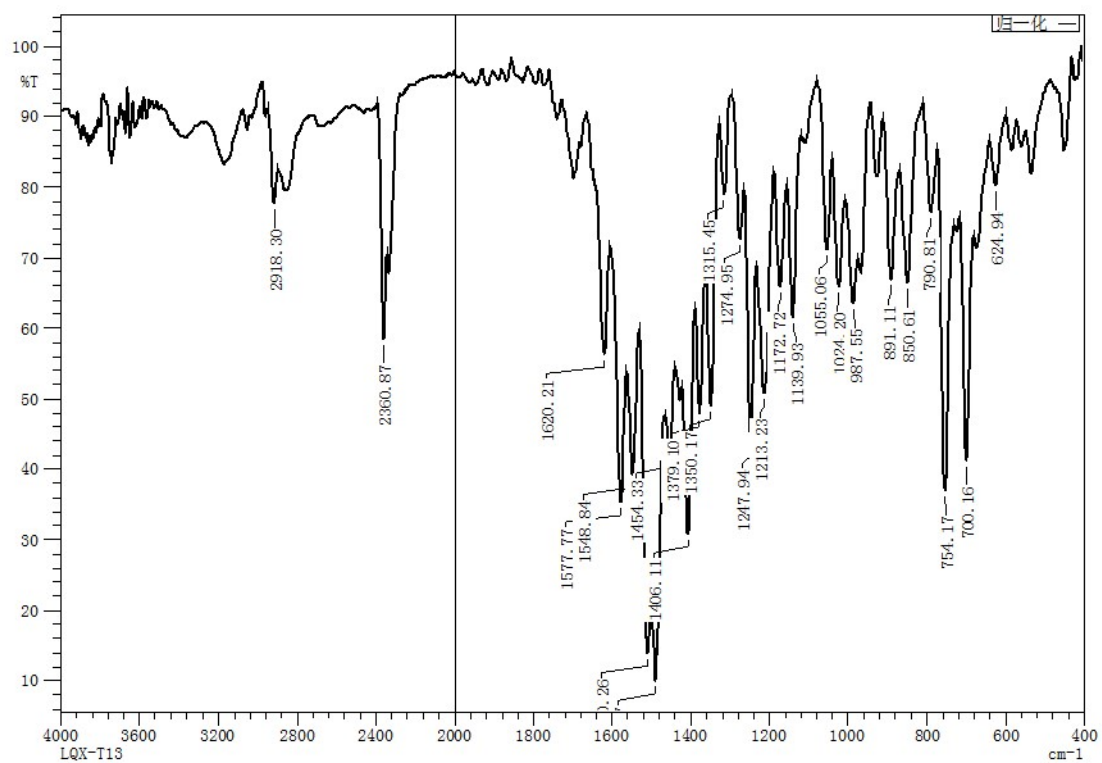
For compound **8k**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



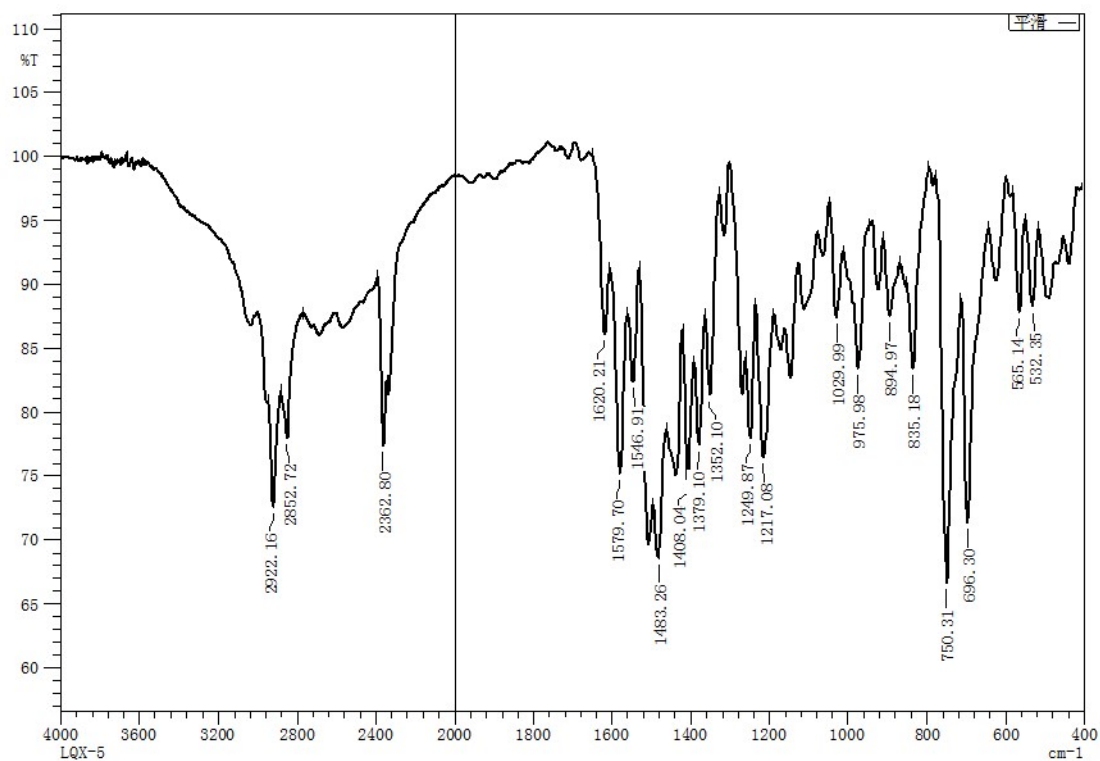
For compound **8l**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



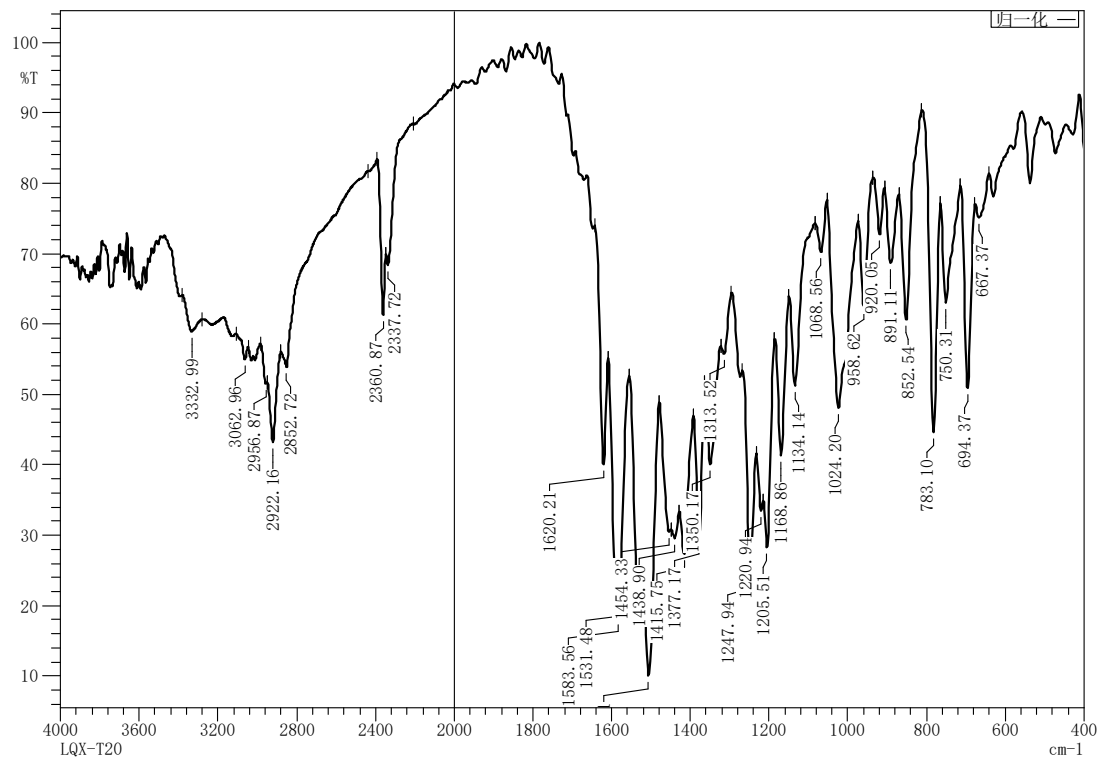
For compound **8m**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



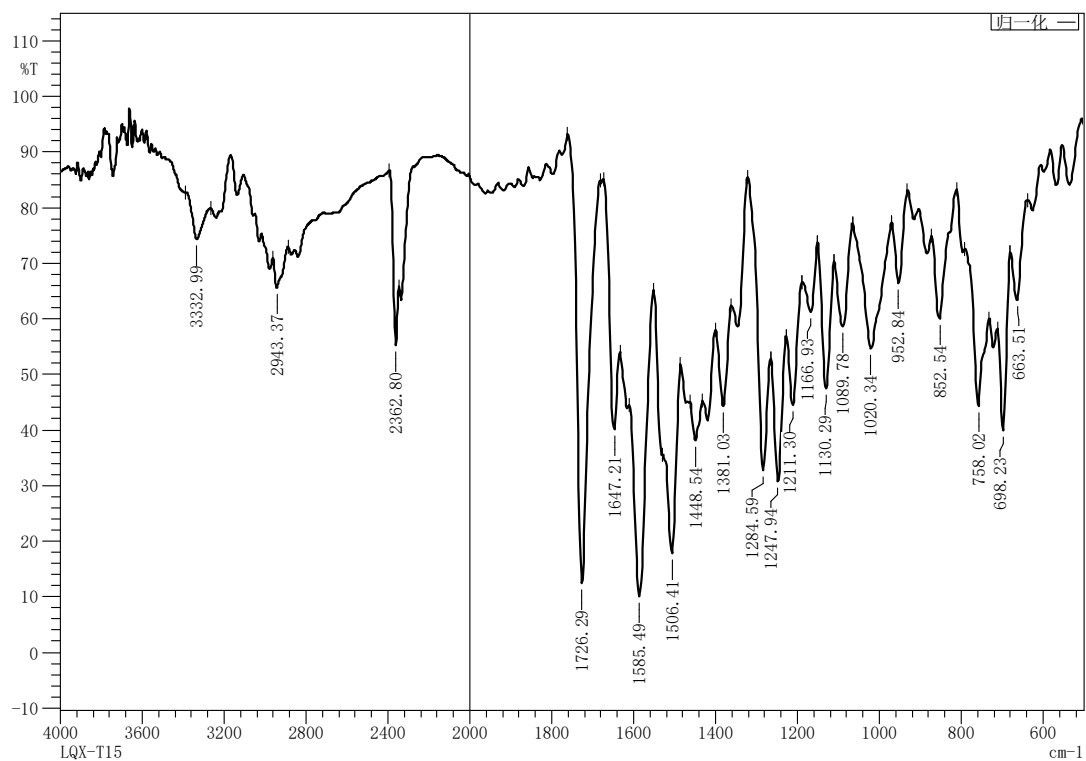
For compound **8n**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



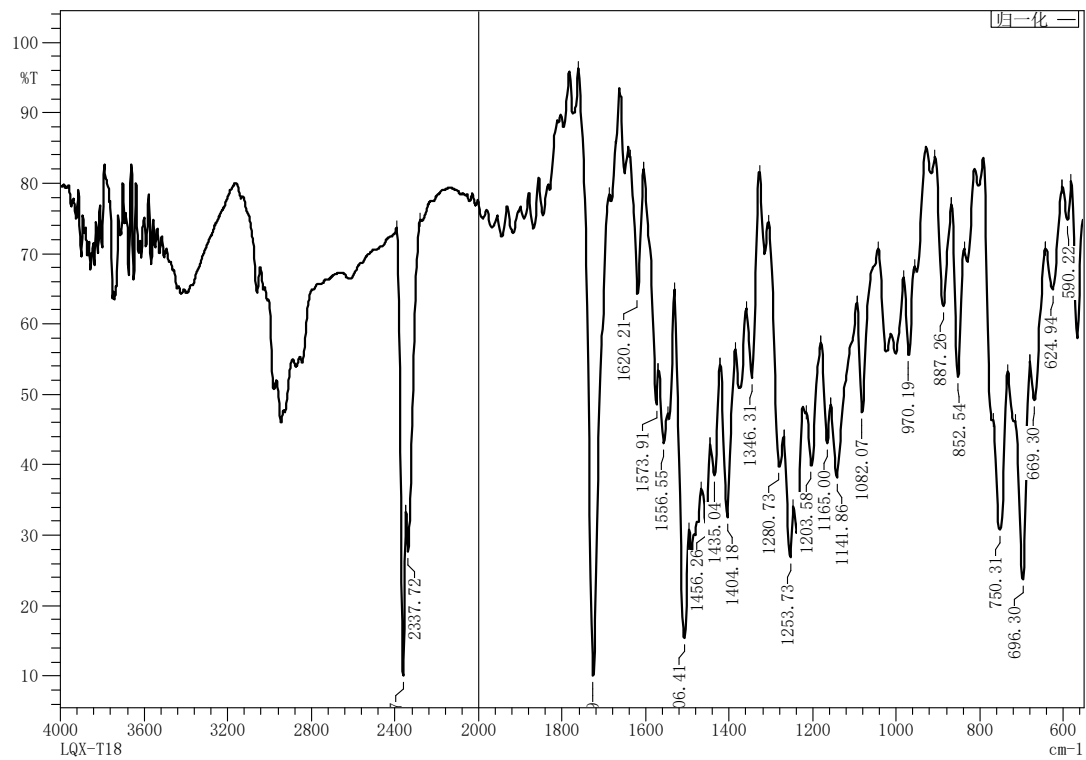
For compound **8o**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:



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

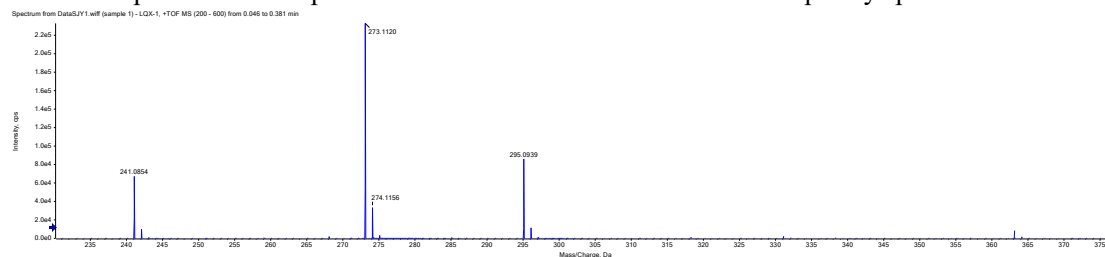


For compound **8q**, IR spectra were recorded on a Thermo Nicolet Nexus 670 FT-IR spectrometer:

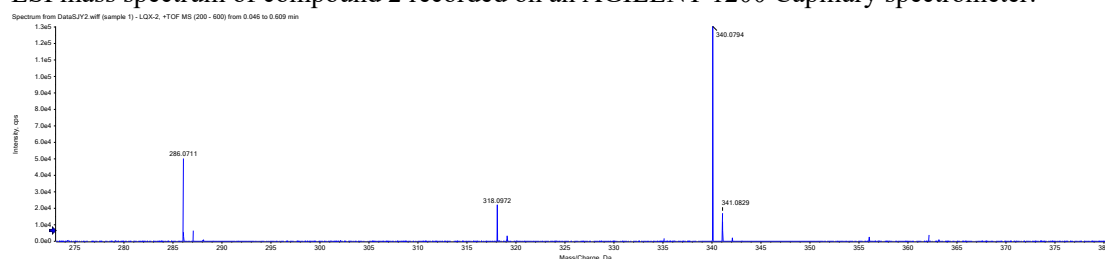


Mass spectra of compounds

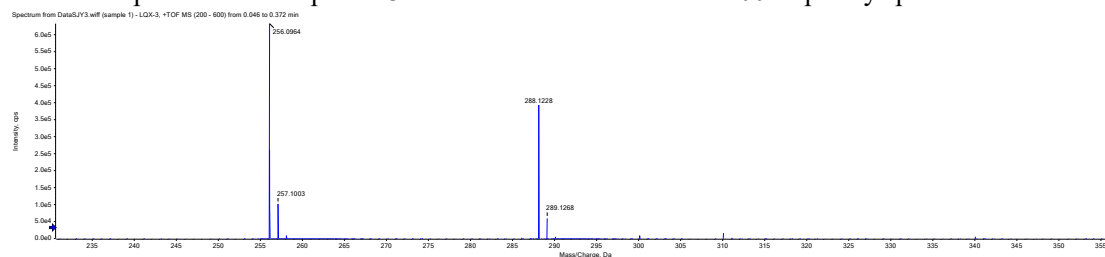
ESI mass spectrum of compound **1** recorded on an AGILENT 1200 Capillary spectrometer:



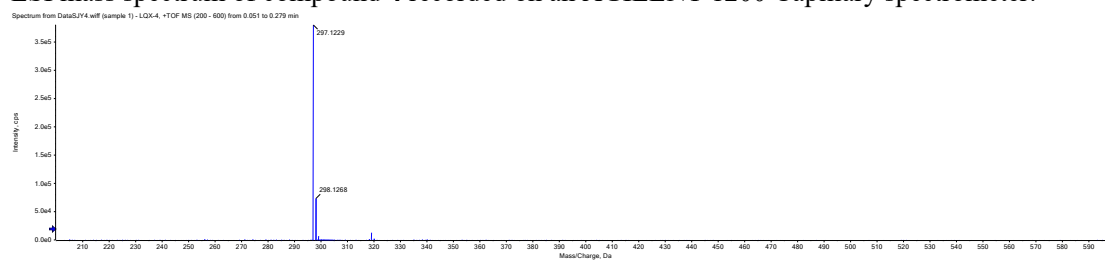
ESI mass spectrum of compound **2** recorded on an AGILENT 1200 Capillary spectrometer:



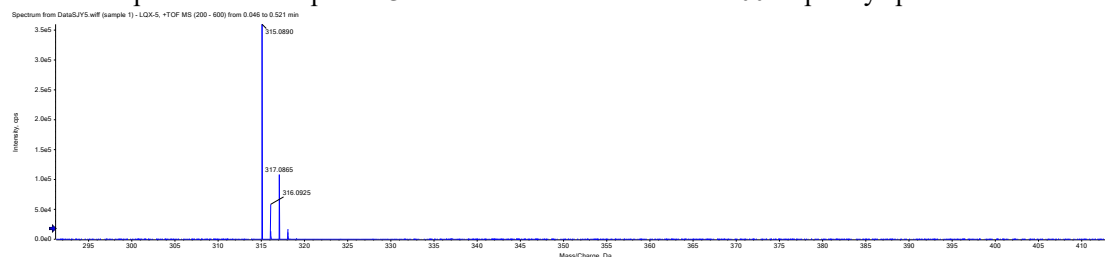
ESI mass spectrum of compound **3** recorded on an AGILENT 1200 Capillary spectrometer:



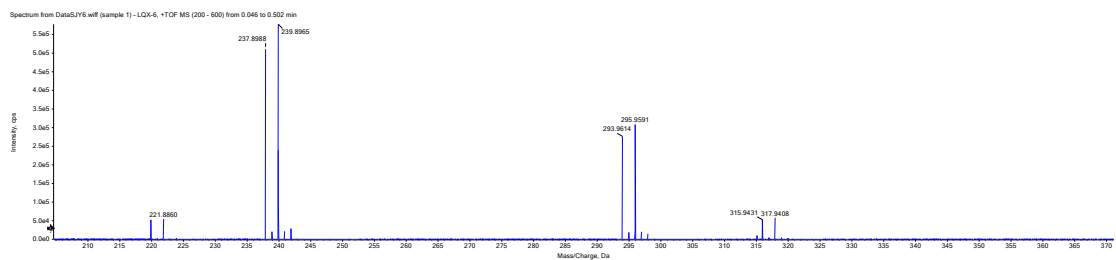
ESI mass spectrum of compound **4** recorded on an AGILENT 1200 Capillary spectrometer:



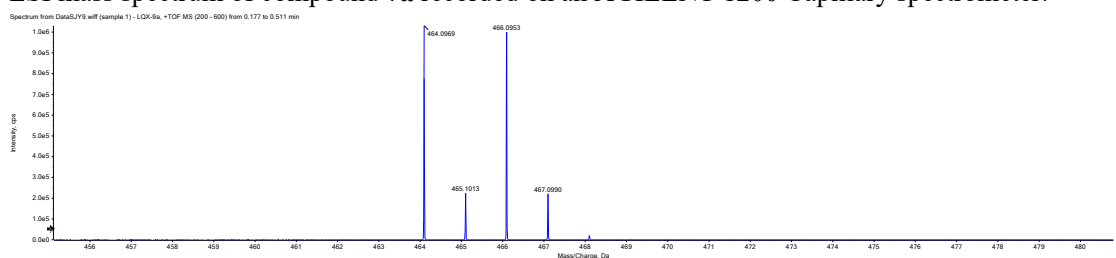
ESI mass spectrum of compound **5** recorded on an AGILENT 1200 Capillary spectrometer:



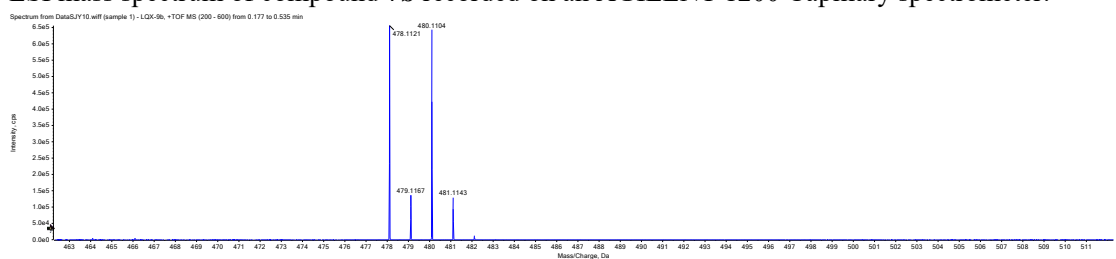
ESI mass spectrum of compound **6** recorded on an AGILENT 1200 Capillary spectrometer:



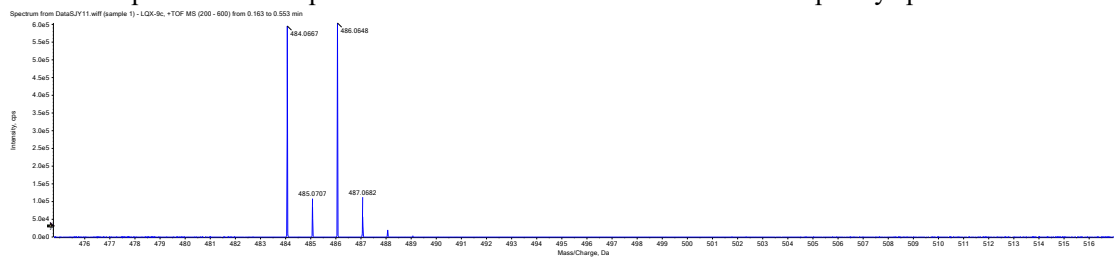
ESI mass spectrum of compound **7a** recorded on an AGILENT 1200 Capillary spectrometer:



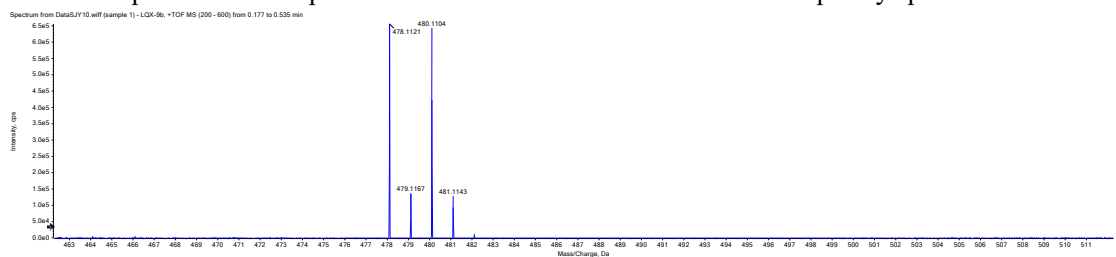
ESI mass spectrum of compound **7b** recorded on an AGILENT 1200 Capillary spectrometer:



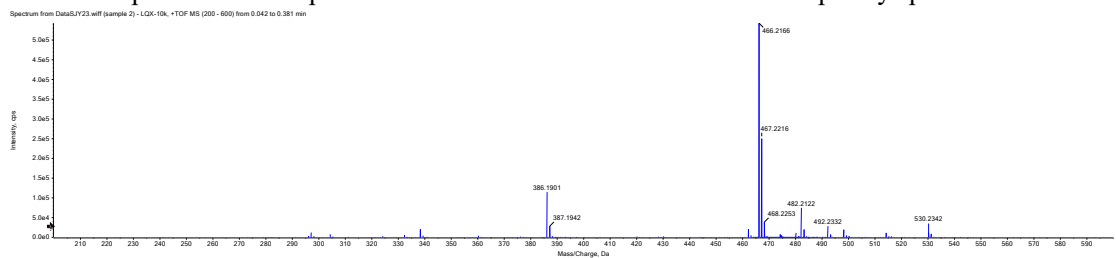
ESI mass spectrum of compound **7c** recorded on an AGILENT 1200 Capillary spectrometer:



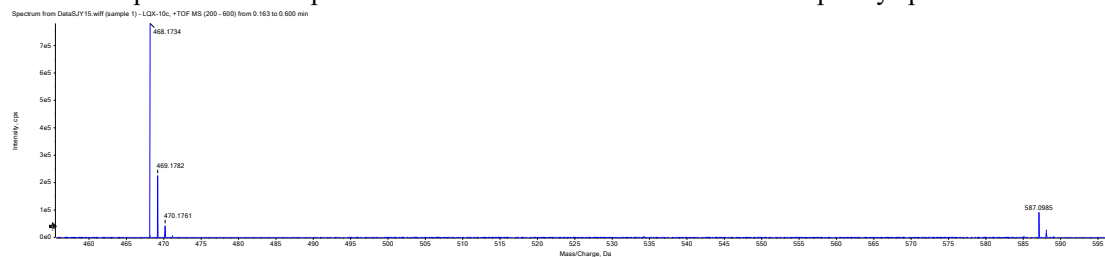
ESI mass spectrum of compound **8a** recorded on an AGILENT 1200 Capillary spectrometer:



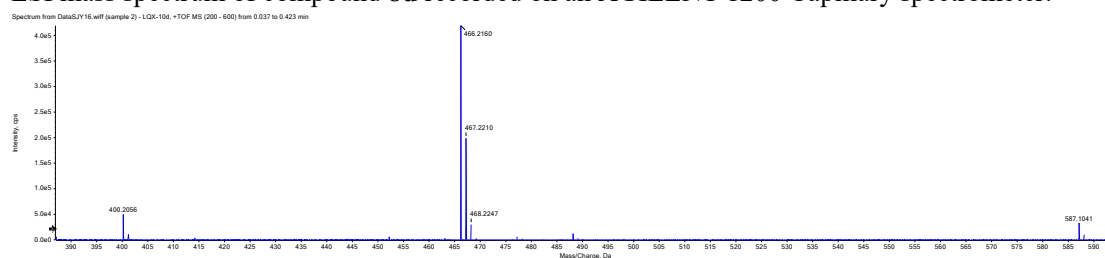
ESI mass spectrum of compound **8b** recorded on an AGILENT 1200 Capillary spectrometer:



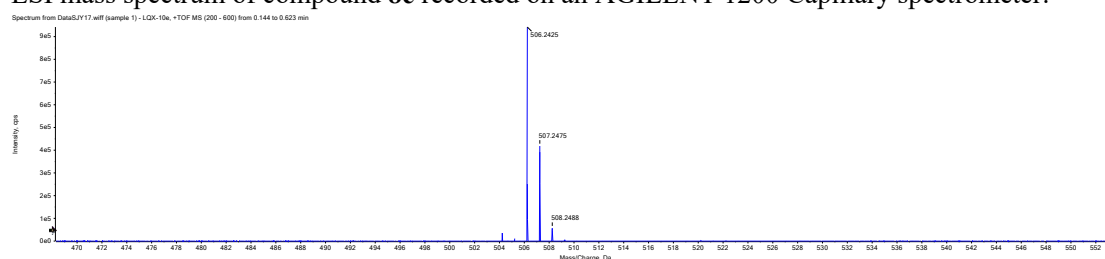
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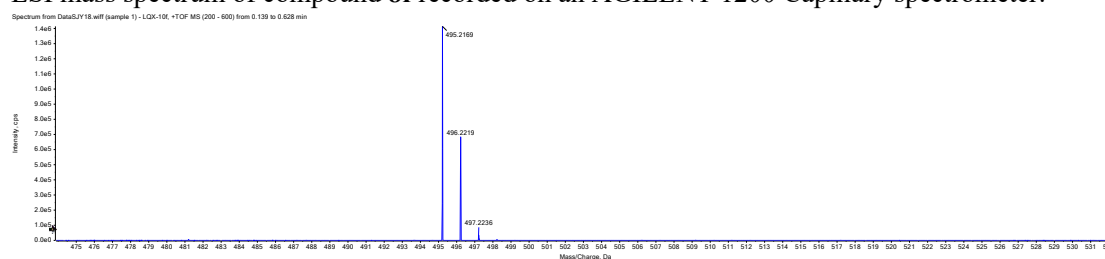
ESI mass spectrum of compound **8d** recorded on an AGILENT 1200 Capillary spectrometer:



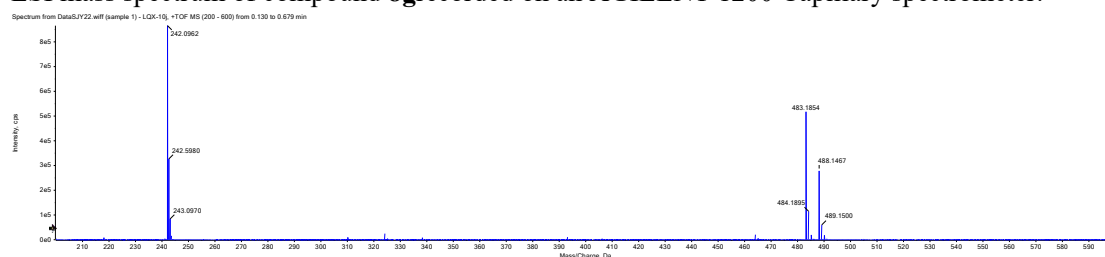
ESI mass spectrum of compound **8e** recorded on an AGILENT 1200 Capillary spectrometer:



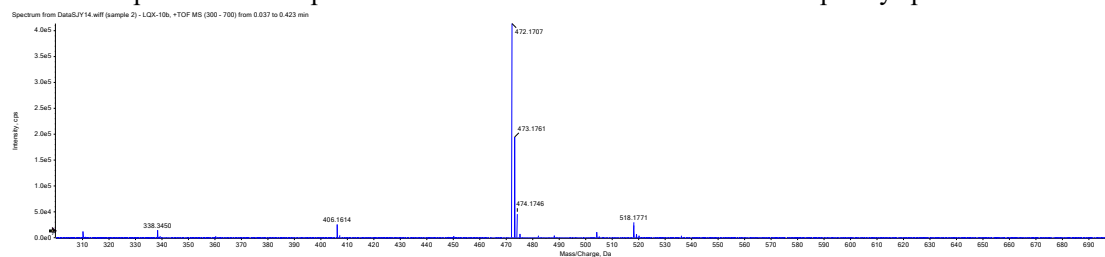
ESI mass spectrum of compound **8f** recorded on an AGILENT 1200 Capillary spectrometer:



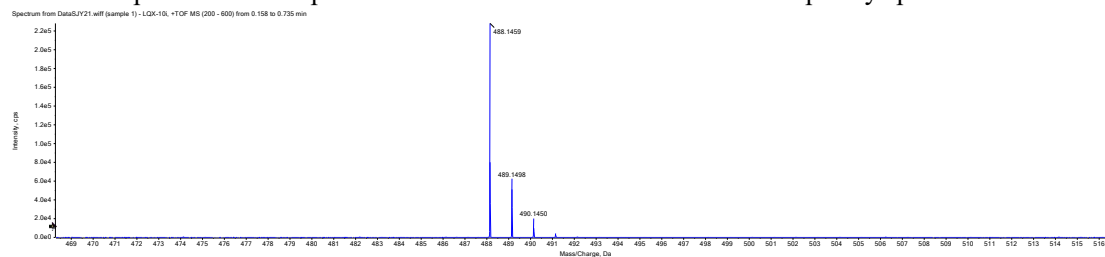
ESI mass spectrum of compound **8g** recorded on an AGILENT 1200 Capillary spectrometer:



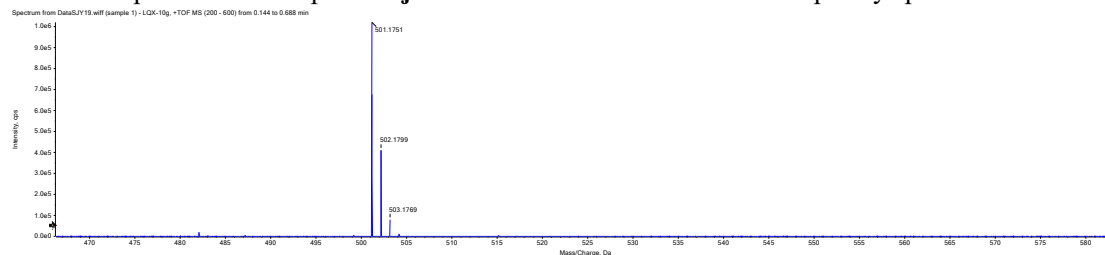
ESI mass spectrum of compound **8h** recorded on an AGILENT 1200 Capillary spectrometer:



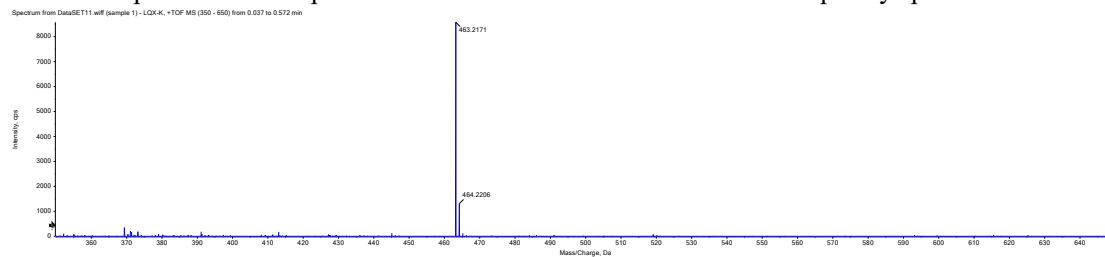
ESI mass spectrum of compound **8i** recorded on an AGILENT 1200 Capillary spectrometer:



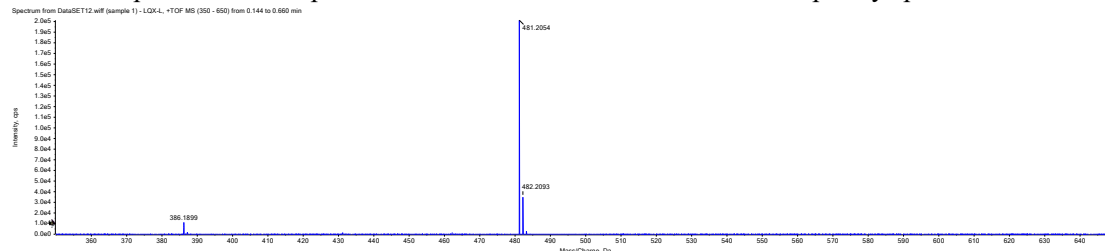
ESI mass spectrum of compound **8j** recorded on an AGILENT 1200 Capillary spectrometer:



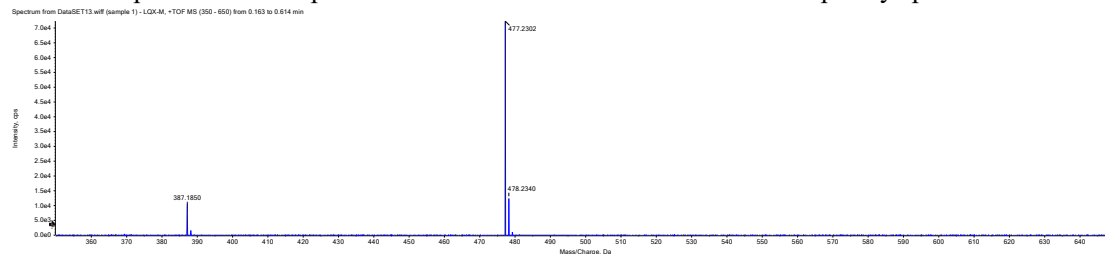
ESI mass spectrum of compound **8k** recorded on an AGILENT 1200 Capillary spectrometer:



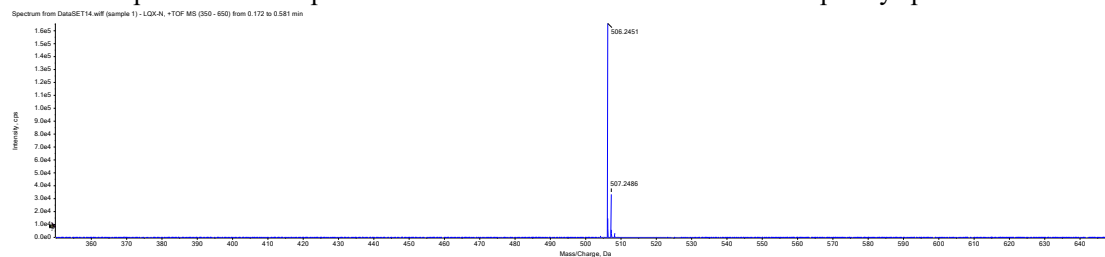
ESI mass spectrum of compound **8l** recorded on an AGILENT 1200 Capillary spectrometer:



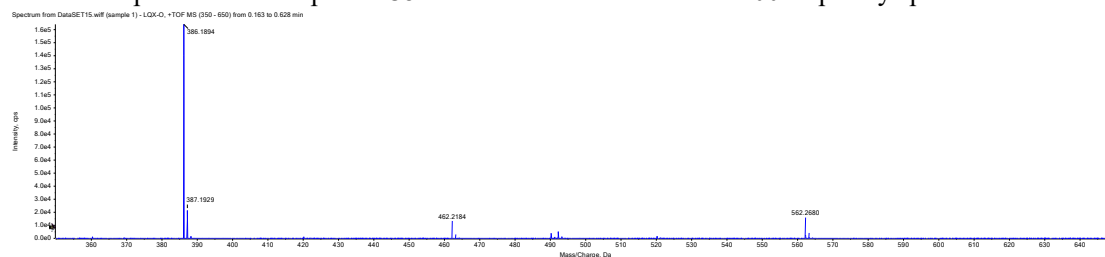
ESI mass spectrum of compound **8m** recorded on an AGILENT 1200 Capillary spectrometer:



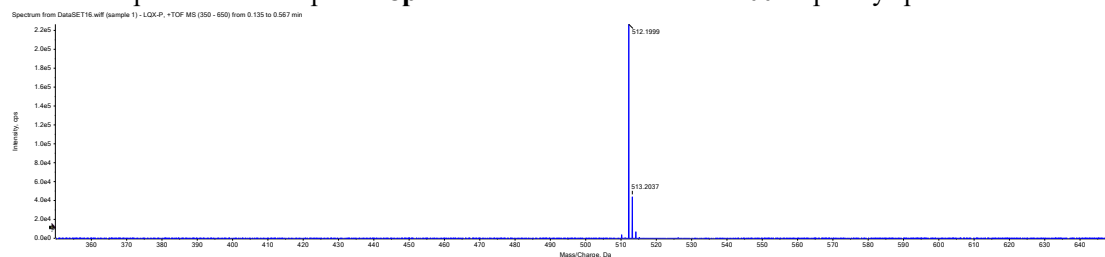
ESI mass spectrum of compound **8n** recorded on an AGILENT 1200 Capillary spectrometer:



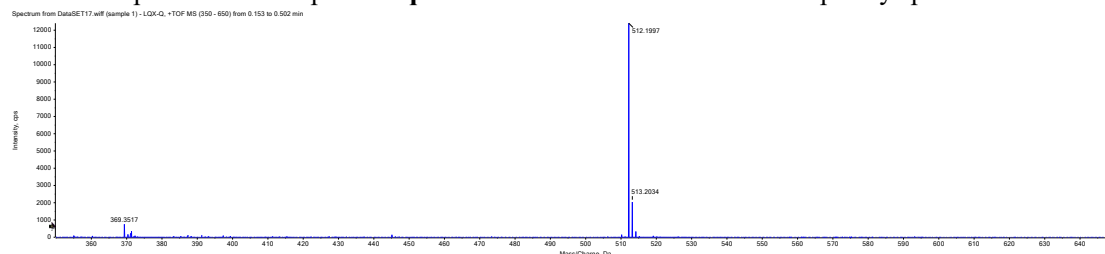
ESI mass spectrum of compound **8o** recorded on an AGILENT 1200 Capillary spectrometer:



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

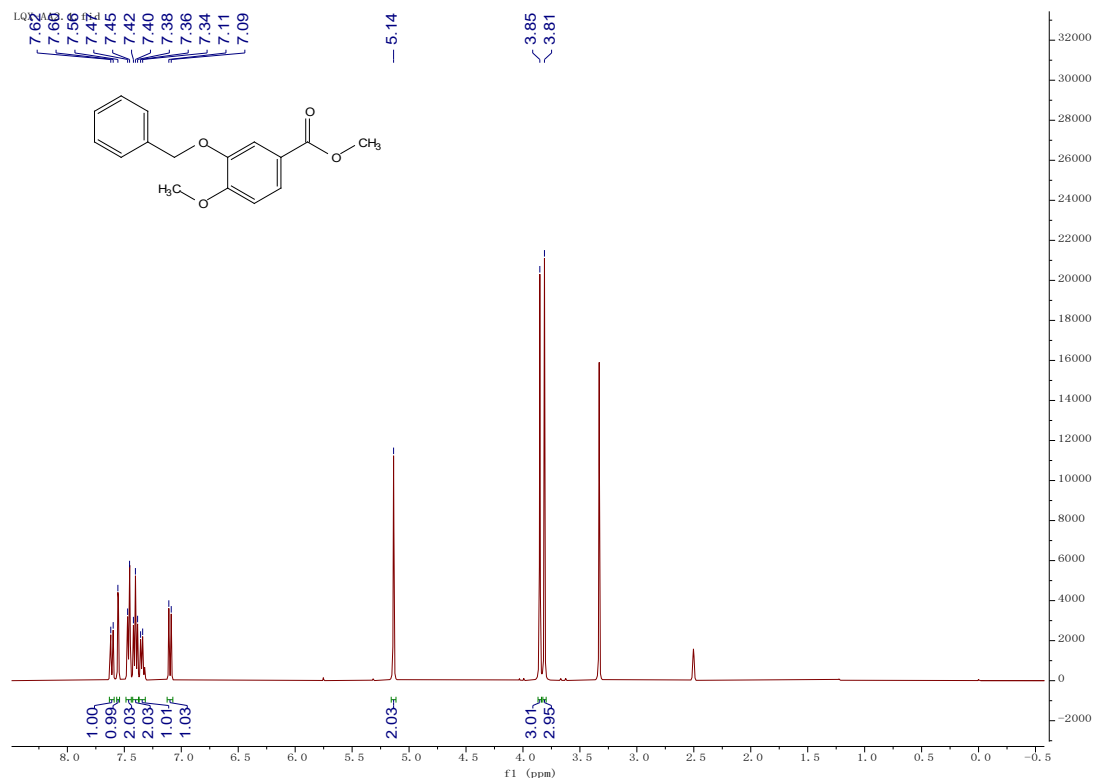


ESI mass spectrum of compound **8q** recorded on an AGILENT 1200 Capillary spectrometer:

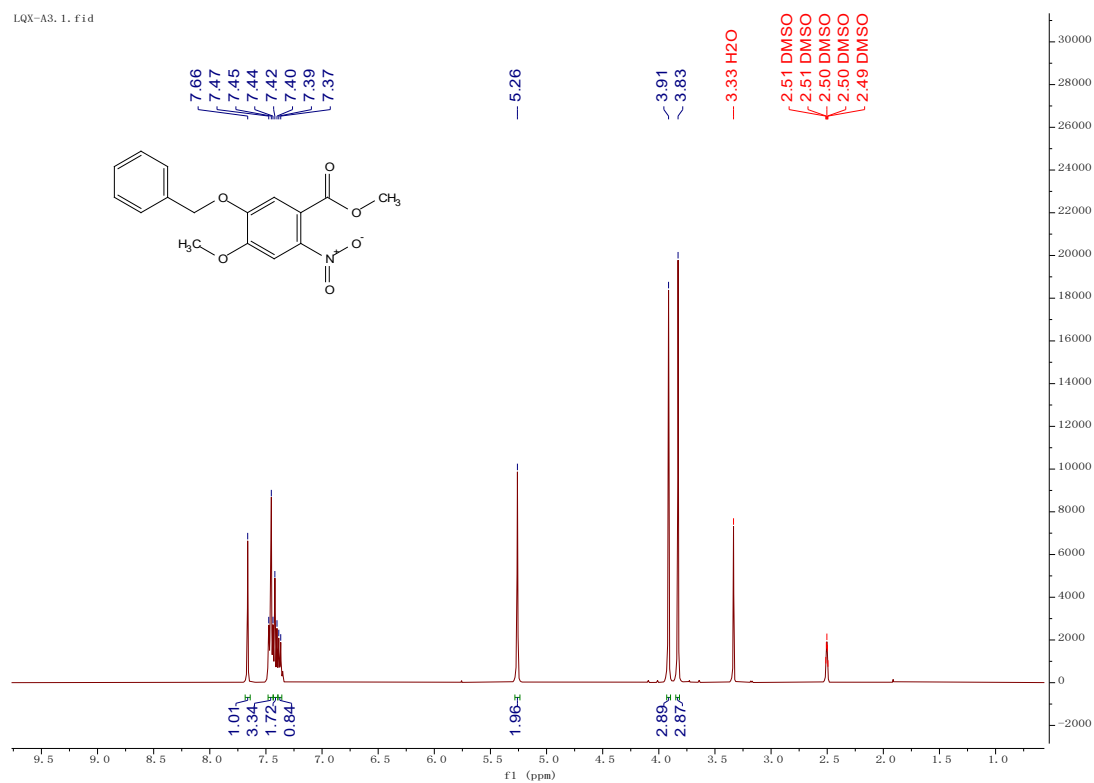


¹H NMR (600MHz) of compounds

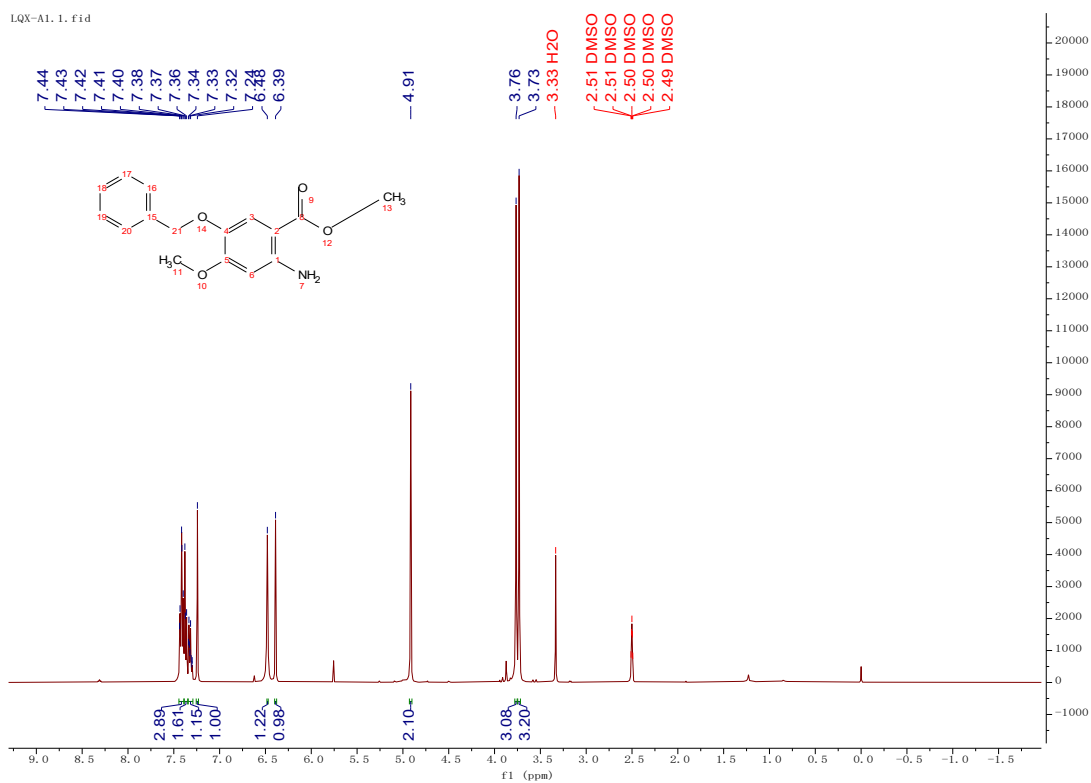
¹H NMR of compound 1



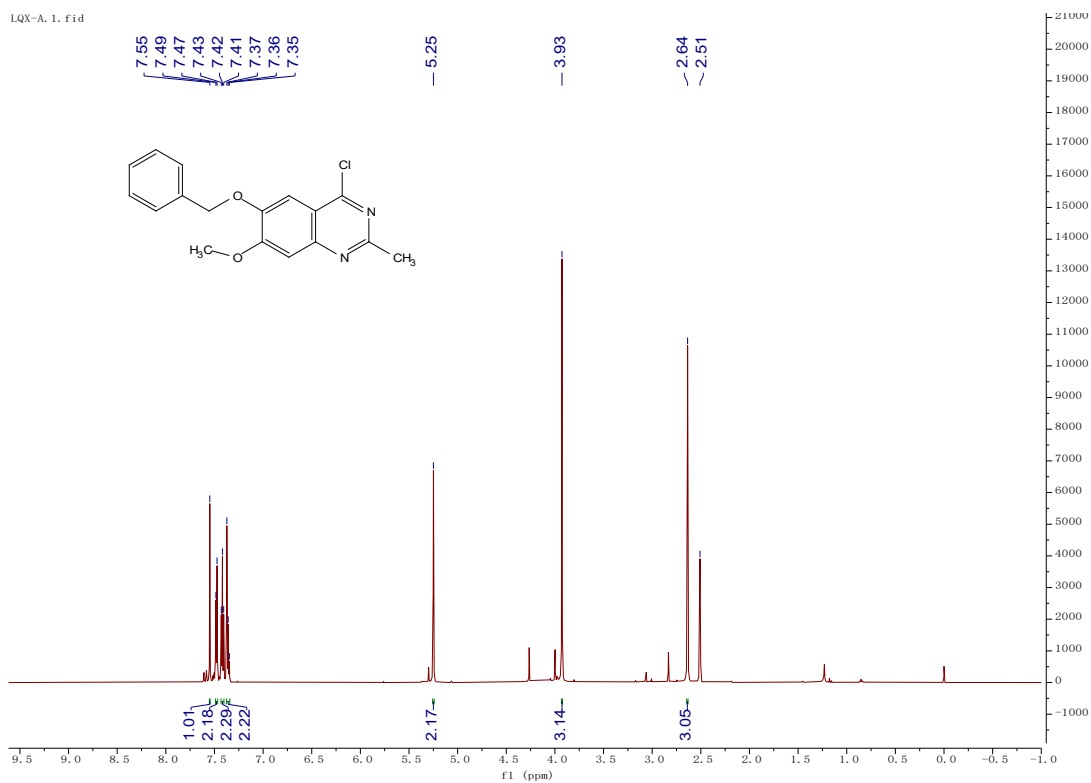
¹H NMR of compound 2



¹H NMR of compound 3

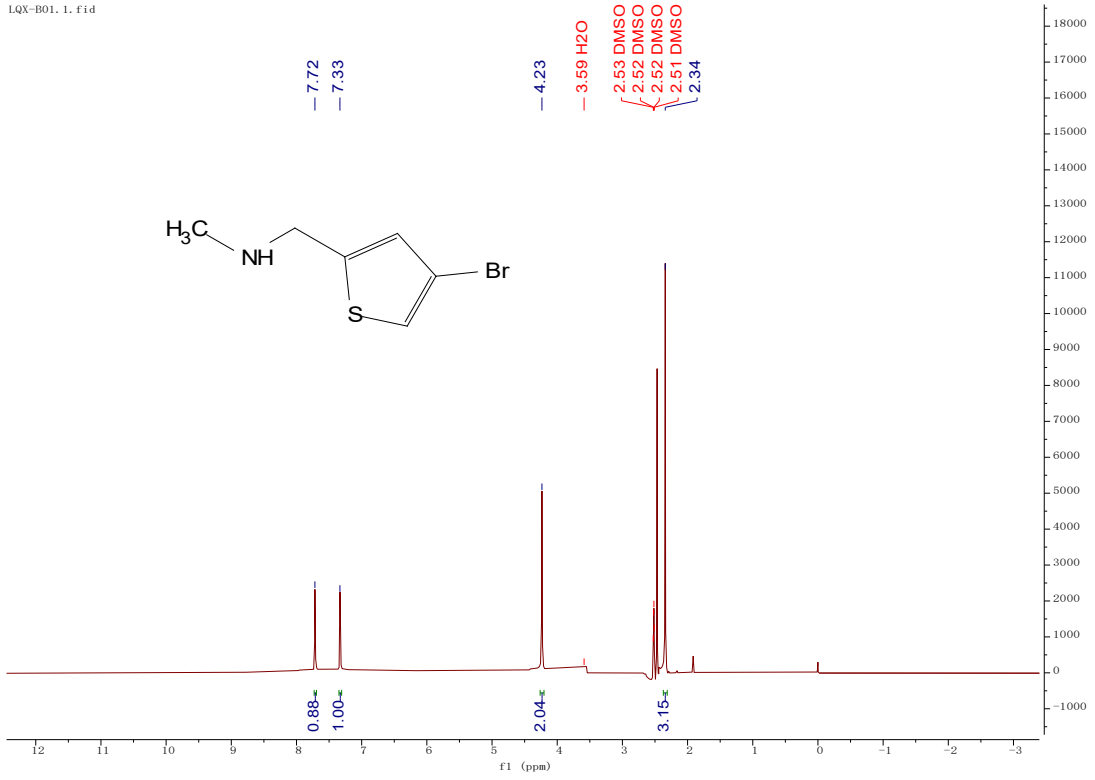


¹H NMR of compound 5



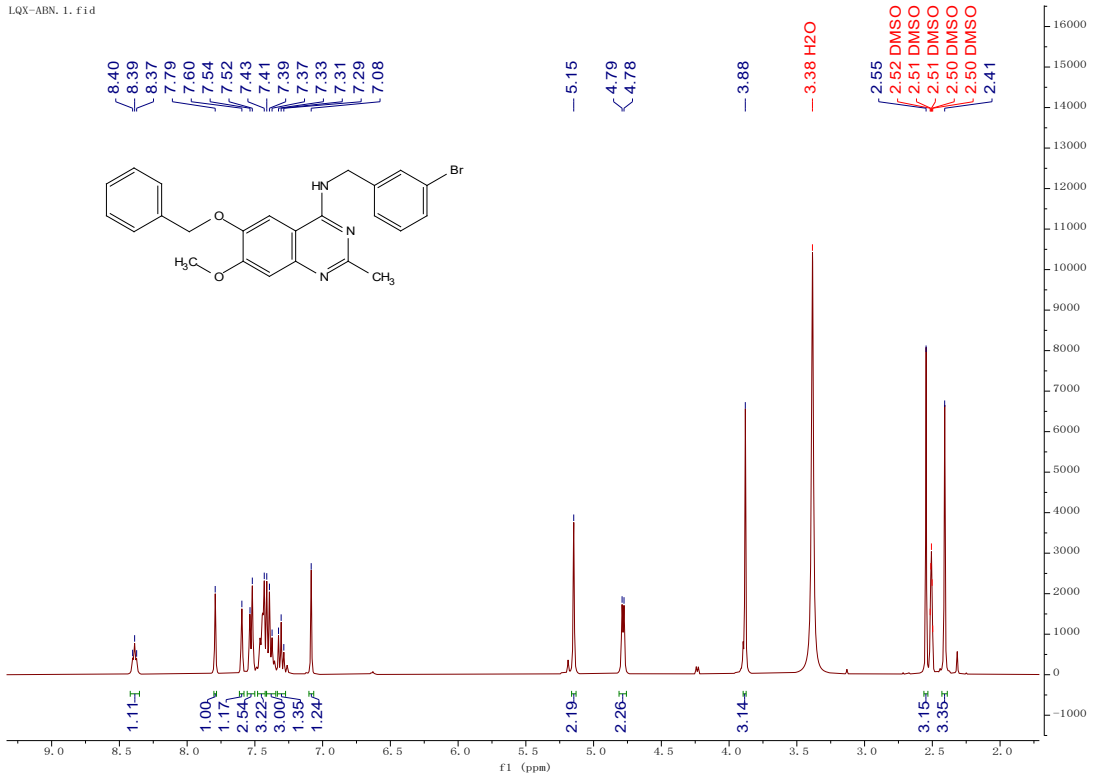
¹H NMR of compound 6

LQX-B01. 1. fid

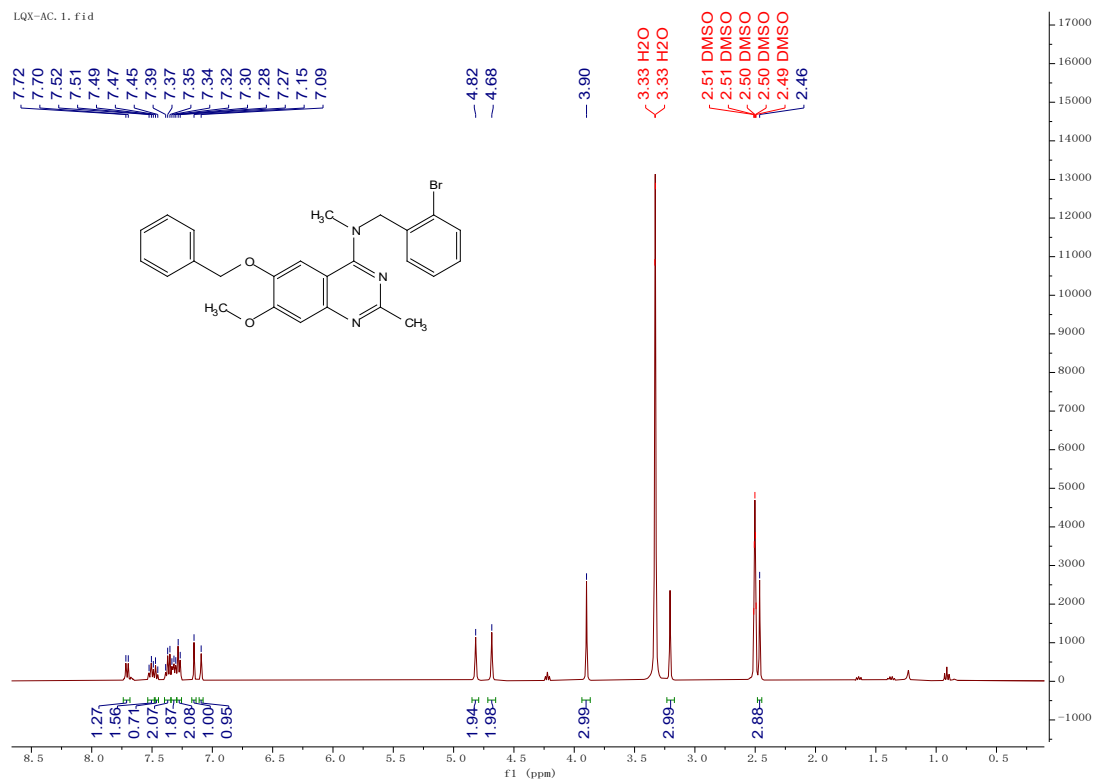


¹H NMR of compound 7a

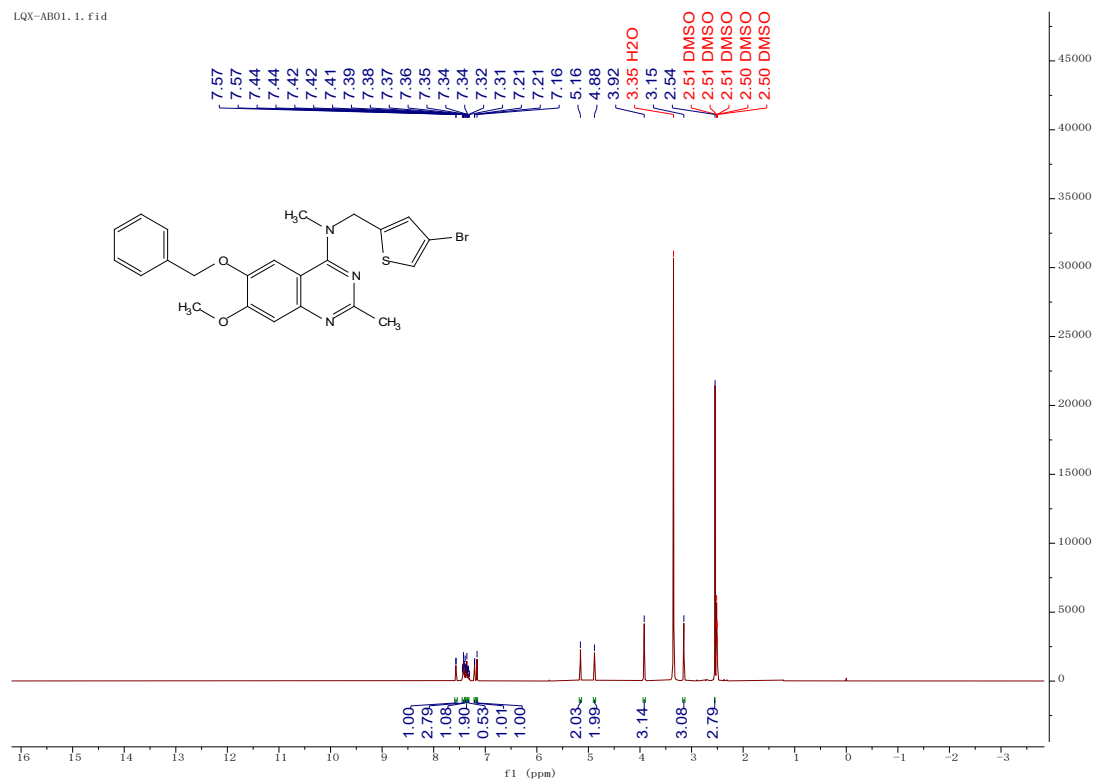
LQX-ABN. 1. fid



¹H NMR of compound 7b

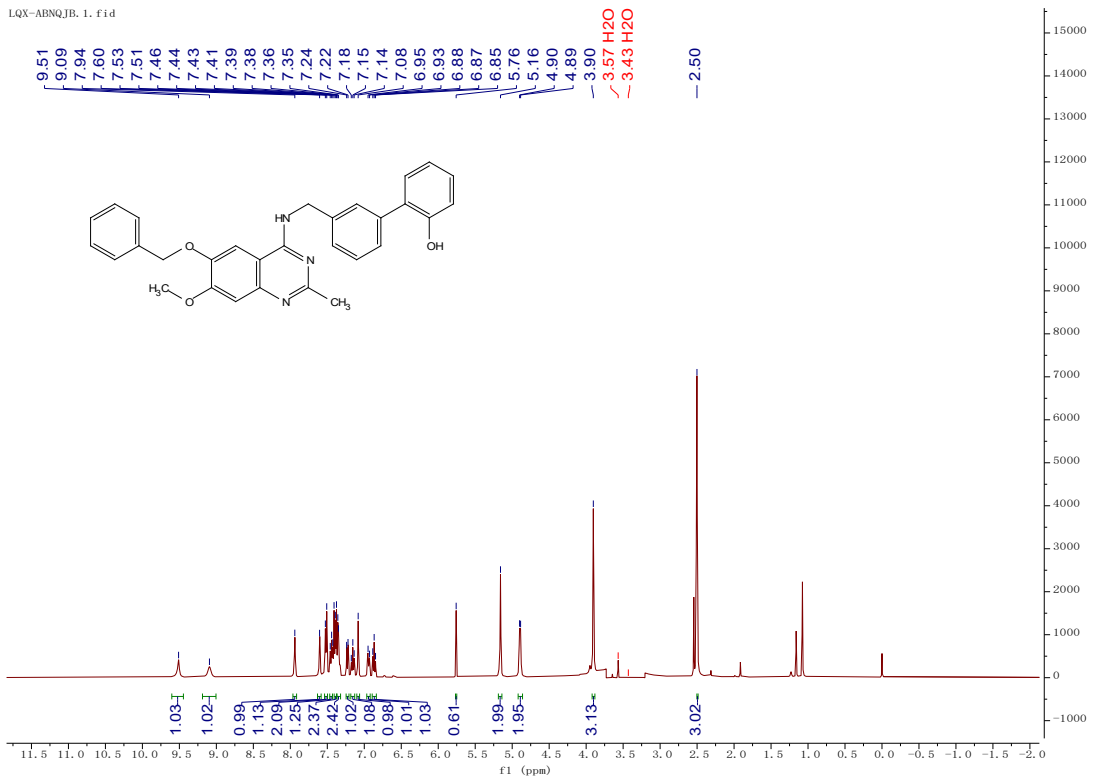


¹H NMR of compound 7c



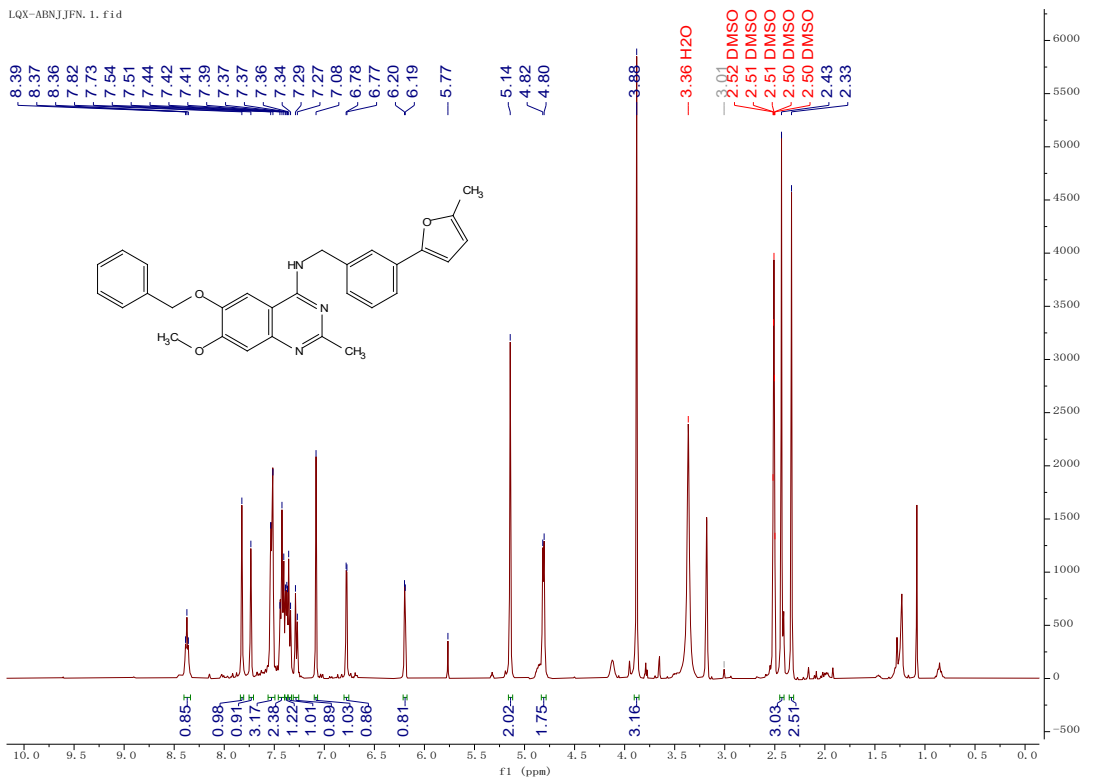
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LQX-ABNQB. 1. F1d

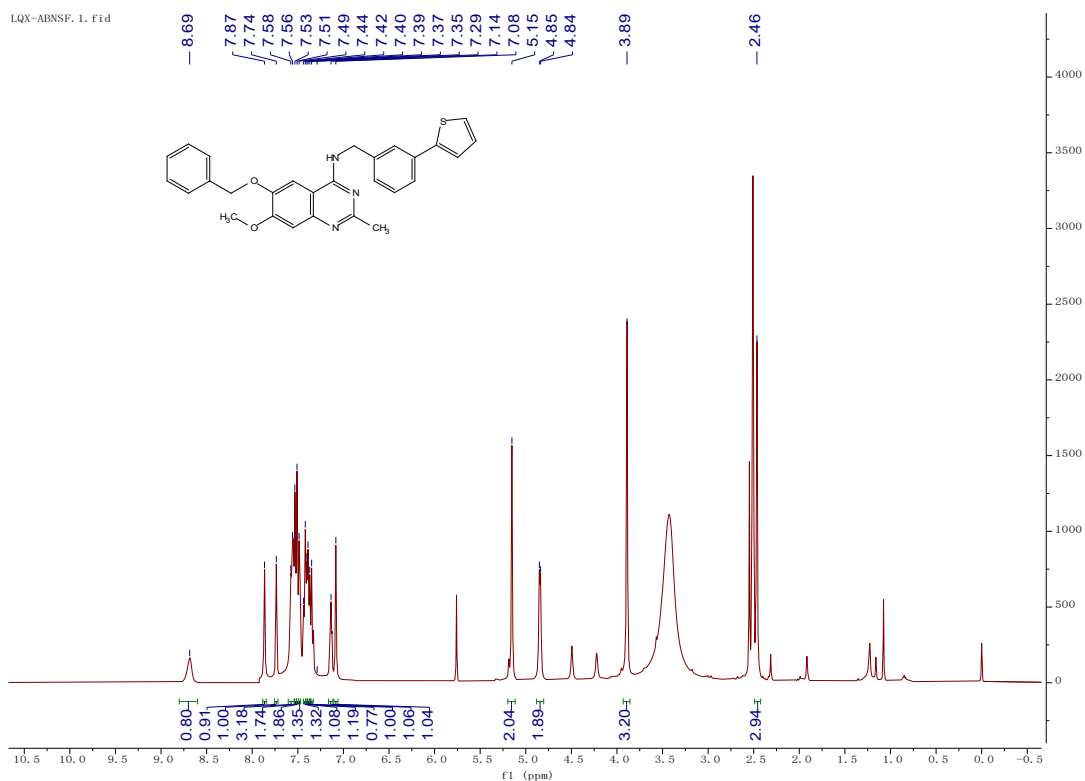


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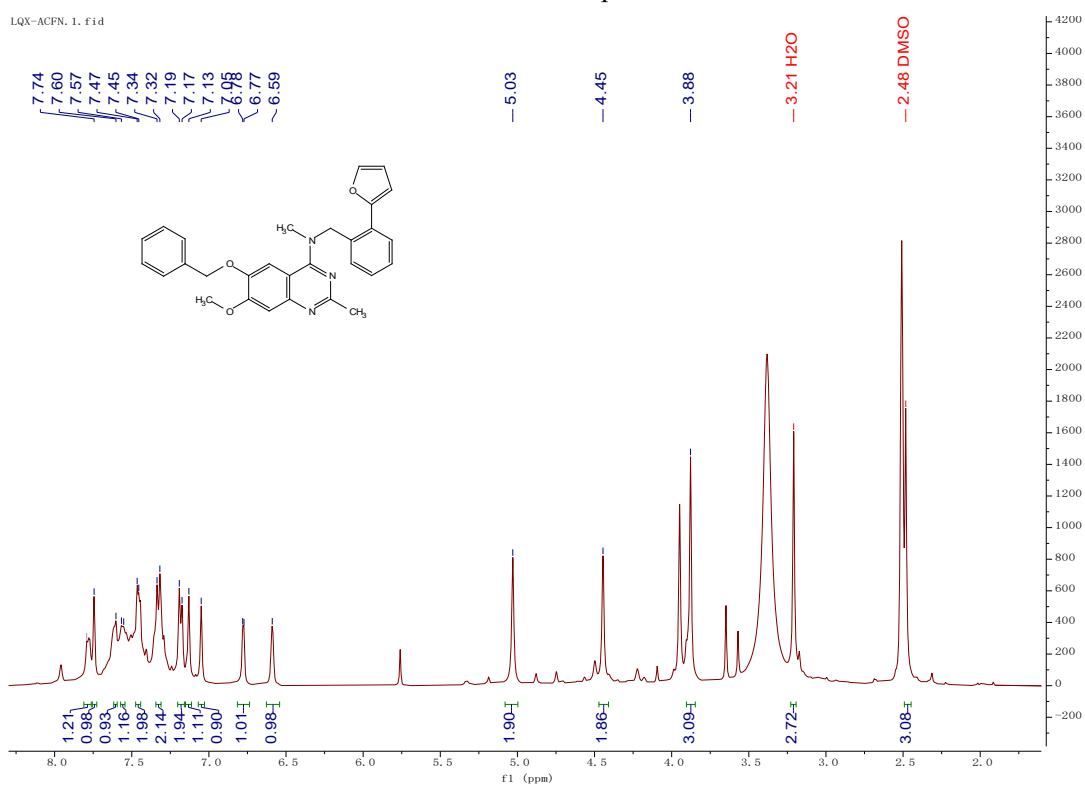
LQX-ABNJFN. 1. F1d



¹H NMR of compound **8c**

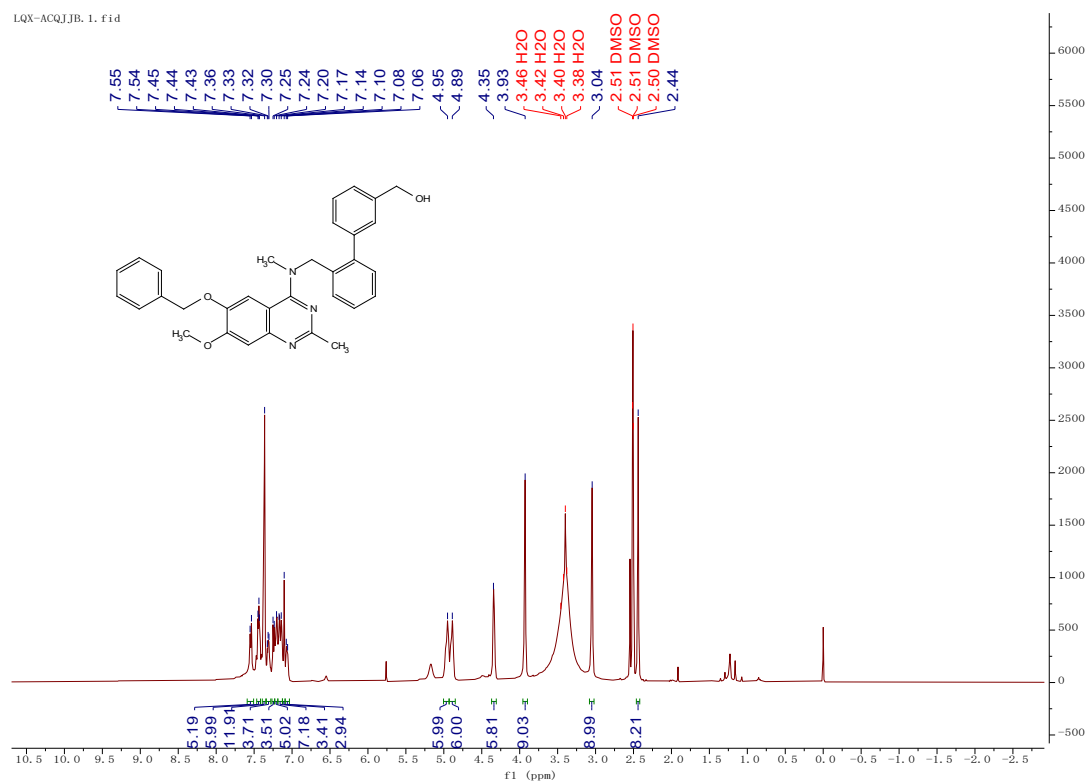


¹H NMR of compound **8d**



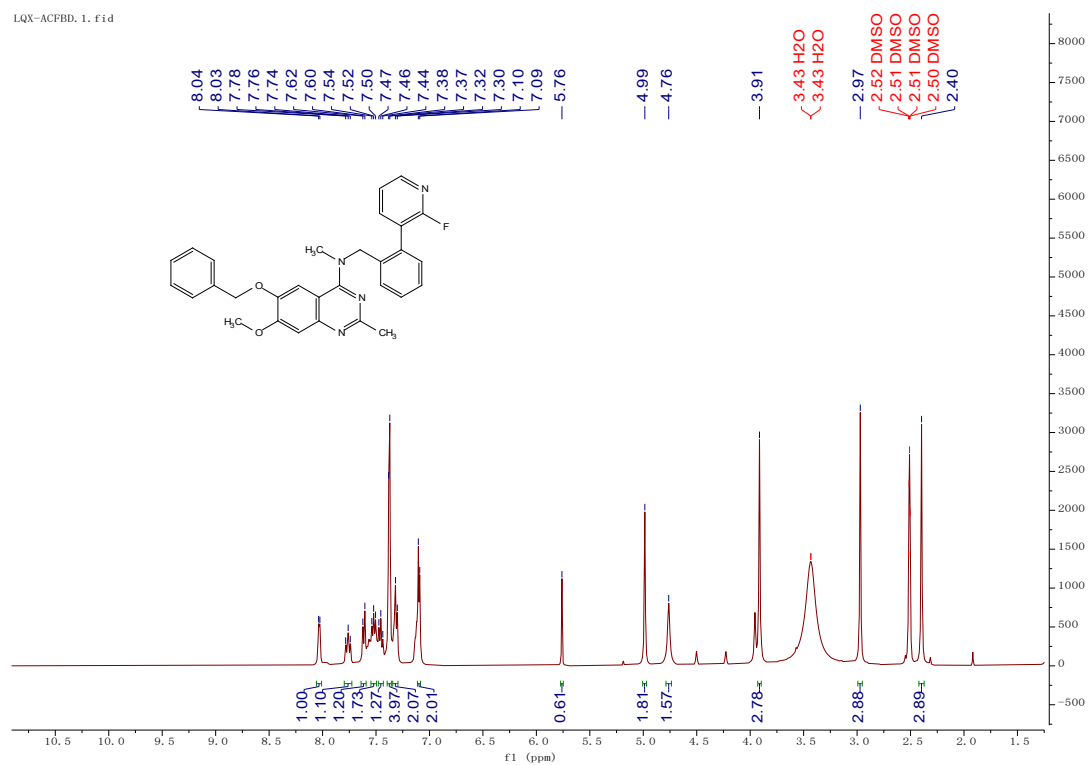
¹H NMR of compound **8e**

LQX-ACQJJB. 1. F1d

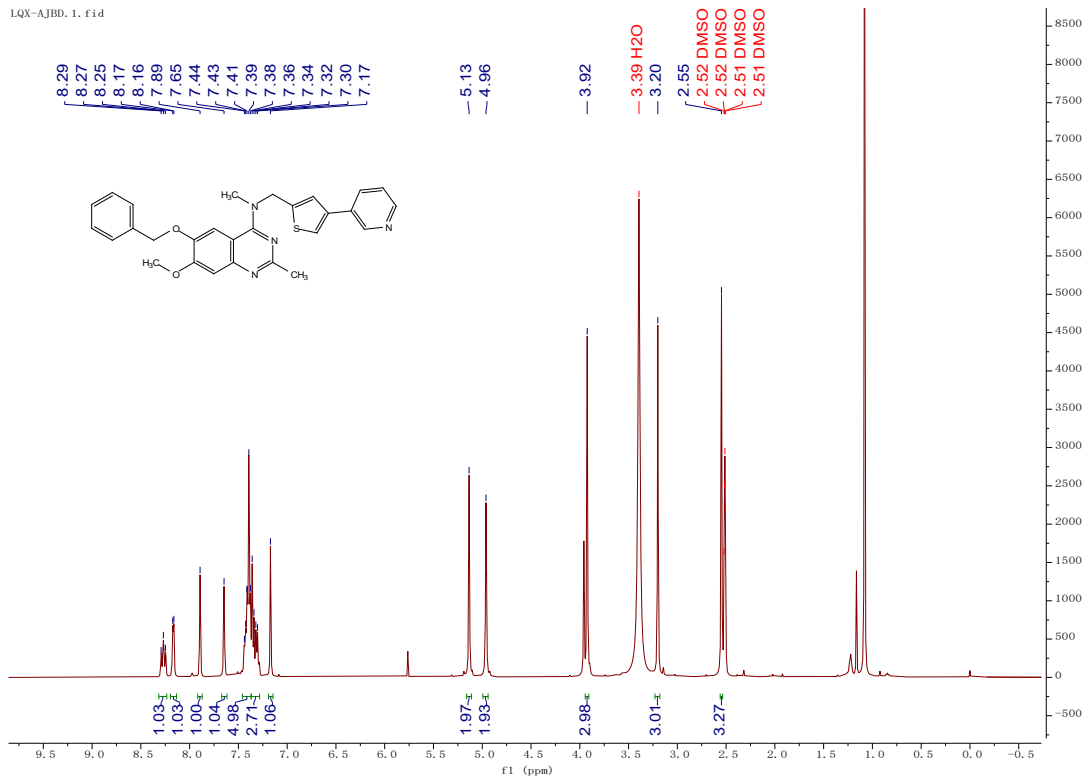


¹H NMR of compound **8f**

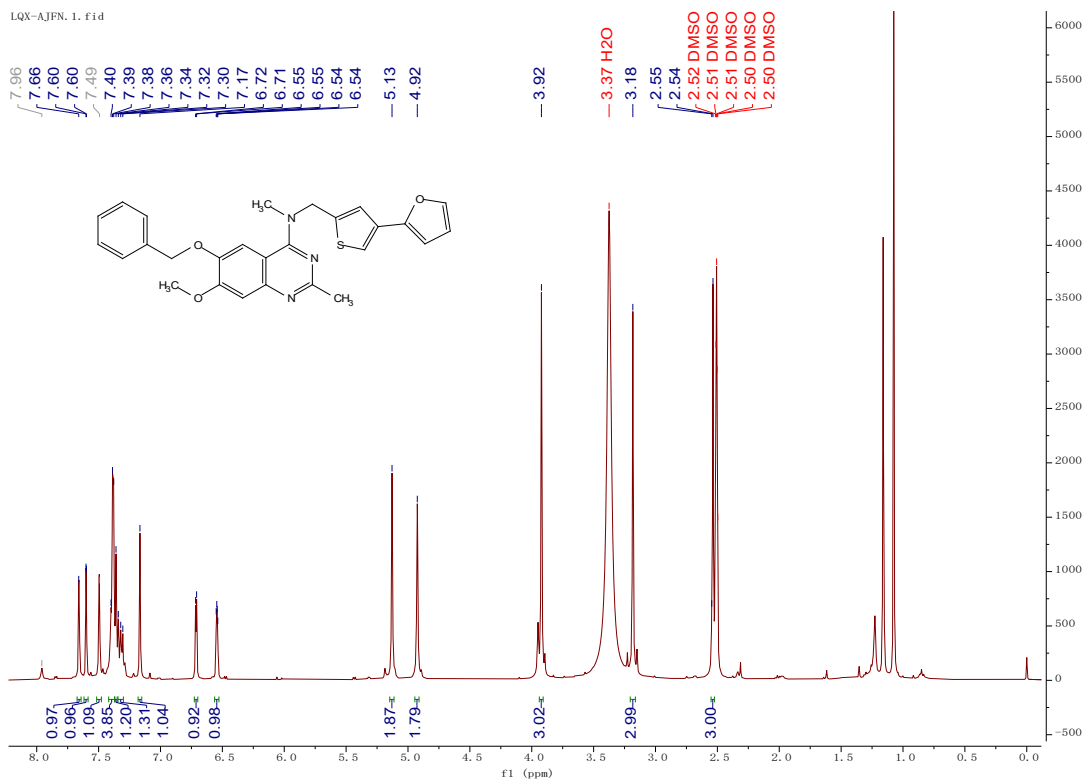
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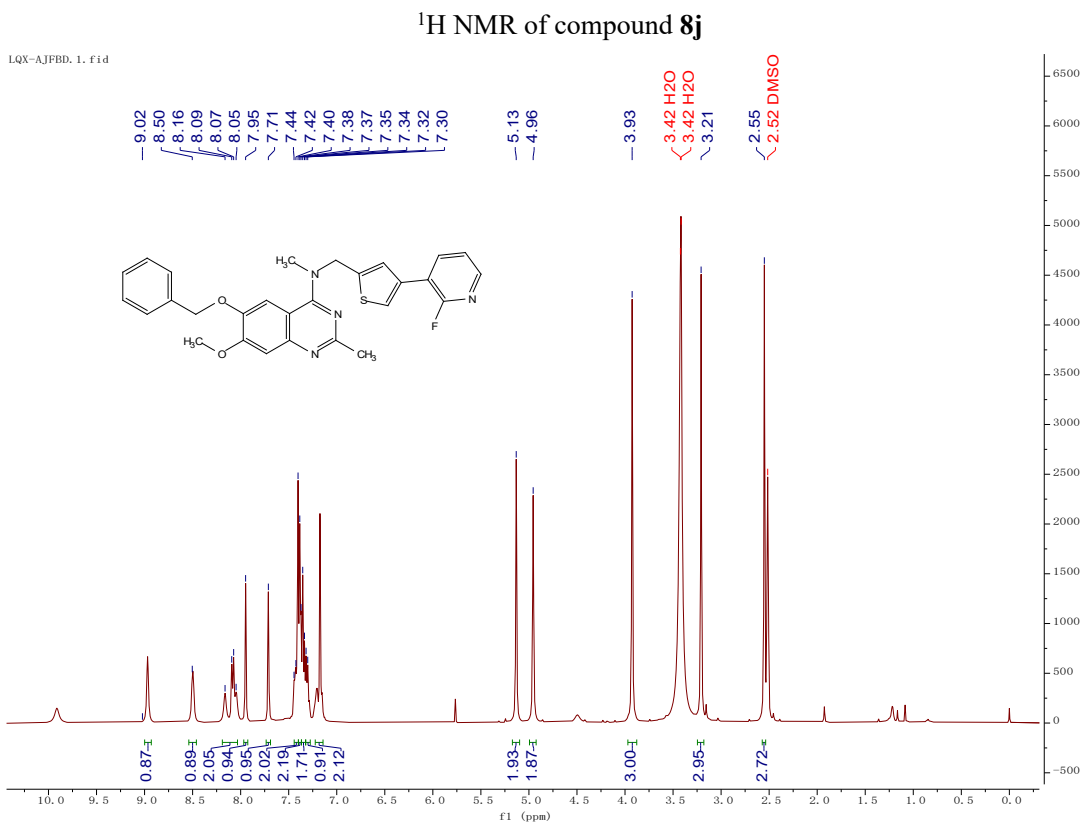
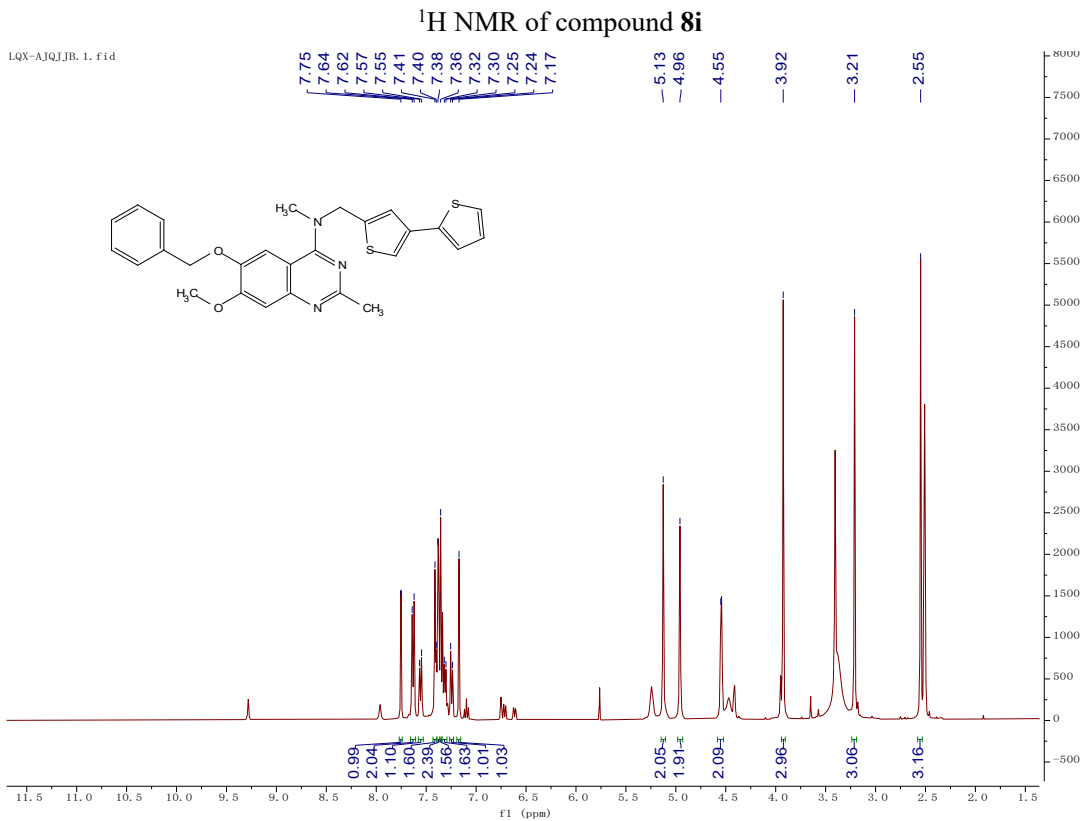


¹H NMR of compound 8g

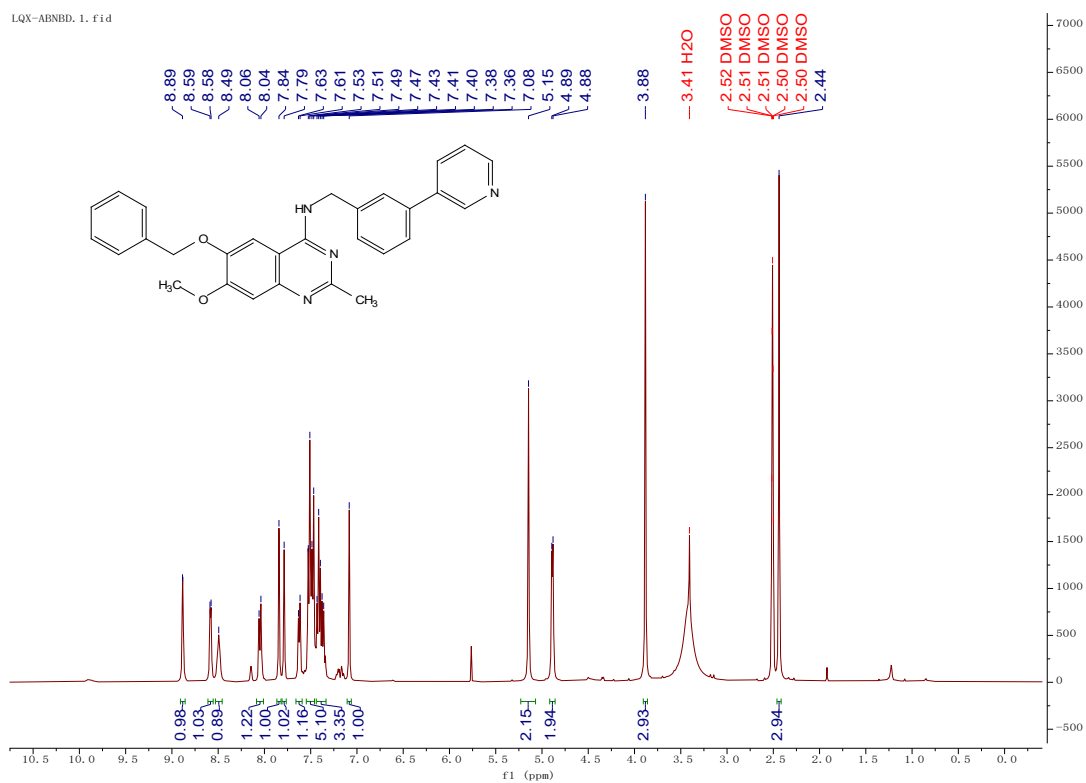


¹H NMR of compound 8h

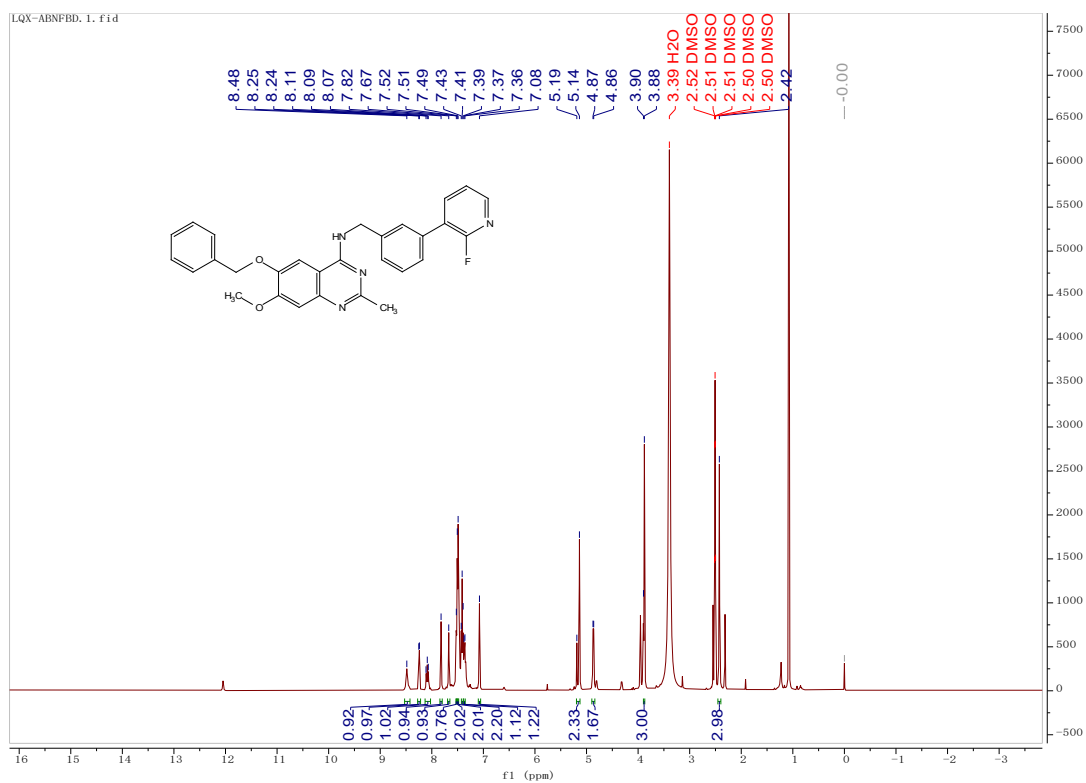




¹H NMR of compound **8k**

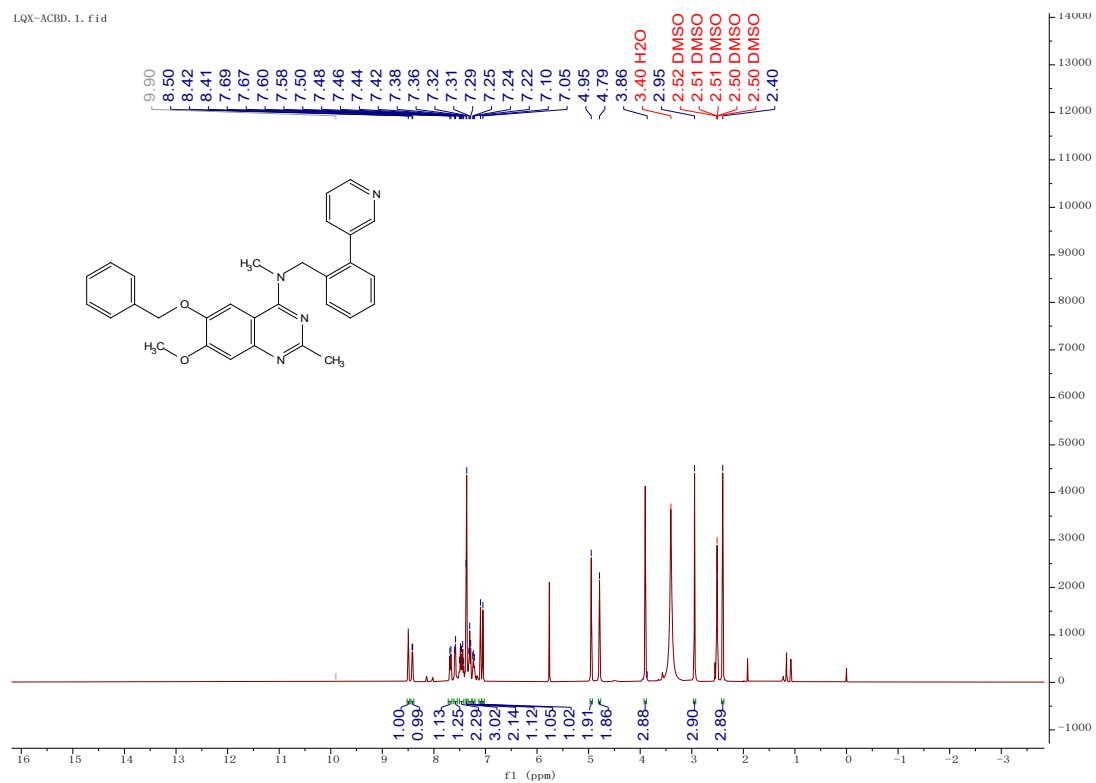


¹H NMR of compound **8l**



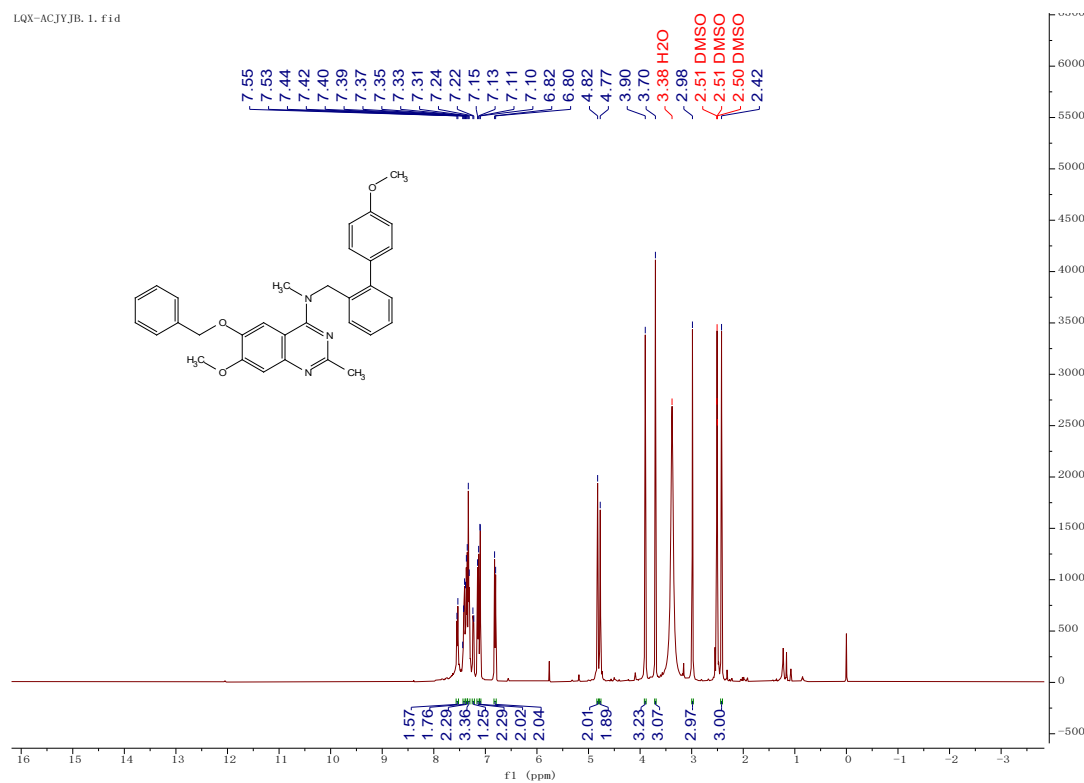
¹H NMR of compound 8m

LQX-ACBD. 1. F1d



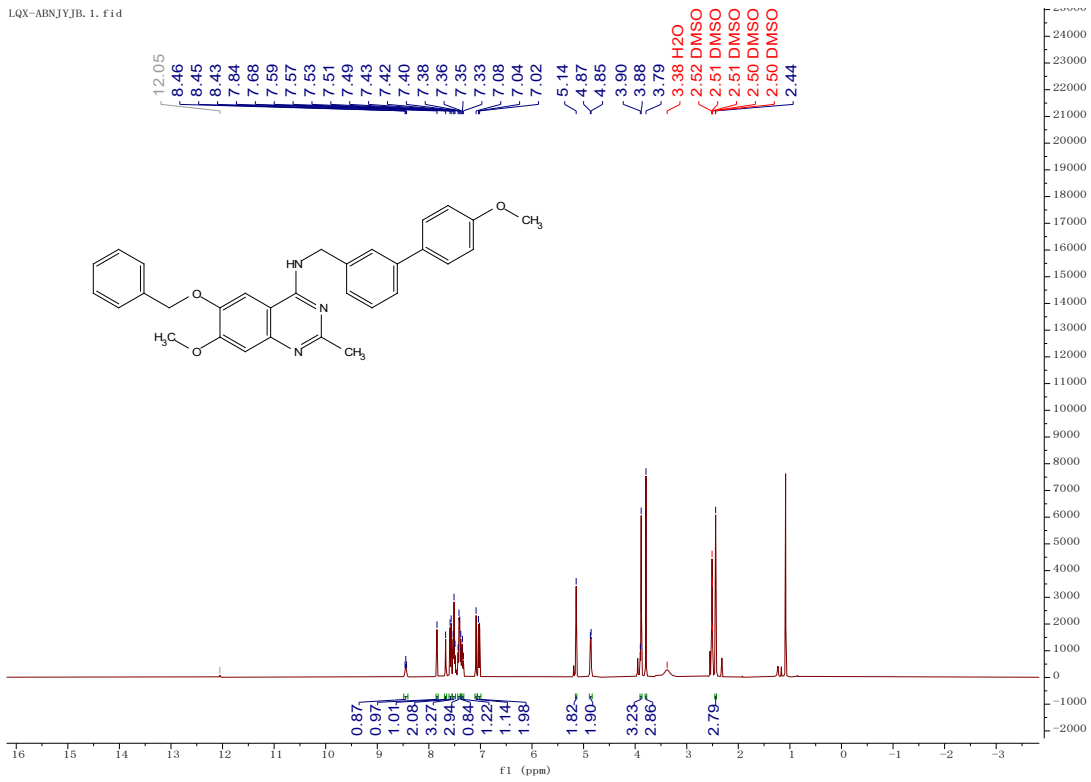
¹H NMR of compound 8n

LQX-ACJYJB. 1. F1d



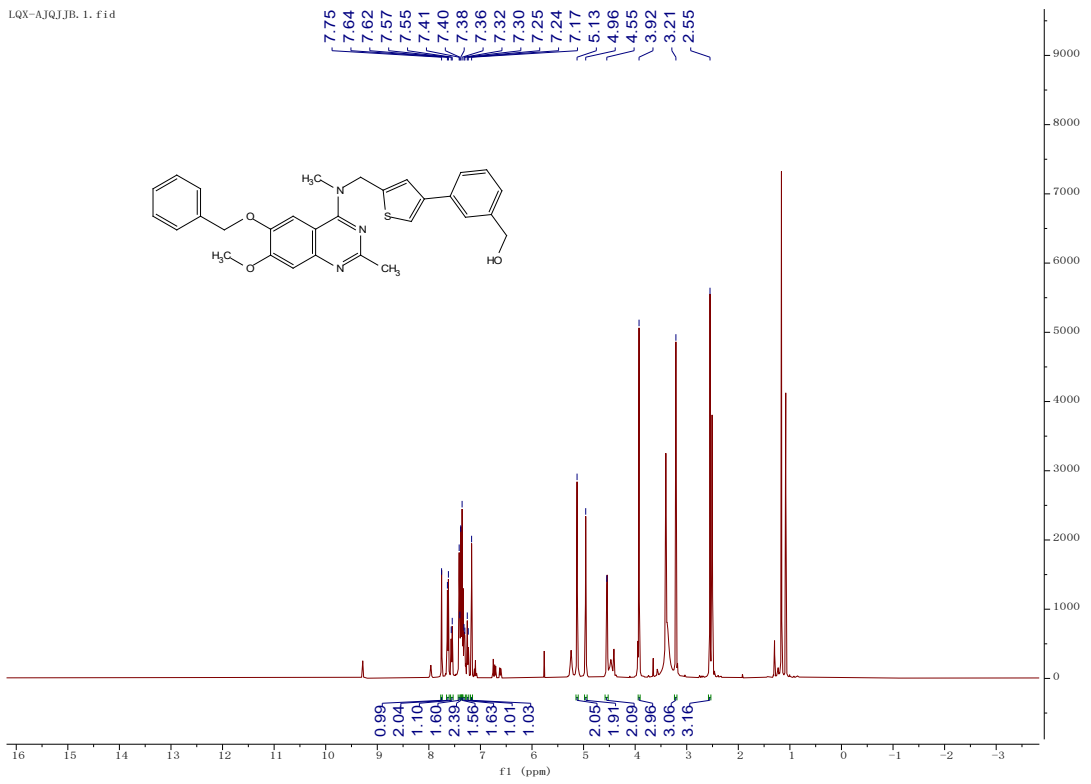
¹H NMR of compound **8o**

LQX-ABNJYJB. 1. fid

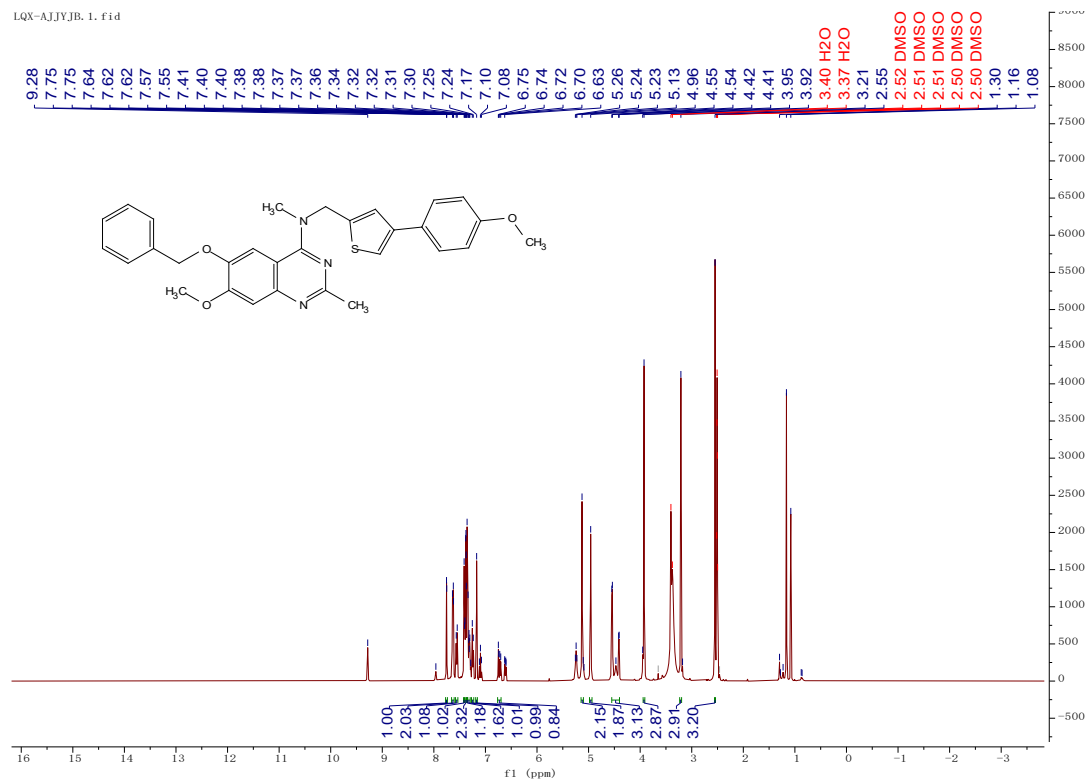


¹H NMR of compound **8p**

LQX-AJQJJB. 1. fid

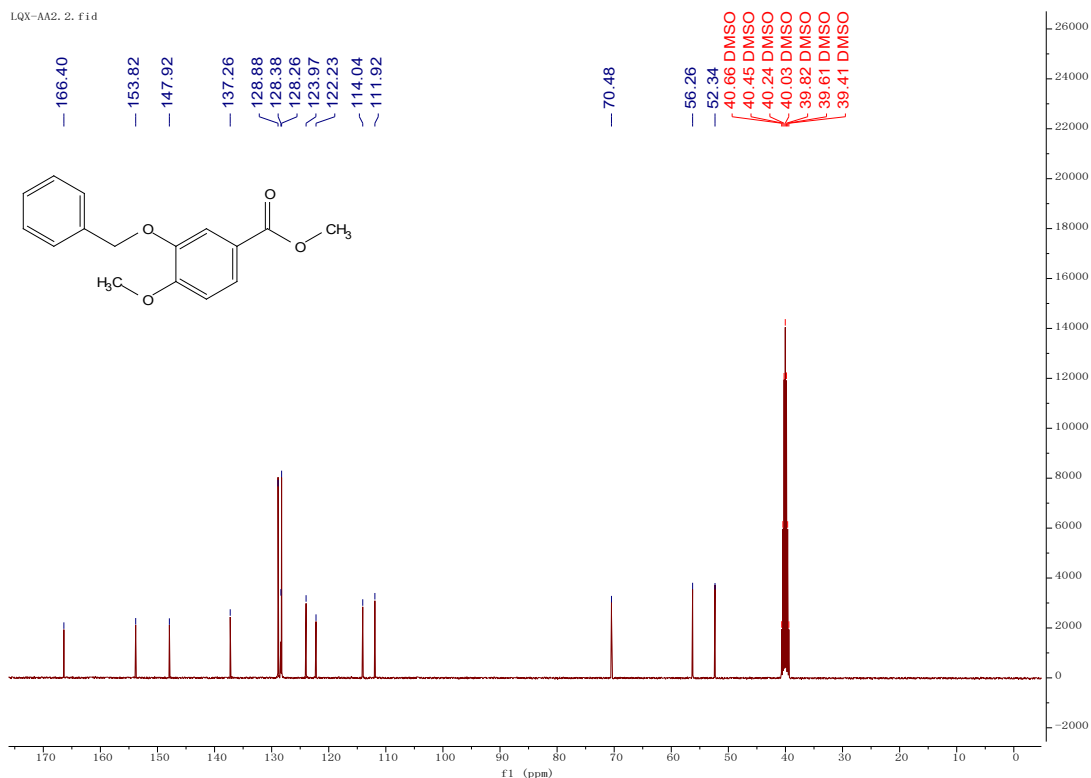


¹H NMR of compound 8q

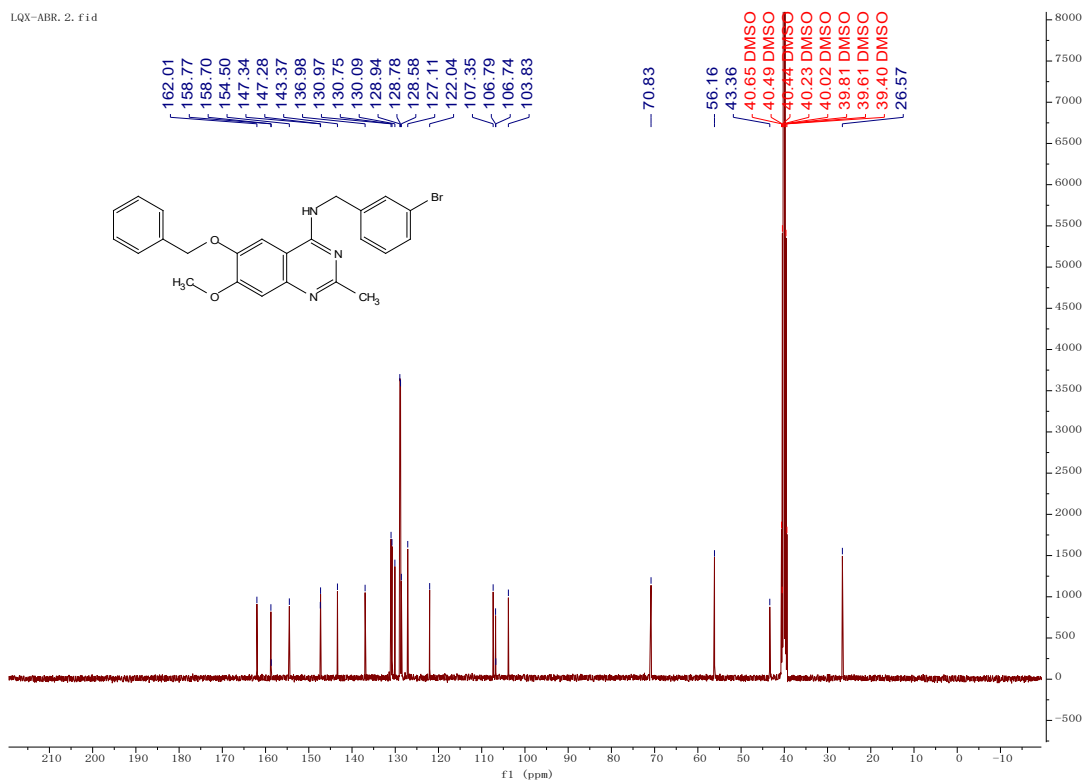


¹³C NMR (150MHz) of compounds

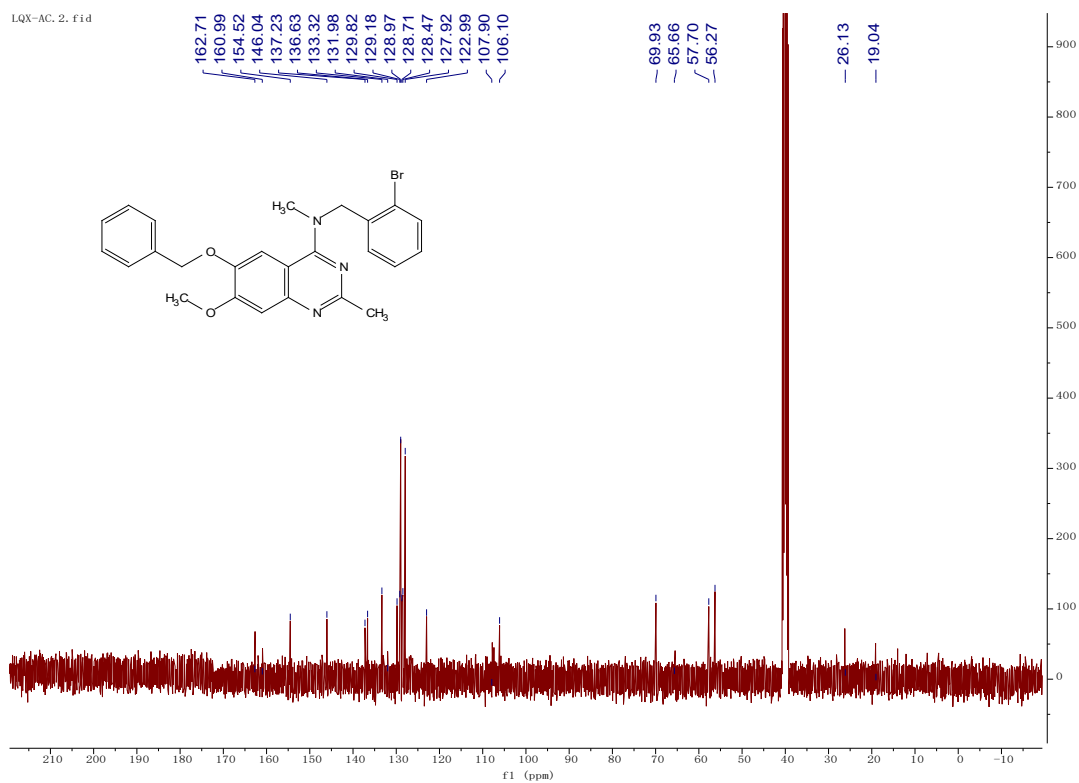
¹³C NMR of compound 1



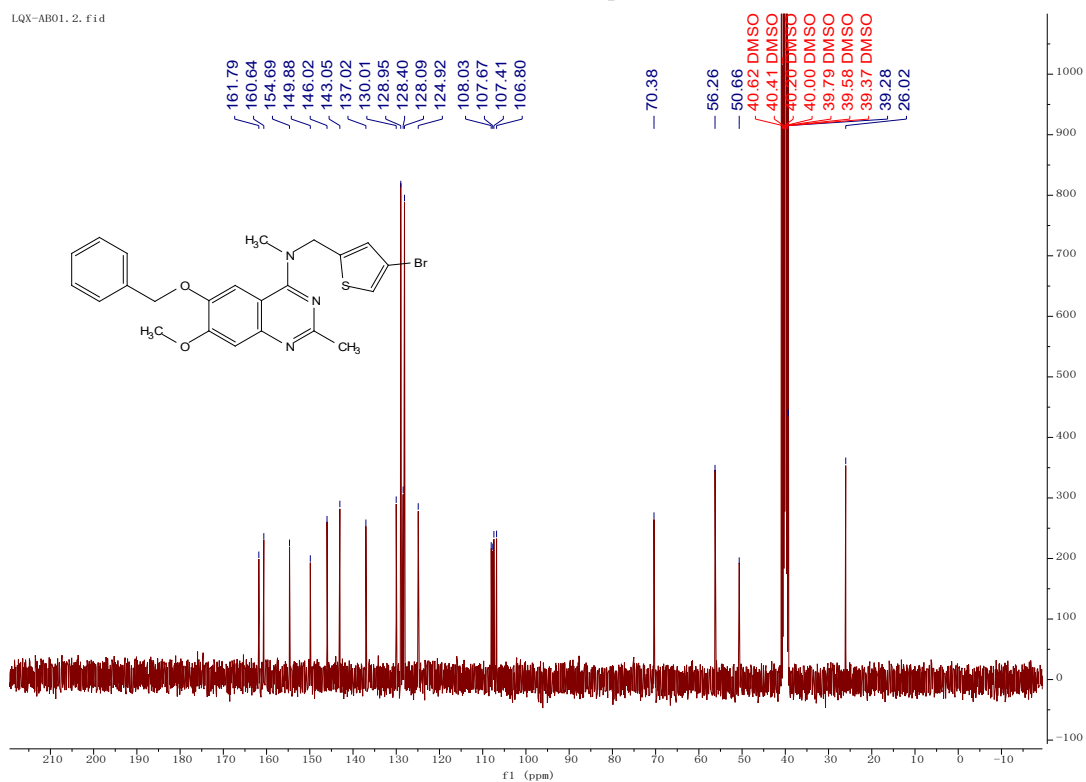
¹³C NMR of compound 7a



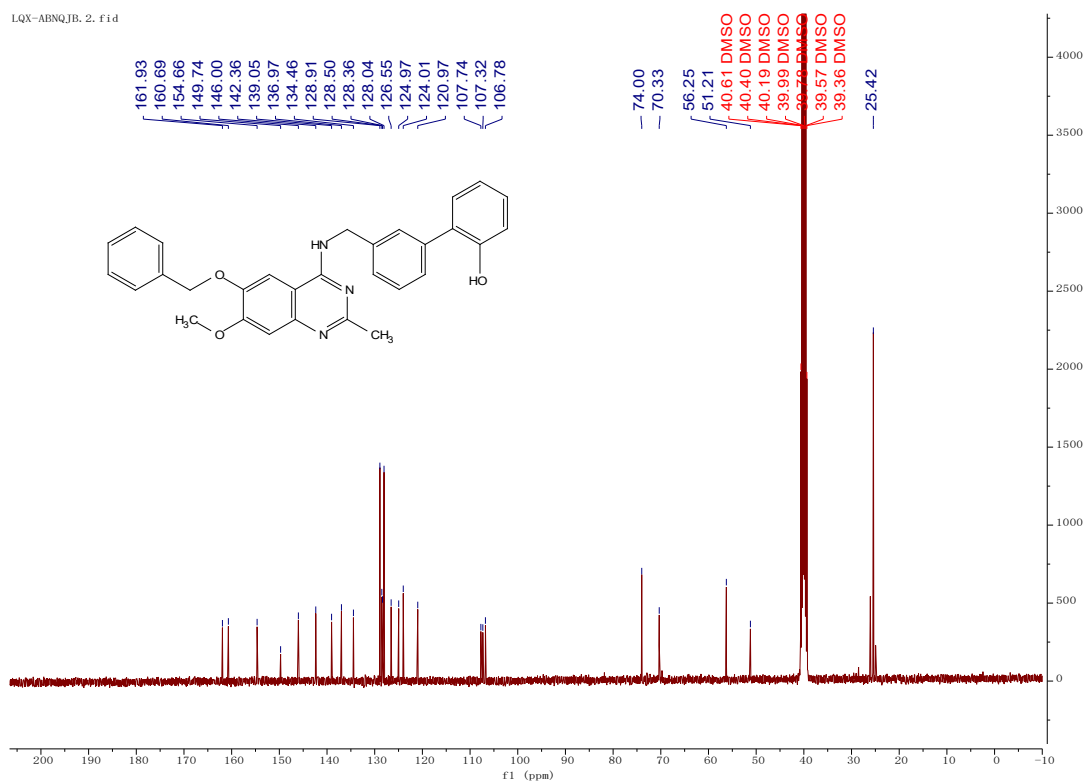
¹³C NMR of compound 7b



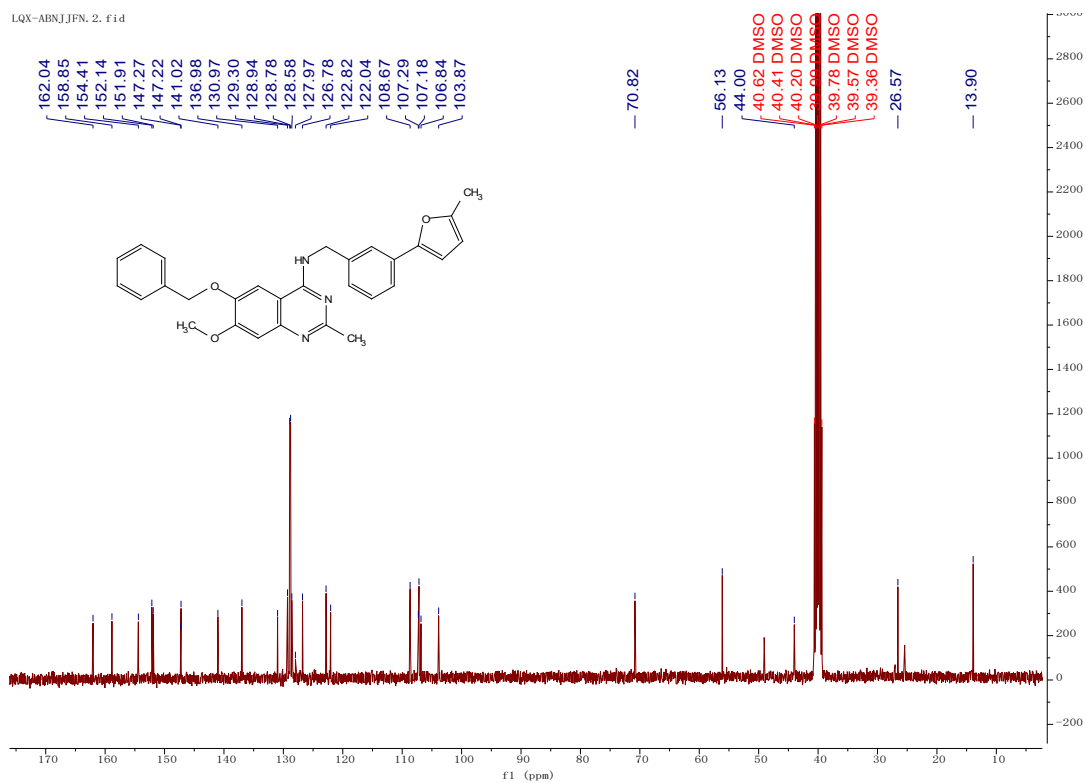
¹³C NMR of compound 7c



¹³C NMR of compound 8a

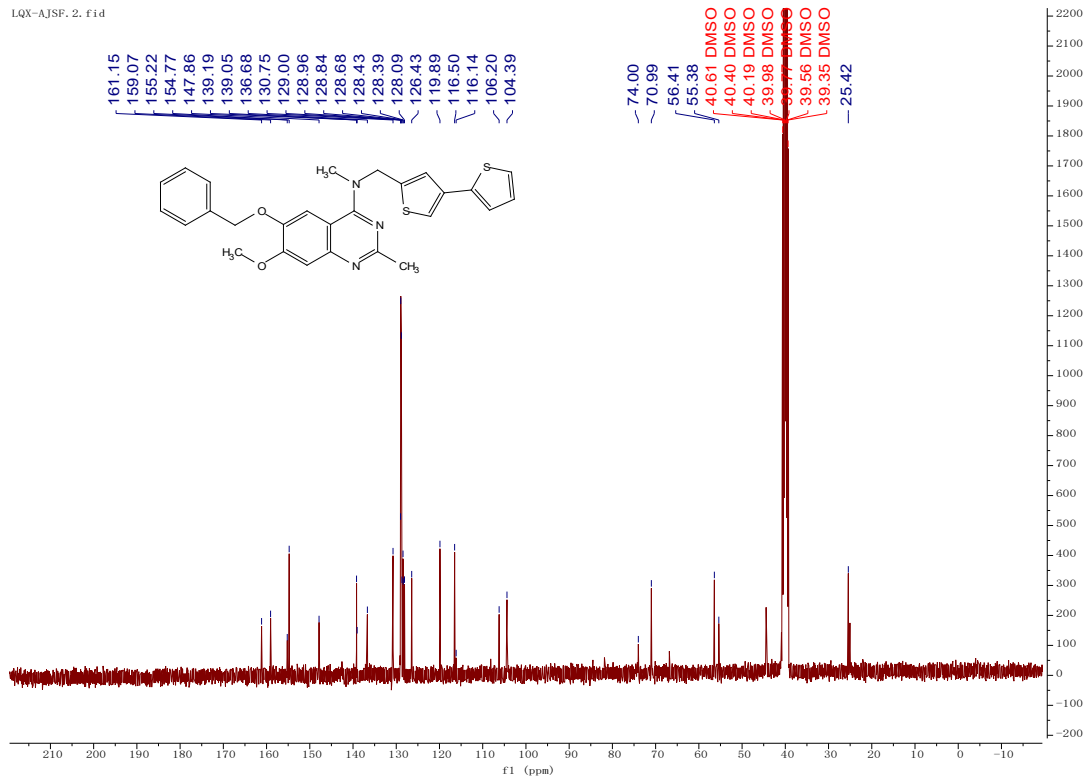


¹³C NMR of compound 8b



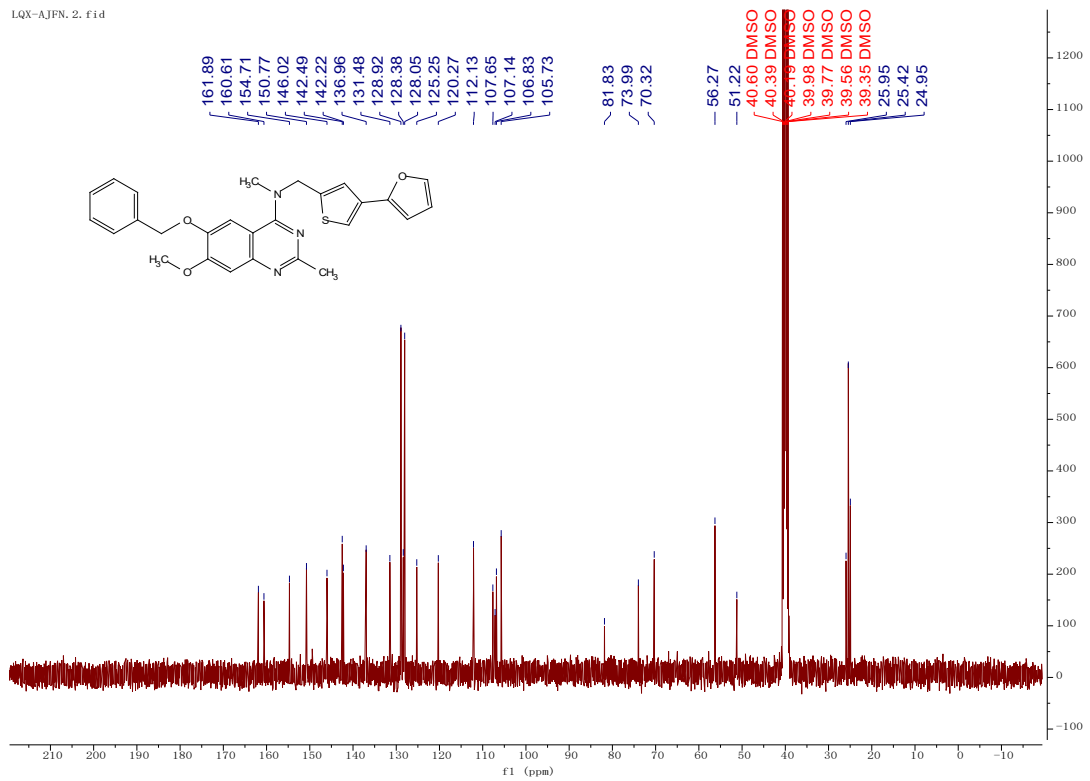
¹³C NMR of compound 8c

LQX-AJSF. 2. fid



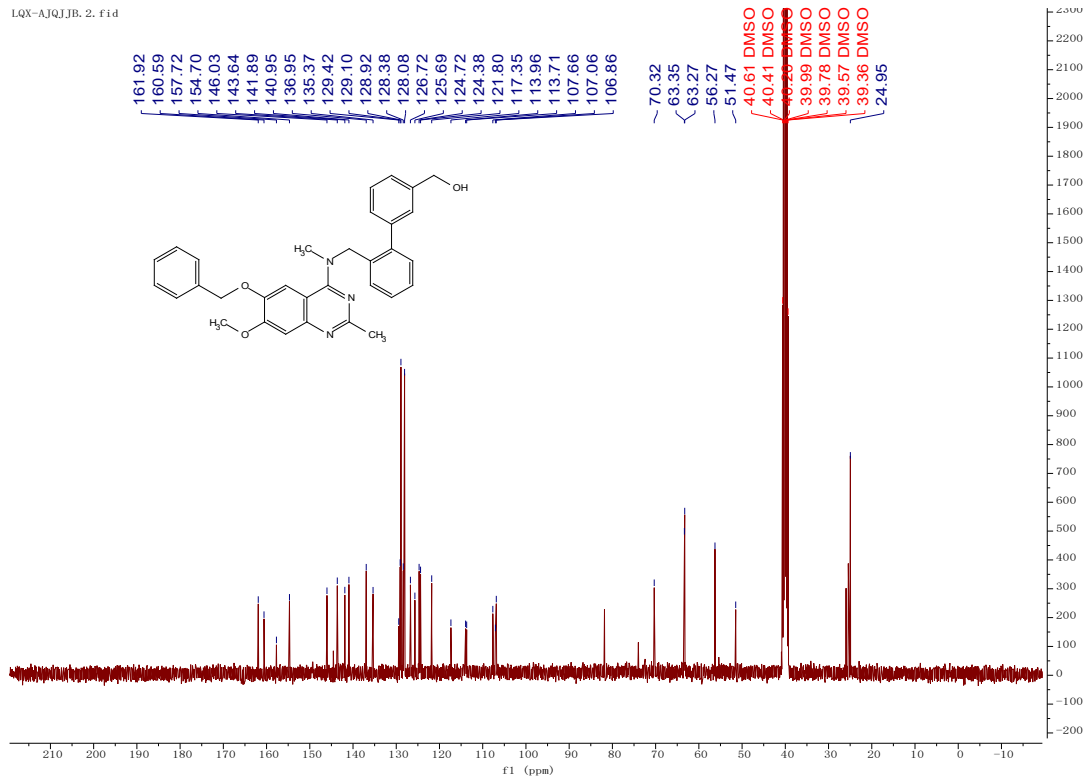
¹³C NMR of compound 8d

LQX-AJFN. 2. fid



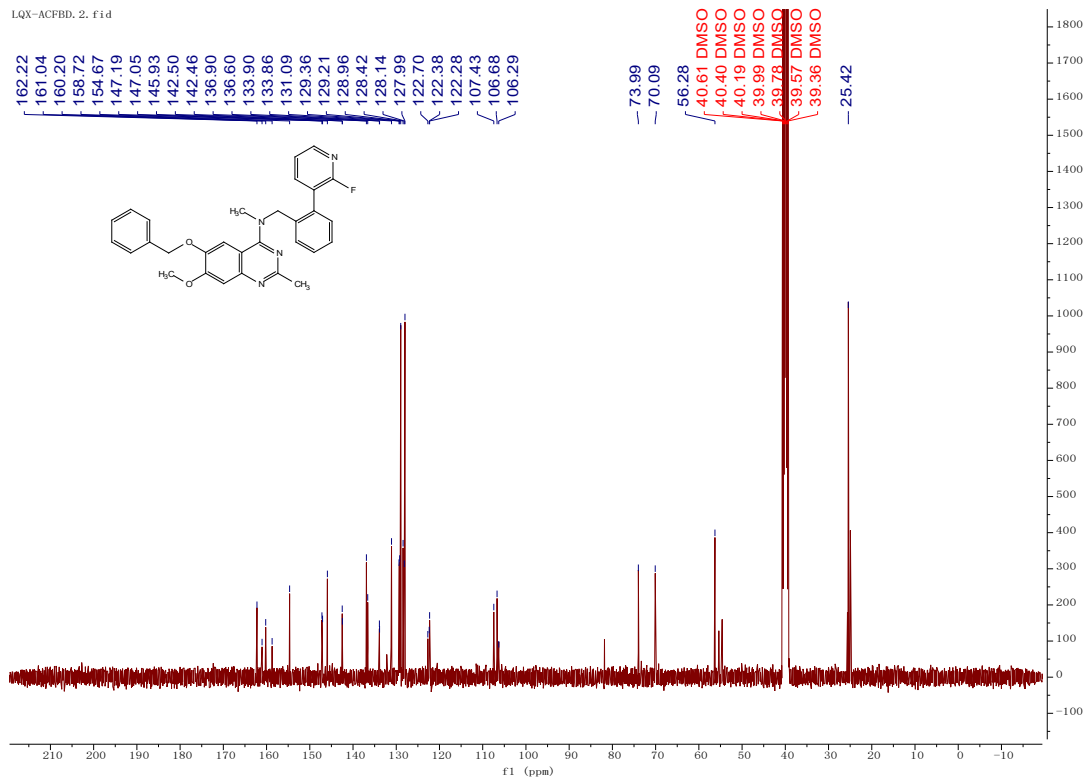
¹³C NMR of compound **8e**

LQX-AJQJJB. 2. F1d

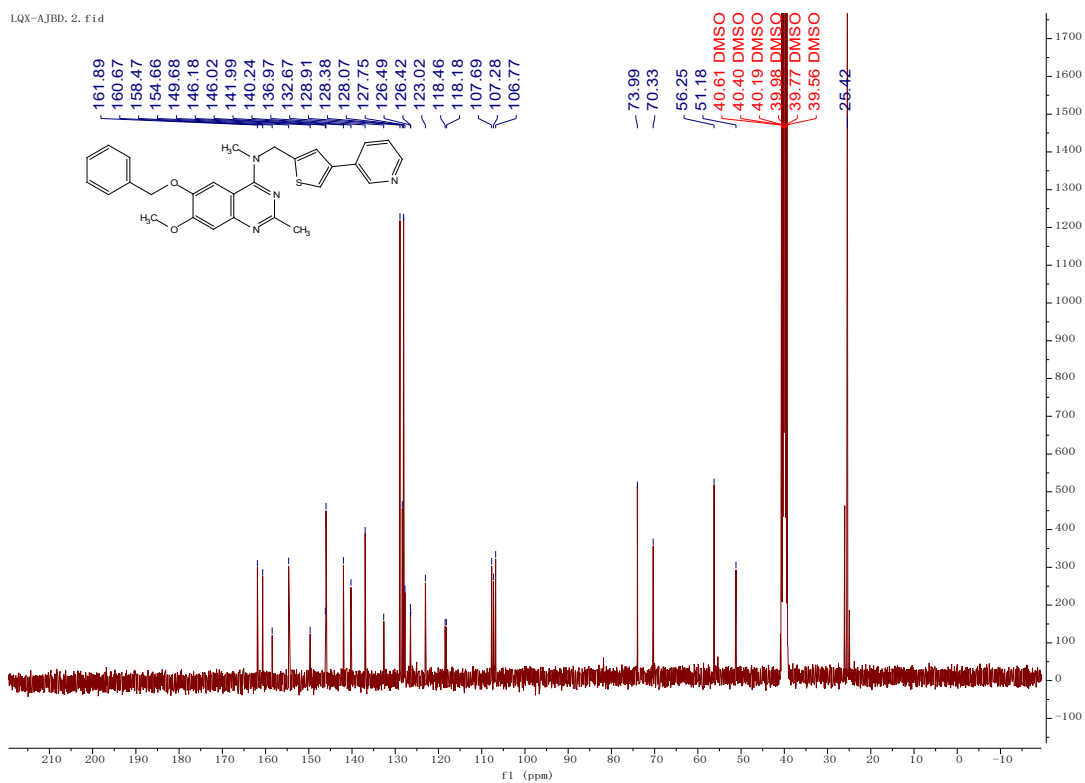


¹³C NMR of compound **8f**

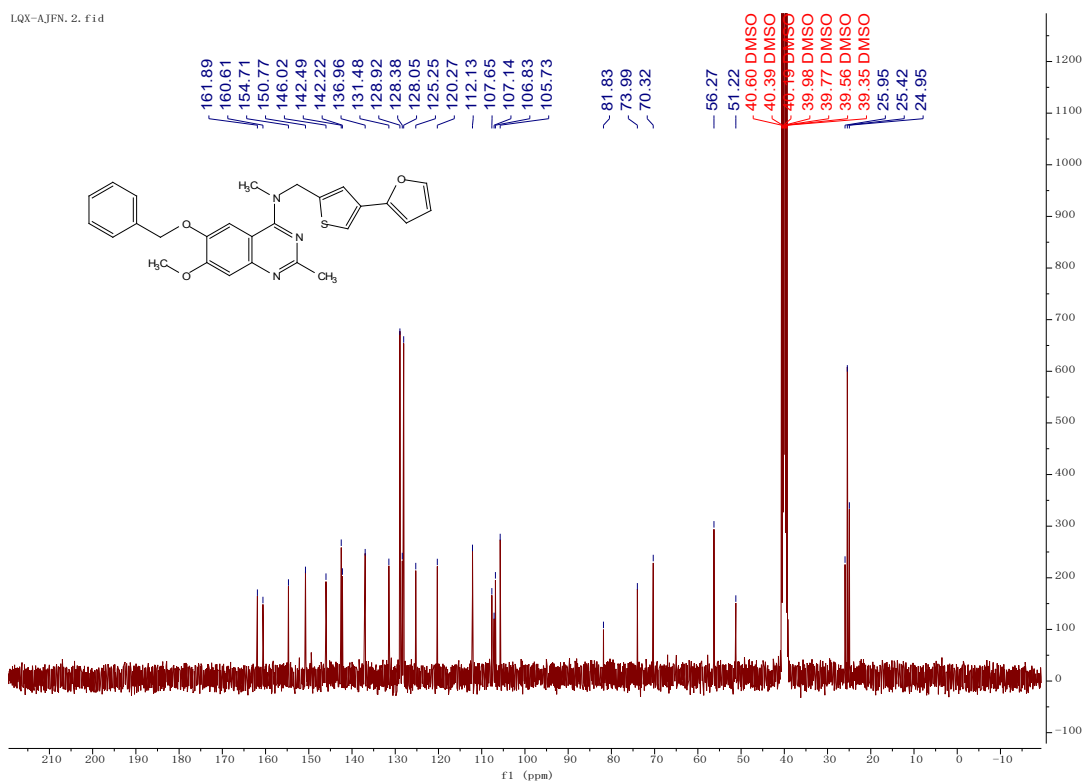
LQX-ACFBD. 2. f1d



¹³C NMR of compound 8g

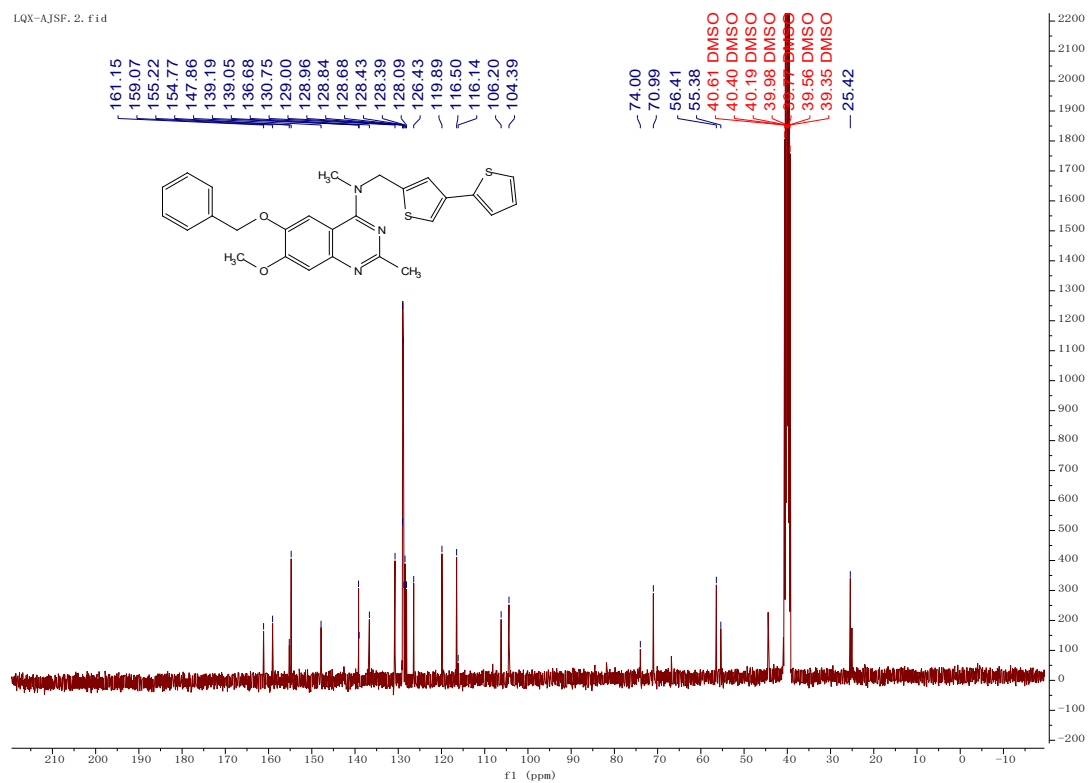


¹³C NMR of compound 8h



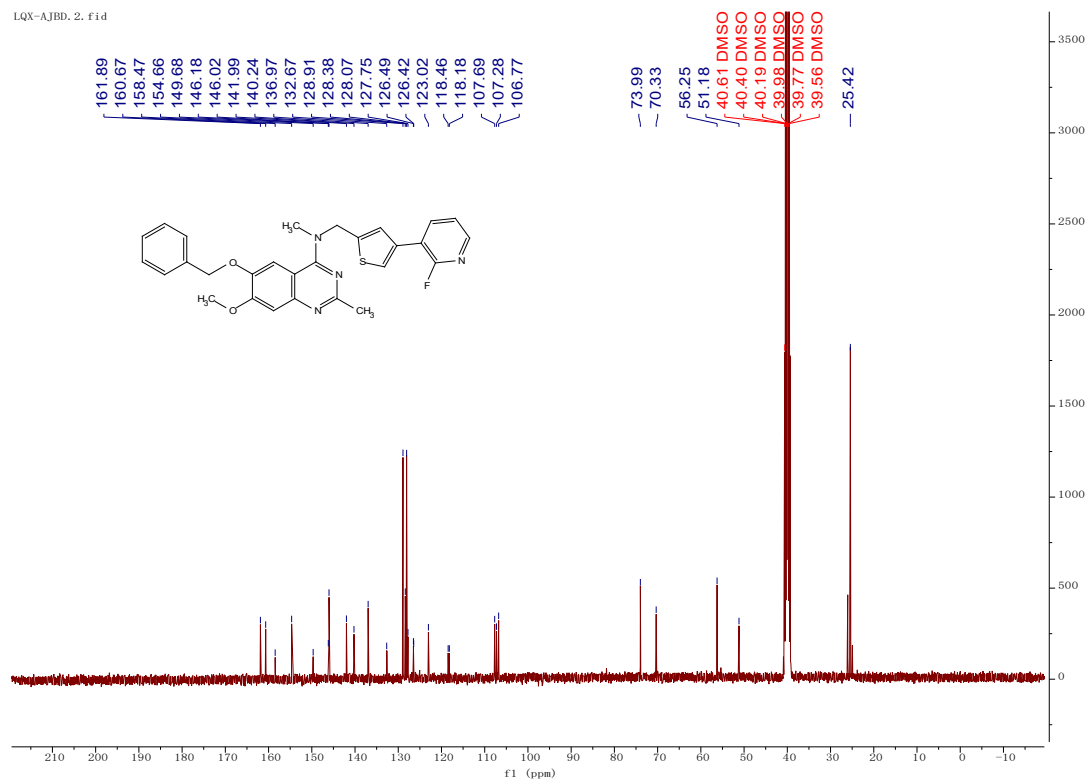
¹³C NMR of compound **8i**

LQX-AJSF. 2. fid

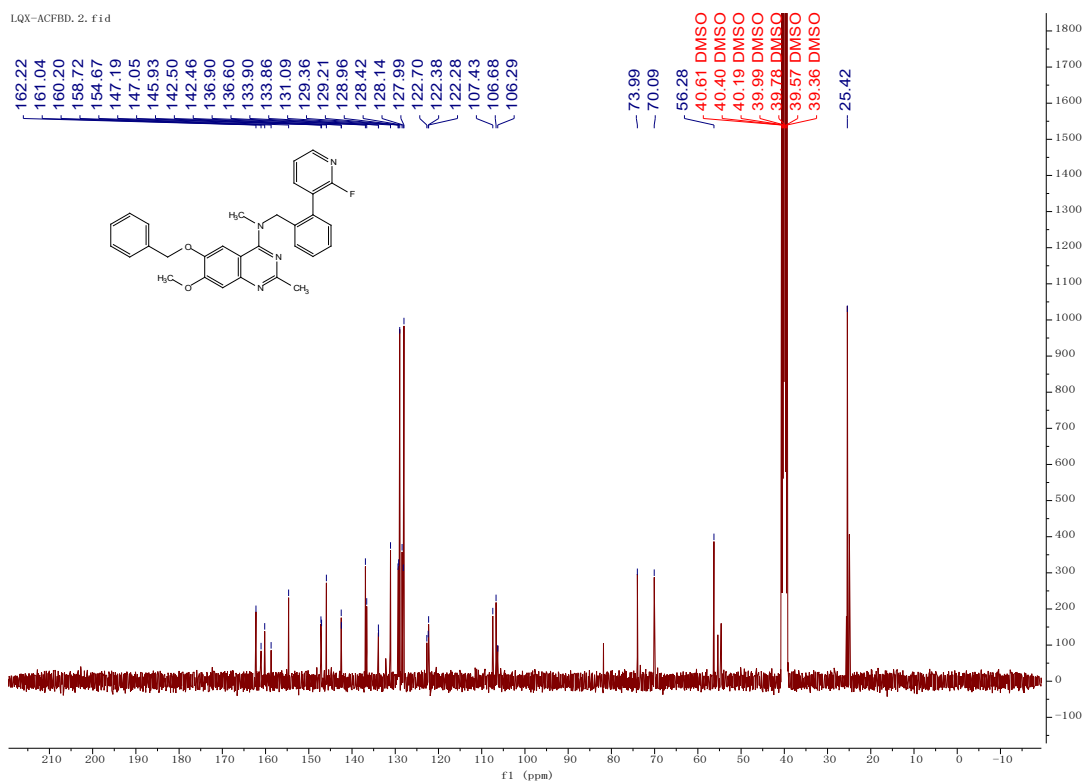


¹³C NMR of compound **8j**

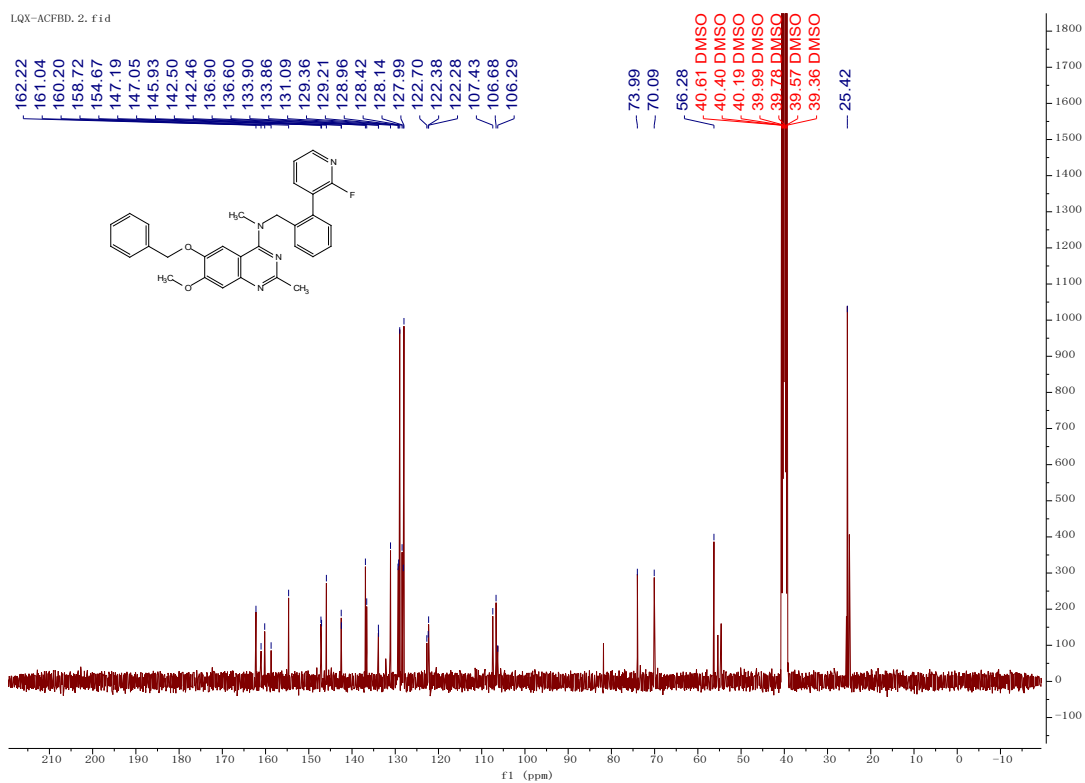
LQX-AJBD. 2. fid



¹³C NMR of compound 8k

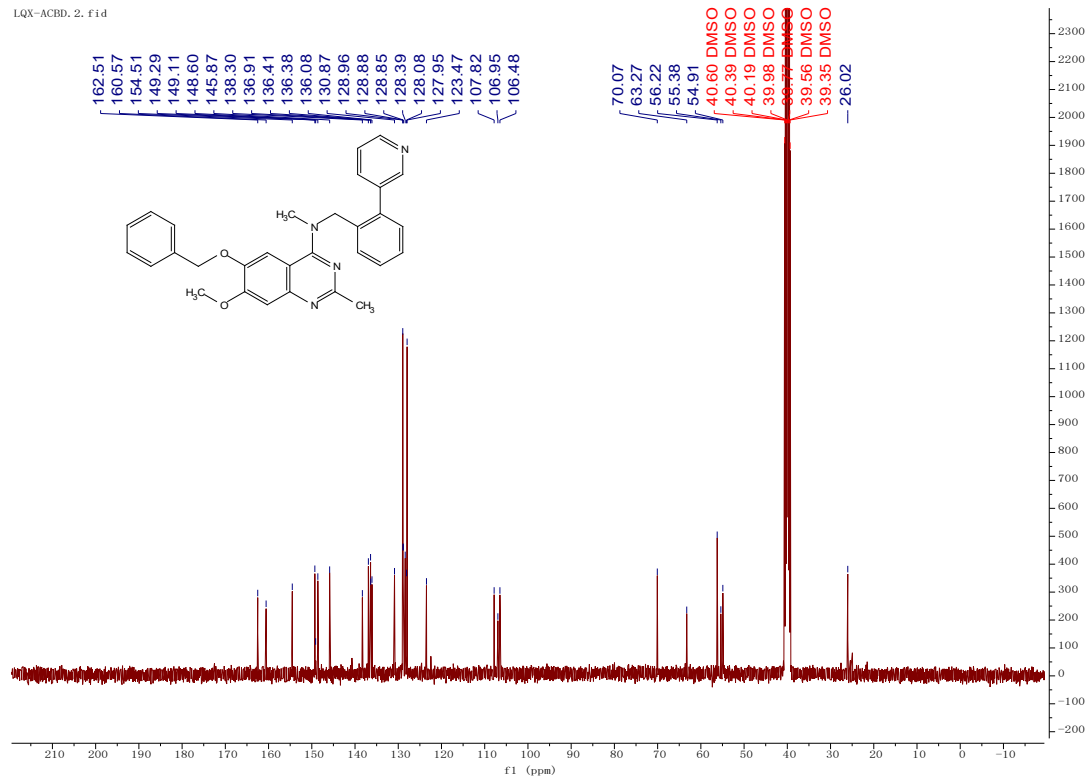


¹³C NMR of compound 8l



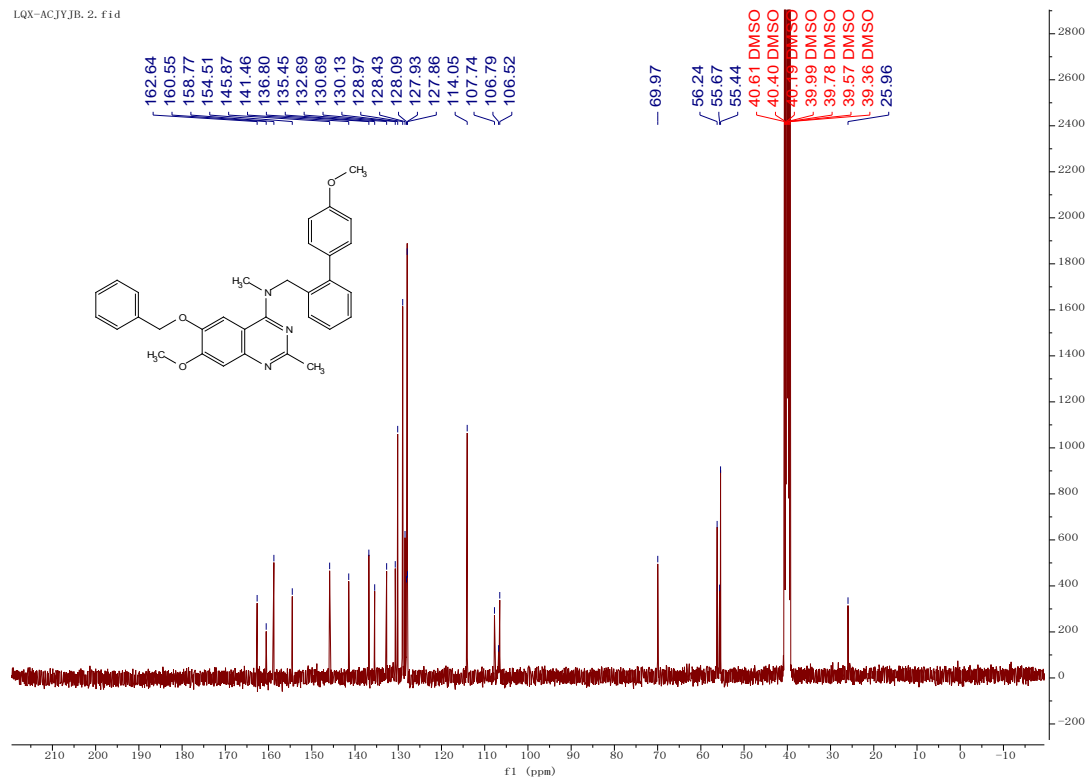
¹³C NMR of compound **8m**

LQX-ACBD. 2. Fid

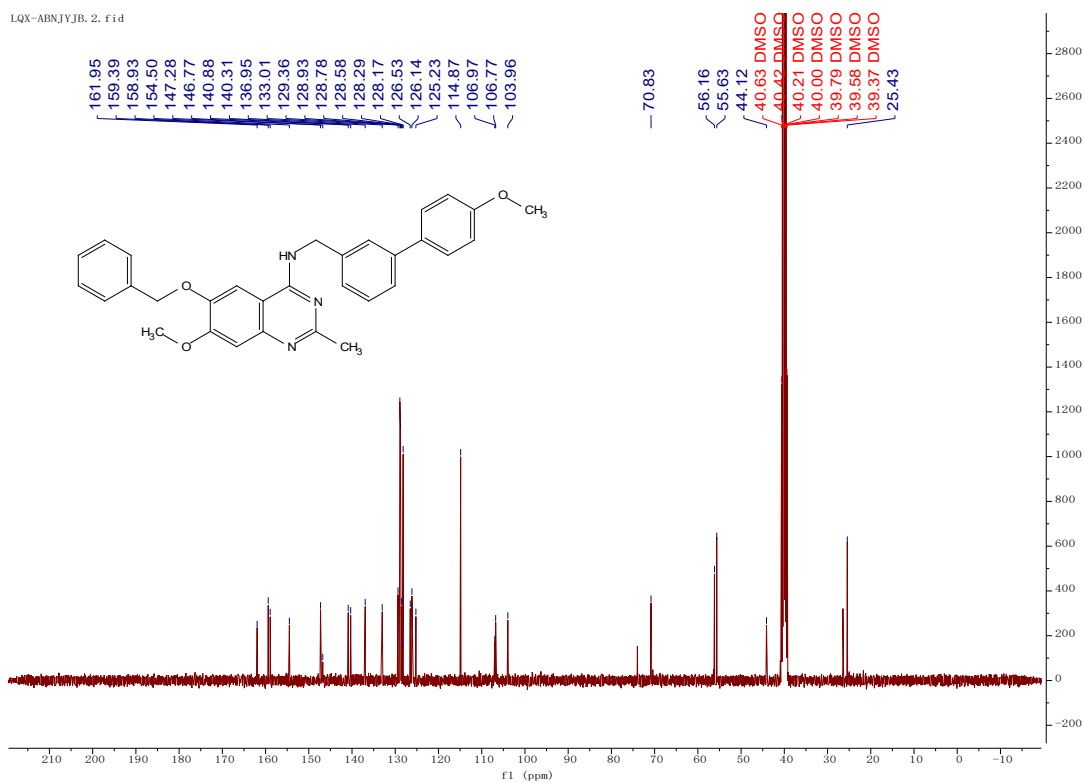


¹³C NMR of compound **8n**

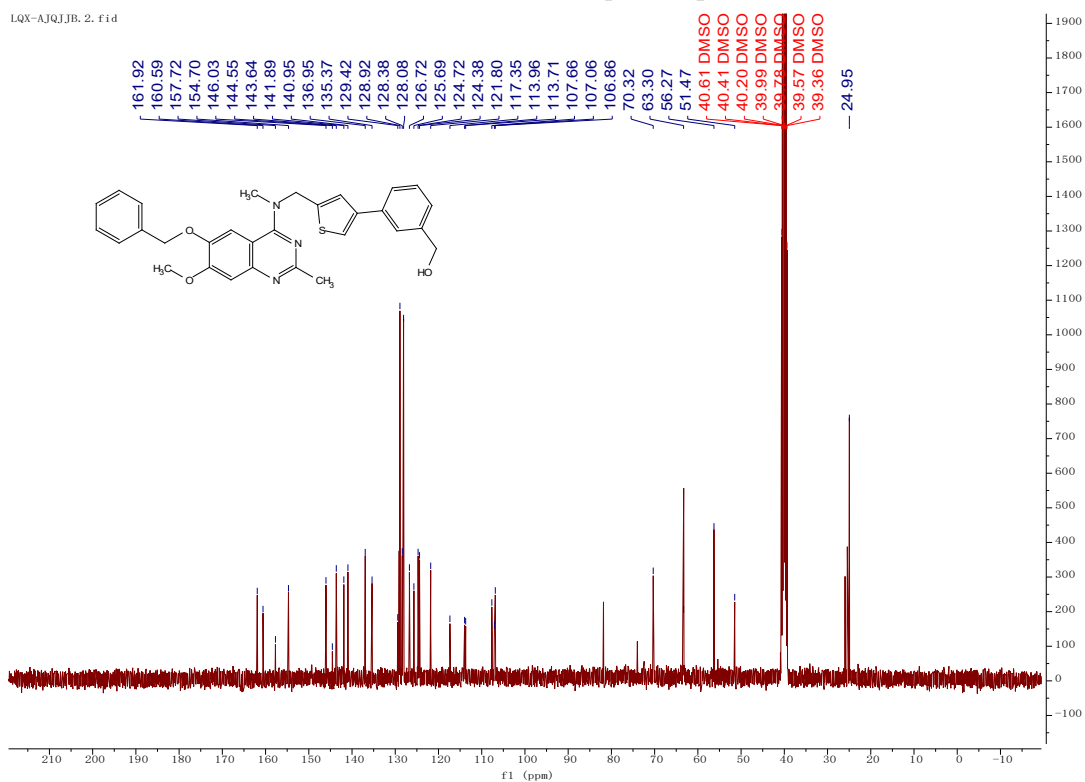
LQX-ACJYJB. 2. Fid



¹³C NMR of compound **8o**



¹³C NMR of compound **8p**



¹³C NMR of compound **8q**

LQX-AJJYJB. 2. Fid

