

Supplementary Information

Design, synthesis, anti-inflammatory evaluation, and molecular docking studies of novel quinazoline-4(3H)-one-2-carbothioamide derivatives

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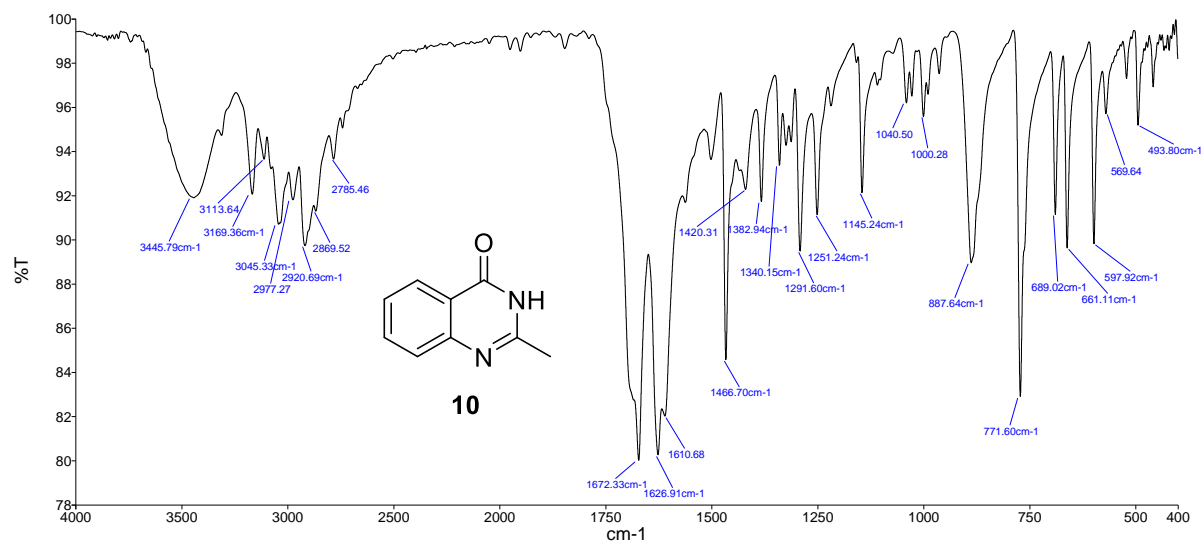
^dInstitute of Chemistry, Vietnam Academy of Science and Technology, Hanoi, Vietnam.

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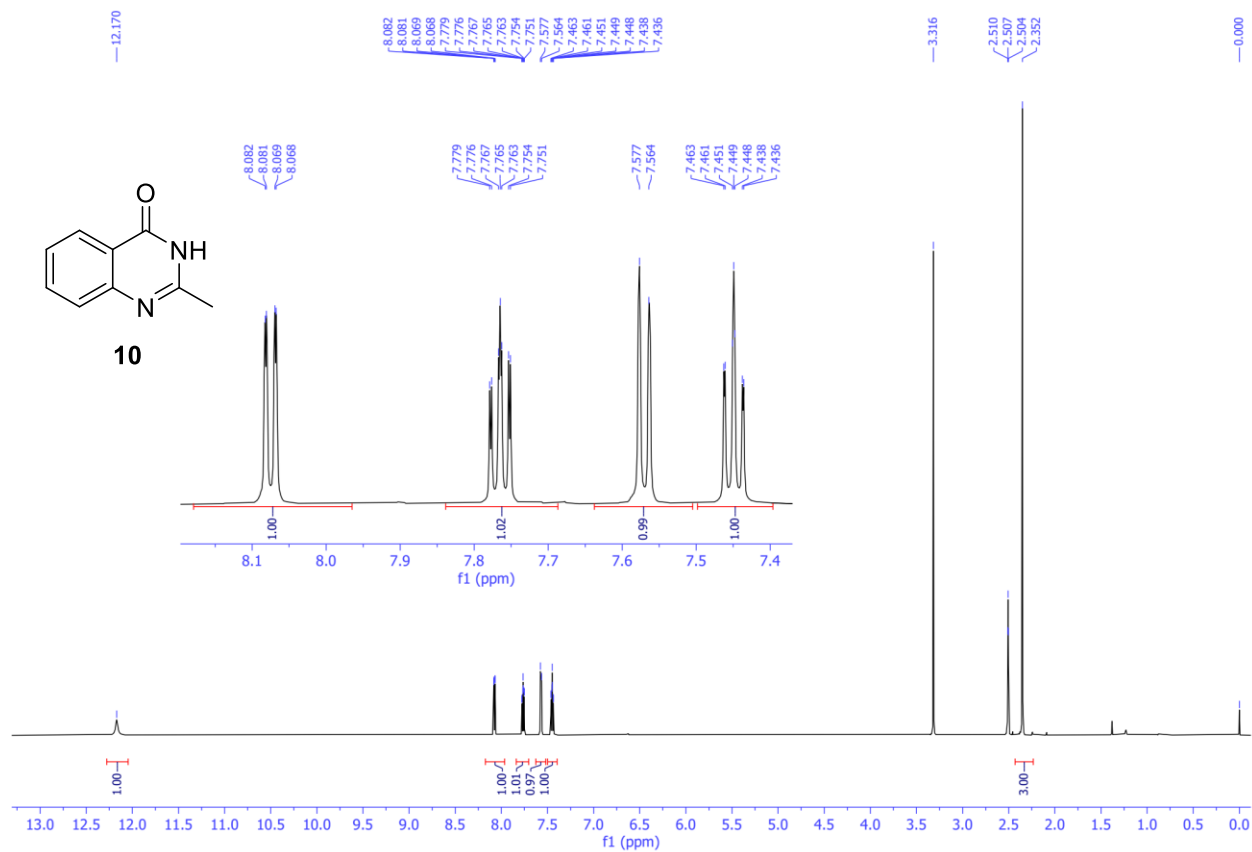
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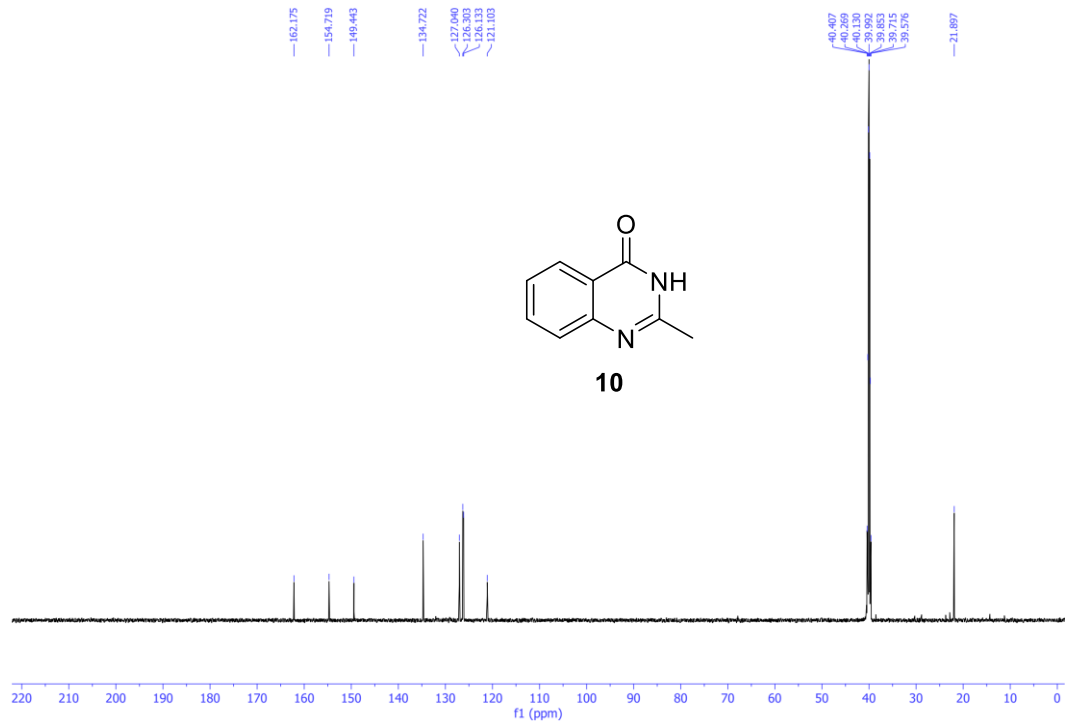
IR spectra of compound **10**



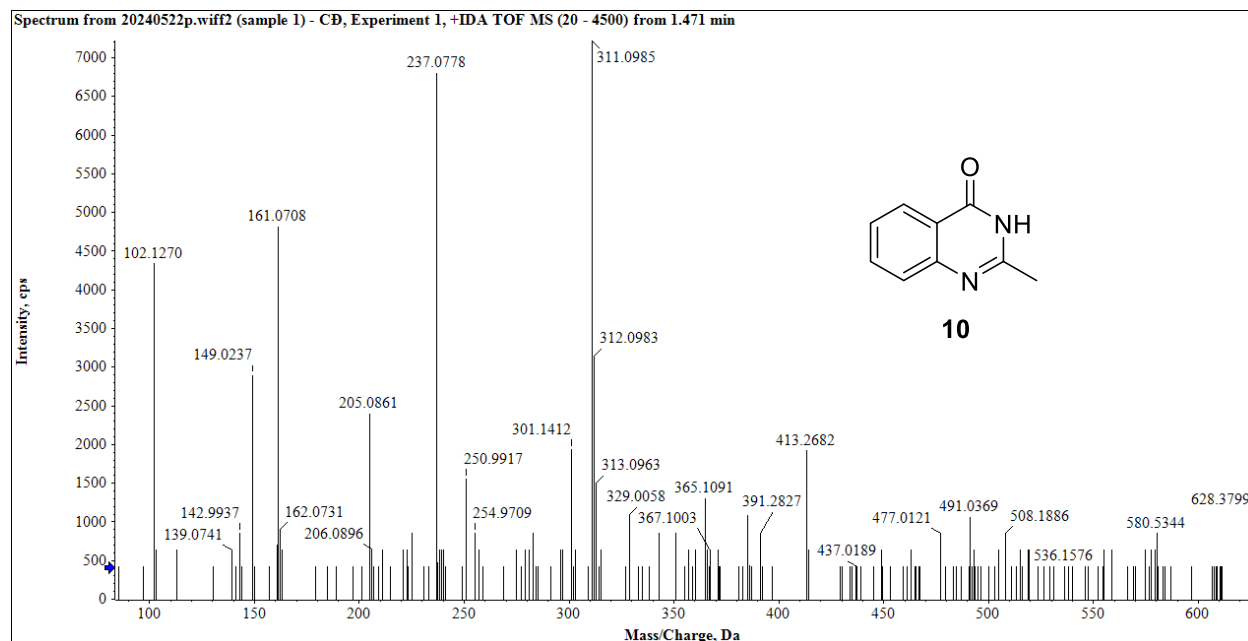
¹H NMR (DMSO-*d*₆, 600 MHz) spectrum of compound **10**



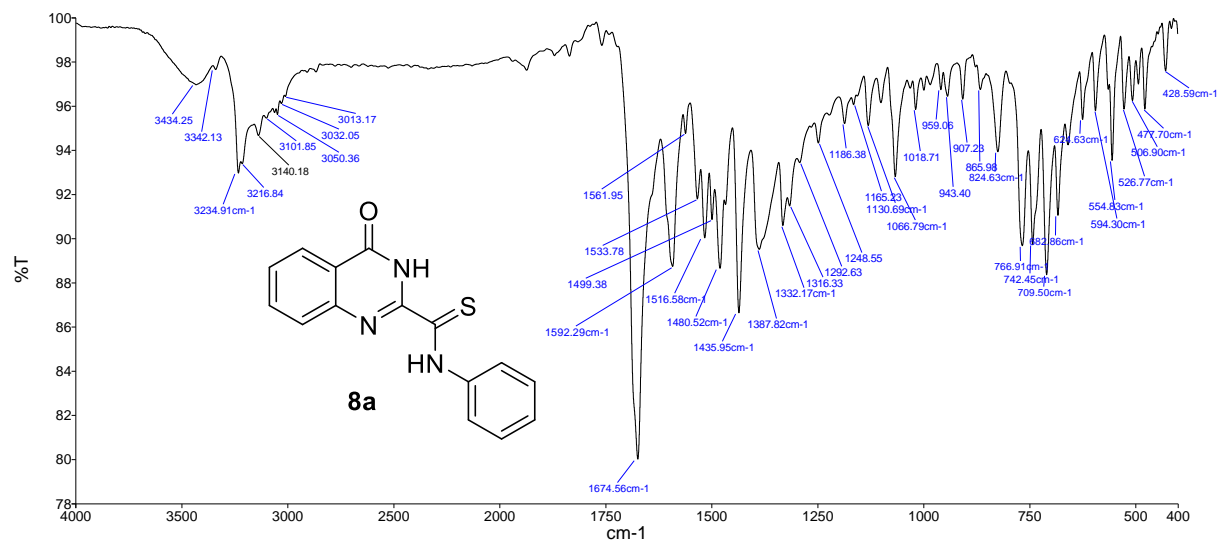
¹³C NMR (DMSO-*d*₆, 150 MHz) spectrum of compound **10**



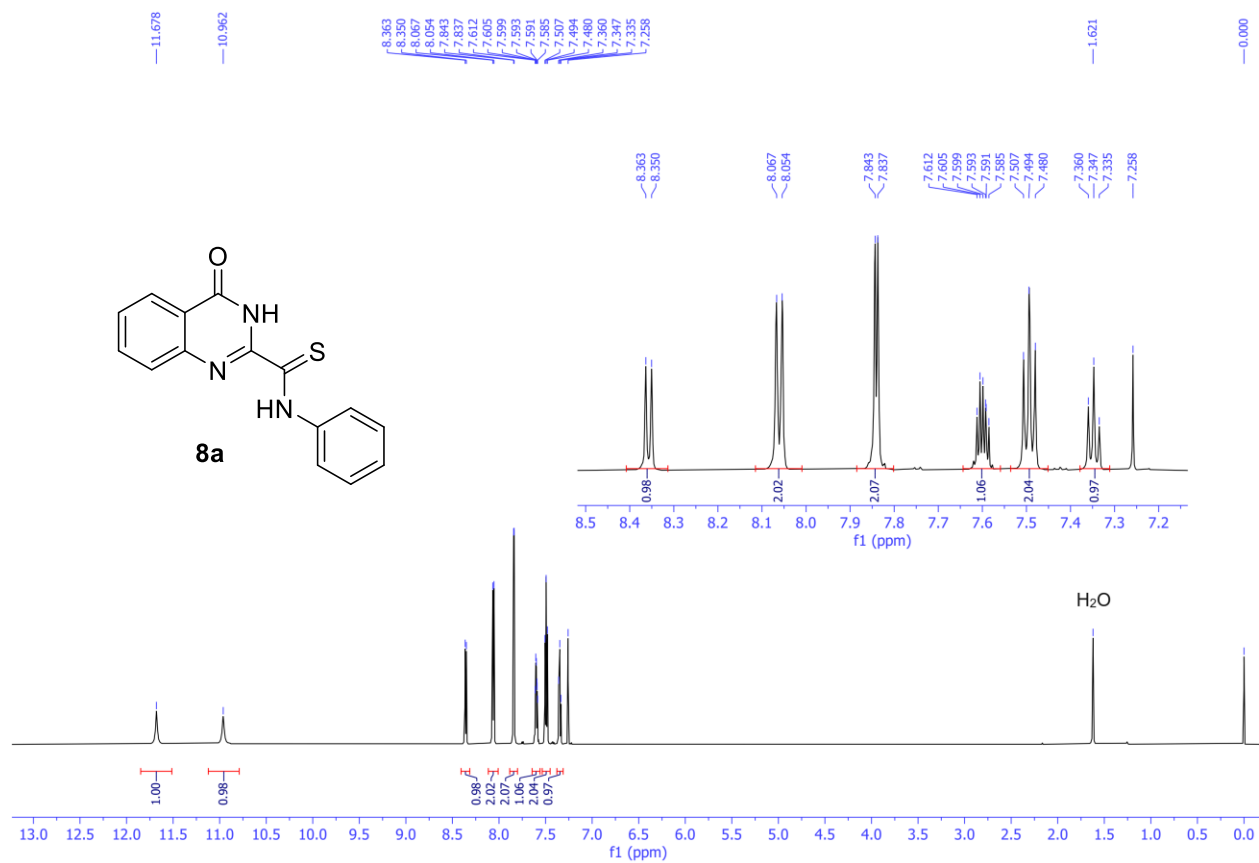
HRMS spectrum of compound **10**



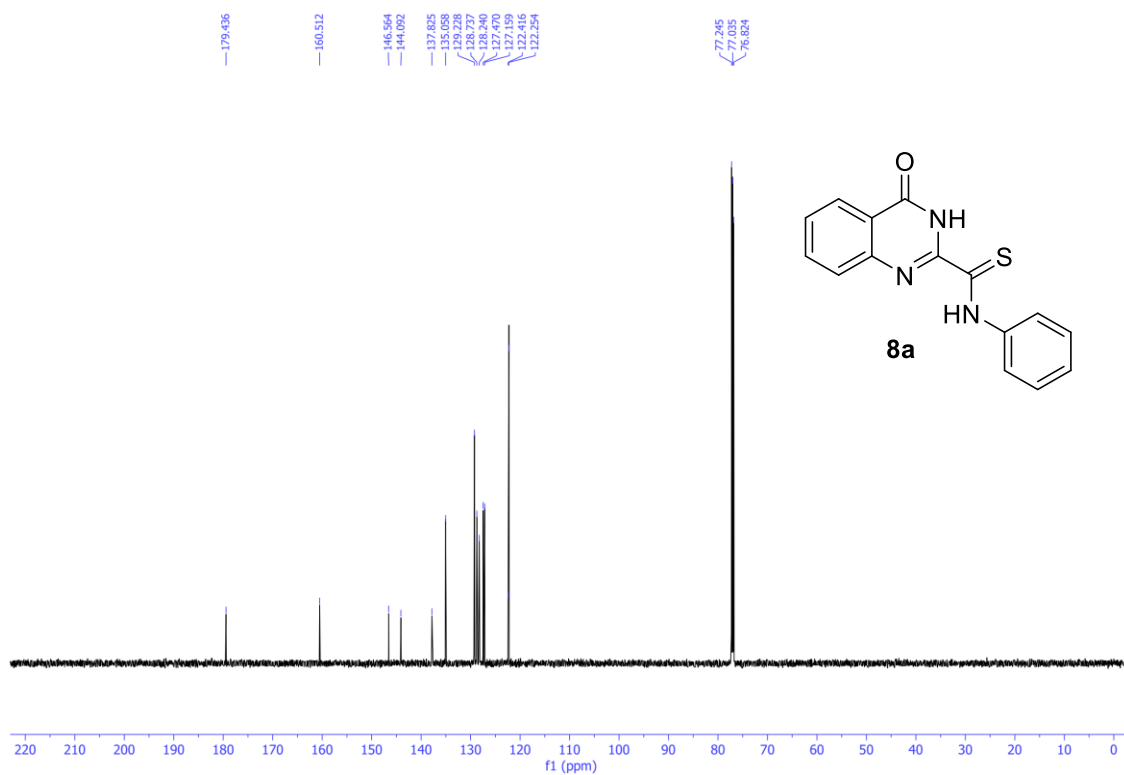
IR spectra of compound **8a**



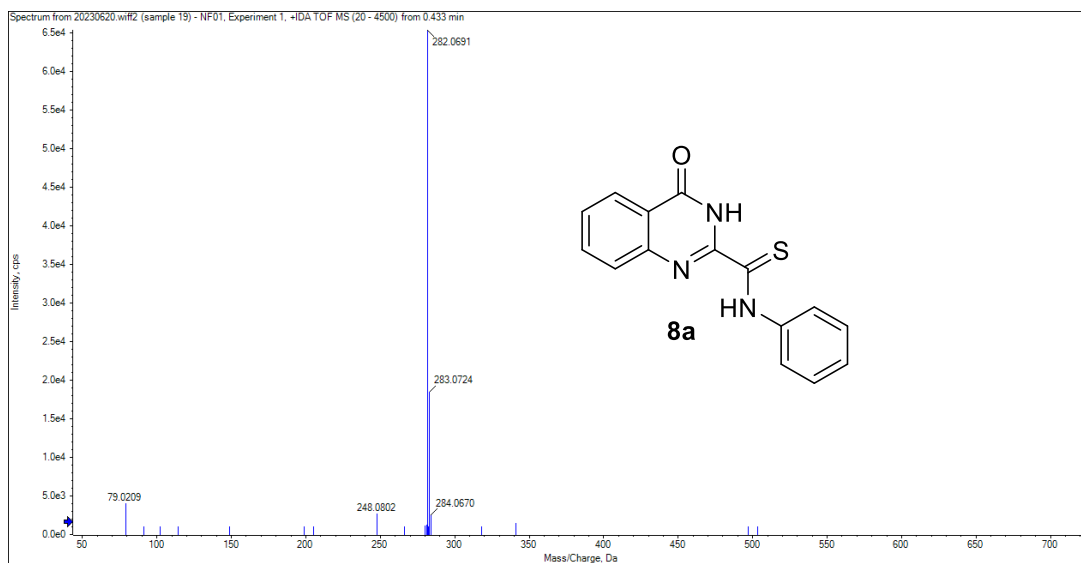
¹H NMR (CDCl₃, 600 MHz) spectrum of compound **8a**



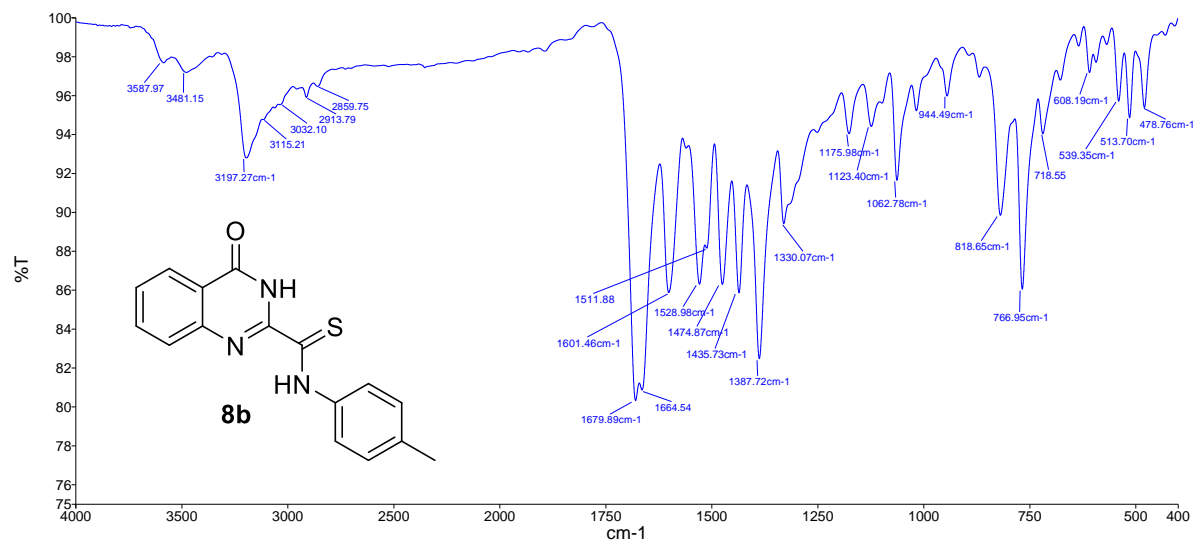
^{13}C NMR (CDCl_3 , 150 MHz) spectrum of compound **8a**



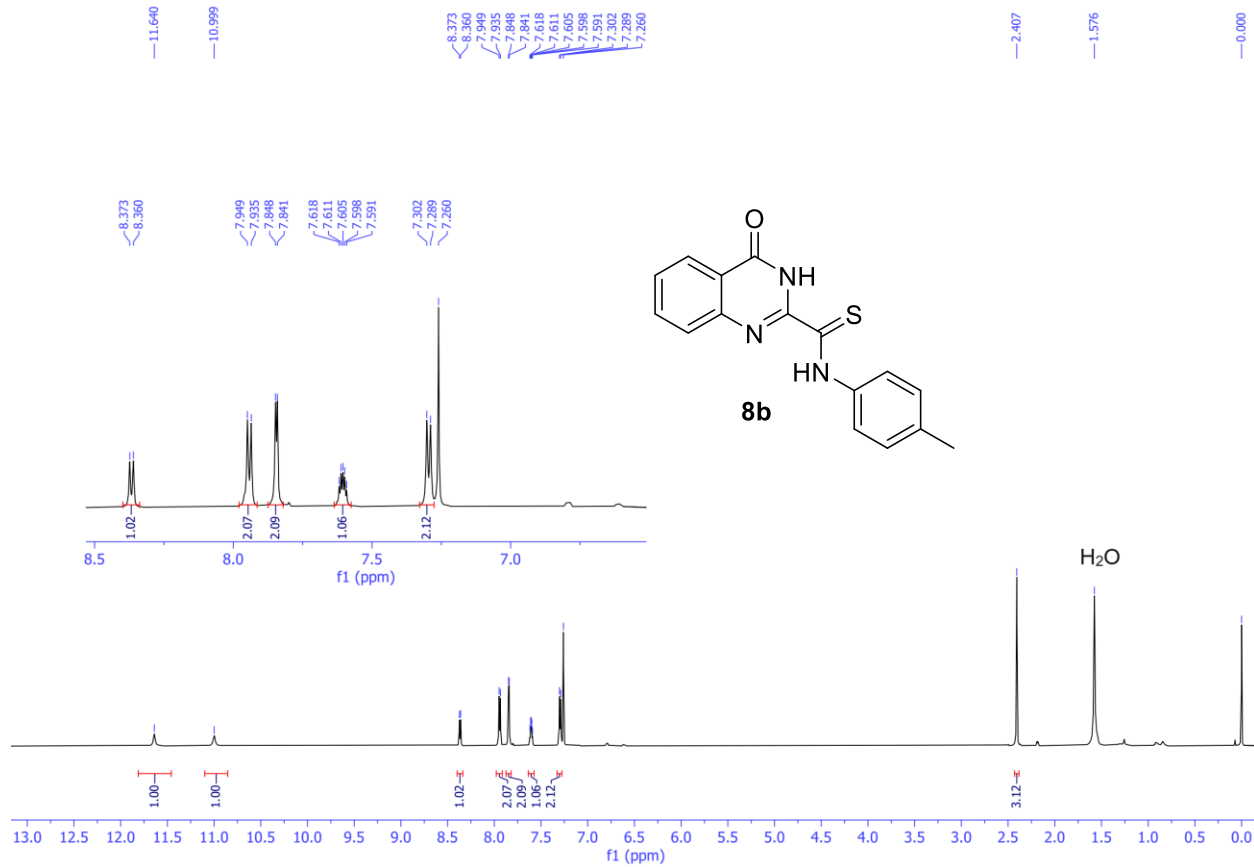
HRMS spectrum of compound **8a**



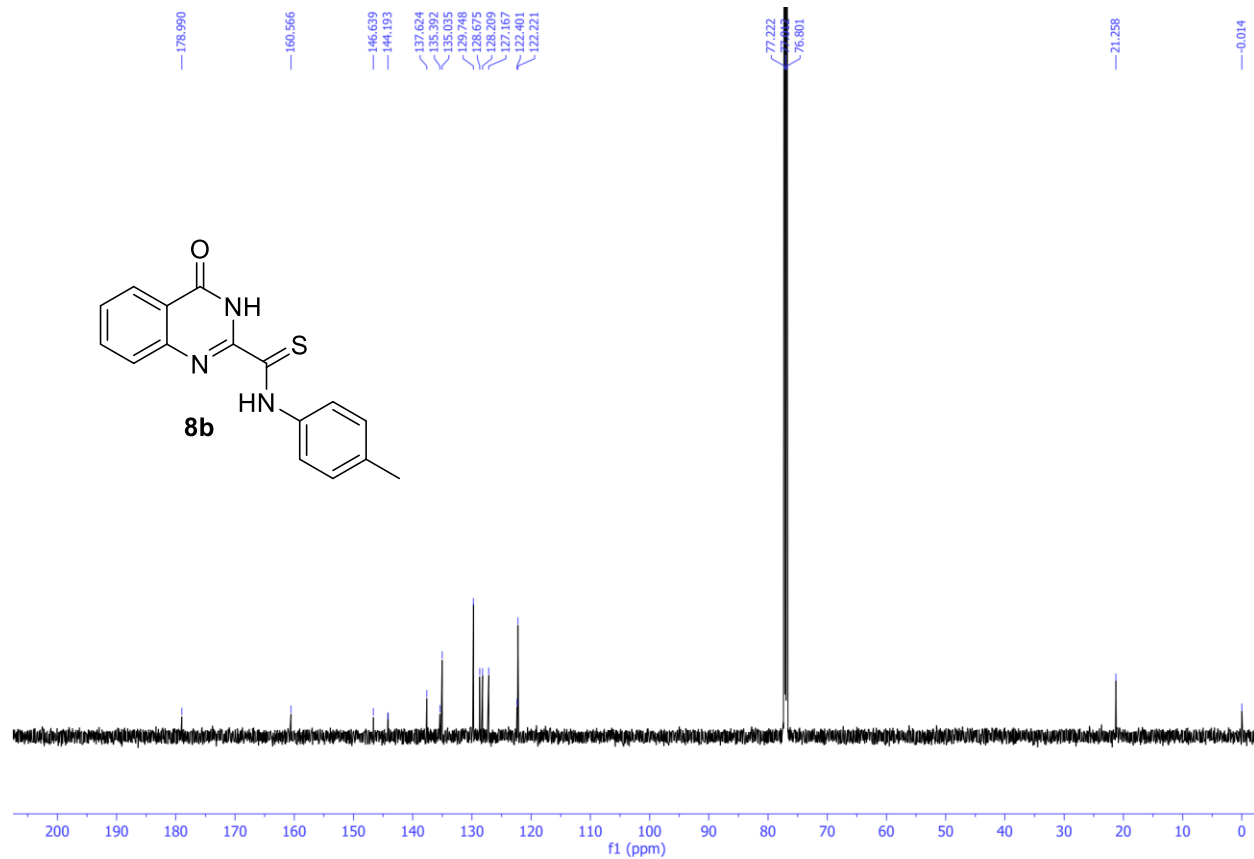
IR spectra of compound **8b**



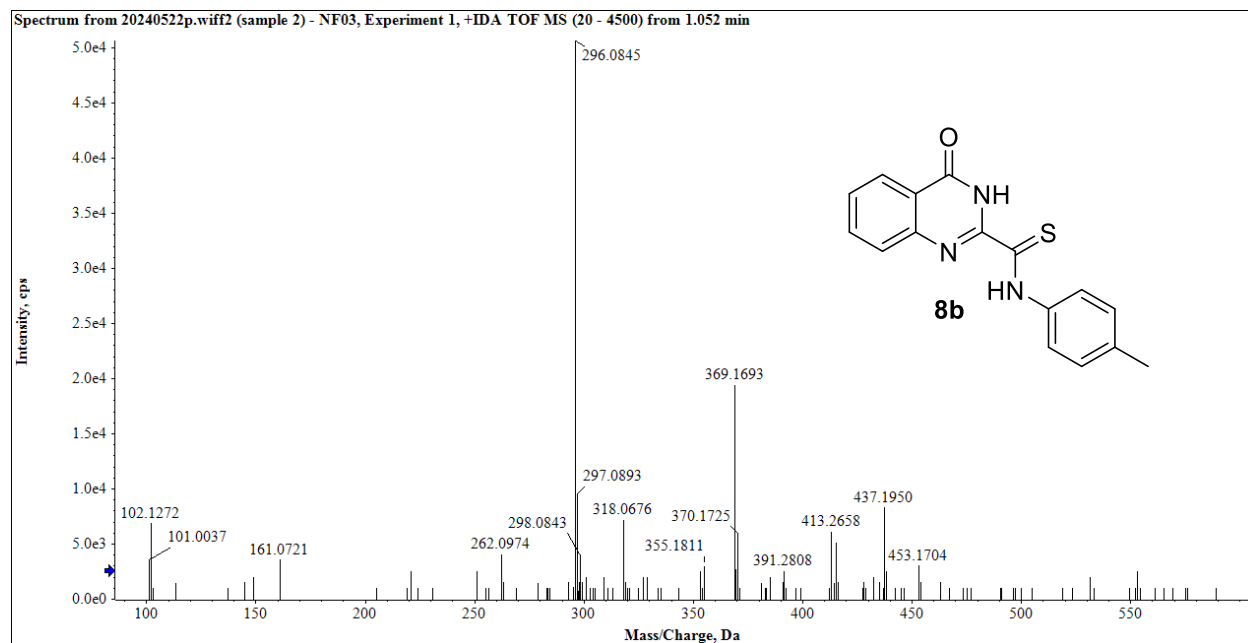
¹H NMR (CDCl₃, 600 MHz) spectrum of compound **8b**



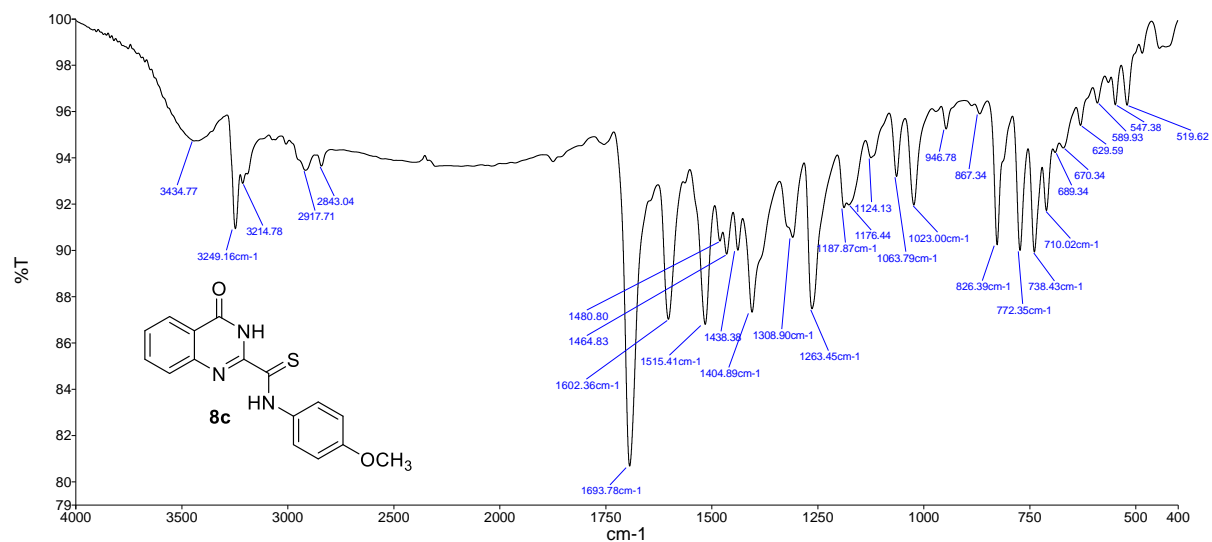
^{13}C NMR (CDCl_3 , 150 MHz) spectrum of compound **8b**



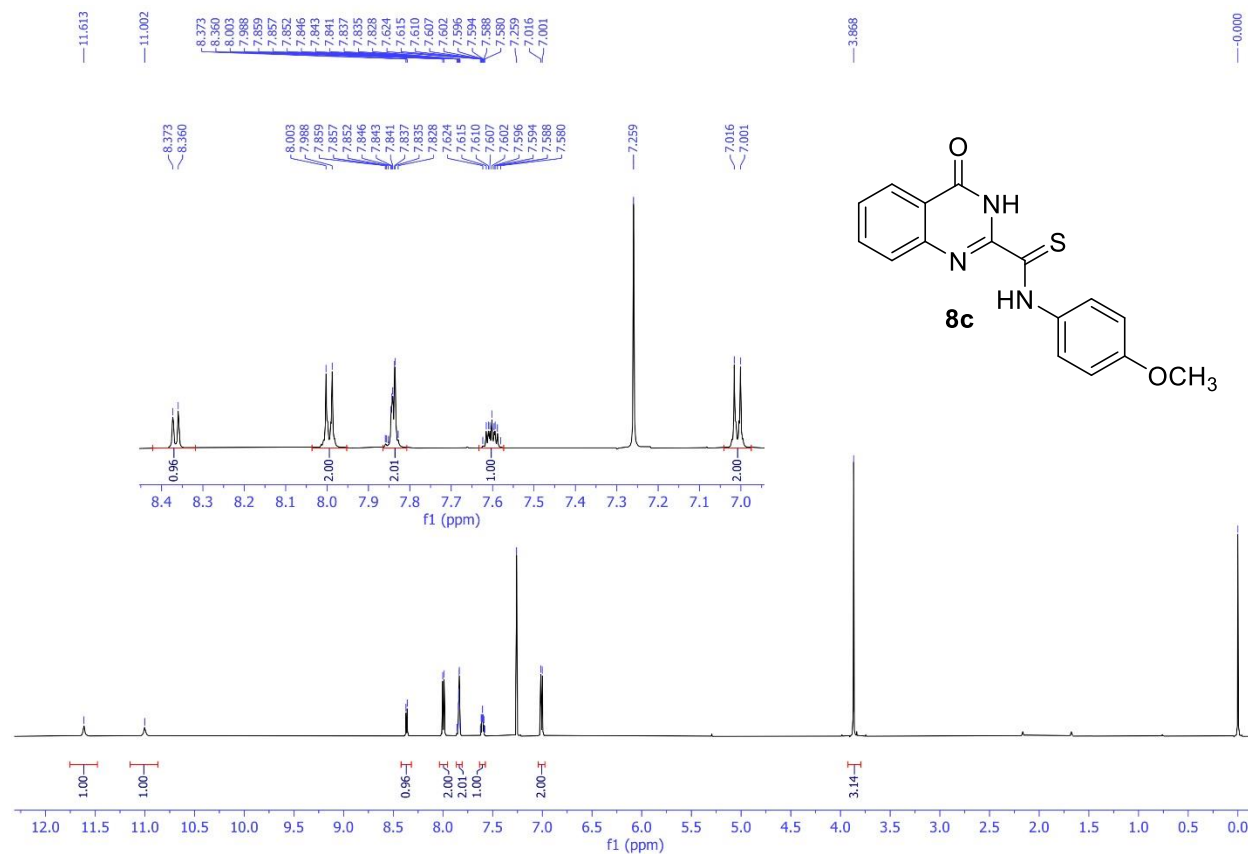
HRMS spectrum of compound **8b**



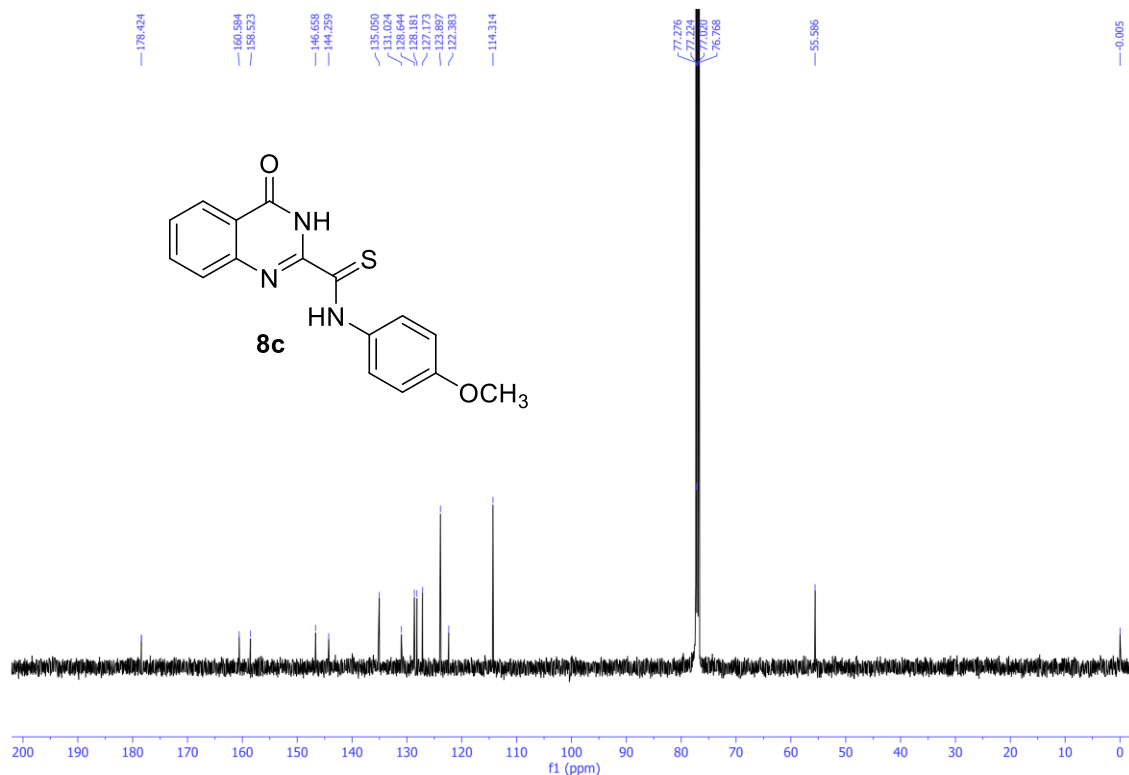
IR spectra of compound **8c**



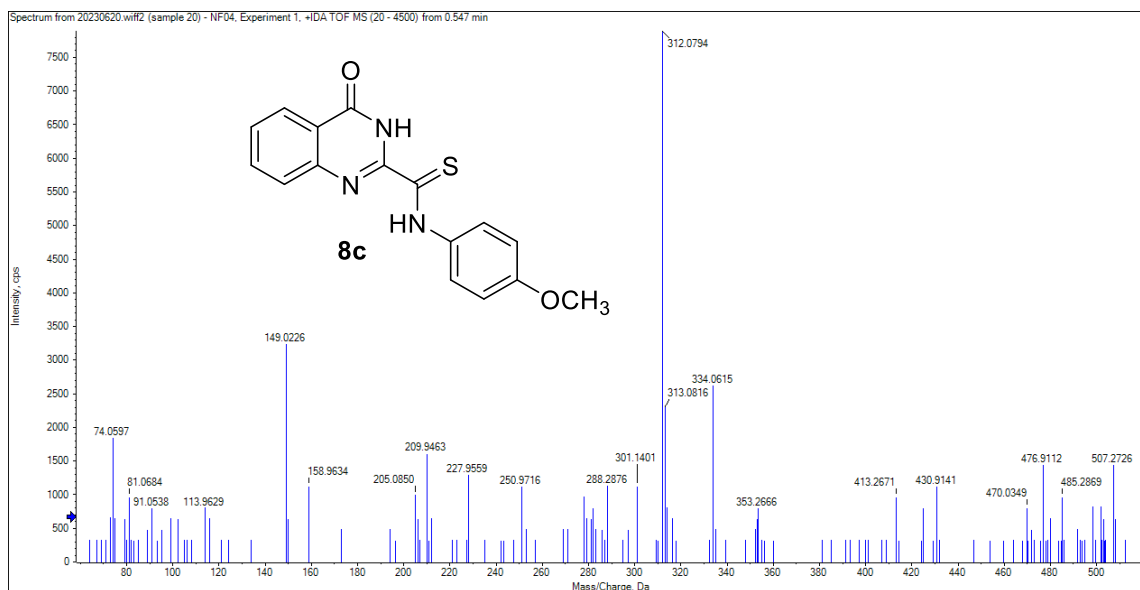
^1H NMR (CDCl_3 , 600 MHz) spectrum of compound **8c**



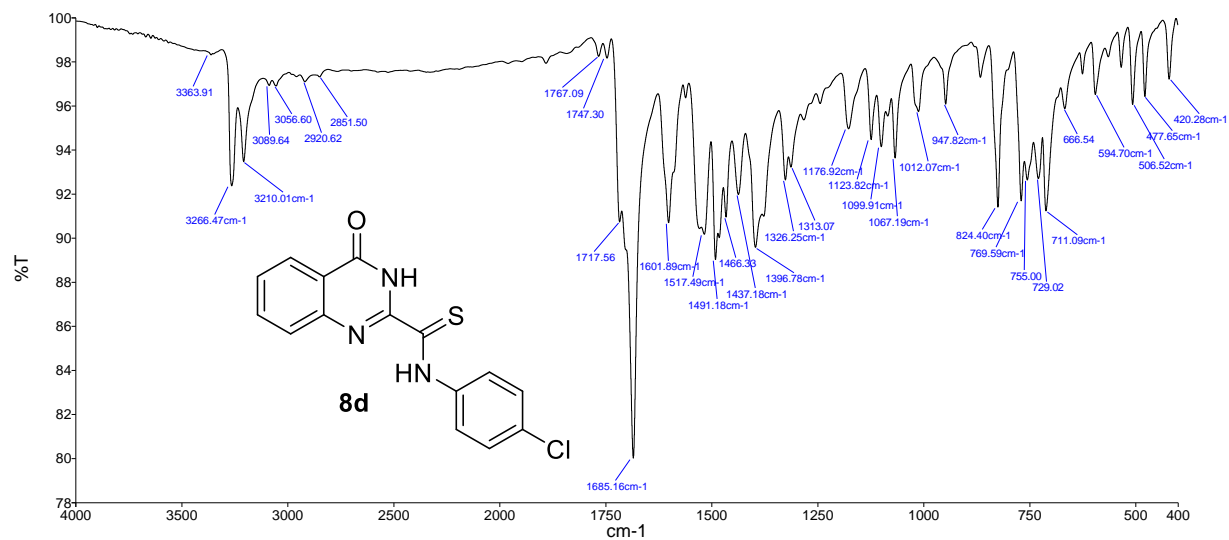
^{13}C NMR (CDCl_3 , 125 MHz) spectrum of compound **8c**



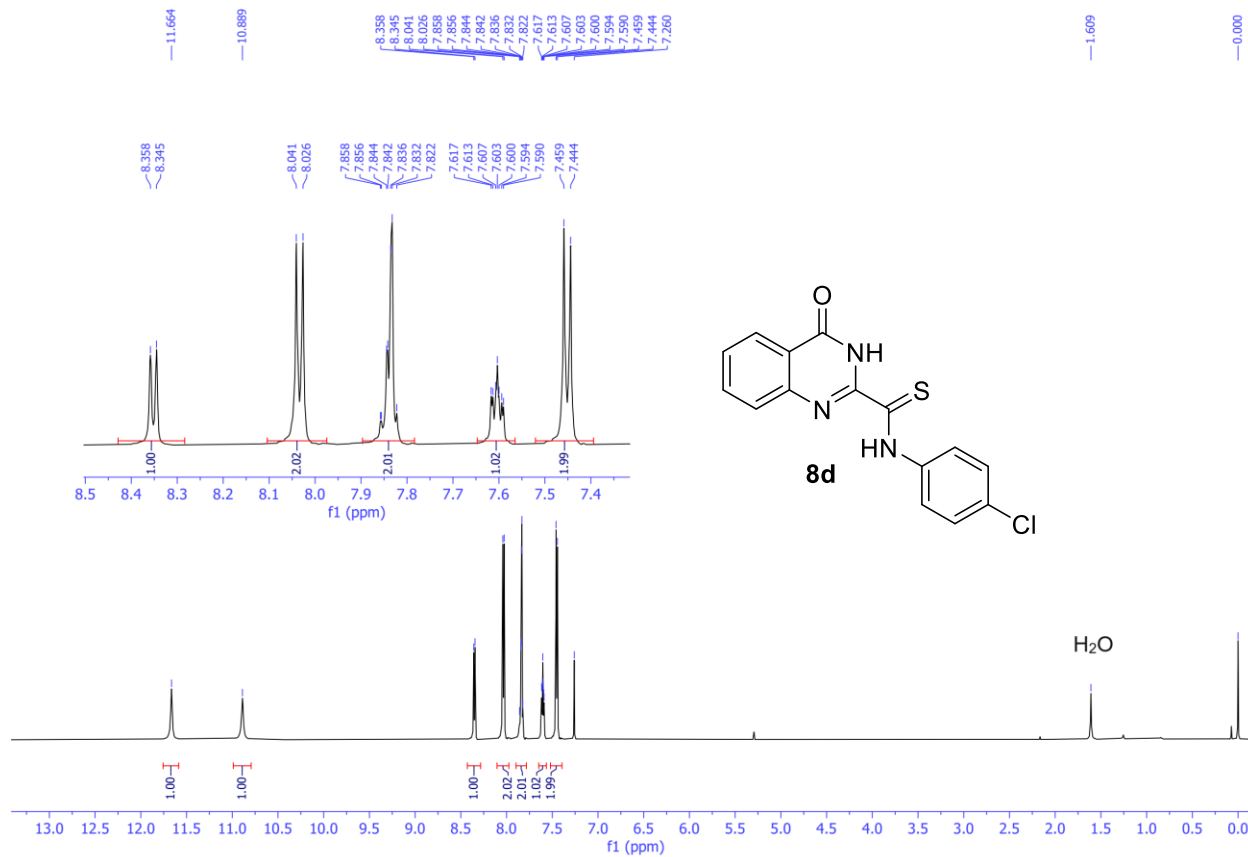
HRMS spectrum of compound **8c**



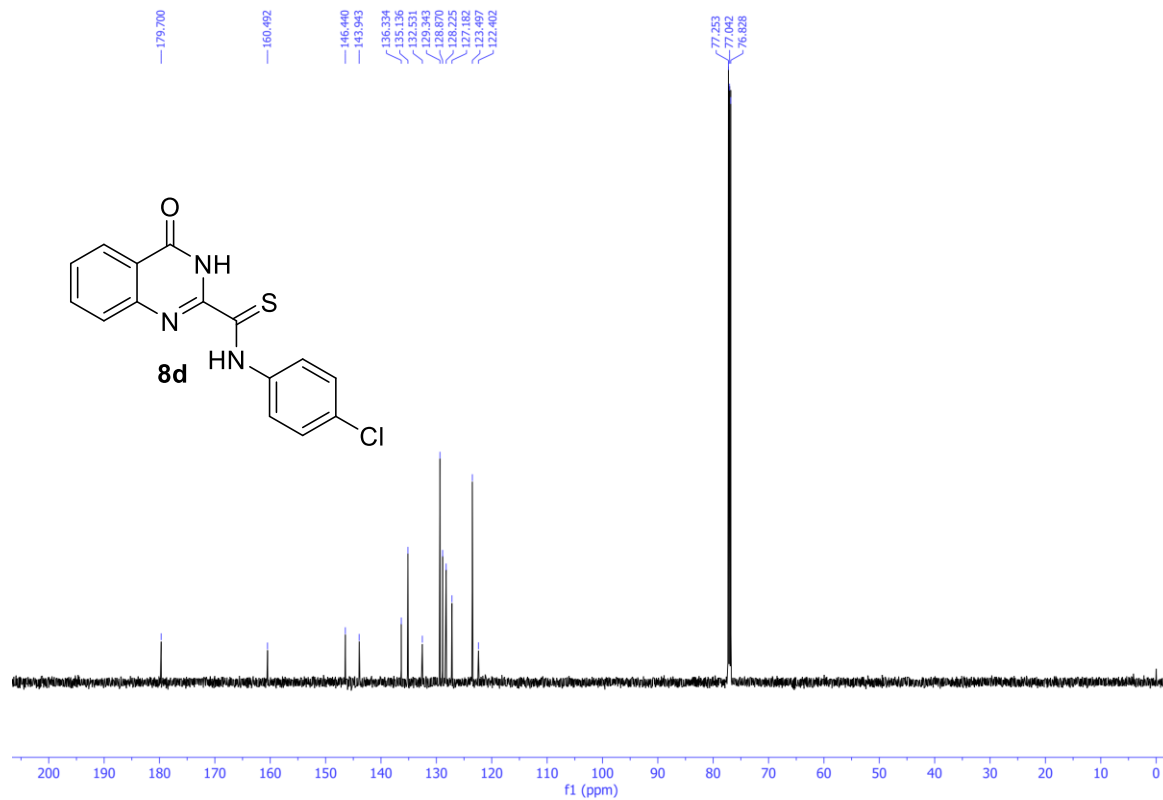
IR of spectra compound **8d**



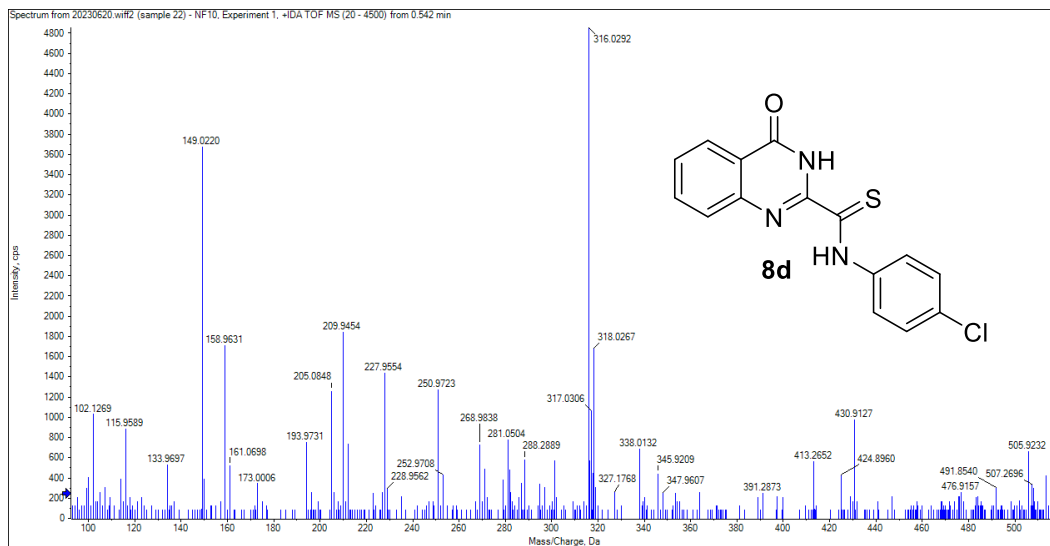
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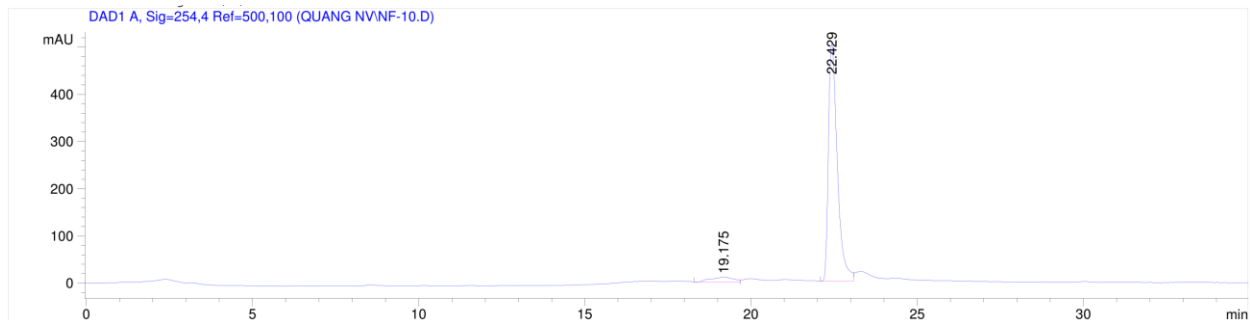
^{13}C NMR (CDCl_3 , 150 MHz) spectrum of compound **8d**



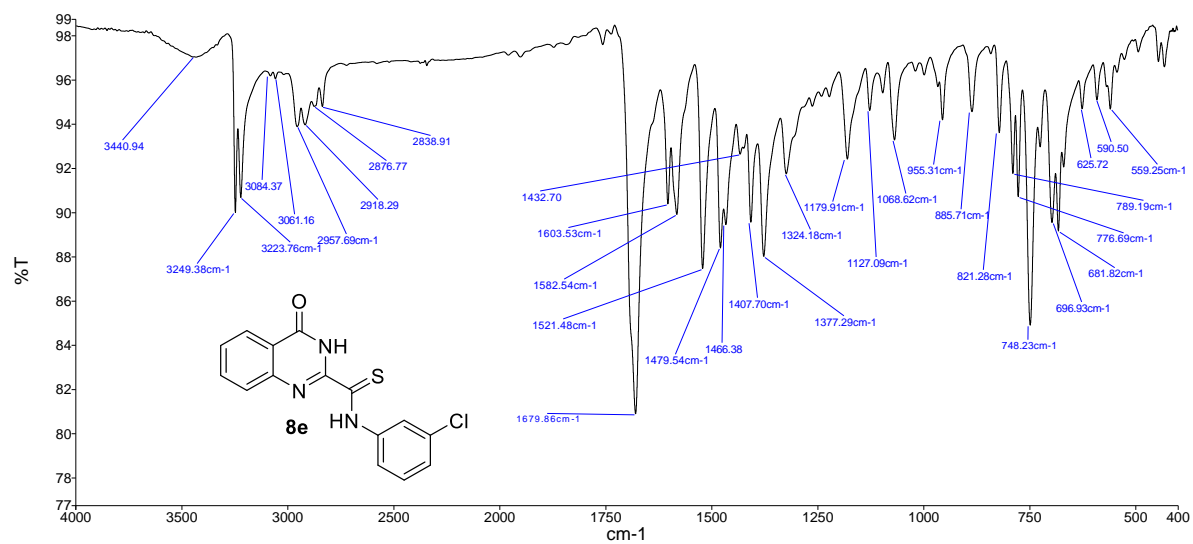
HRMS spectrum of compound **8d**



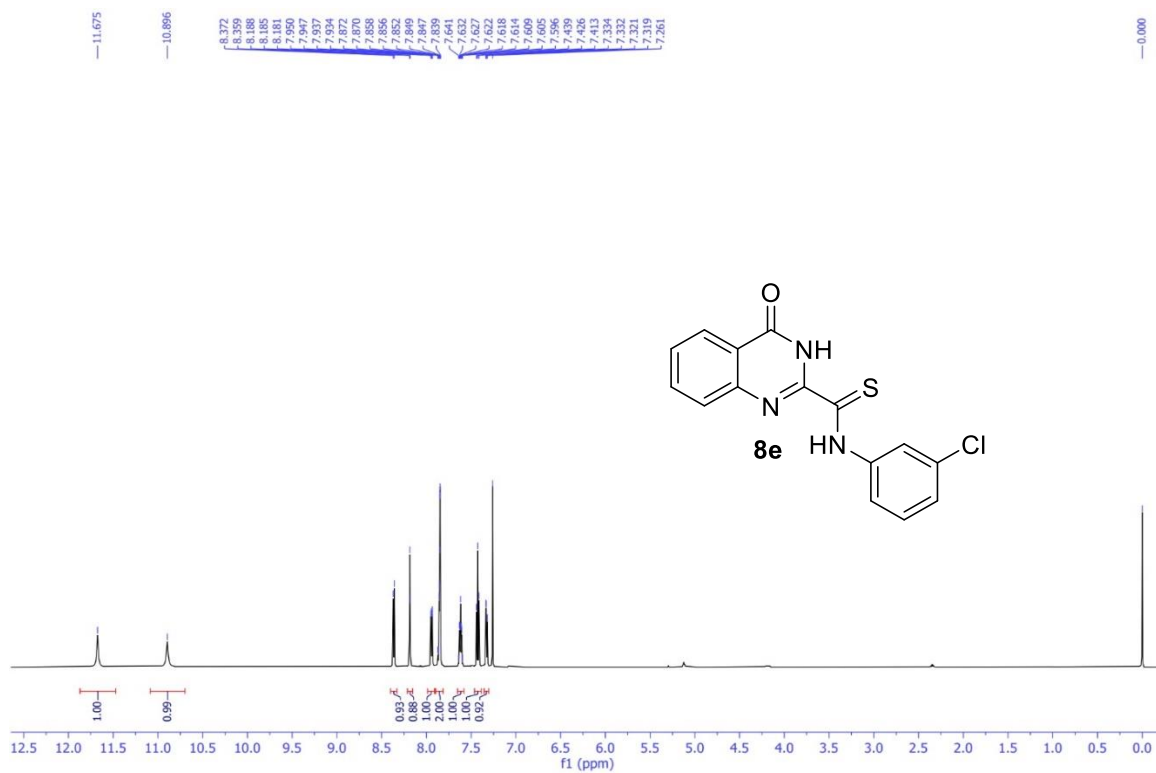
HPLC analysis of compound **8d**



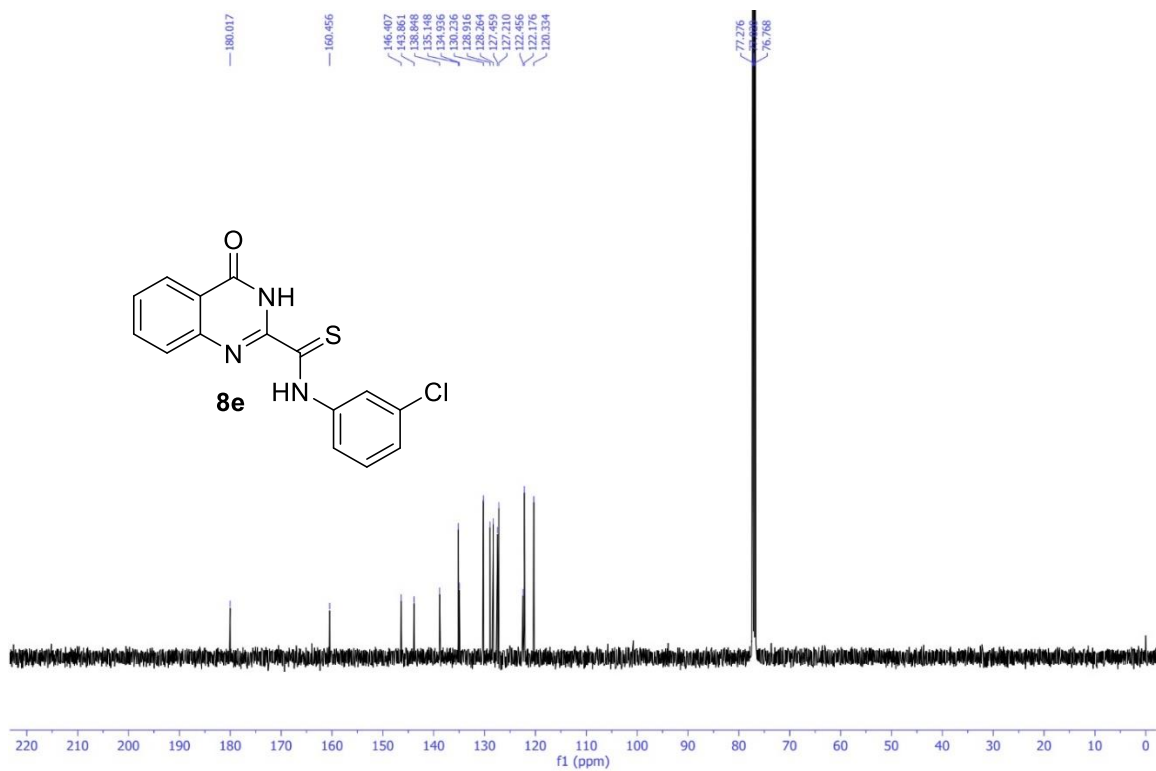
IR of spectra compound **8e**



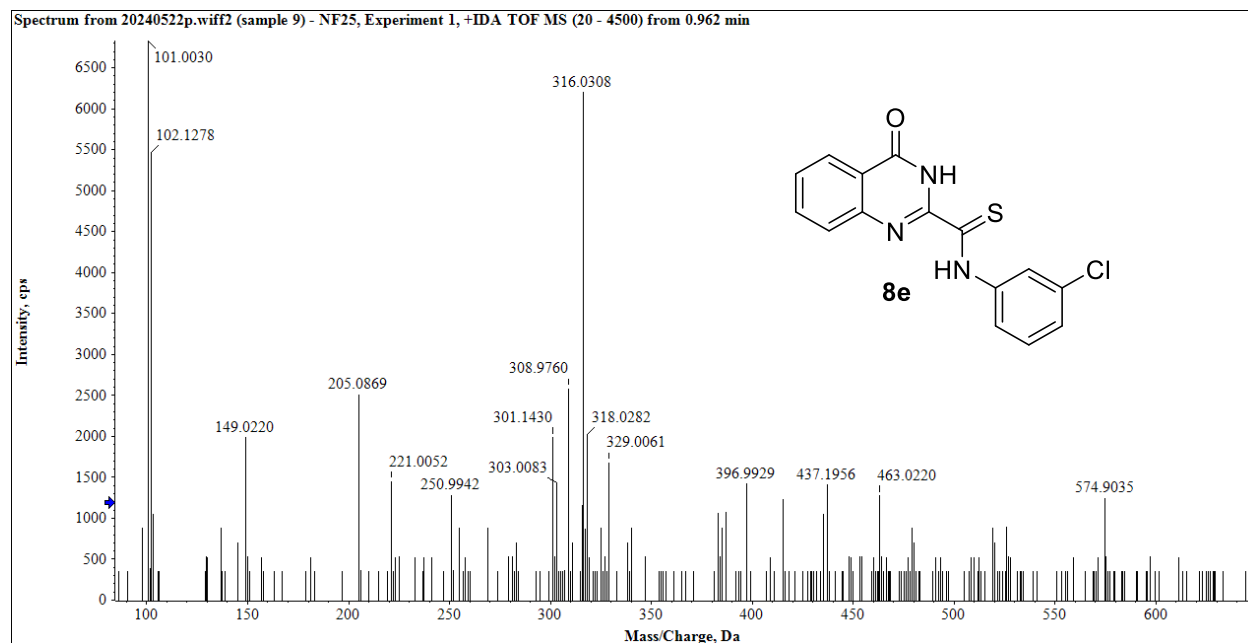
¹H NMR (CDCl₃, 600 MHz) spectrum of compound **8e**



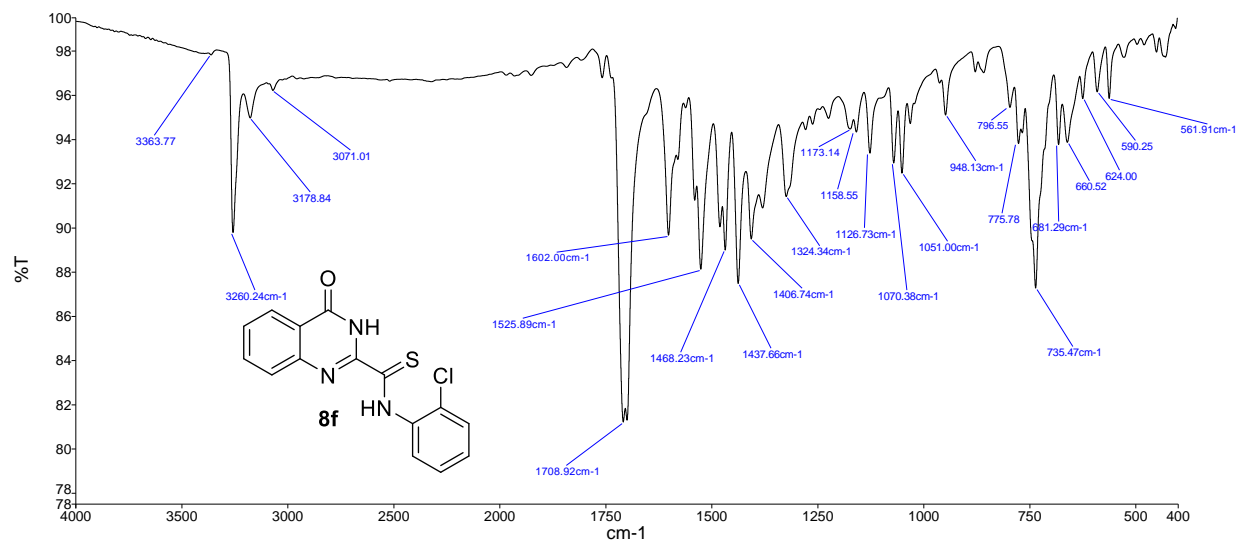
¹³C NMR (CDCl₃, 600 MHz) spectrum of compound **8e**



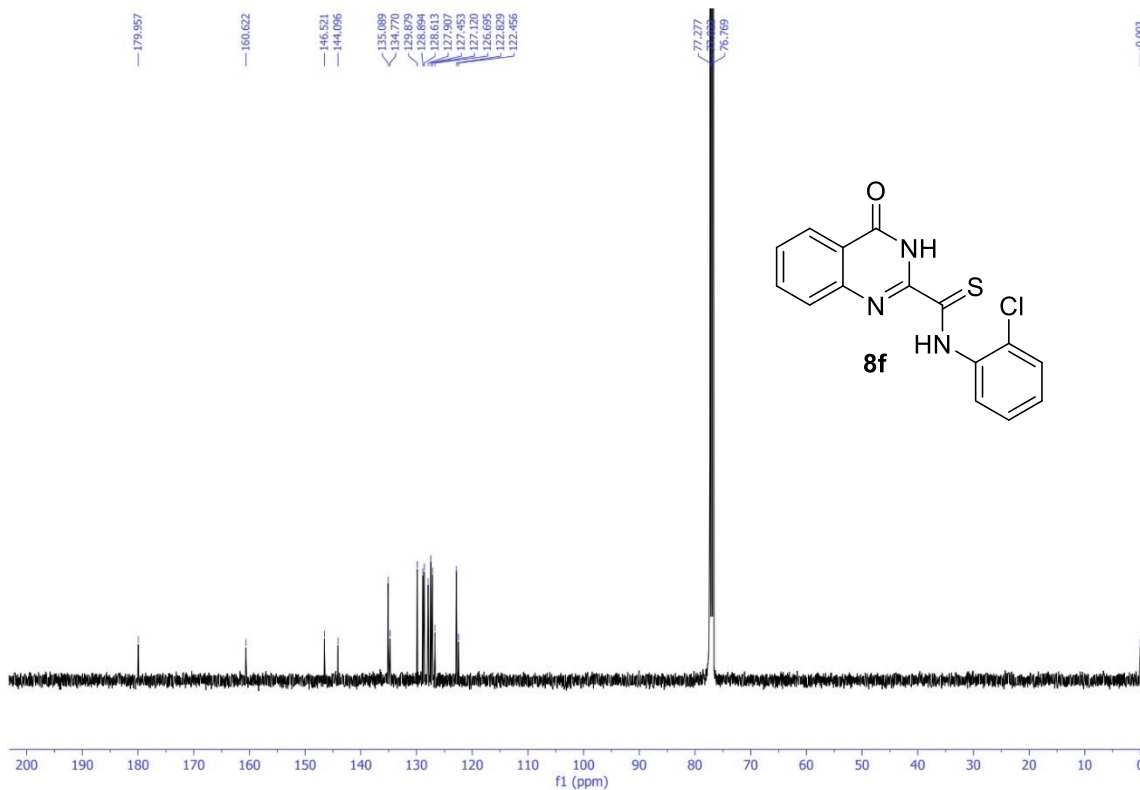
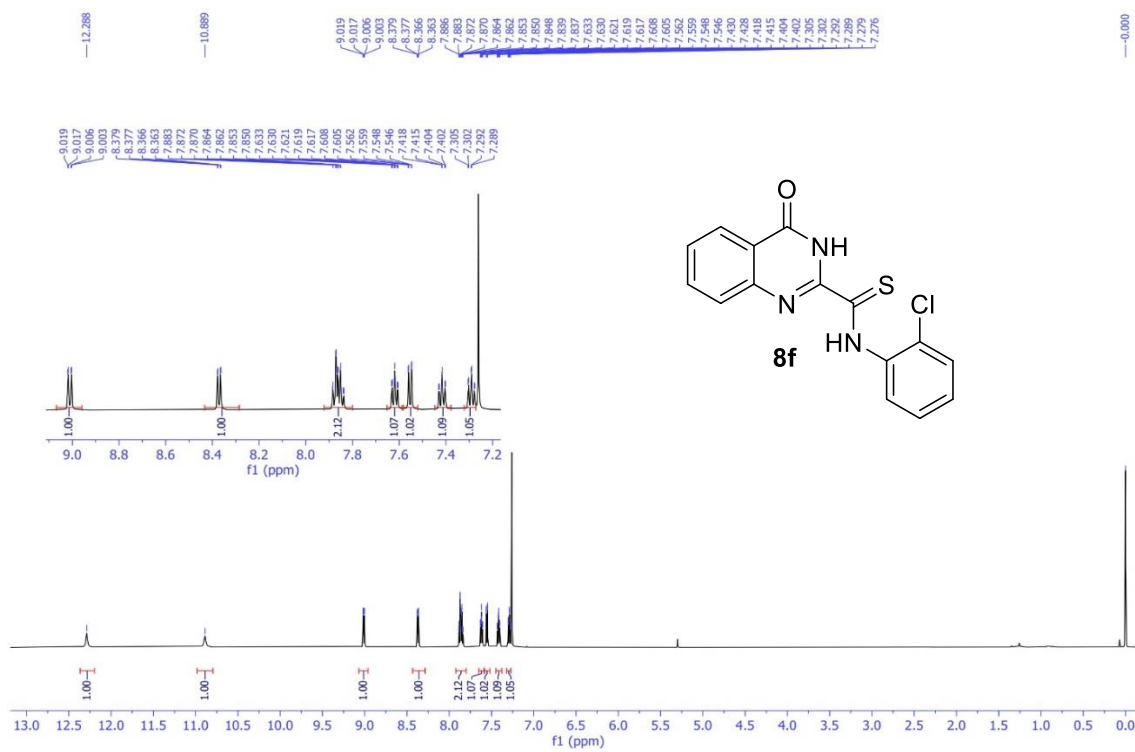
HRMS spectrum of compound **8e**



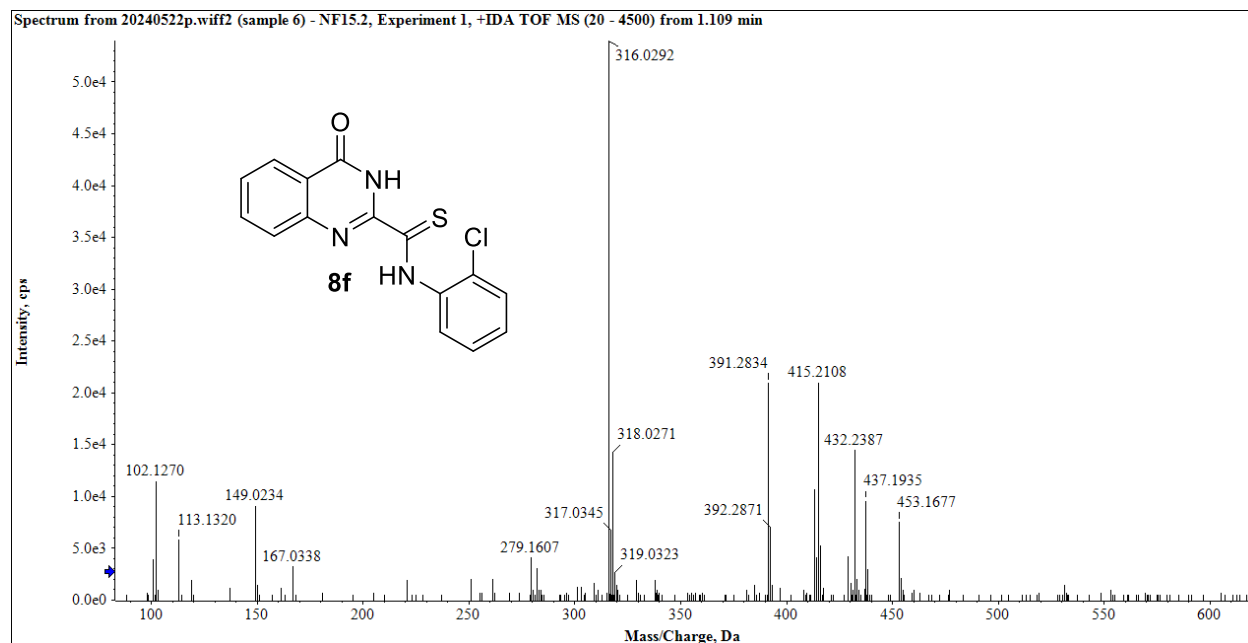
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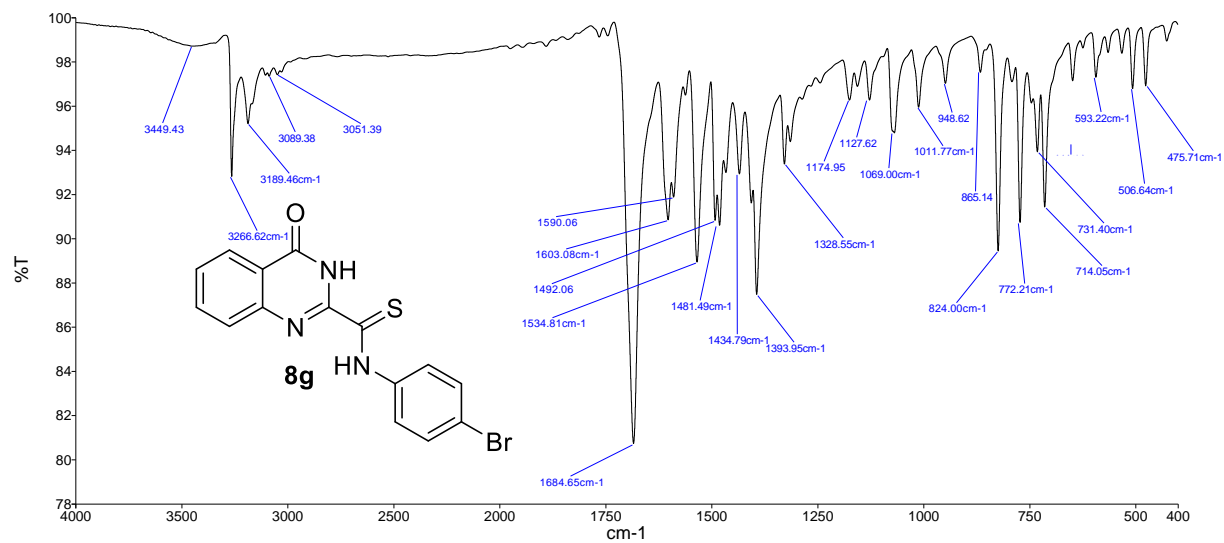
¹H NMR (CDCl₃, 600 MHz) spectrum of compound **8f**



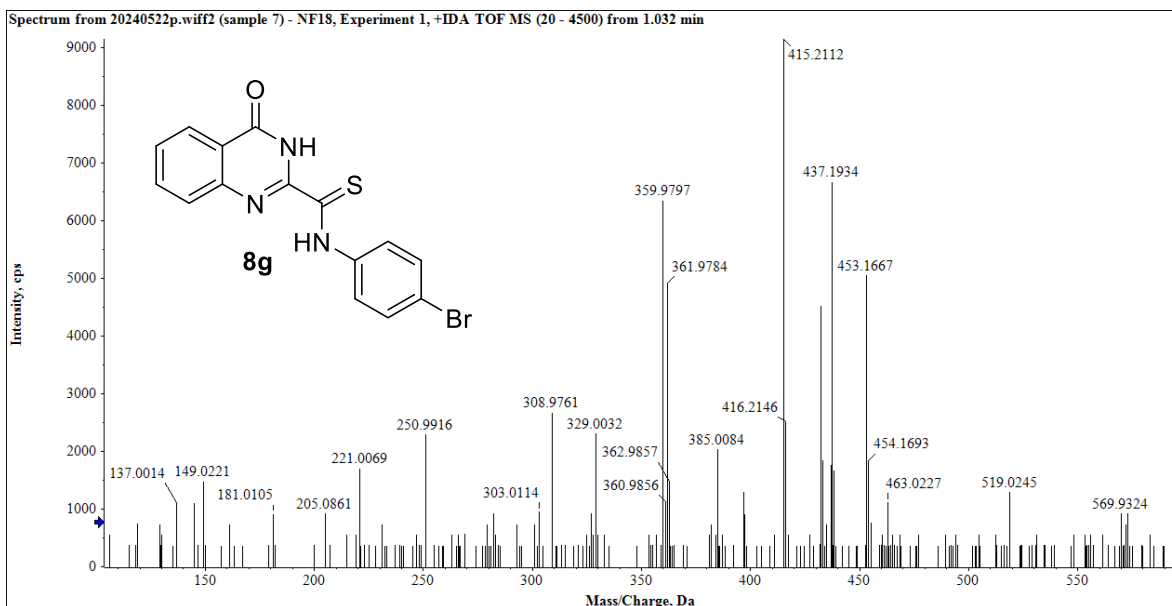
HRMS spectrum of compound **8f**



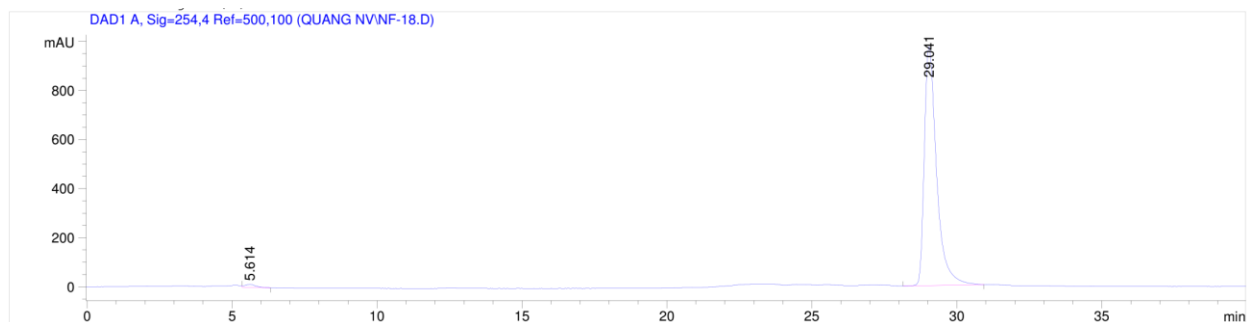
IR of spectra compound **8g**



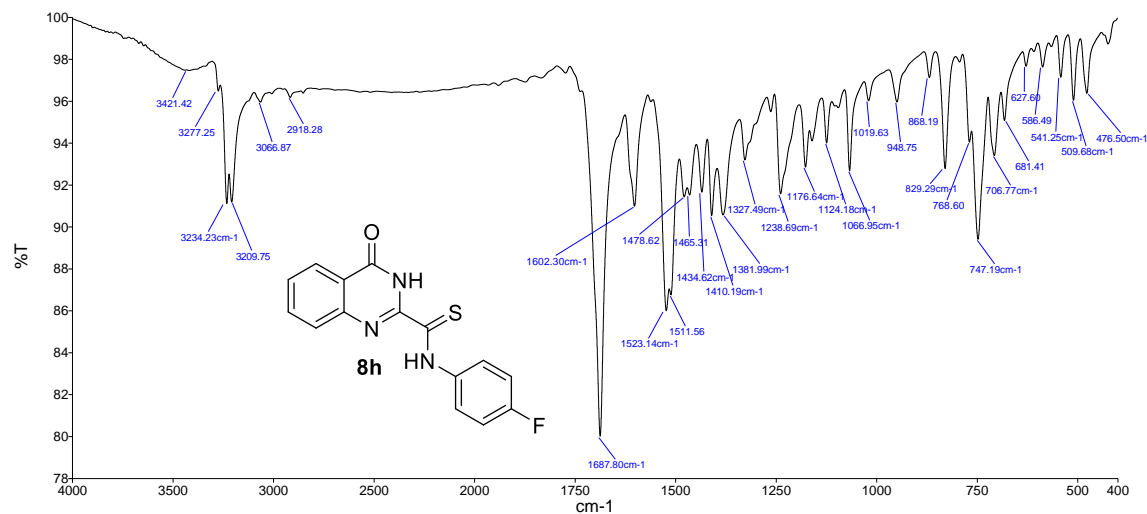
HRMS spectrum of compound **8g**



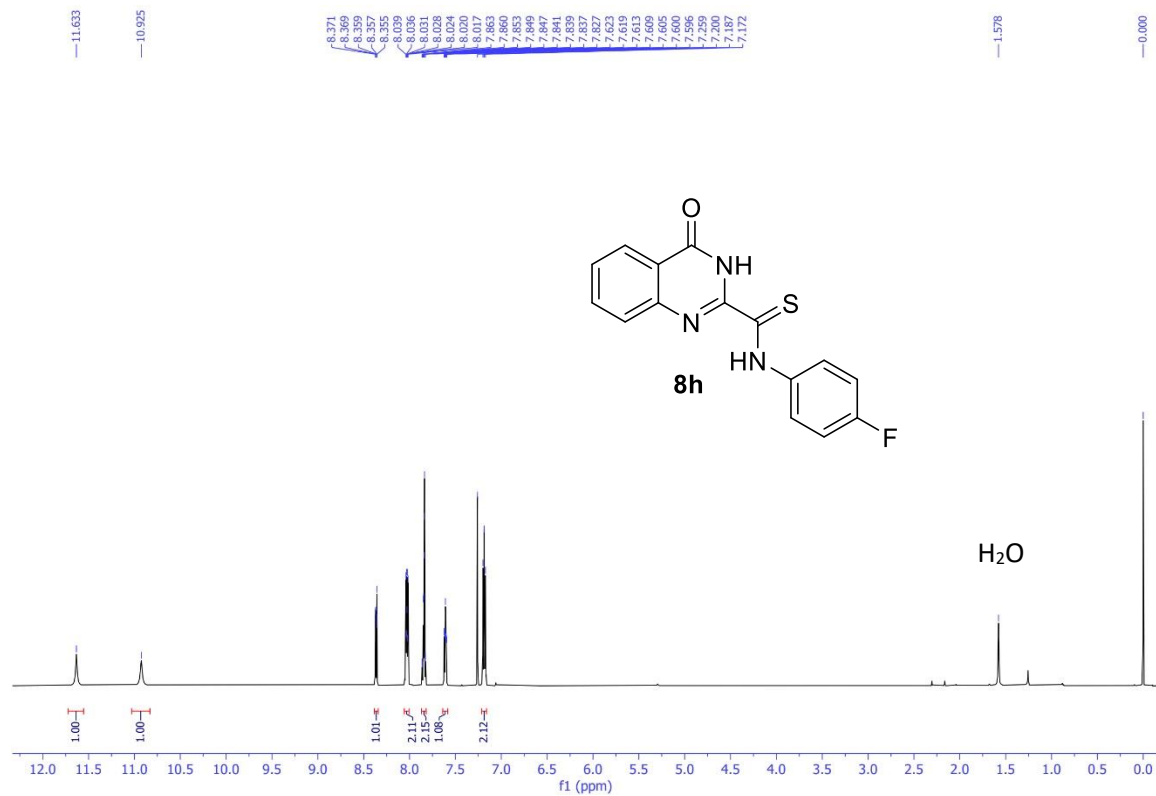
HPLC analysis of compound **8g**



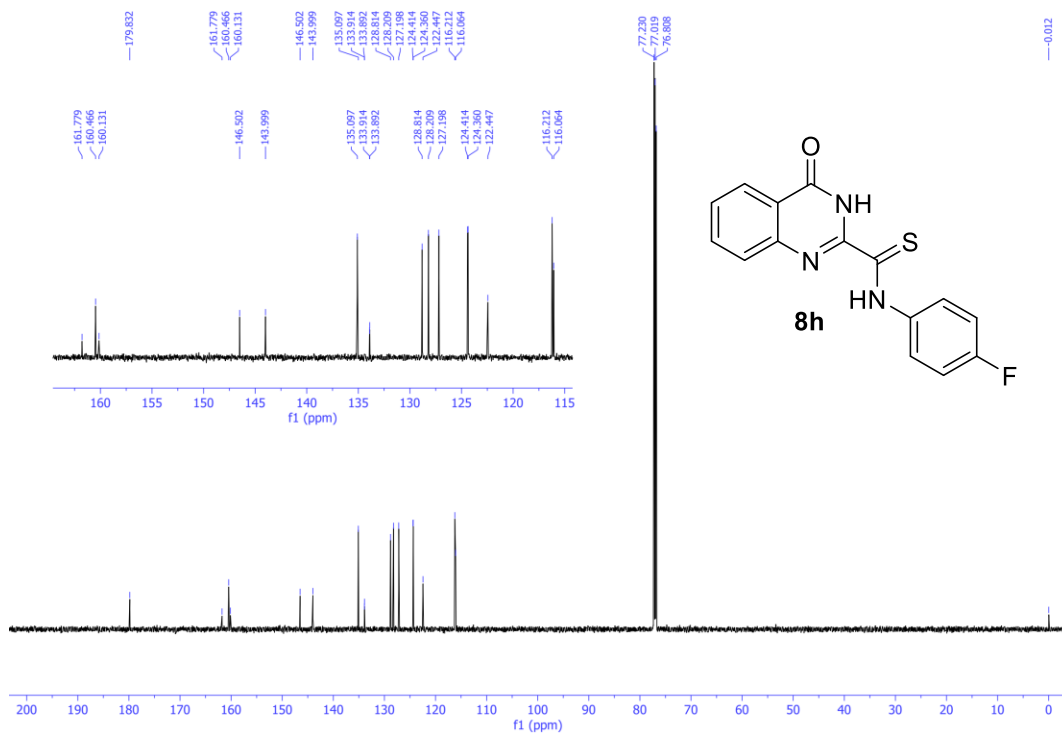
IR of spectra compound **8h**



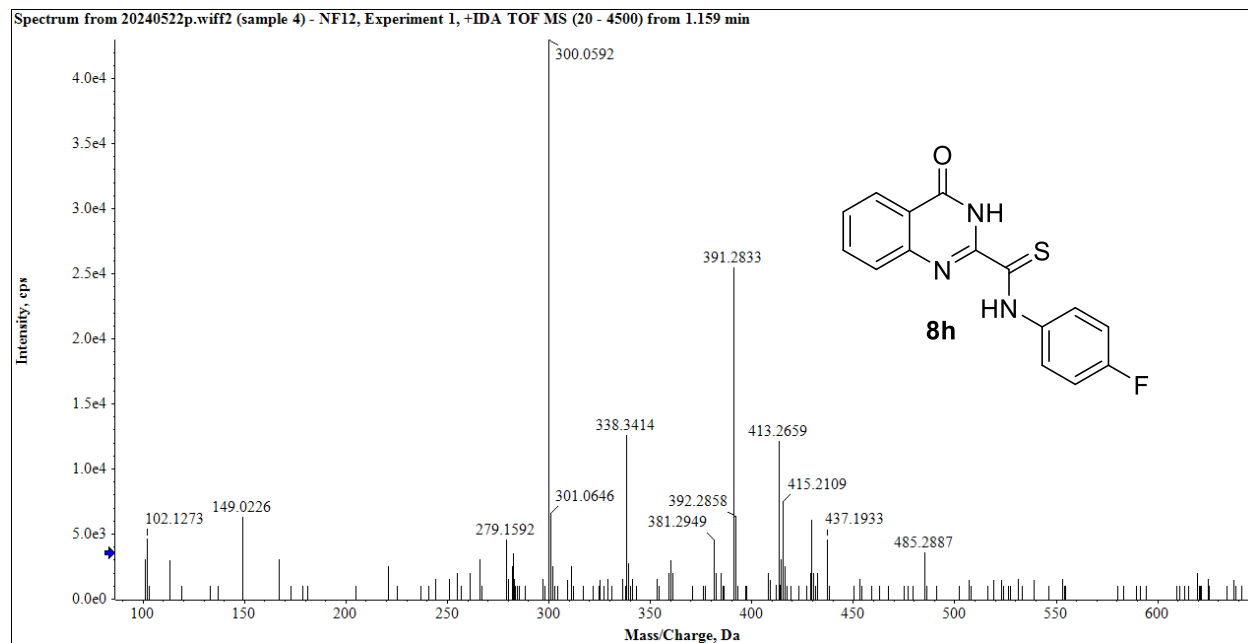
¹H NMR (CDCl₃, 600 MHz) spectrum of **8h**



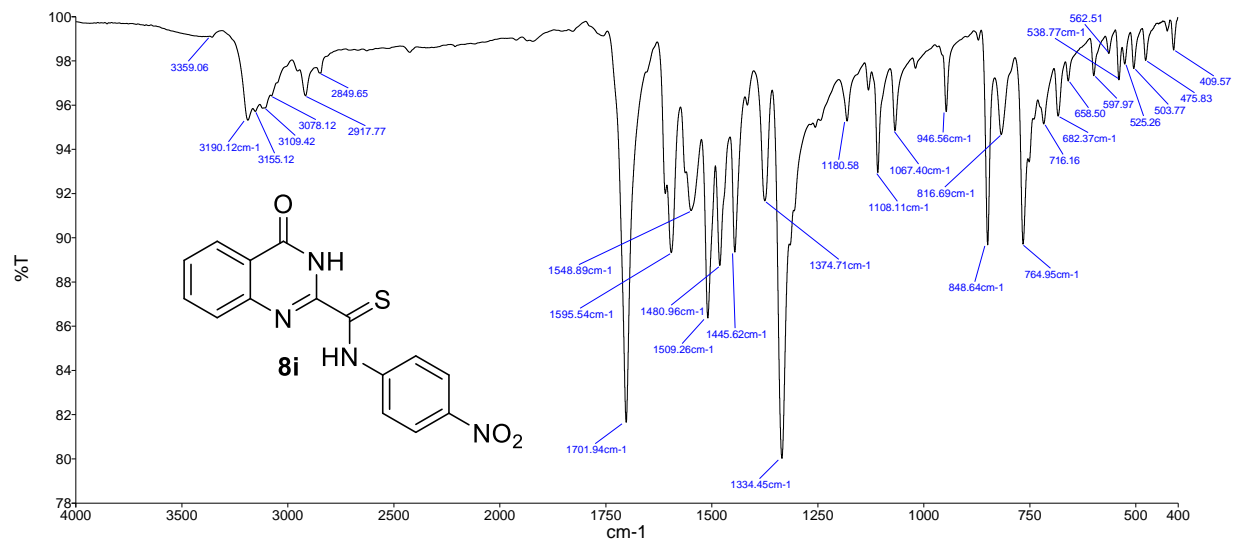
¹³C NMR (CDCl₃, 150 MHz) spectrum of compound **8h**



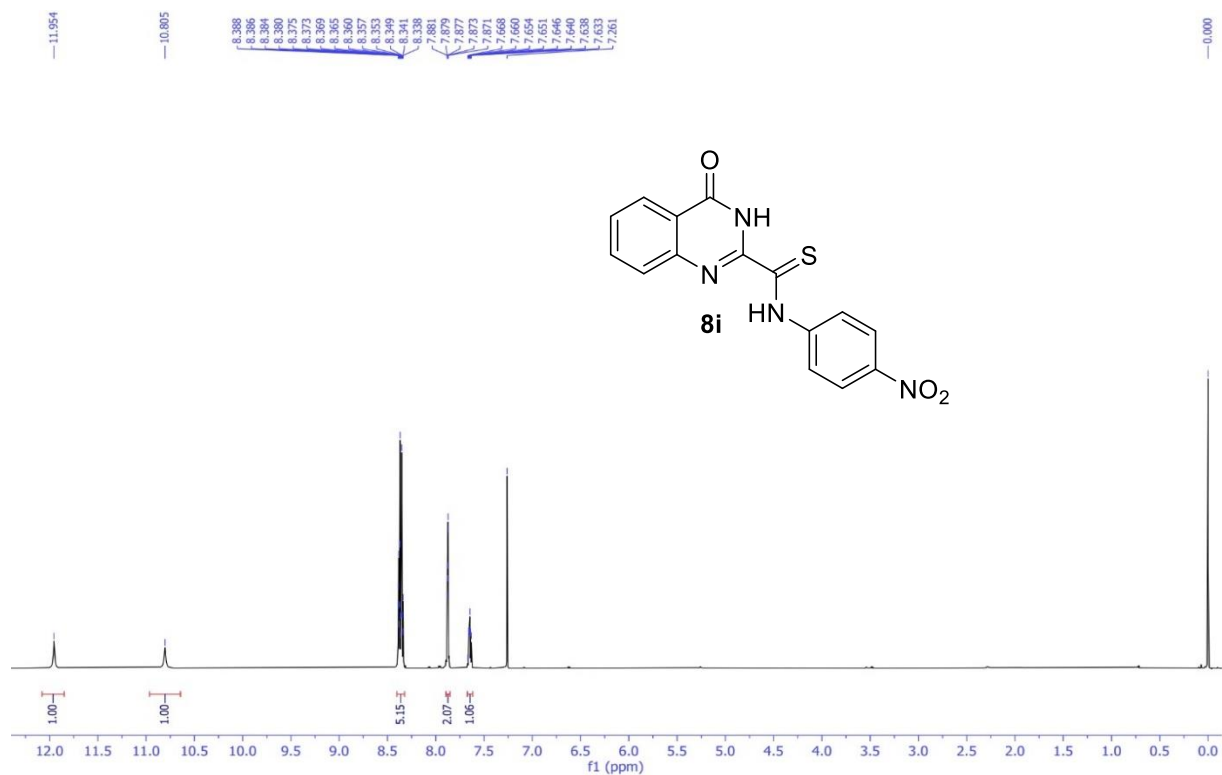
HRMS spectrum of compound **8h**



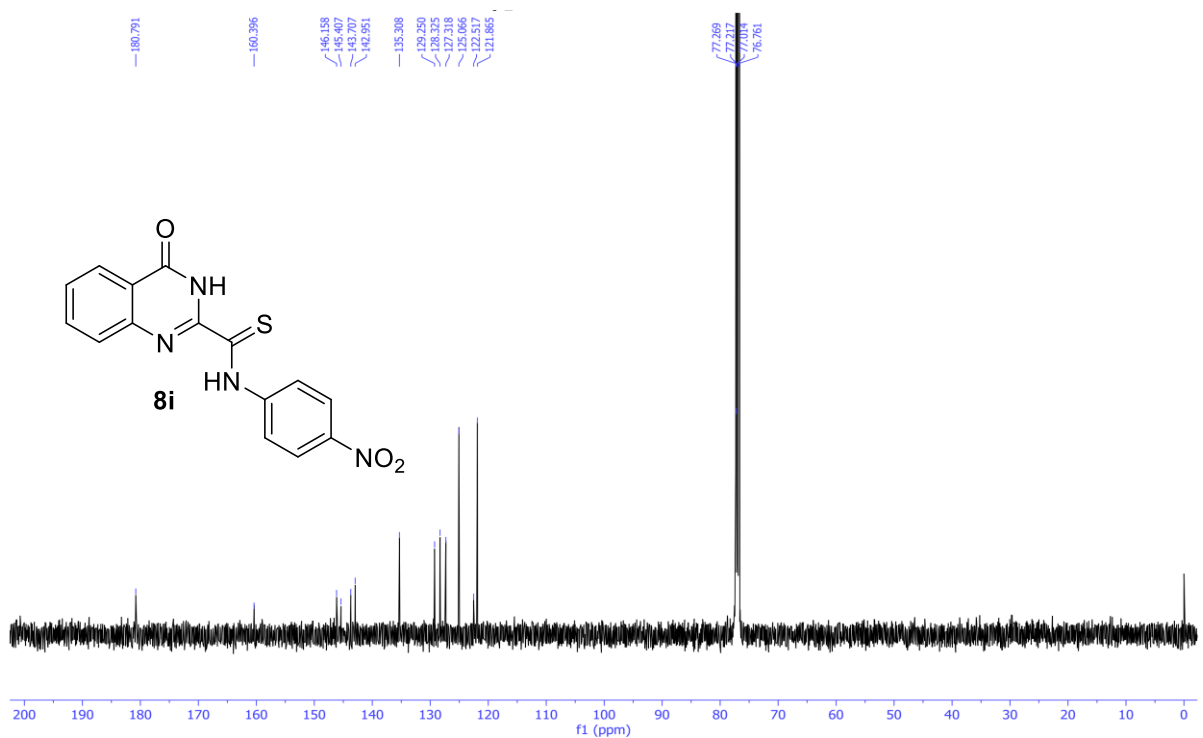
IR of spectra compound **8i**



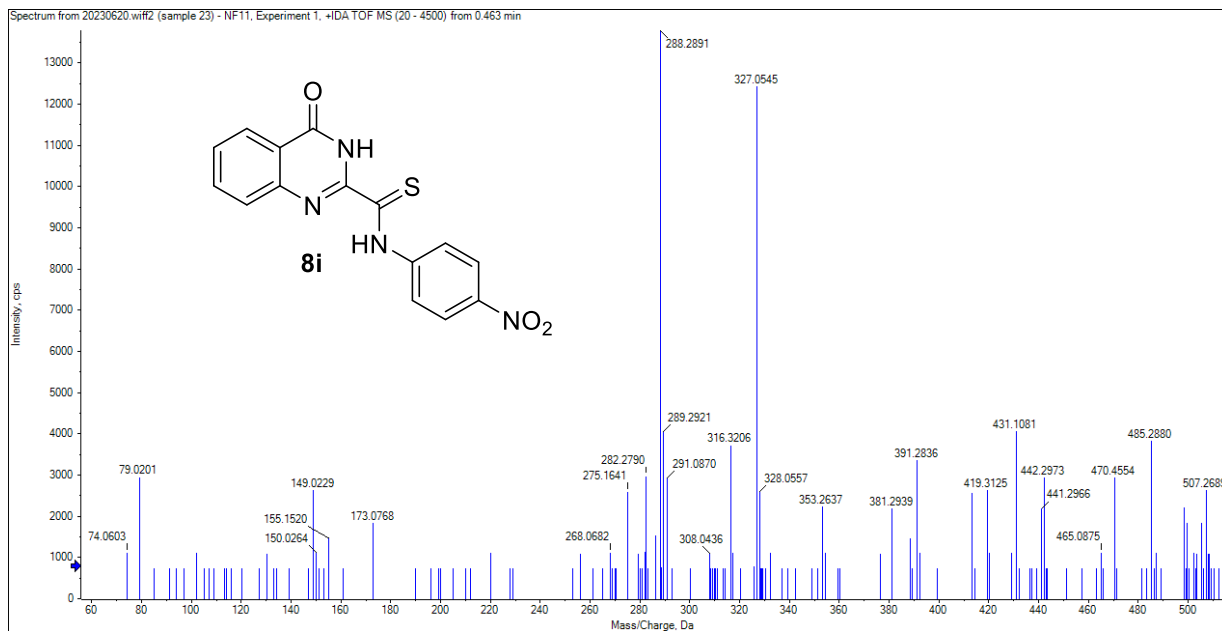
¹H NMR (CDCl₃, 600 MHz) spectrum of compound **8i**



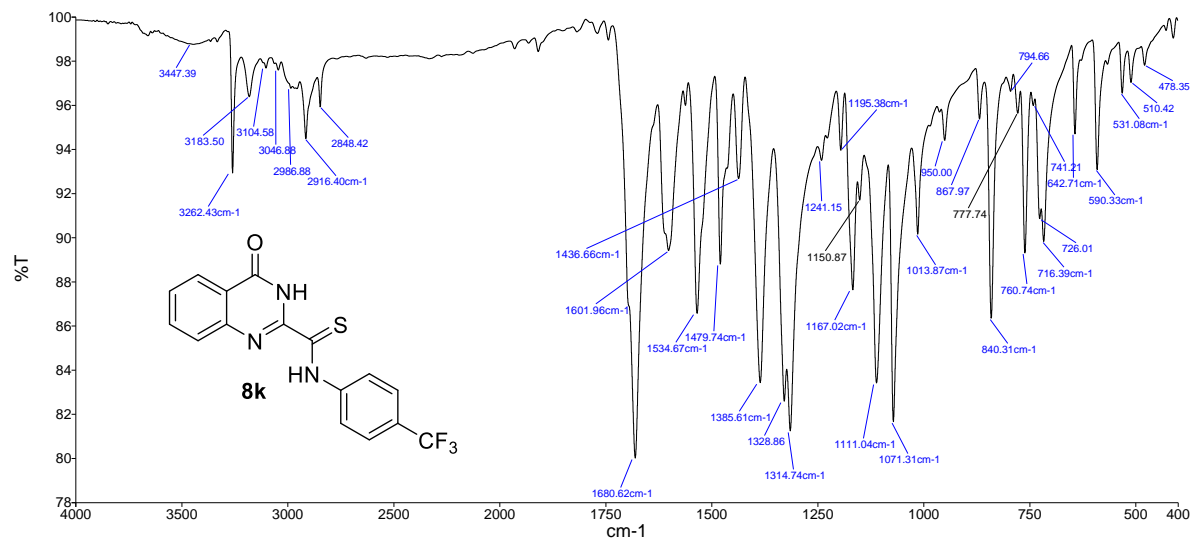
¹³C NMR (CDCl₃, 125 MHz) spectrum of compound **8i**



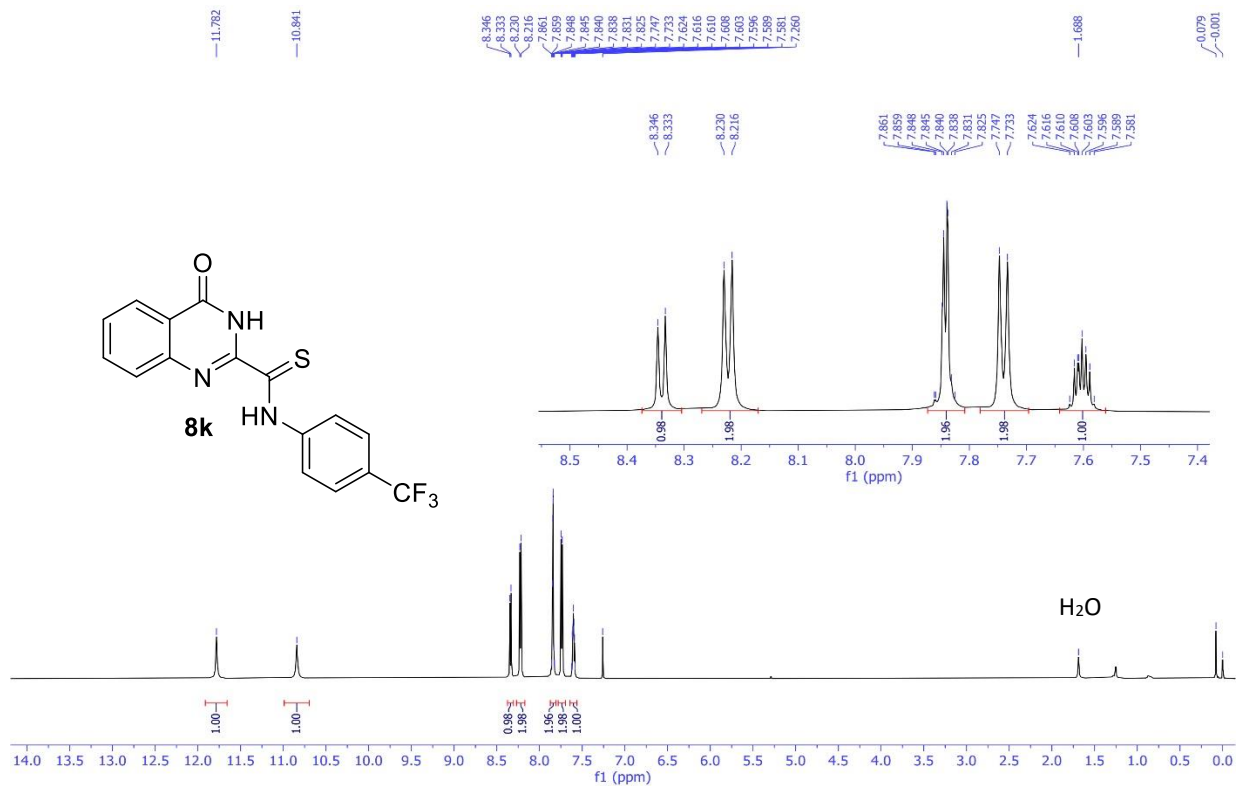
HRMS spectrum of compound **8i**



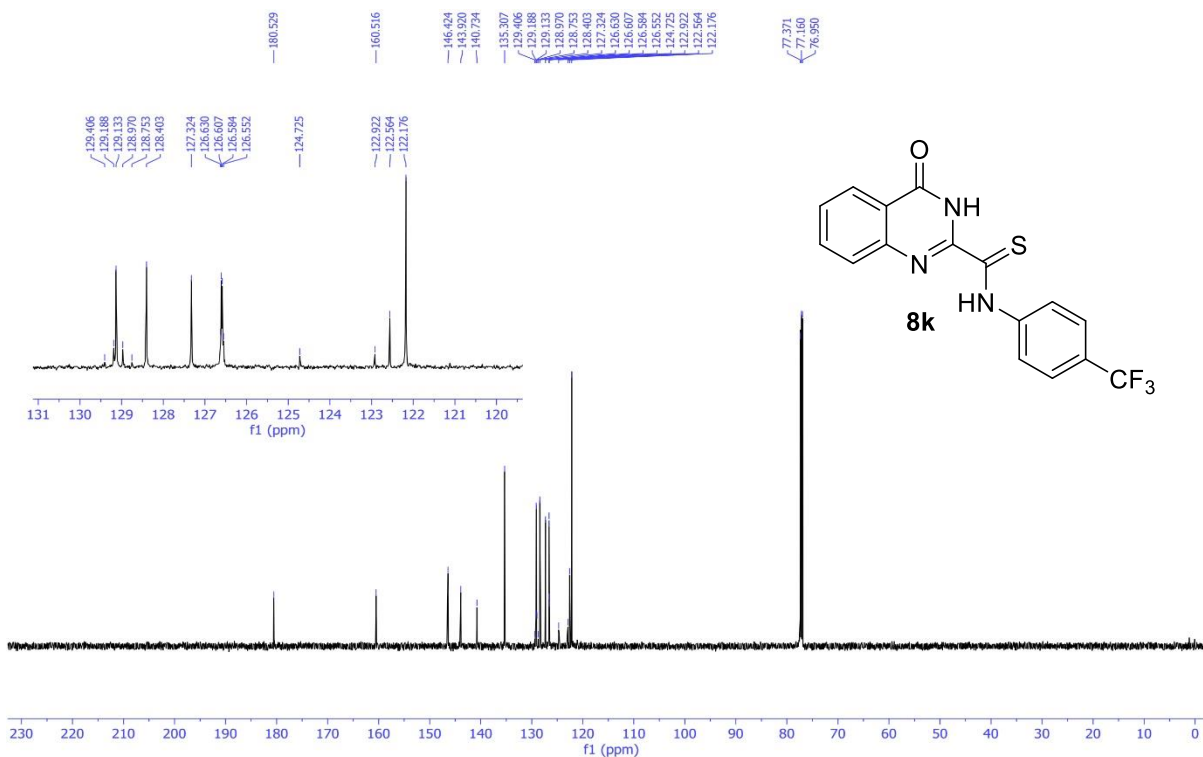
IR of spectra compound **8k**



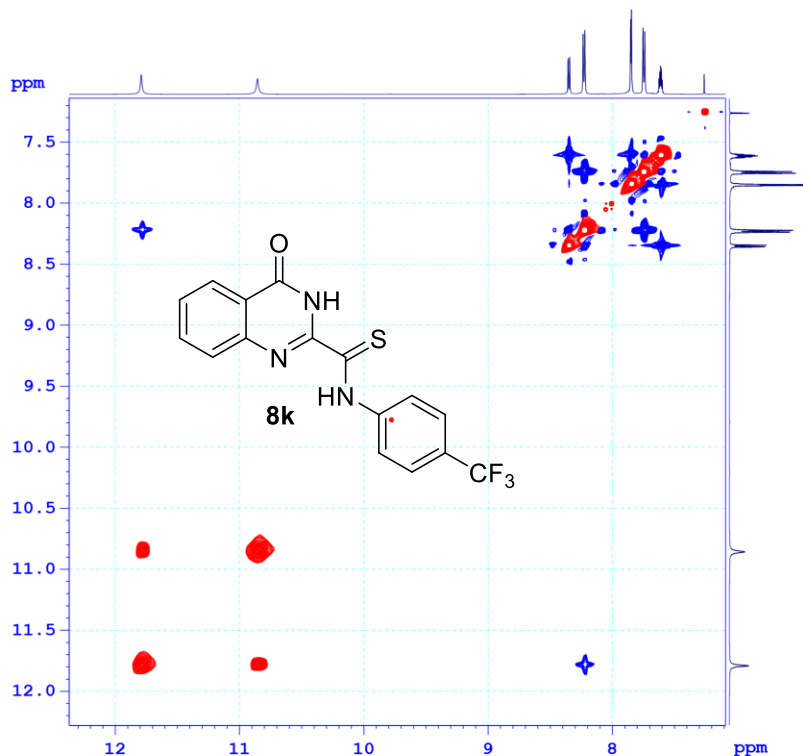
¹H NMR (CDCl₃, 600 MHz) spectrum of compound **8k**



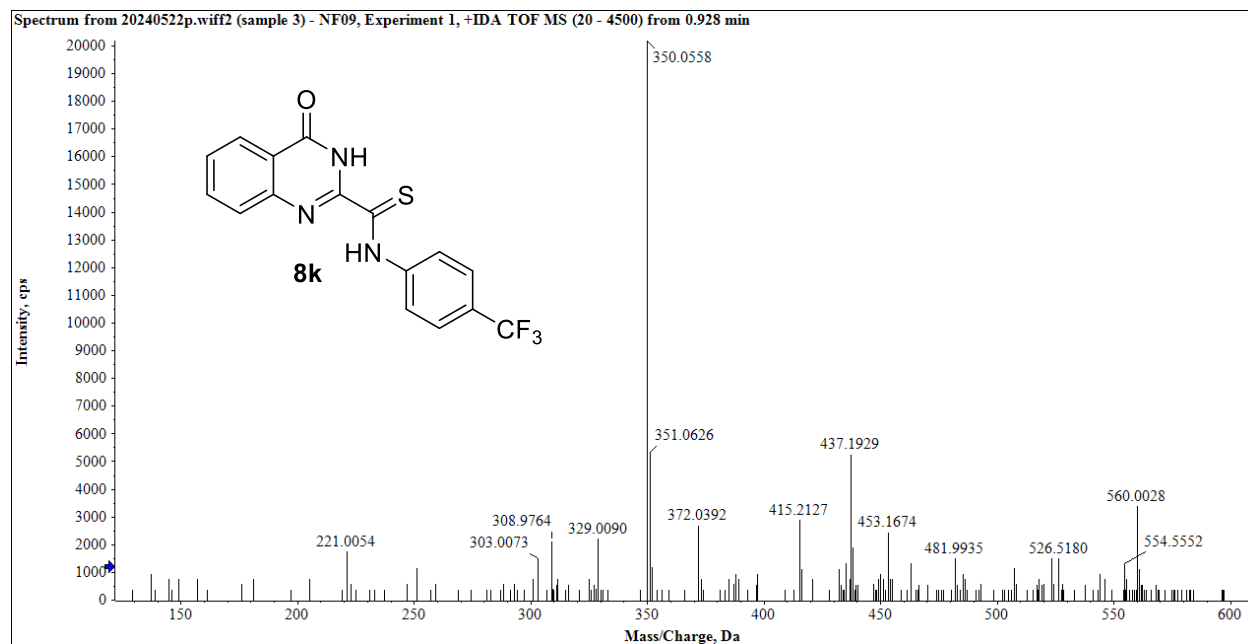
¹³C NMR (CDCl₃, 150 MHz) spectrum of compound **8k**



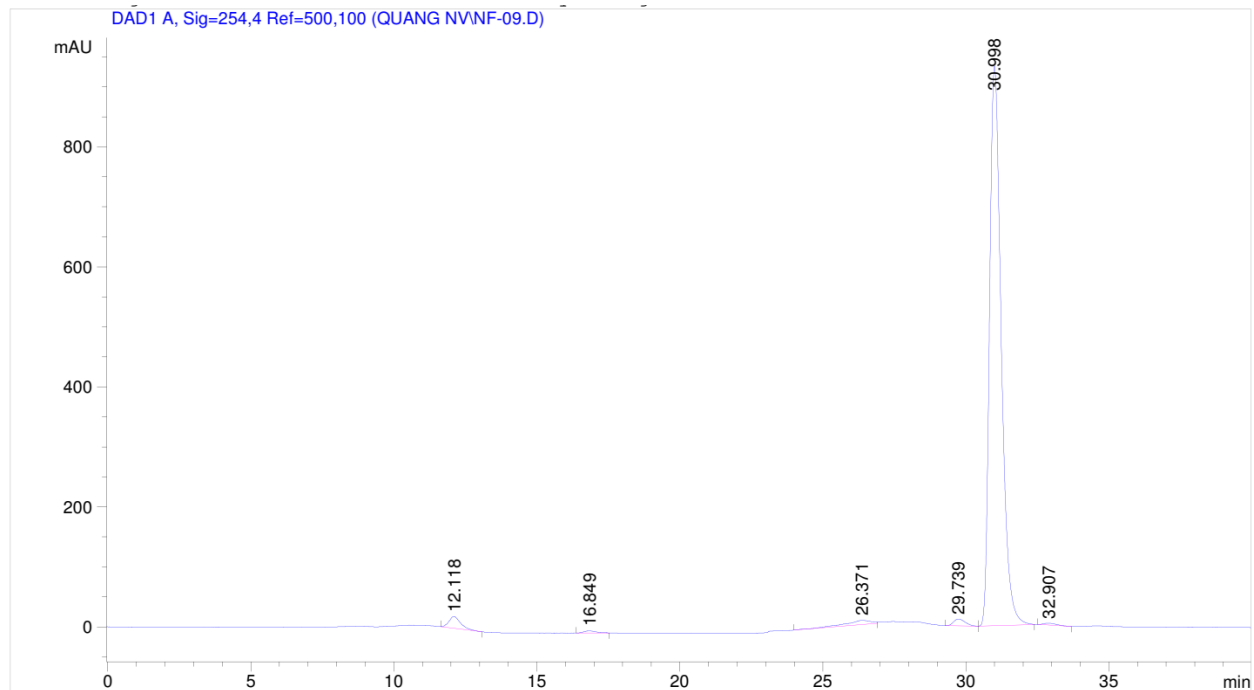
NOESY (CDCl₃) spectrum of compound **8k**



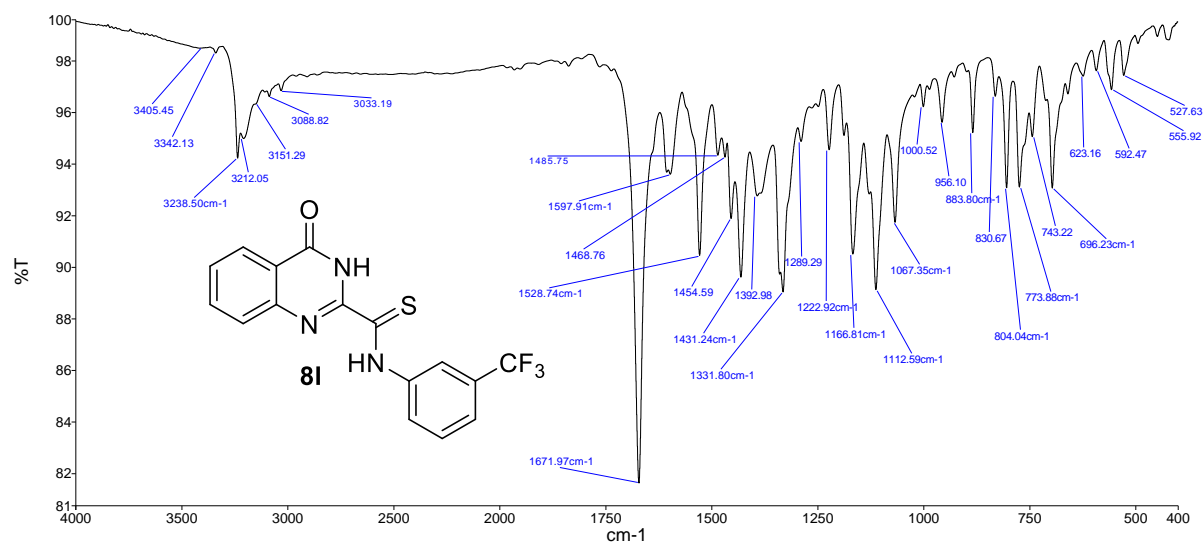
HRMS spectrum of compound **8k**



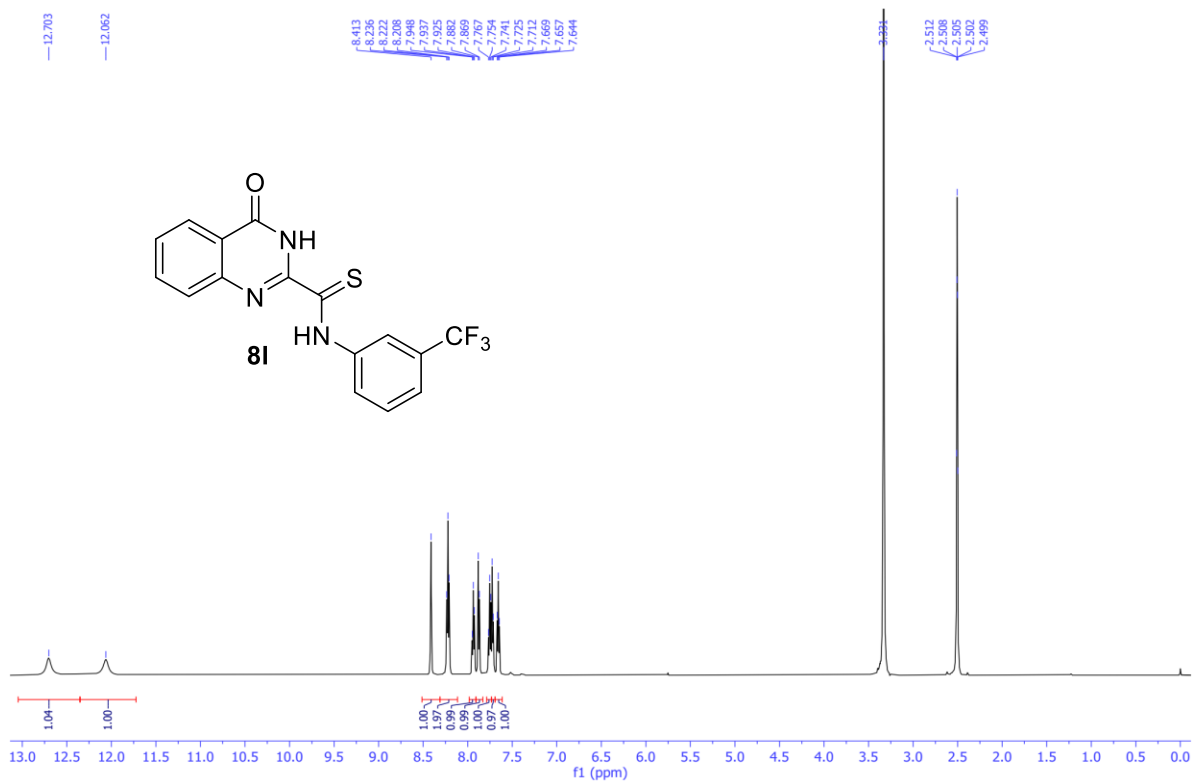
HPLC analysis of compound **8k**



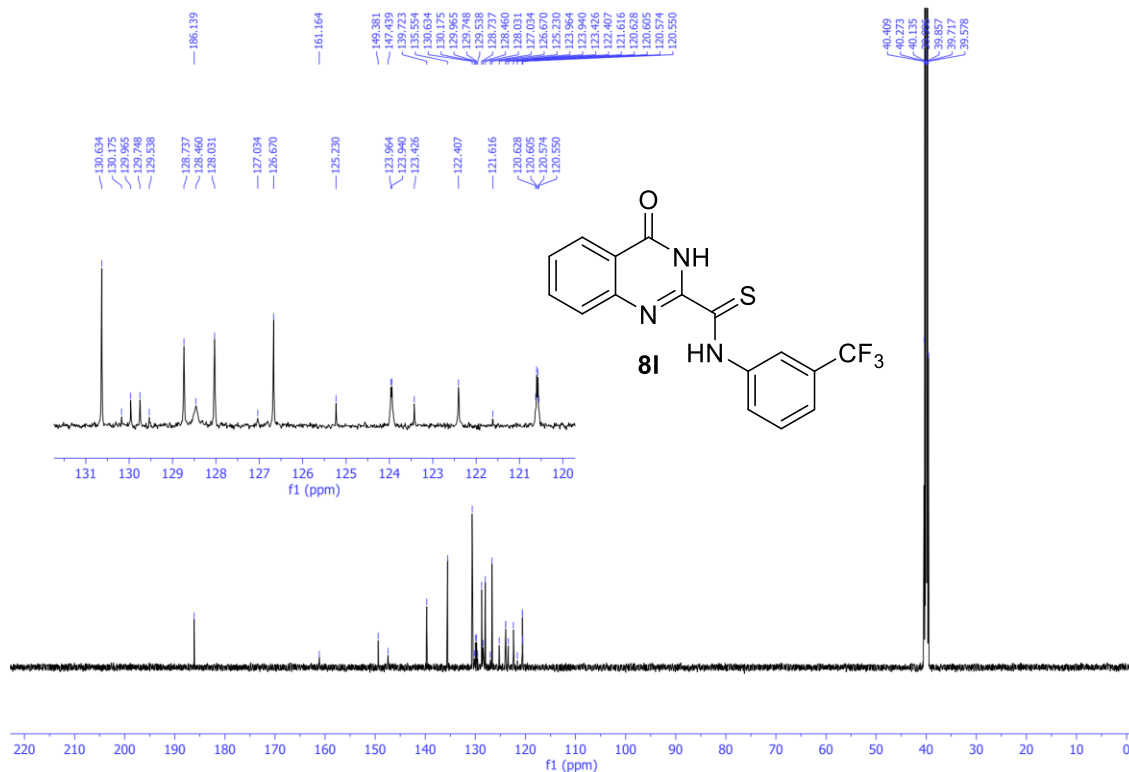
IR of spectra compound **8l**



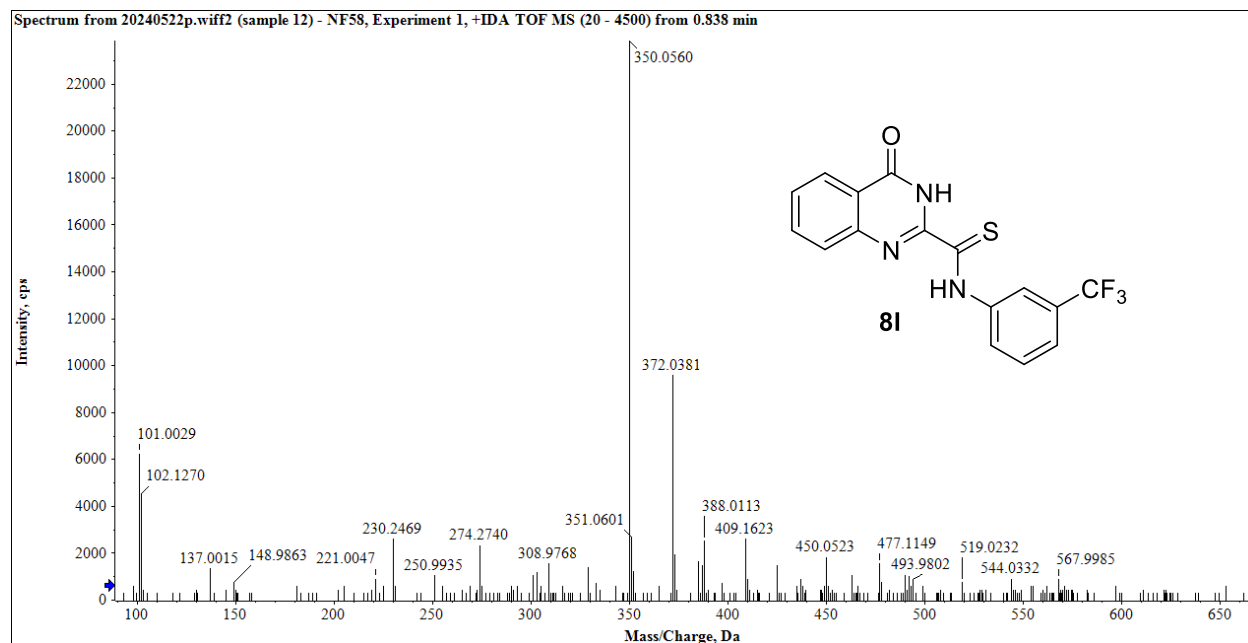
¹H NMR (DMSO-*d*₆, 600 MHz) spectrum of compound **8I**



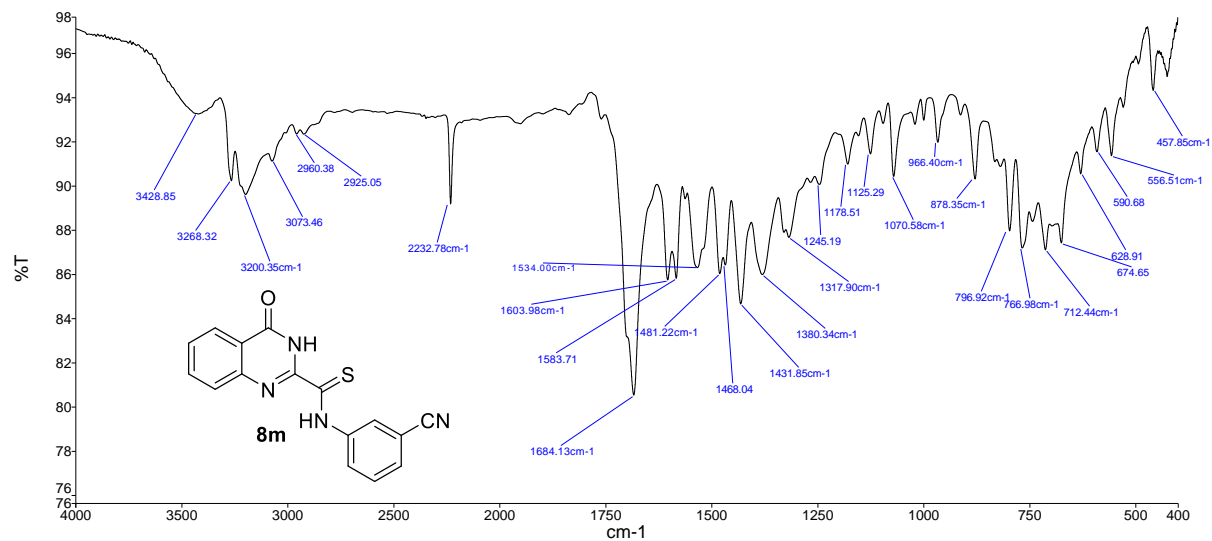
¹³C NMR (DMSO-*d*₆, 150 MHz) spectrum of compound **8I**



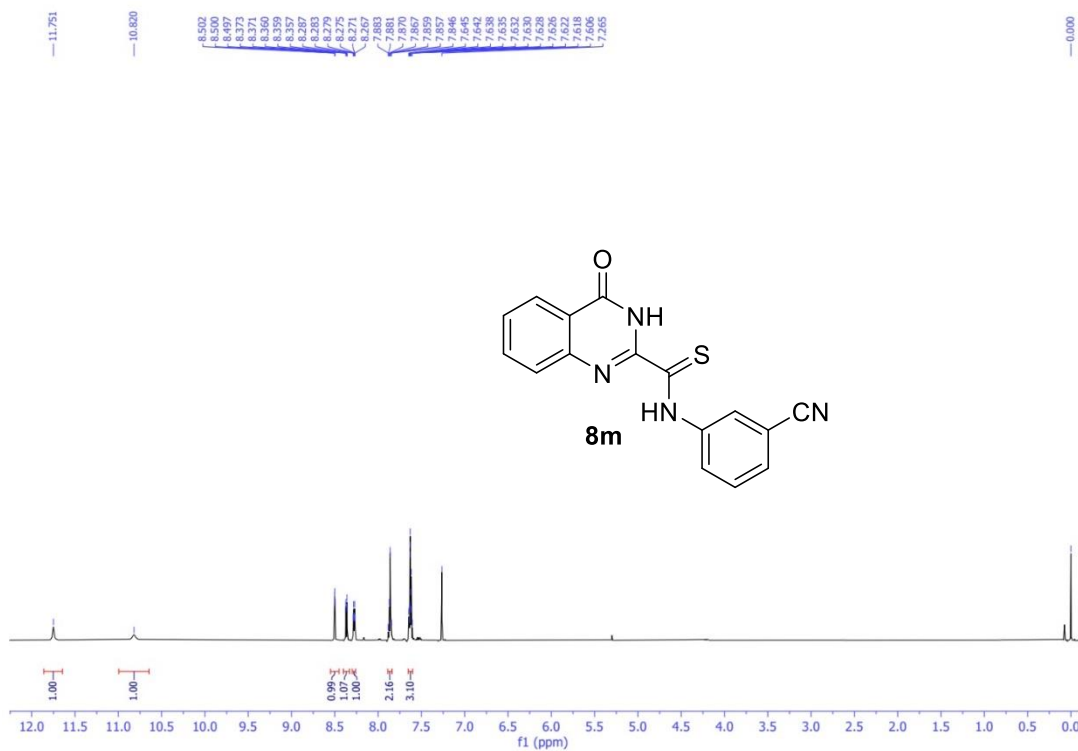
HRMS spectrum of compound **8l**



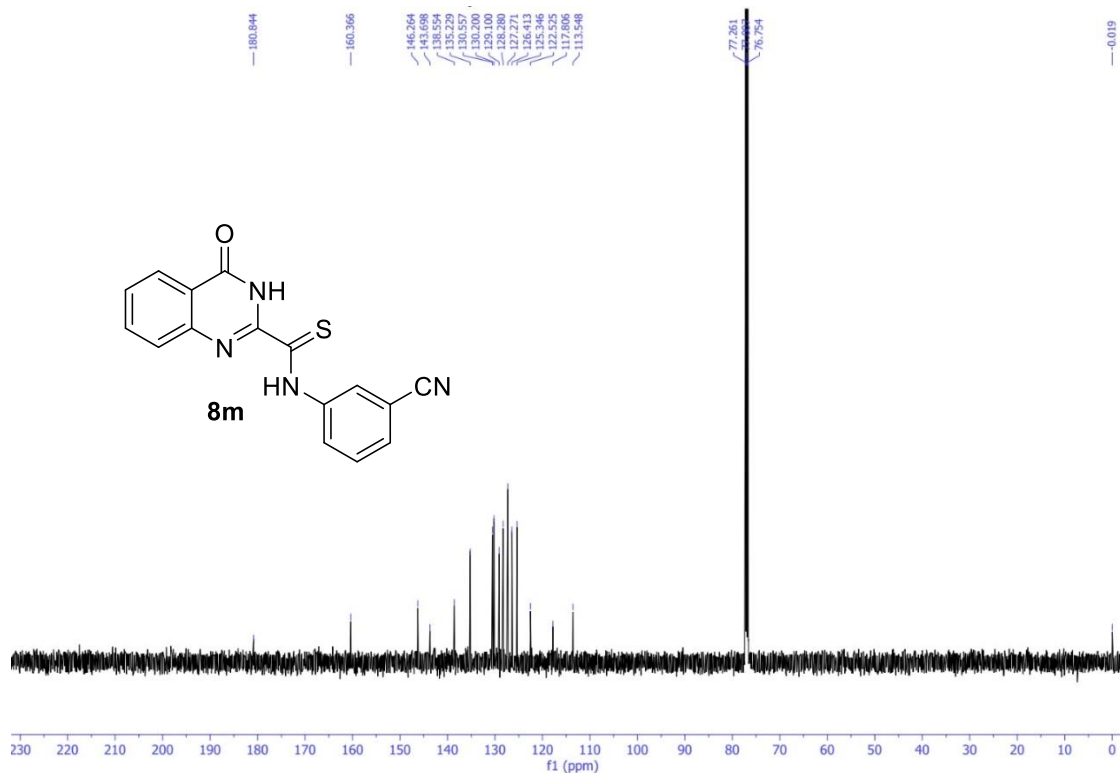
IR of spectra compound **8m**



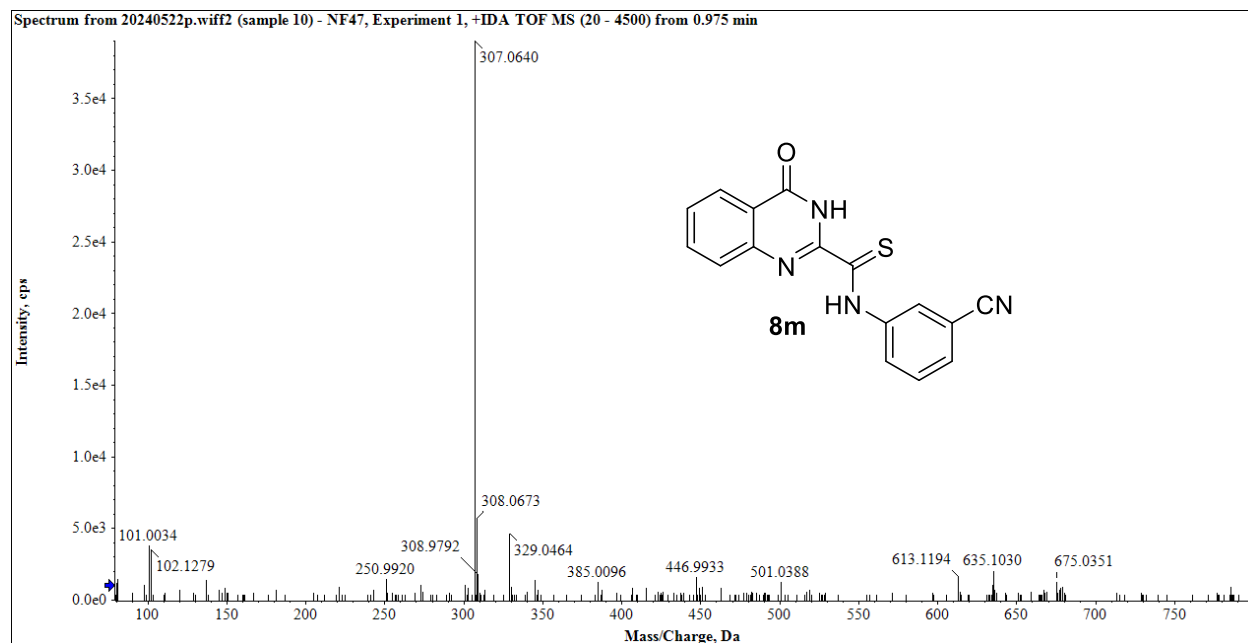
¹H NMR (CDCl₃, 600 MHz) spectrum of compound **8m**



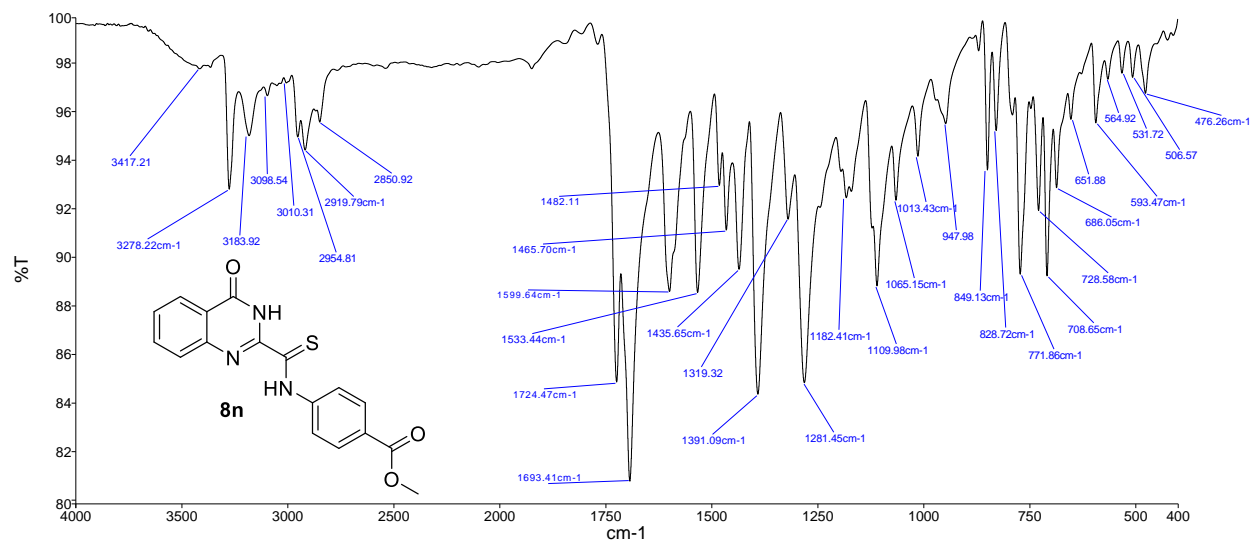
¹³C NMR (CDCl₃, 125 MHz) spectrum of compound **8m**



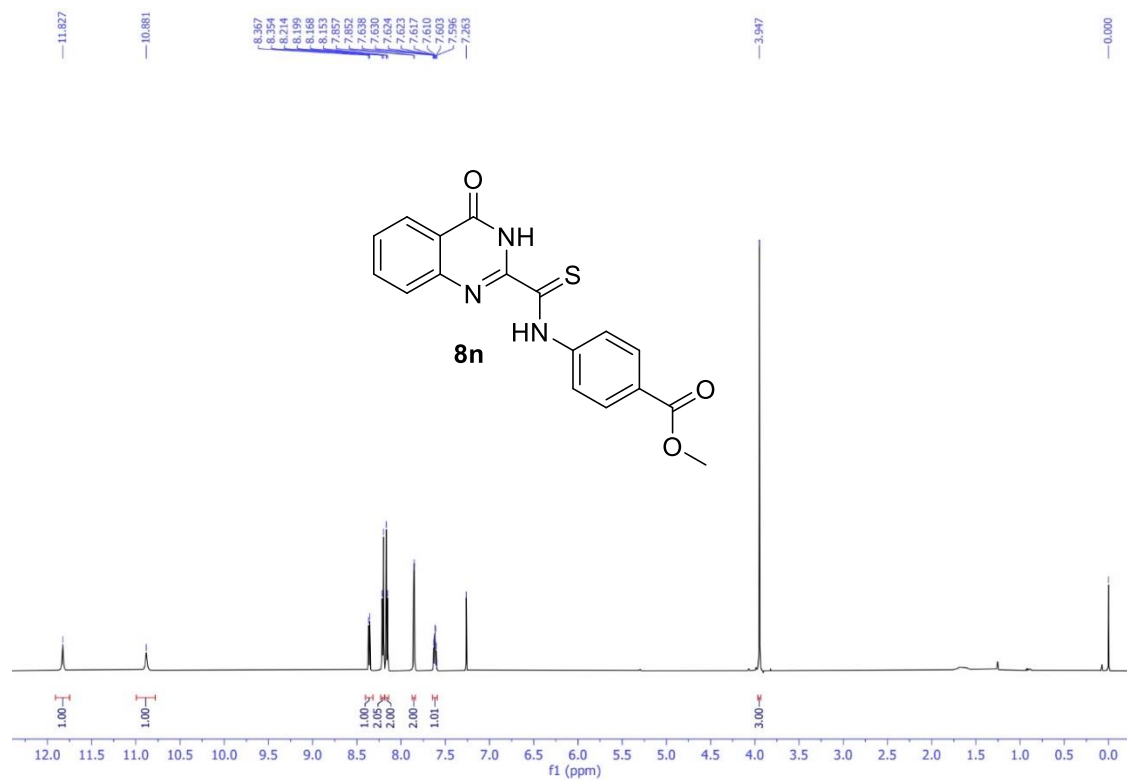
HRMS spectrum of compound **8m**



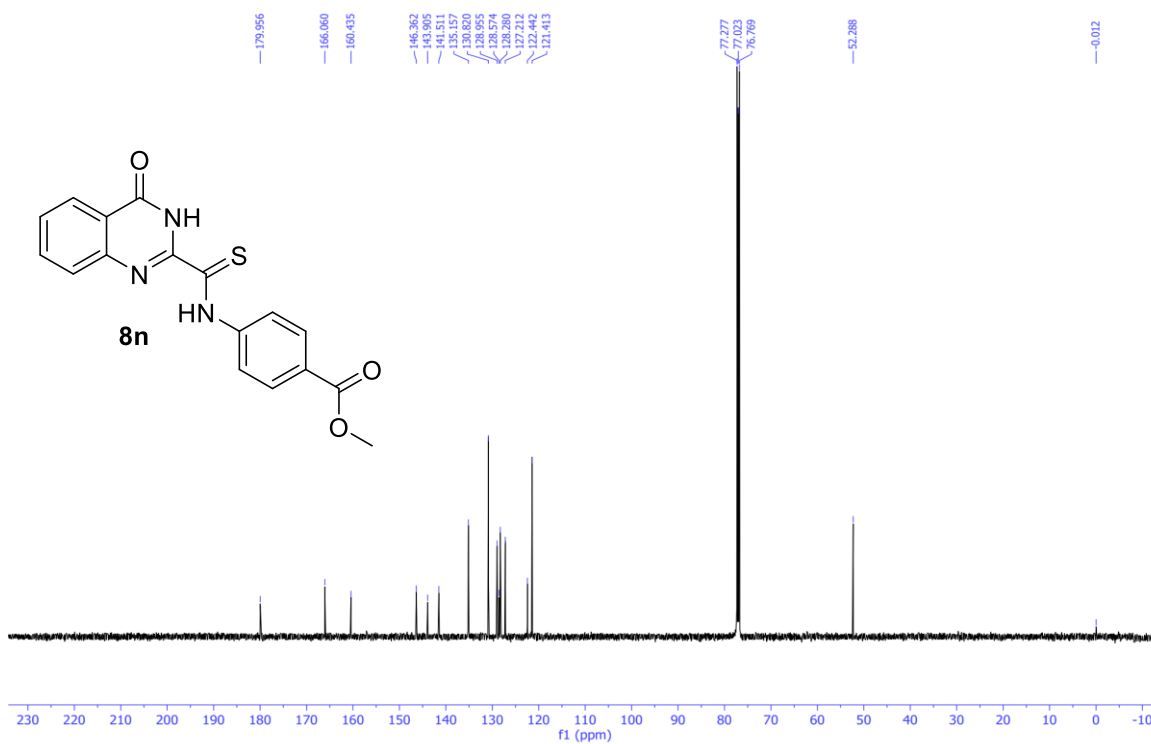
IR of spectra compound **8n**



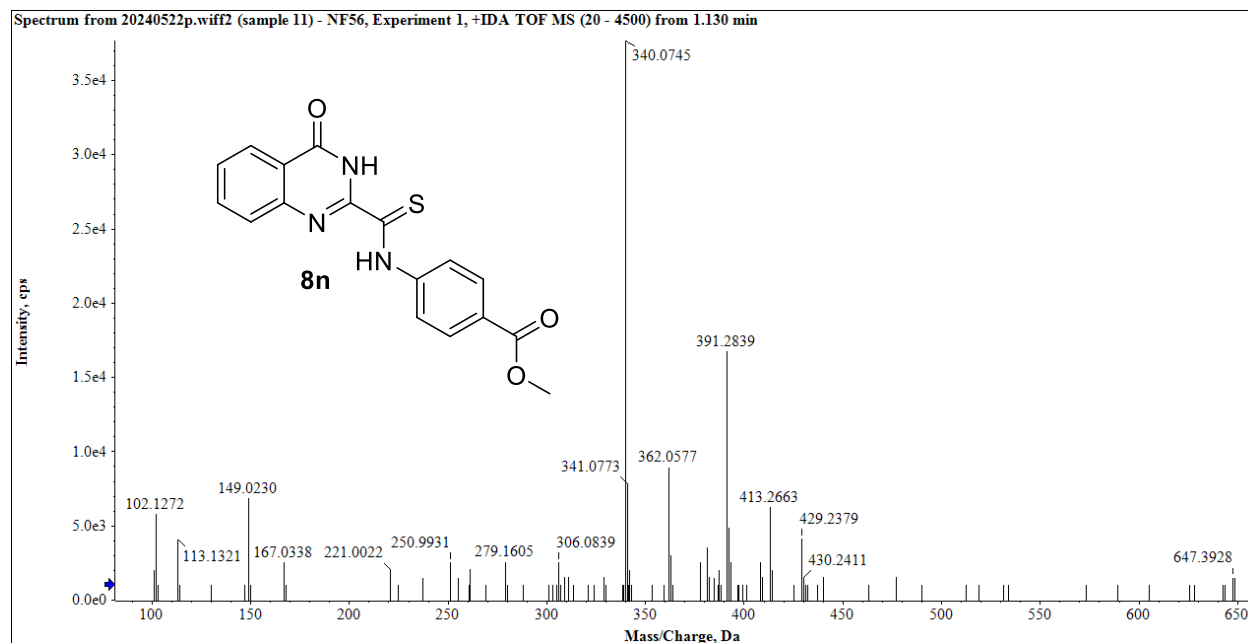
¹H NMR (CDCl₃, 600 MHz) spectrum of compound **8n**



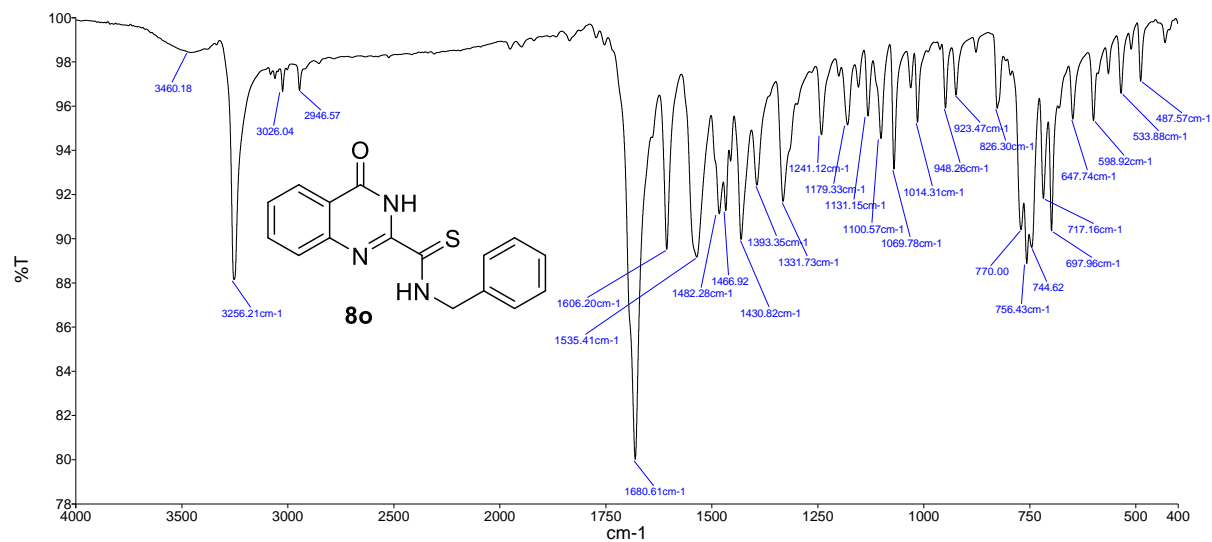
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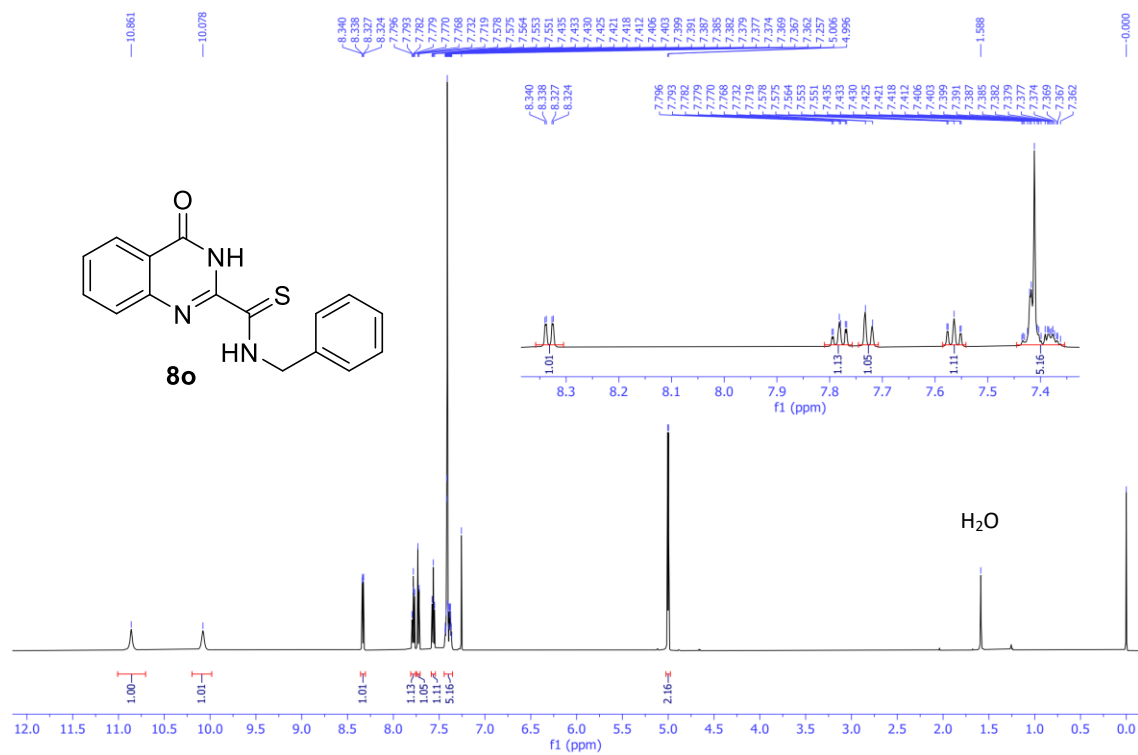
HRMS spectrum of compound **8n**



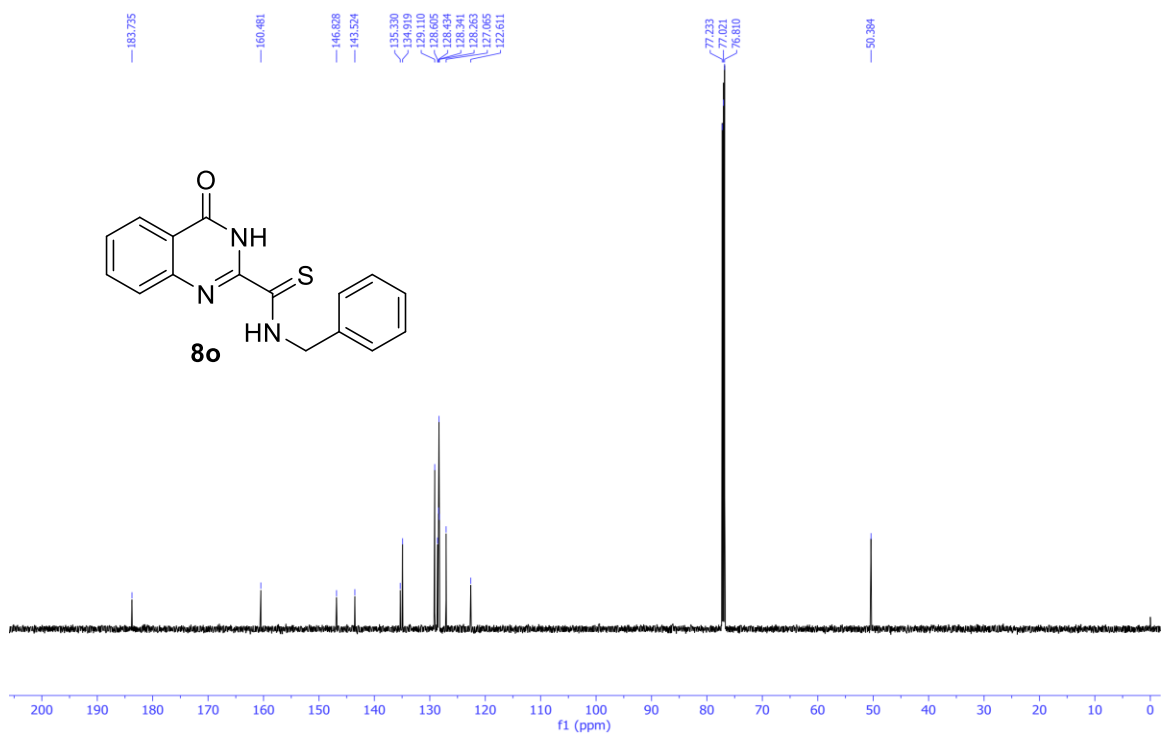
IR of spectra compound **8o**



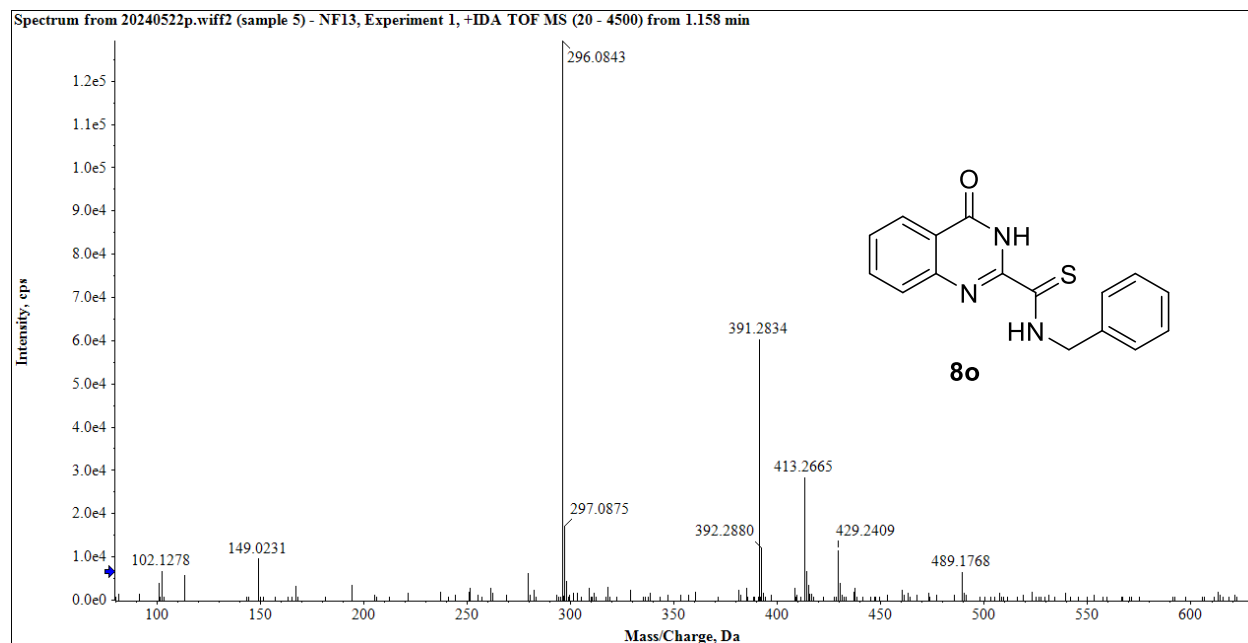
¹H NMR (CDCl₃, 600 MHz) spectrum of compound **8o**



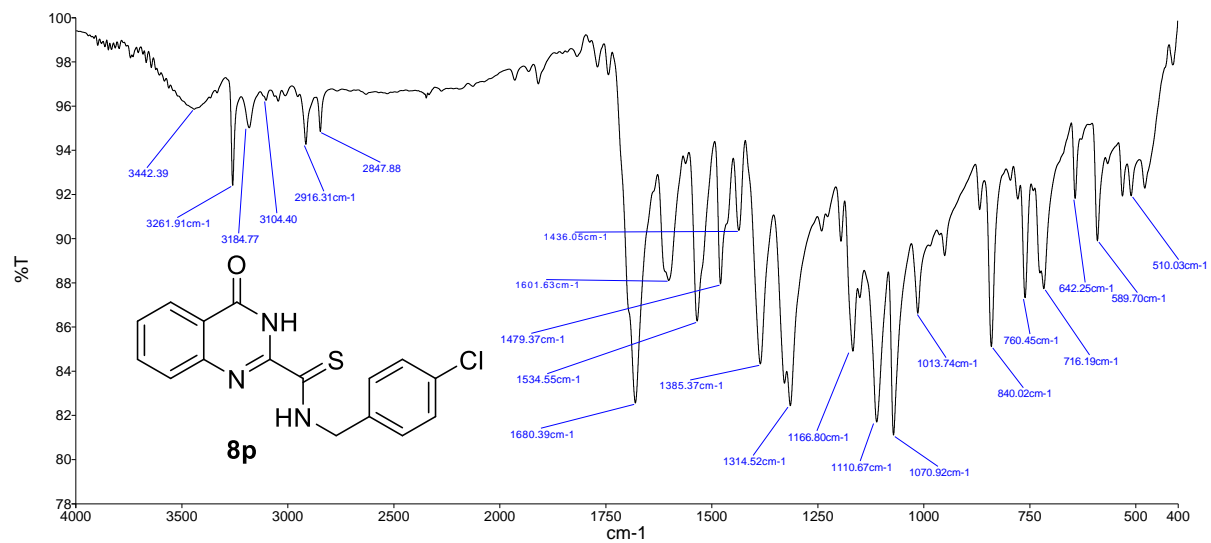
¹³C NMR (CDCl₃, 150 MHz) spectrum compound **8o**



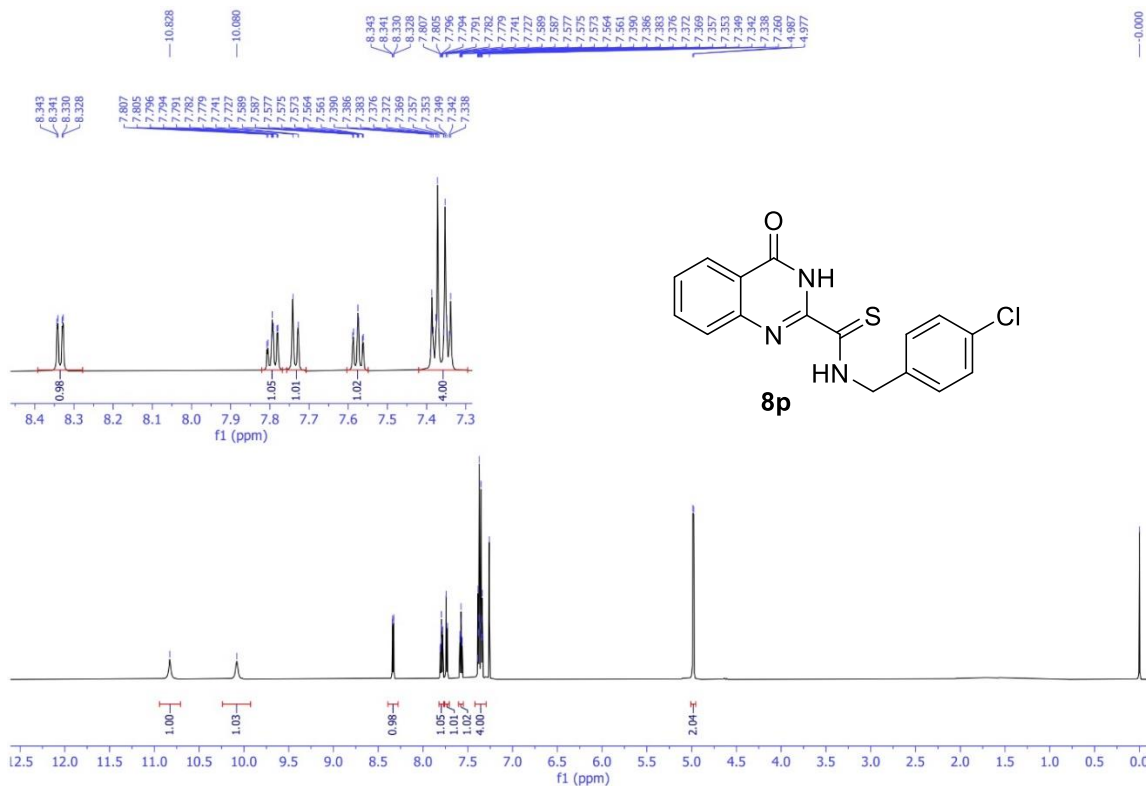
HRMS spectrum of compound **8o**



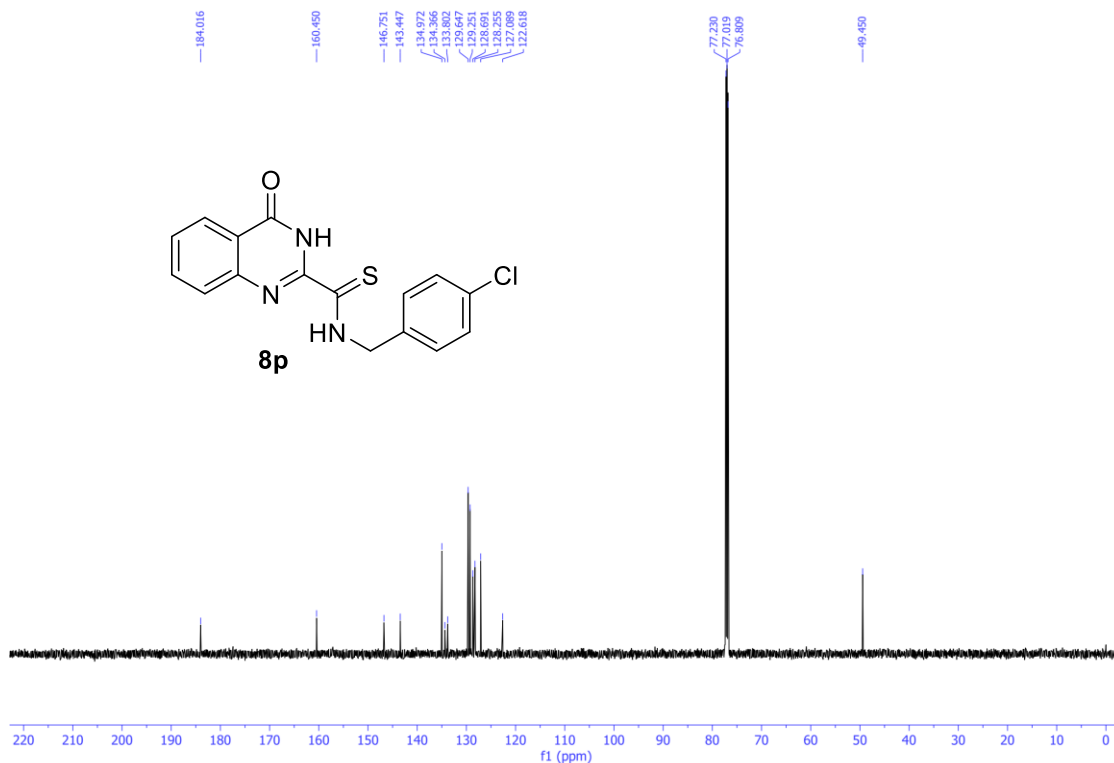
IR of spectra compound **8p**



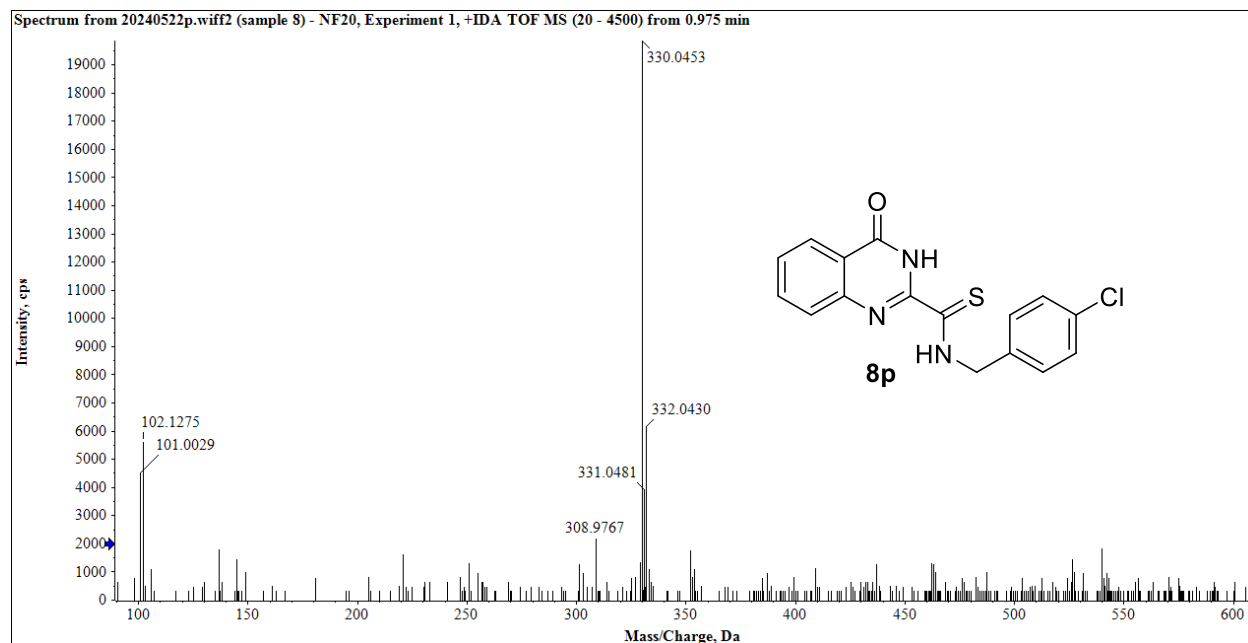
¹H NMR (CDCl₃, 600 MHz) spectrum of compound **8p**



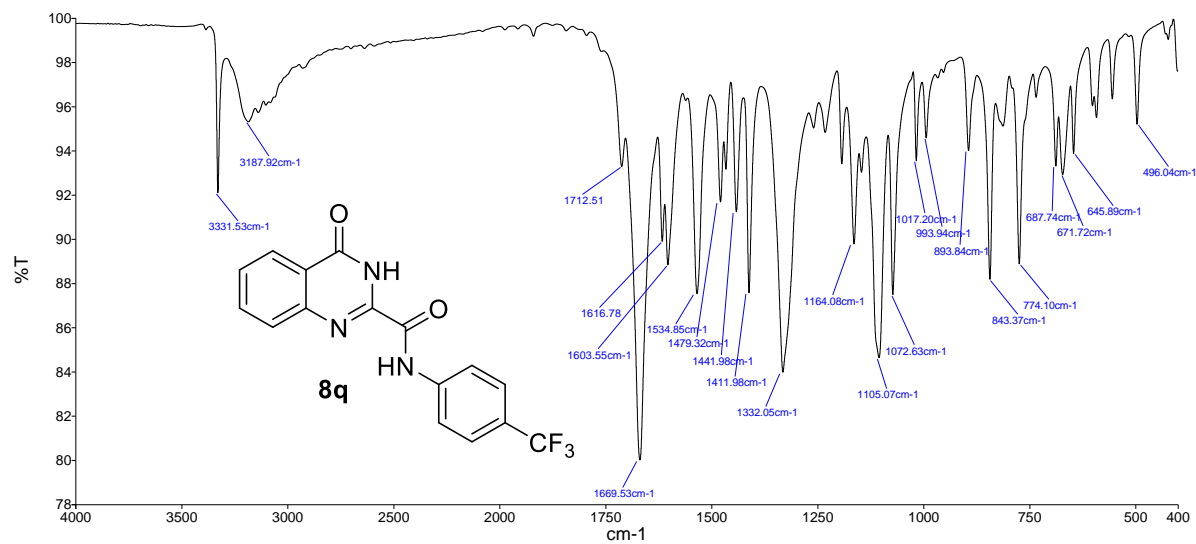
¹³C NMR (CDCl₃, 150 MHz) spectrum compound **8p**



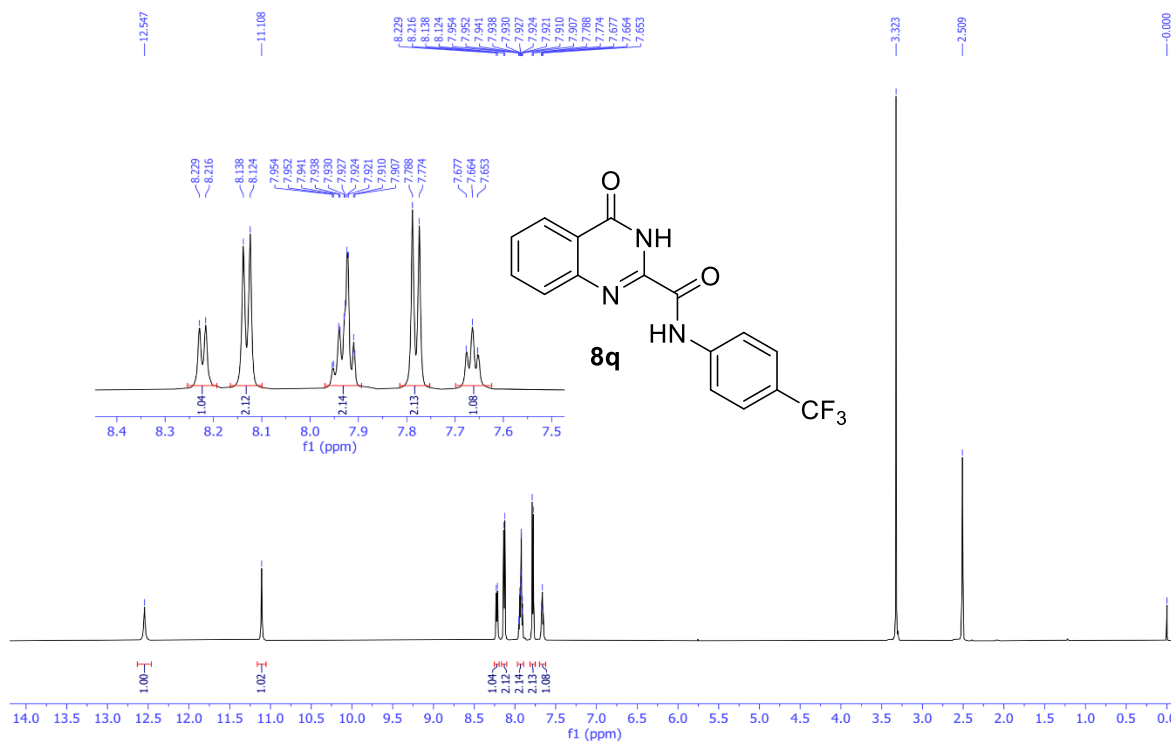
HRMS spectrum of compound **8p**



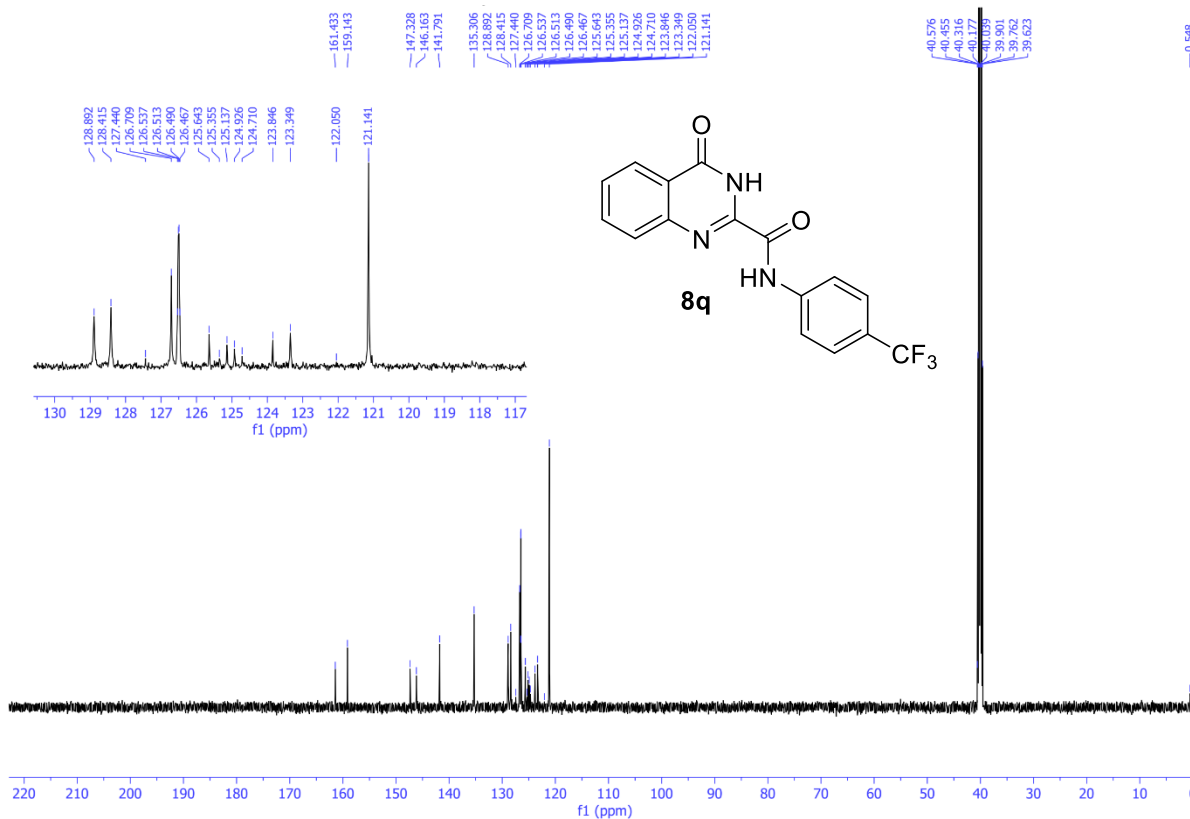
IR of spectra compound **8q**



¹H NMR (DMSO-*d*₆, 600 MHz) spectrum of compound **8q**



¹³C NMR (DMSO-*d*₆, 150 MHz) spectrum compound **8q**



HRMS spectrum of compound **8q**

