

## Supporting information

# Synthesis and Anti-Pim-1/2 Kinase Activity of Potassium 6-oxo-7,13,16,22- tetraazatetracyclo[12.6.2.1<sup>8,12</sup>.0<sup>17,21</sup>]tricos- 1(20),8,10,12(23),14(22),15(16),17,18-octaen-2-yne-15- carboxylate

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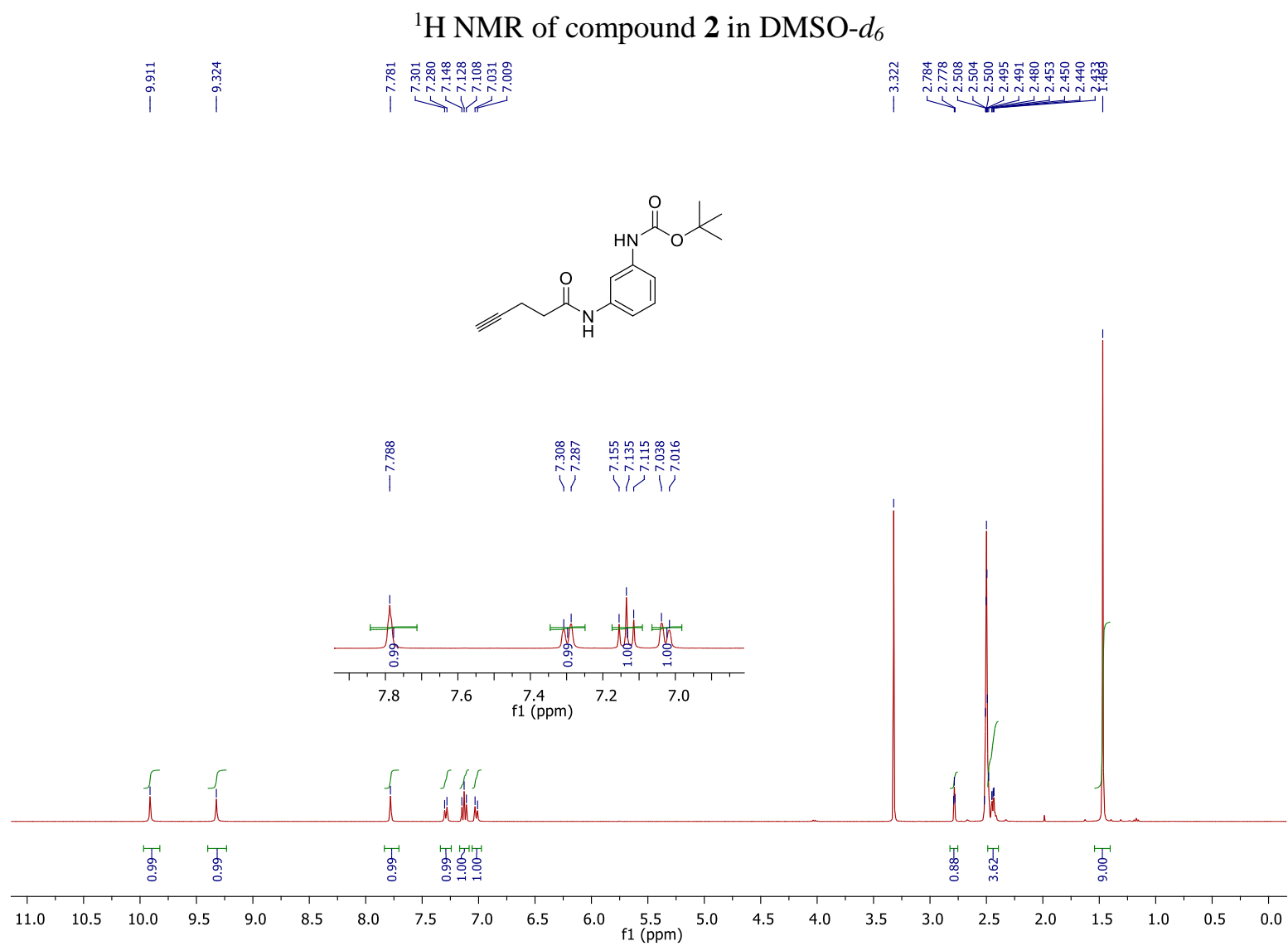
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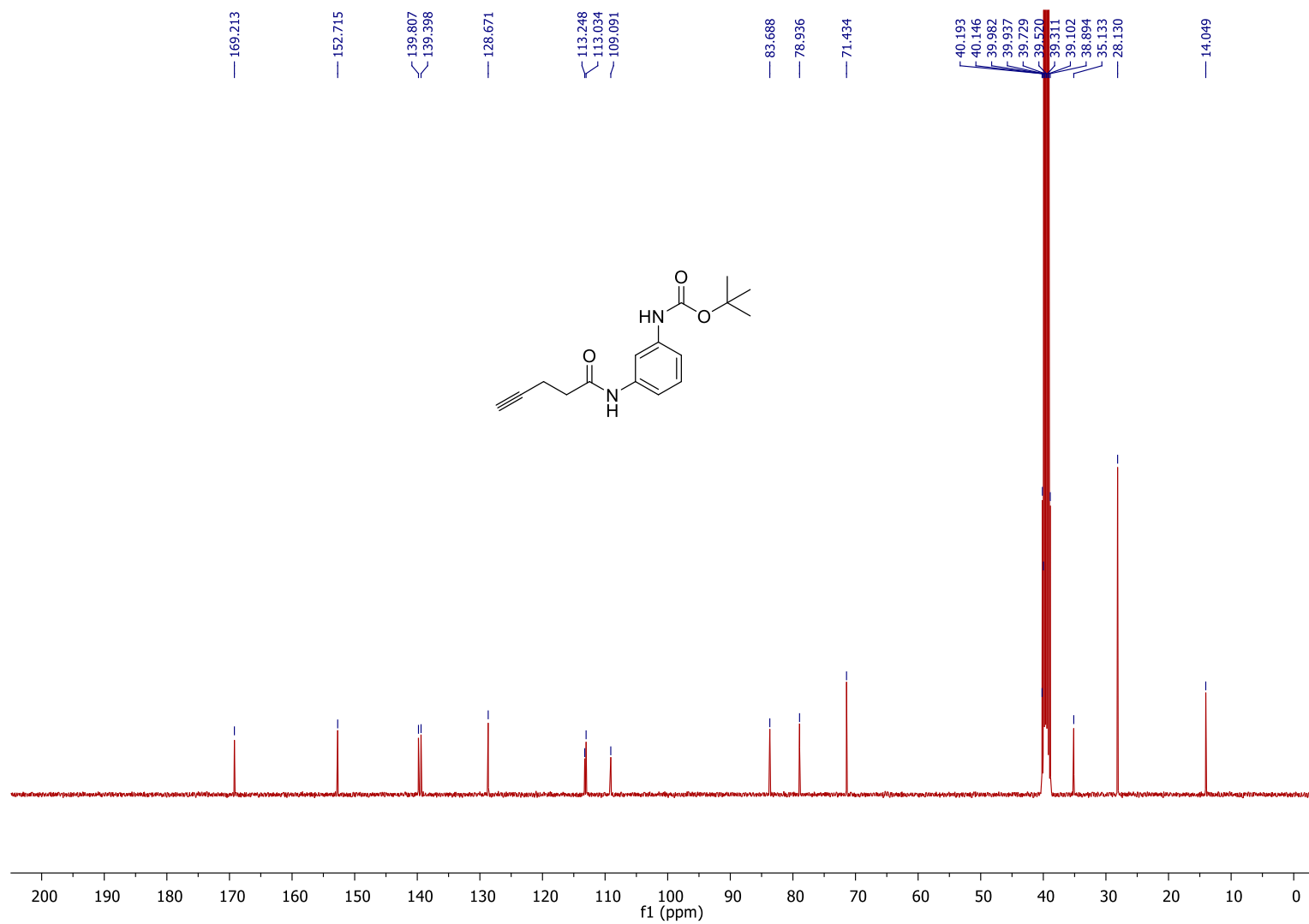
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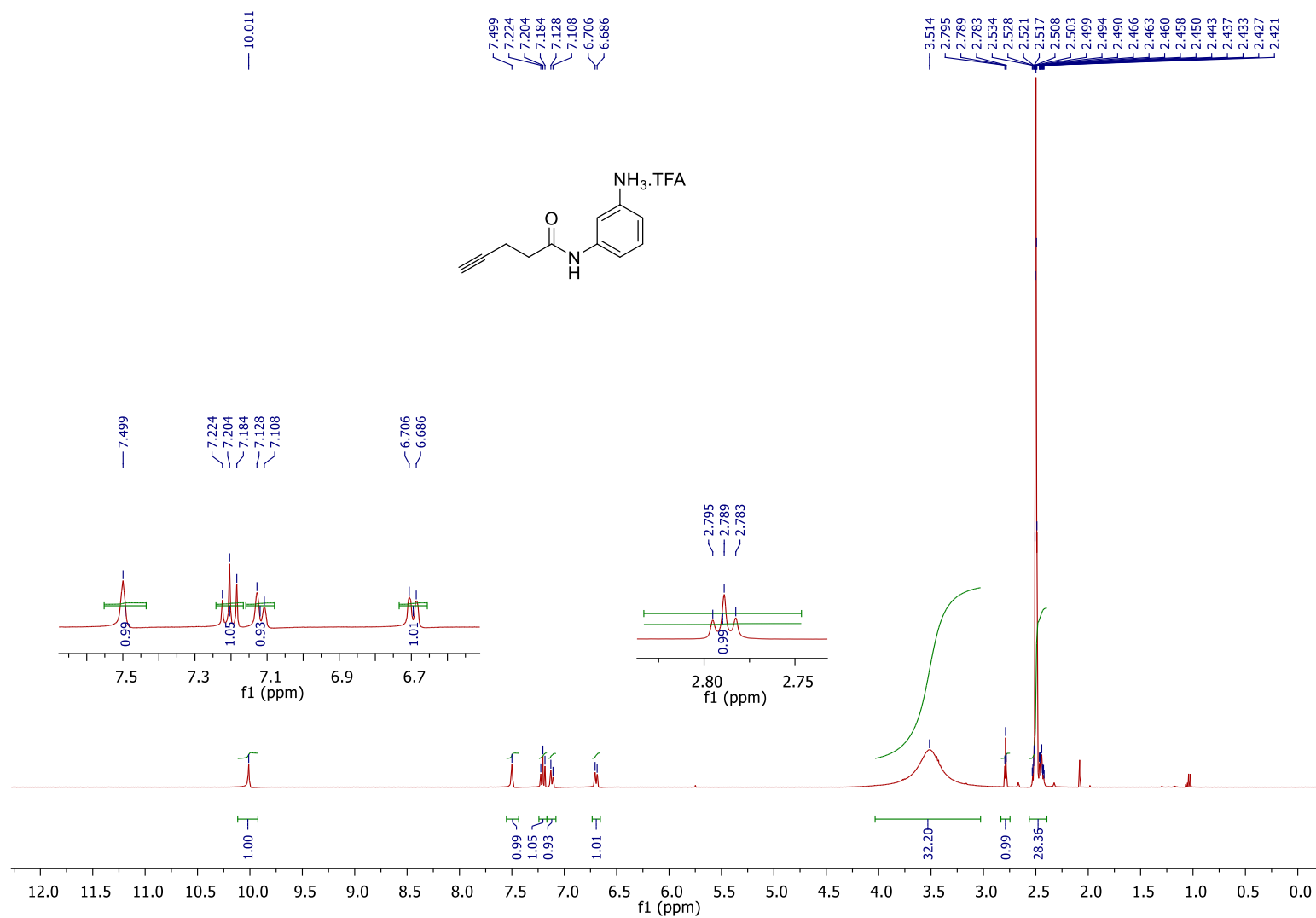
# 1. NMR spectra



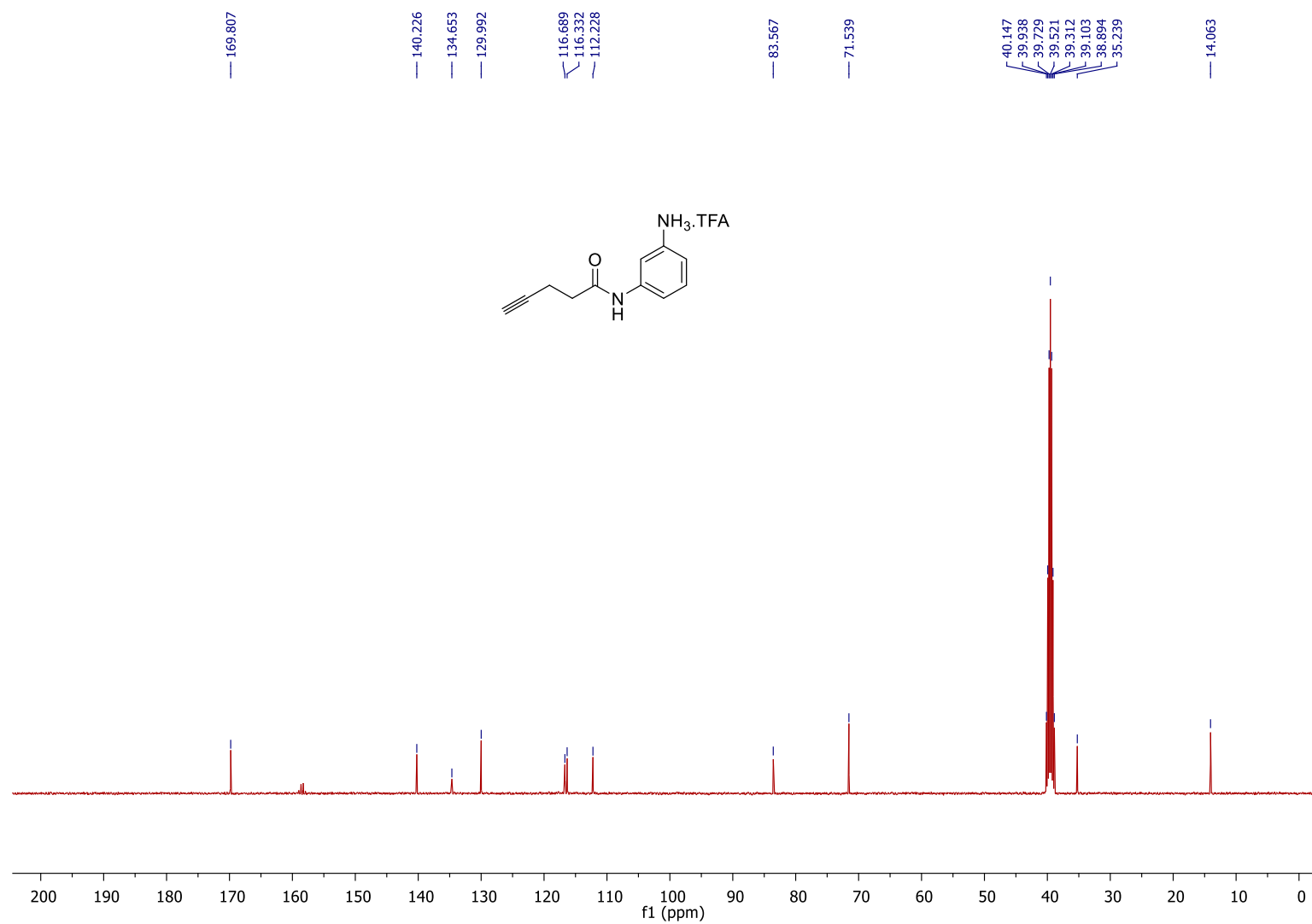
$^{13}\text{C}$  NMR of compound **2** in  $\text{DMSO-}d_6$



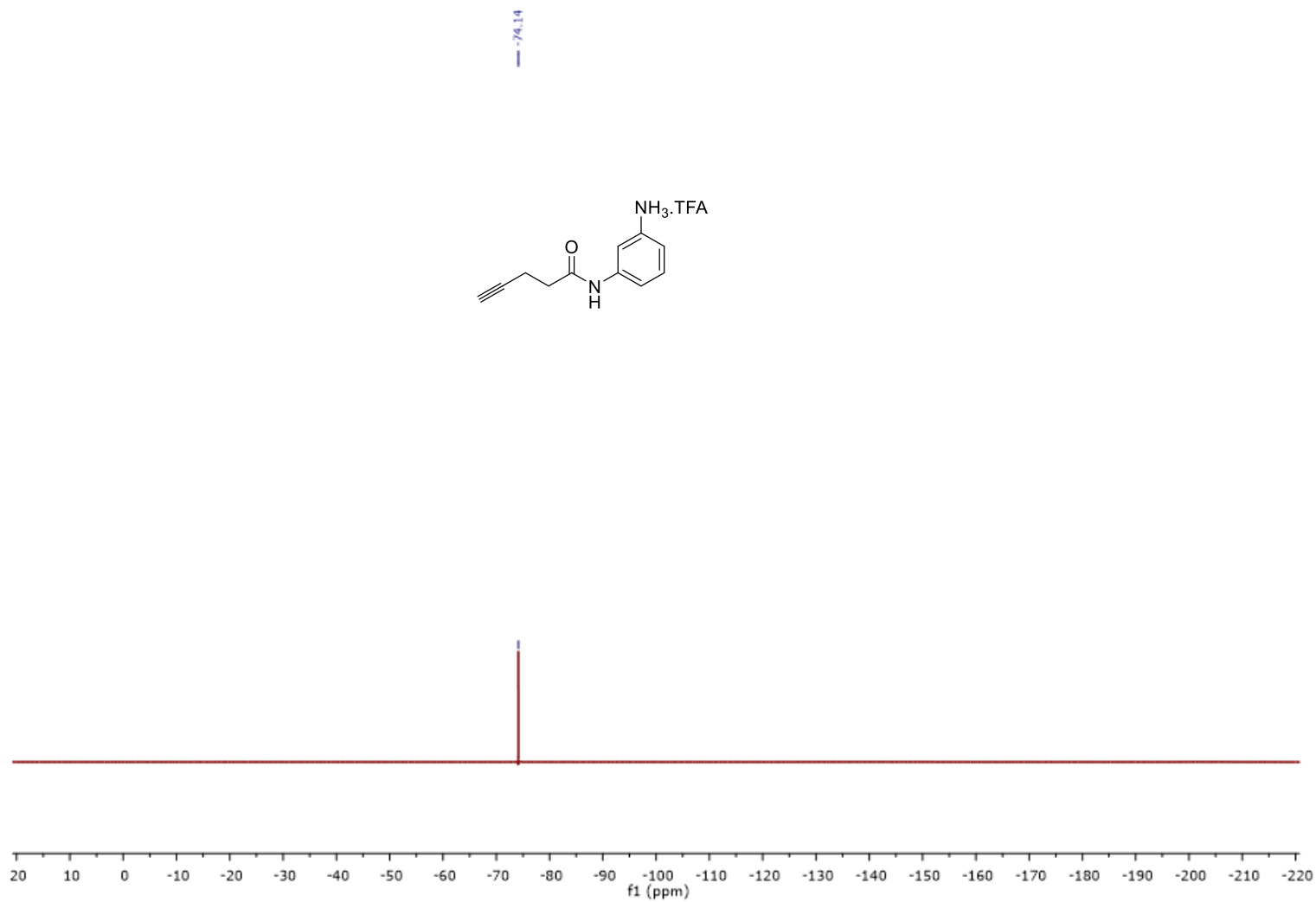
$^1\text{H}$  NMR of compound **3** in  $\text{DMSO-}d_6$



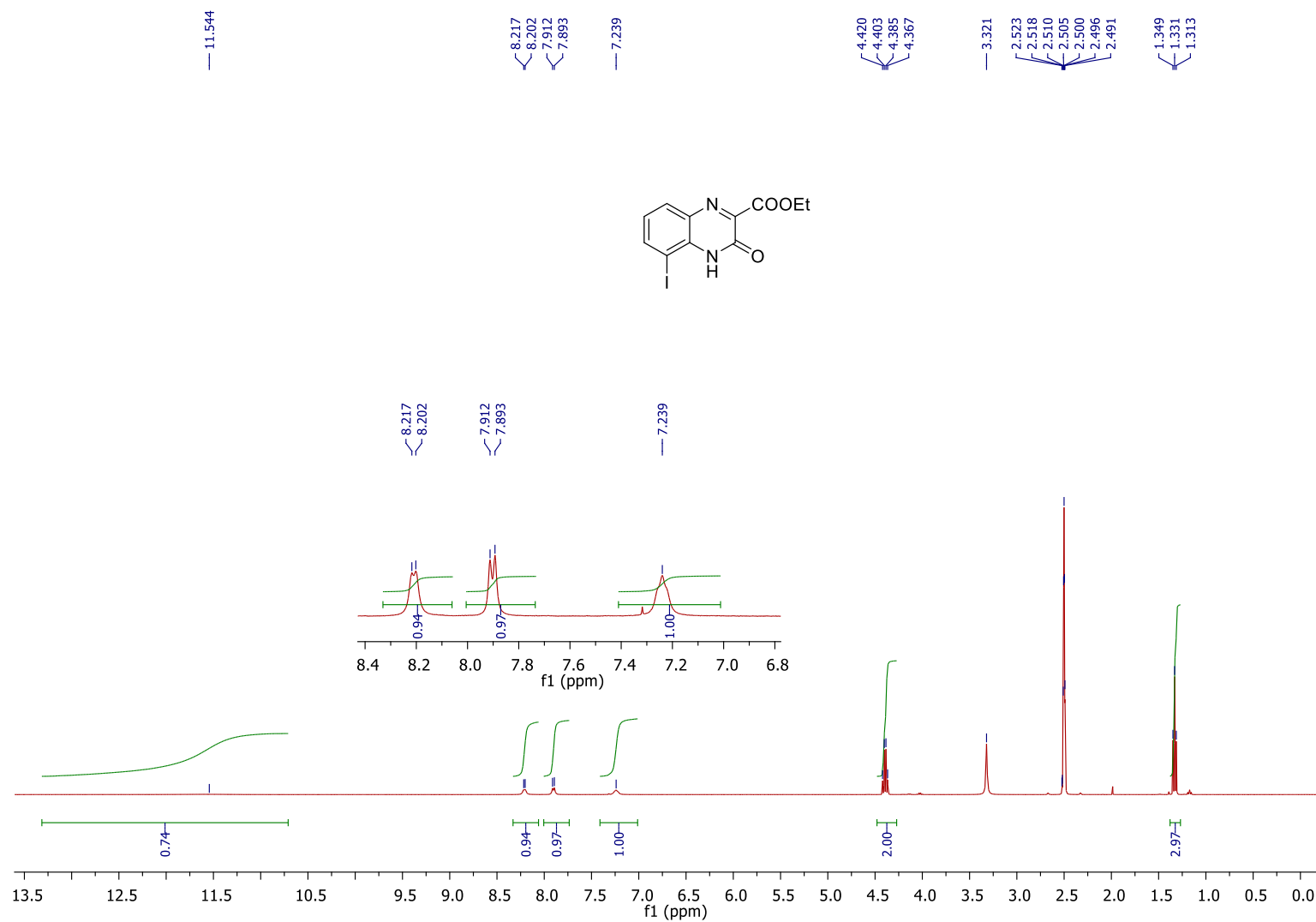
$^{13}\text{C}$  NMR of compound **3** in  $\text{DMSO-}d_6$



$^{19}\text{F}$  NMR of compound **3** in  $\text{DMSO-}d_6$

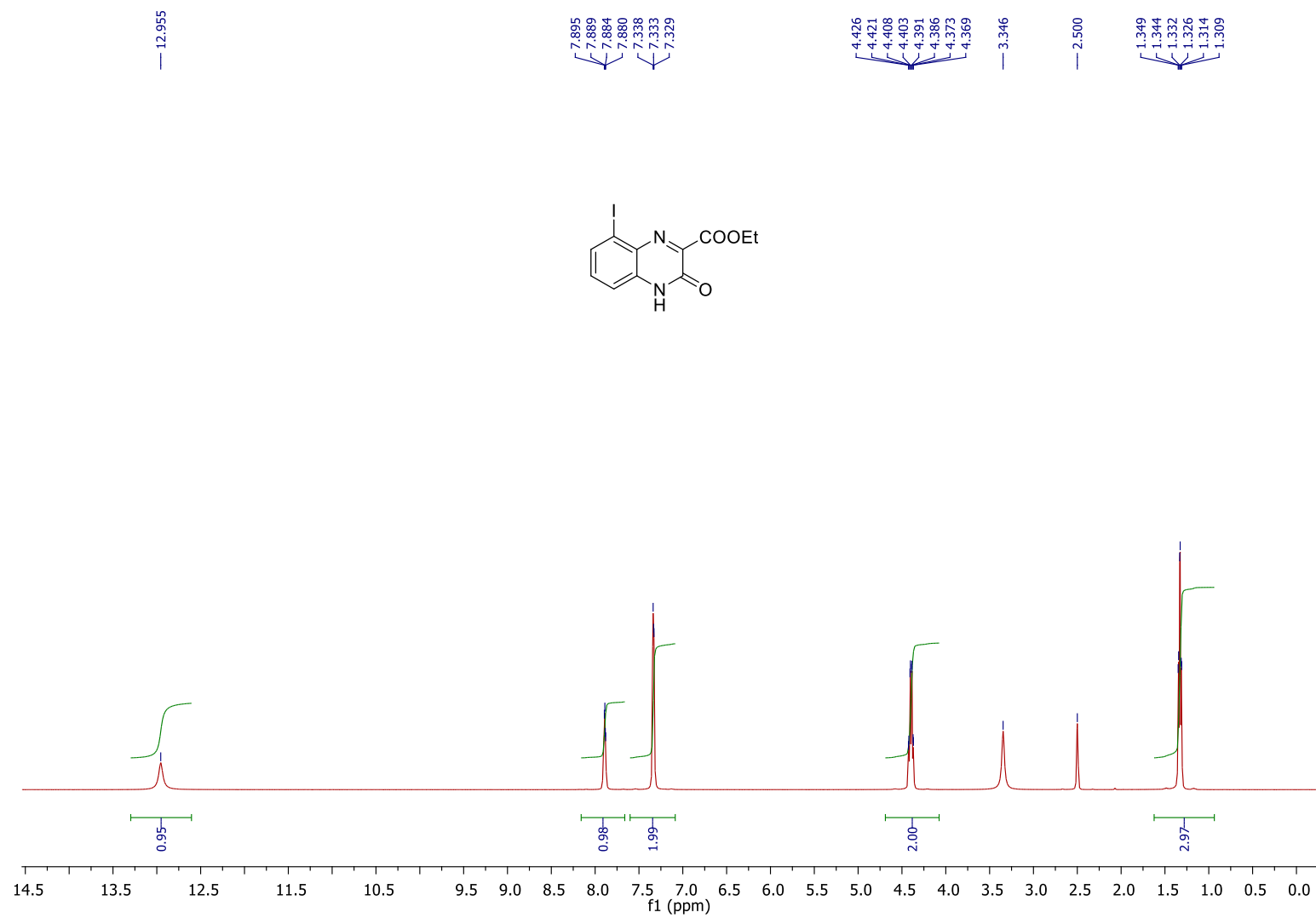


$^1\text{H}$  NMR of compound **4a** in  $\text{DMSO}-d_6$

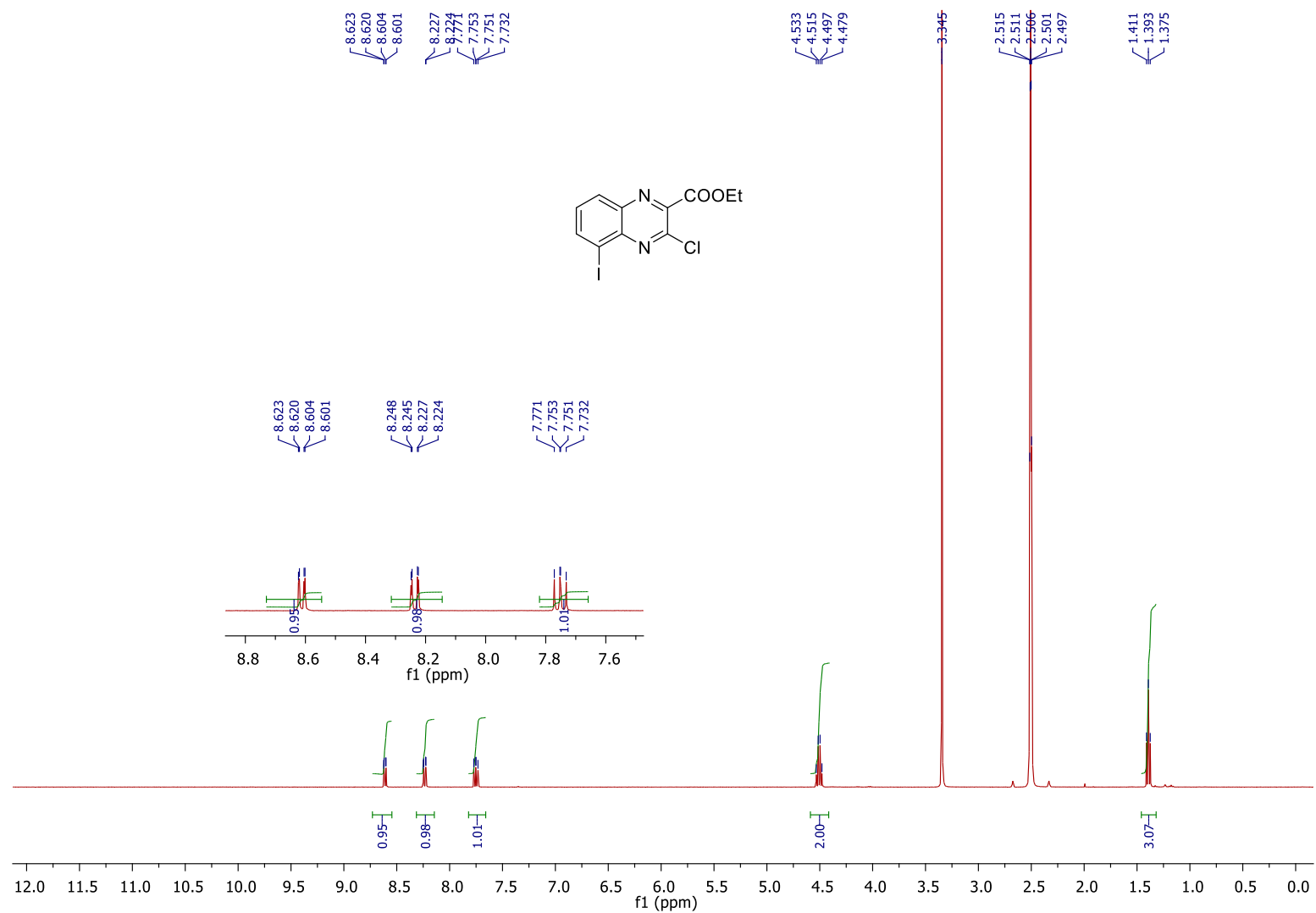




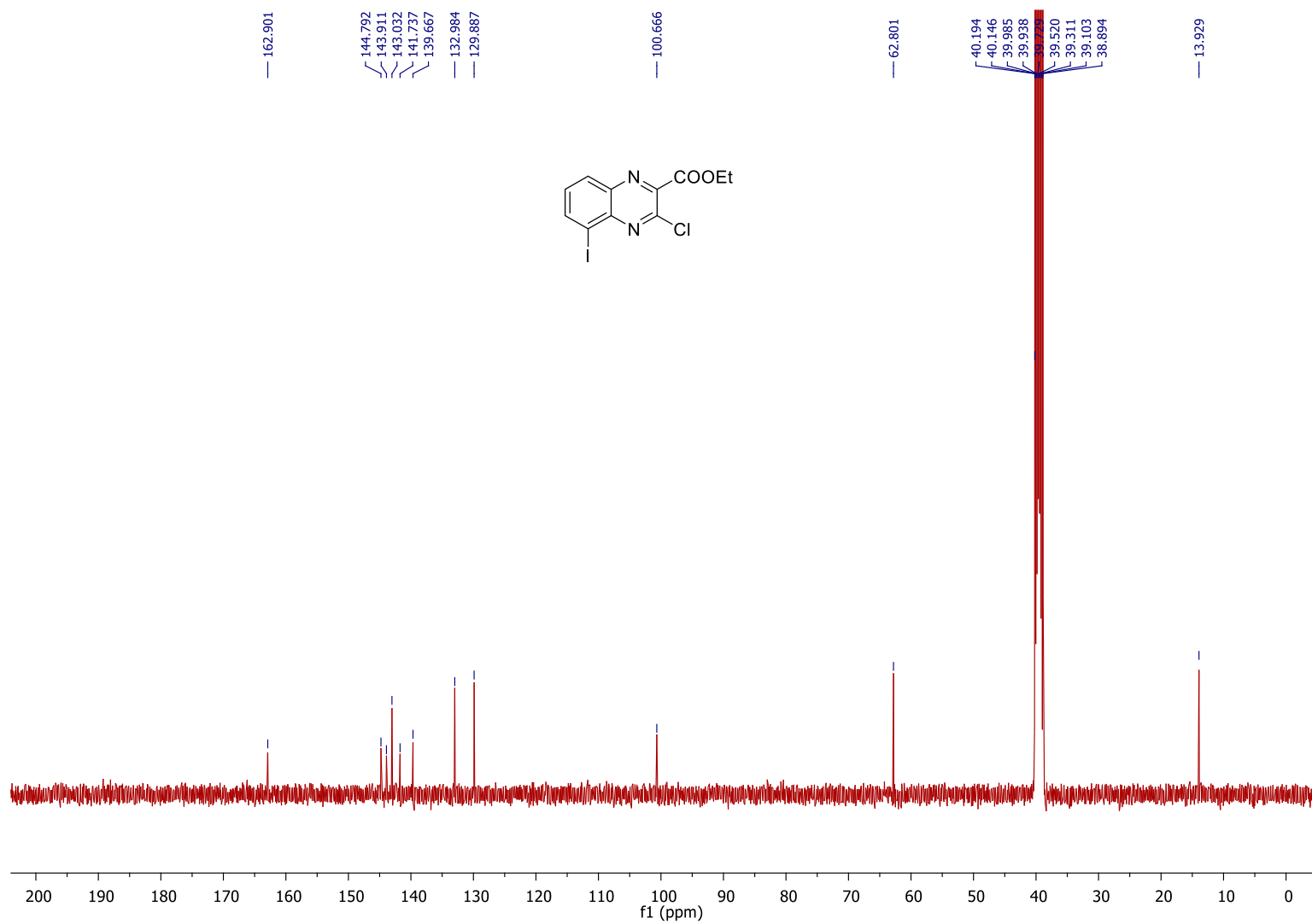
$^1\text{H}$  NMR of compound **4b** in  $\text{DMSO-}d_6$



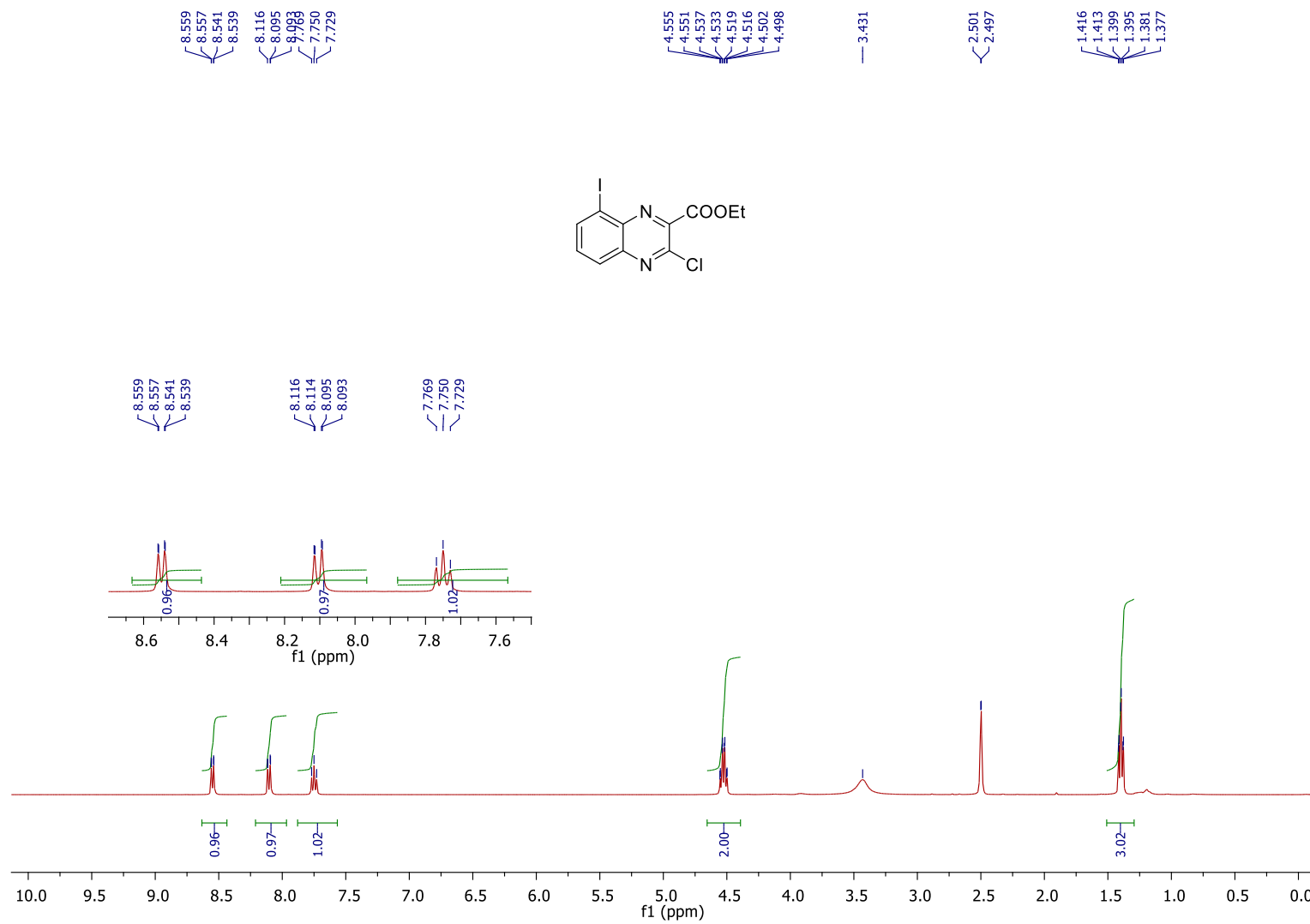
$^1\text{H}$  NMR of compound **5a** in  $\text{DMSO}-d_6$



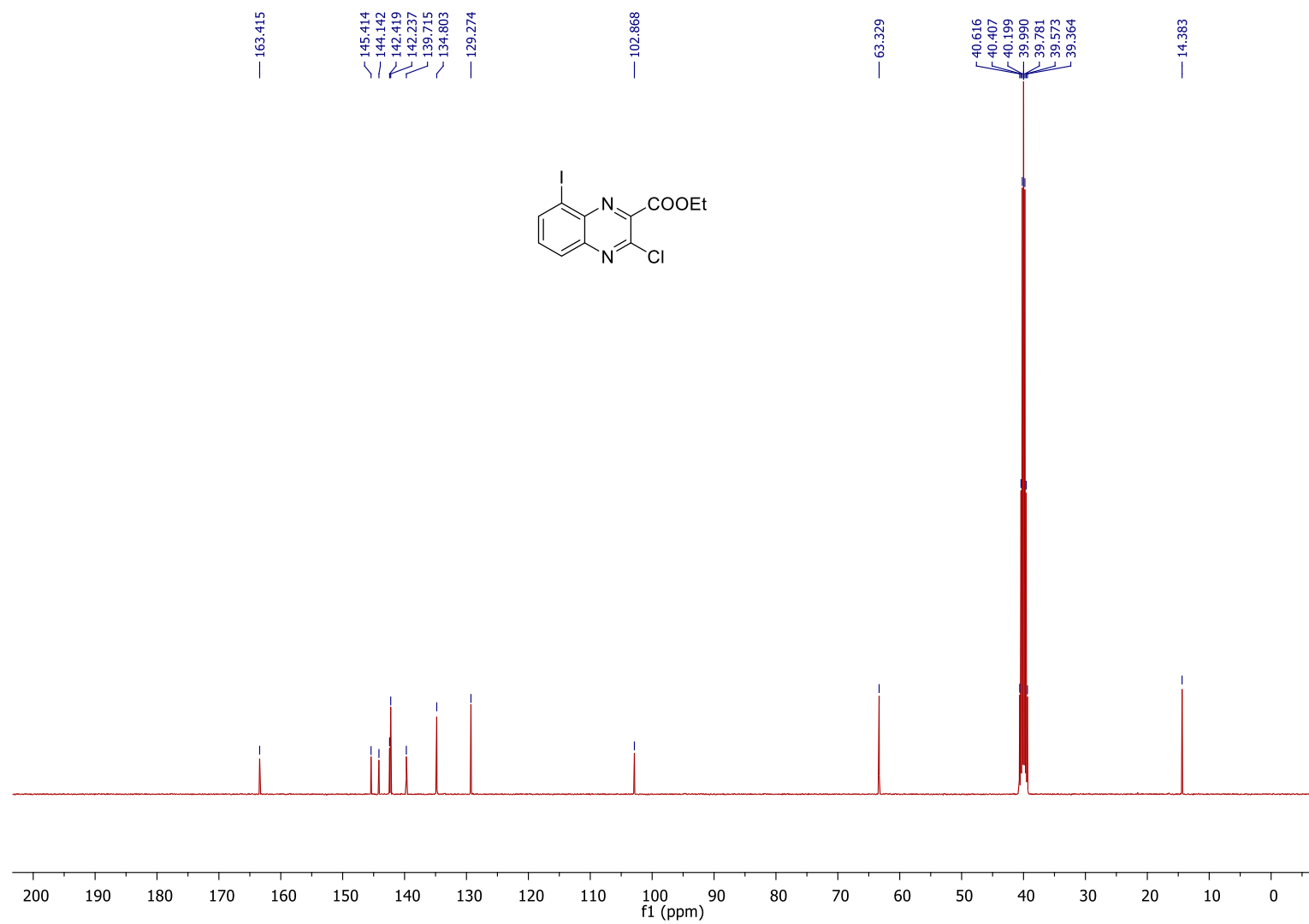
$^{13}\text{C}$  NMR of compound **5a** in  $\text{DMSO}-d_6$



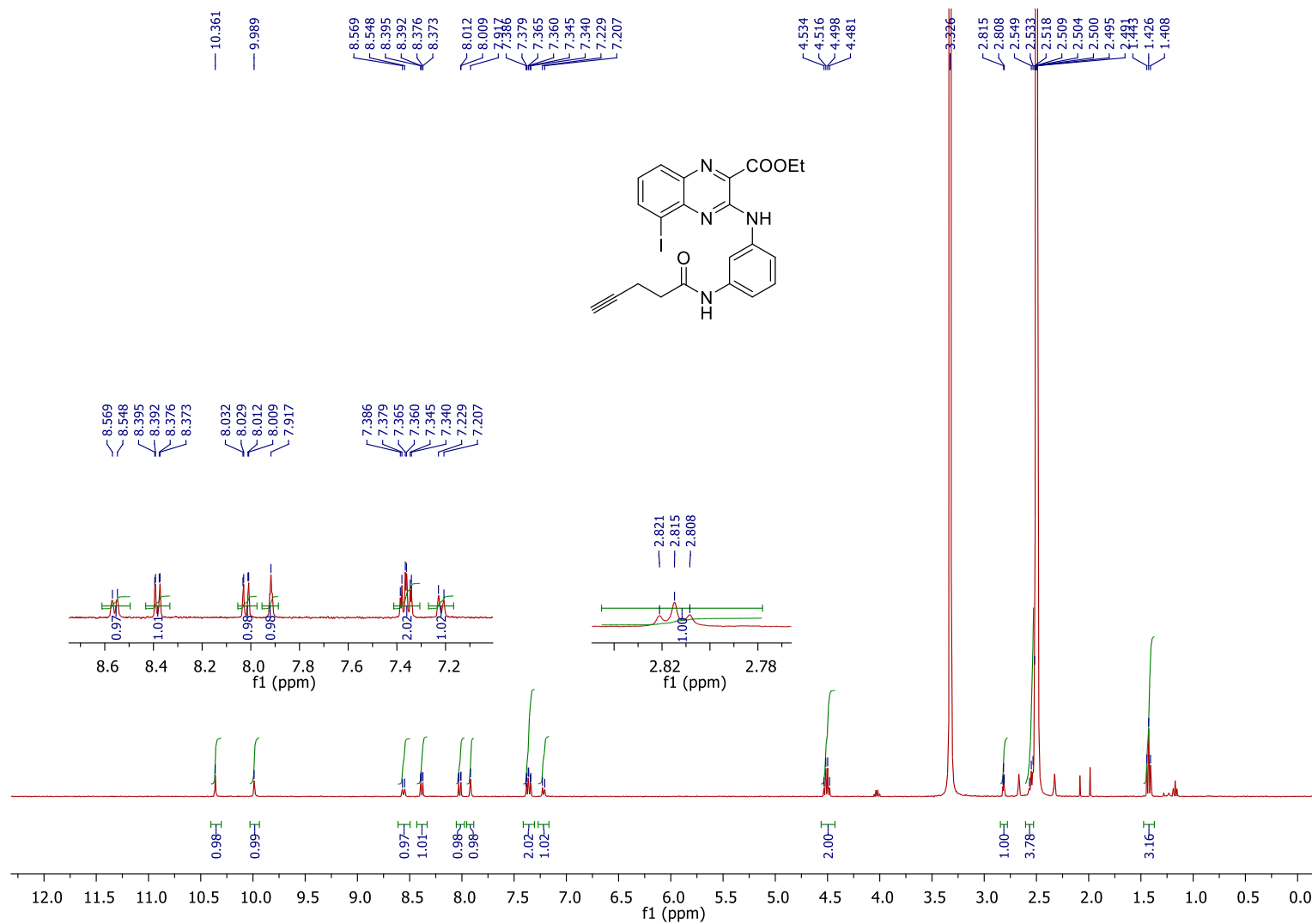
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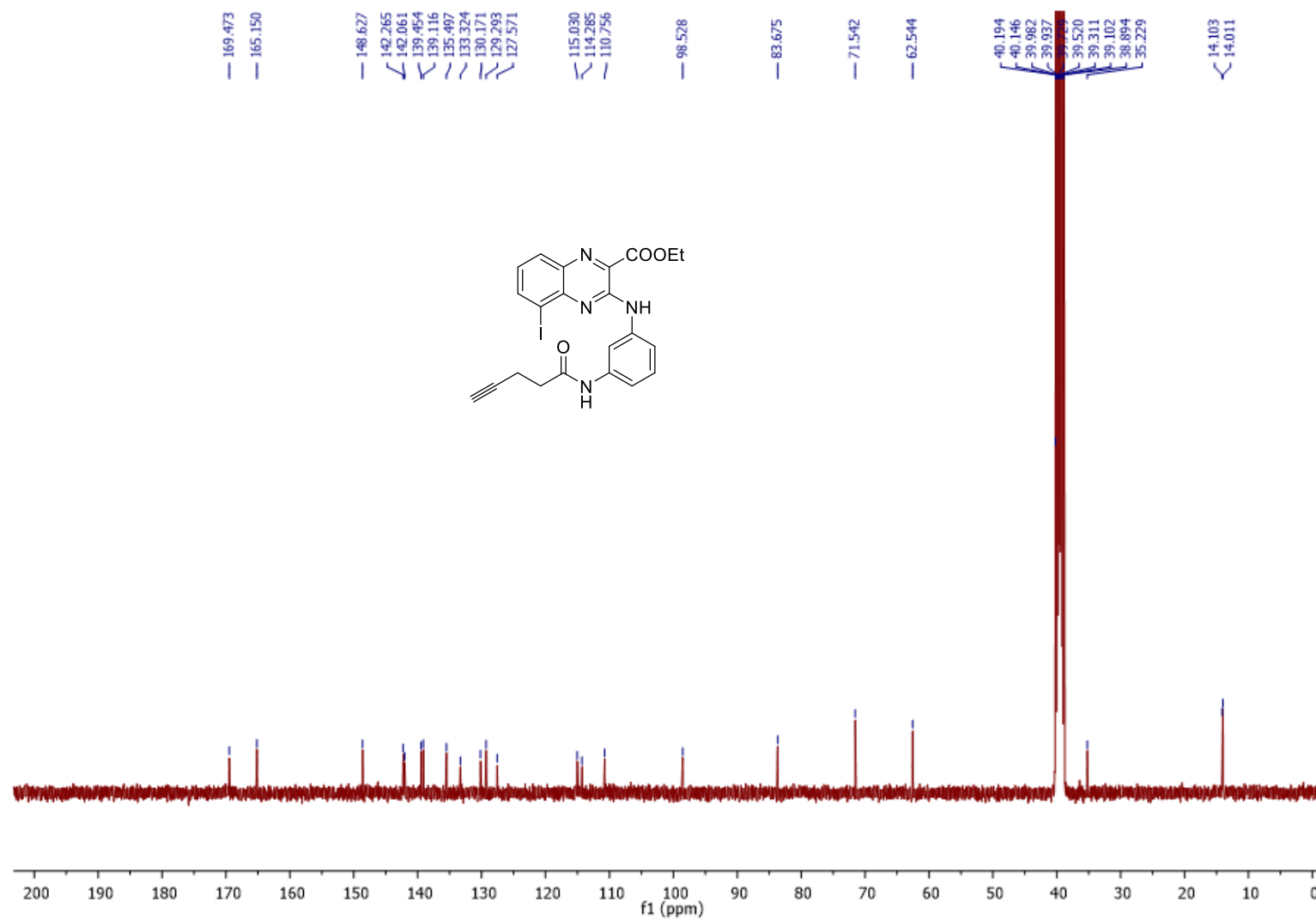
$^{13}\text{C}$  NMR of compound **5b** in  $\text{DMSO-}d_6$



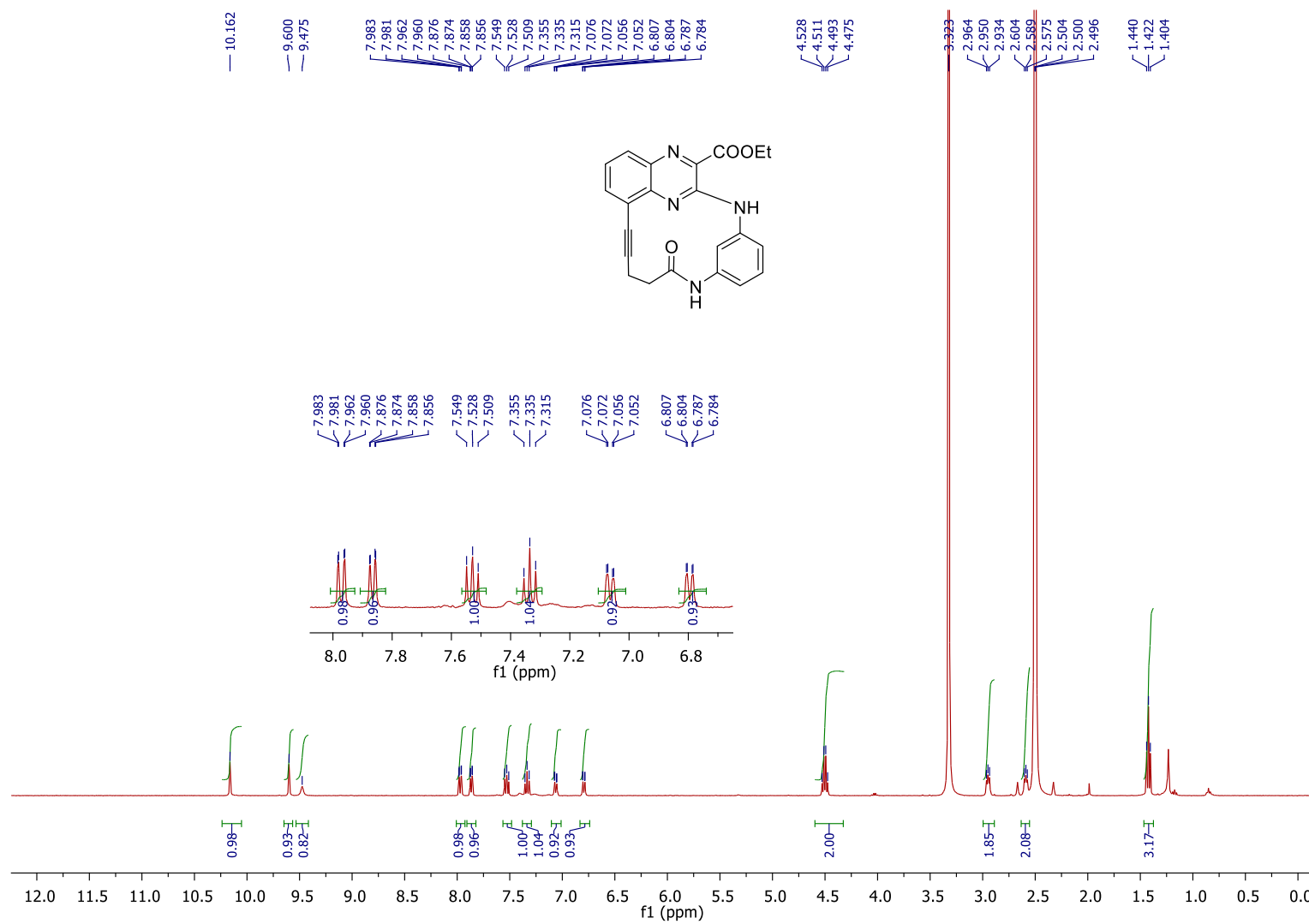
<sup>1</sup>H NMR of compound **6** in DMSO-*d*<sub>6</sub>



$^{13}\text{C}$  NMR of compound **6** in  $\text{DMSO-}d_6$

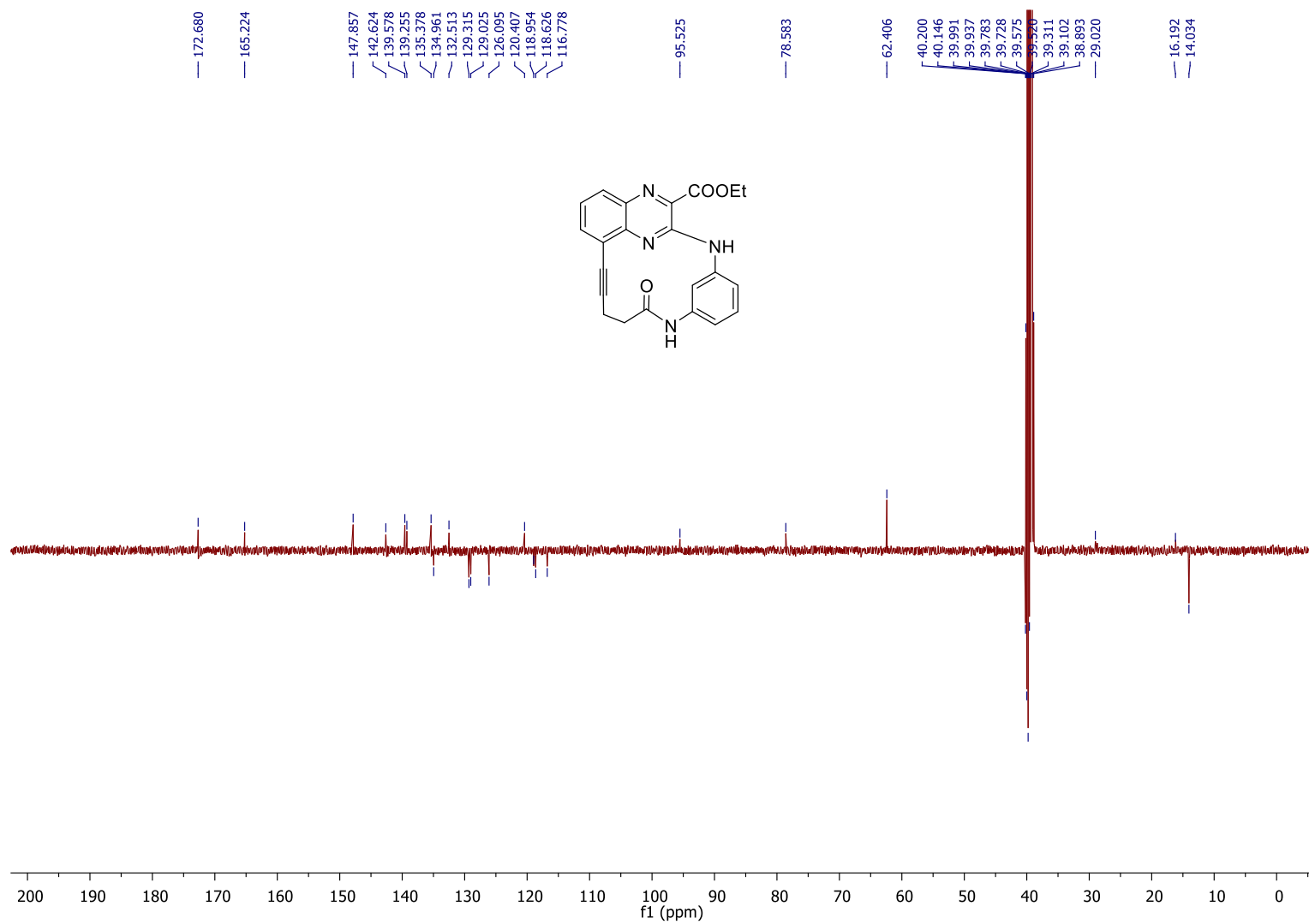


<sup>1</sup>H NMR of compound **7** in DMSO-*d*<sub>6</sub>

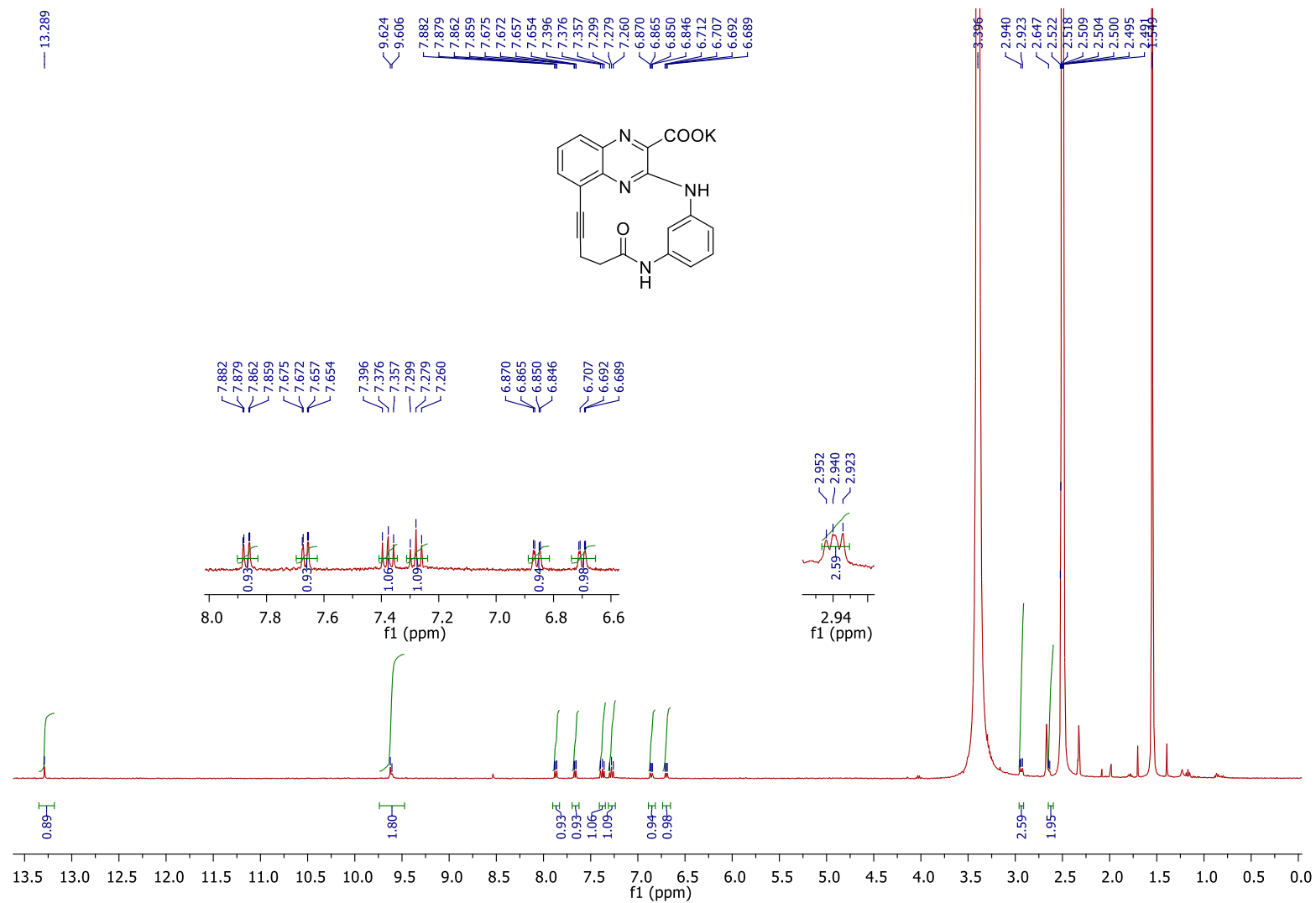




$^{13}\text{C}$  NMR (JMOD) of compound **7** in  $\text{DMSO}-d_6$



<sup>1</sup>H NMR of compound **8** in DMSO-*d*<sub>6</sub>

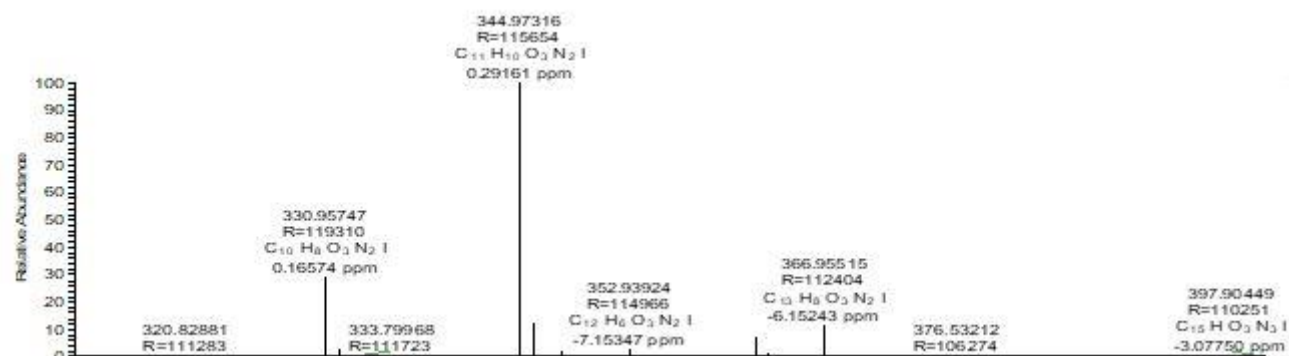


## 2. HRMS spectra

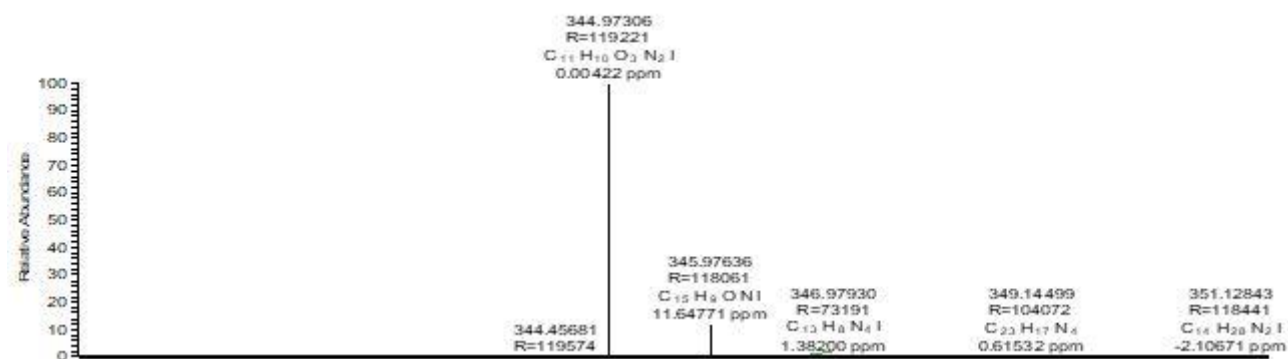
HRMS spectrum of compound **2**



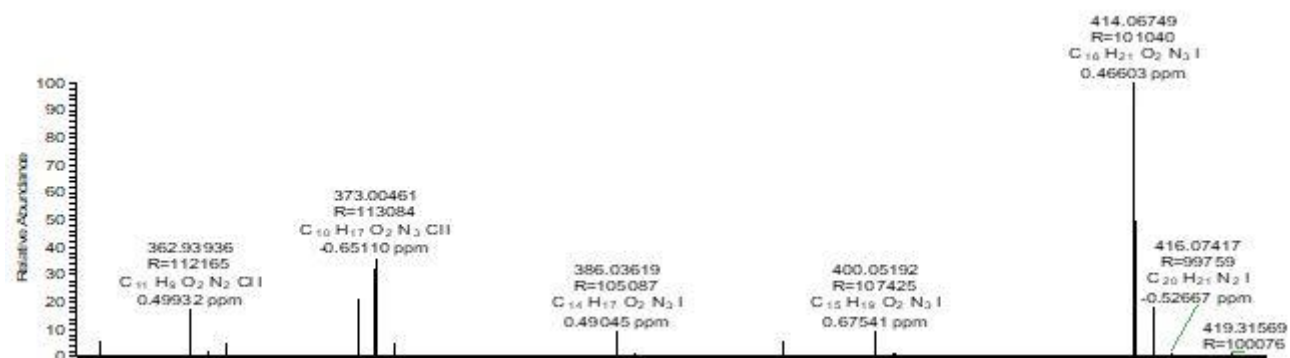
# HRMS spectrum of compound **4a**



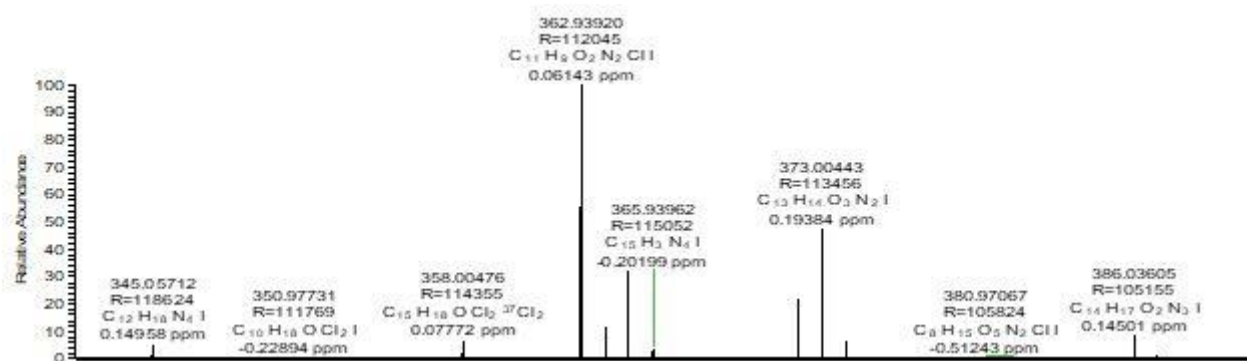
# HRMS spectrum of compound **4b**



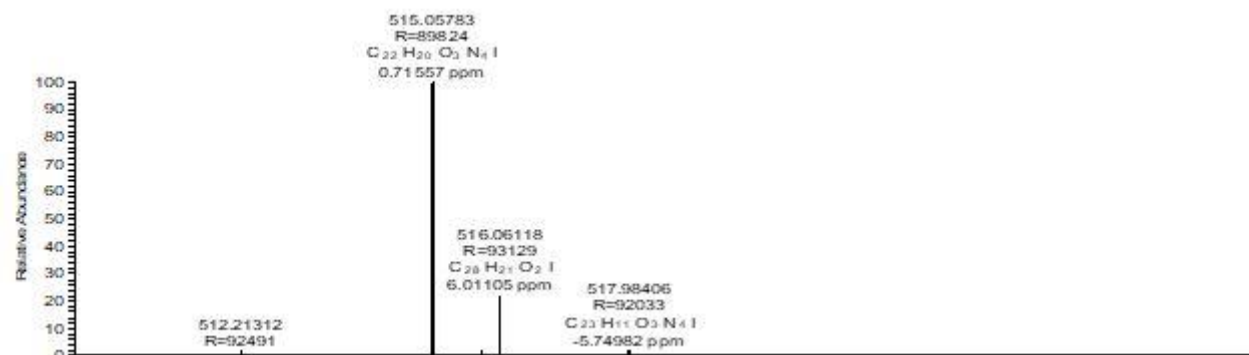
# HRMS spectrum of compound **5a**



# HRMS spectrum of compound **5b**

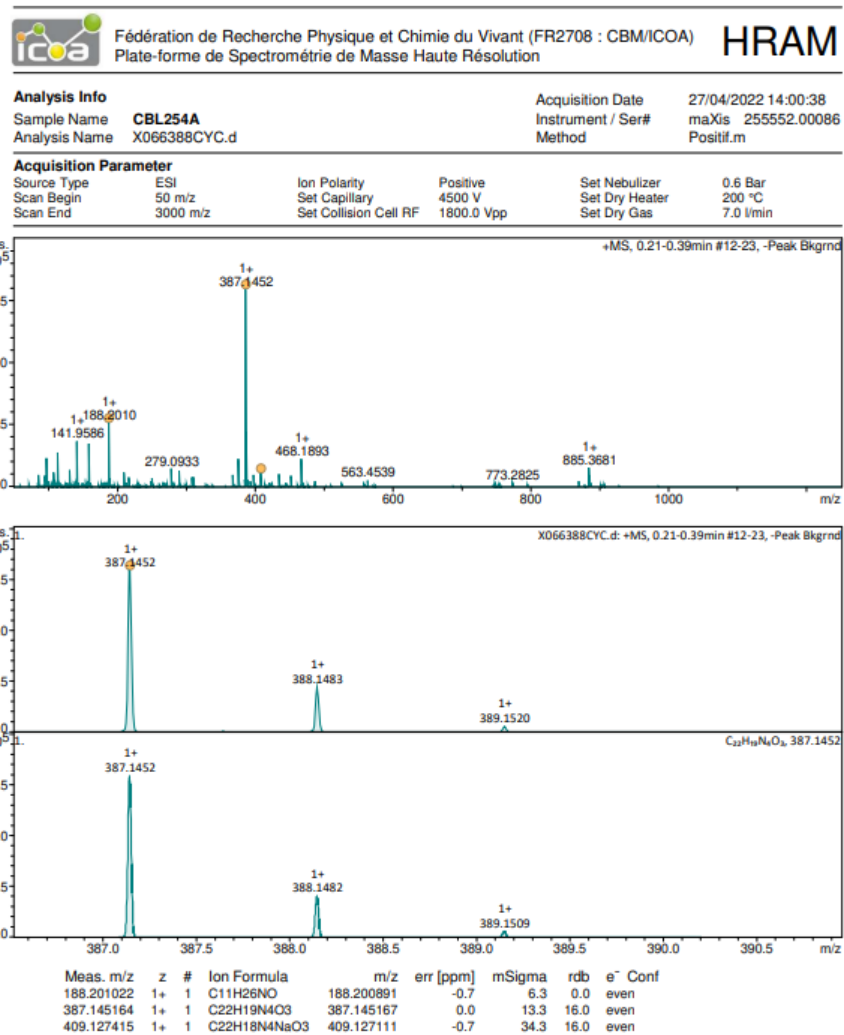


HRMS spectrum of compound **6**





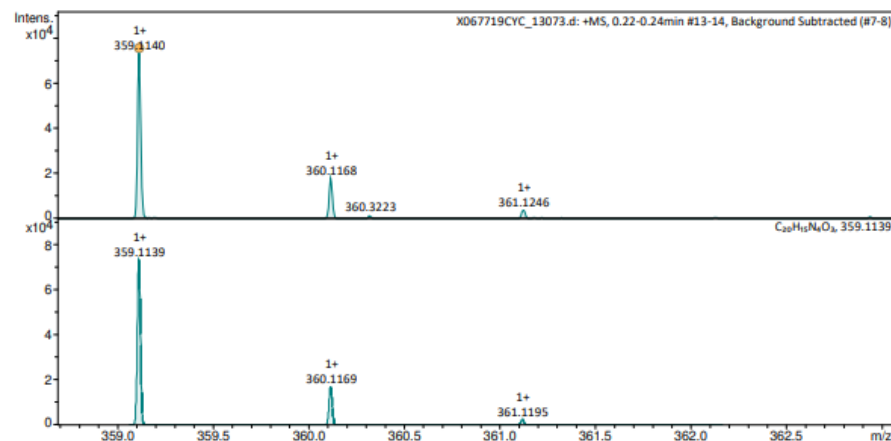
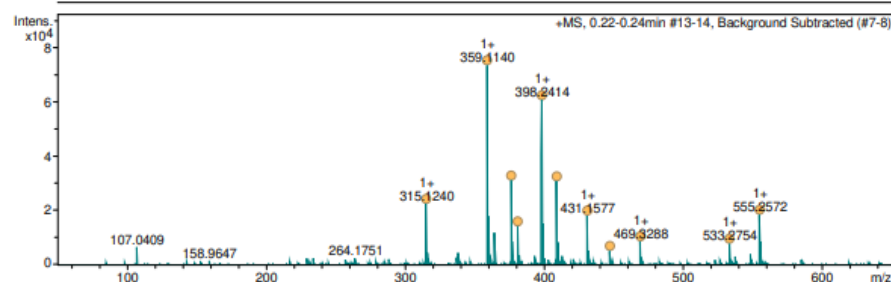
## HRMS spectrum of compound 7



## HRMS spectrum of compound 8

<b>Analysis Info</b>		Acquisition Date	06/07/2022 12:14:30
Sample Name	<b>CBL323b</b>	Instrument / Ser#	maXis 255552.00086
Analysis Name	X067719CYC_13073.d	Method	Positif.m

<b>Acquisition Parameter</b>					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan End	3000 m/z	Set Collision Cell RF	1800.0 Vpp	Set Dry Gas	7.0 l/min



Meas. m/z	z	#	Ion Formula	m/z	err [ppm]	mSigma	rdB	e <sup>-</sup>	Conf
315.124029	1+	1	C19H15N4O	315.124038	0.0	14.8	15.0	even	
359.114011	1+	1	C20H15N4O3	359.113867	-0.4	12.9	16.0	even	
376.259804	1+	1	C21H34N3O3	376.259468	-0.9	22.5	7.0	even	
381.095904	1+	1	C20H14N4NaO3	381.095811	-0.2	26.9	16.0	even	
398.241419	1+	1	C21H33N3NaO3	398.241413	-0.0	4.8	7.0	even	
409.175862	1+	1	C23H25N2O5	409.175798	-0.2	9.5	13.0	even	
431.157745	1+	1	C23H24N2NaO5	431.157743	-0.0	15.7	13.0	even	
447.346736	1+	1	C28H47O4	447.346886	0.3	109.5	6.0	even	