

Synthesis of Pyrazolo[1,5-*a*]quinoxalin-4(5*H*)-ones via One-pot Amidation/N-Arylation Reactions Under Transition Metal-Free Conditions

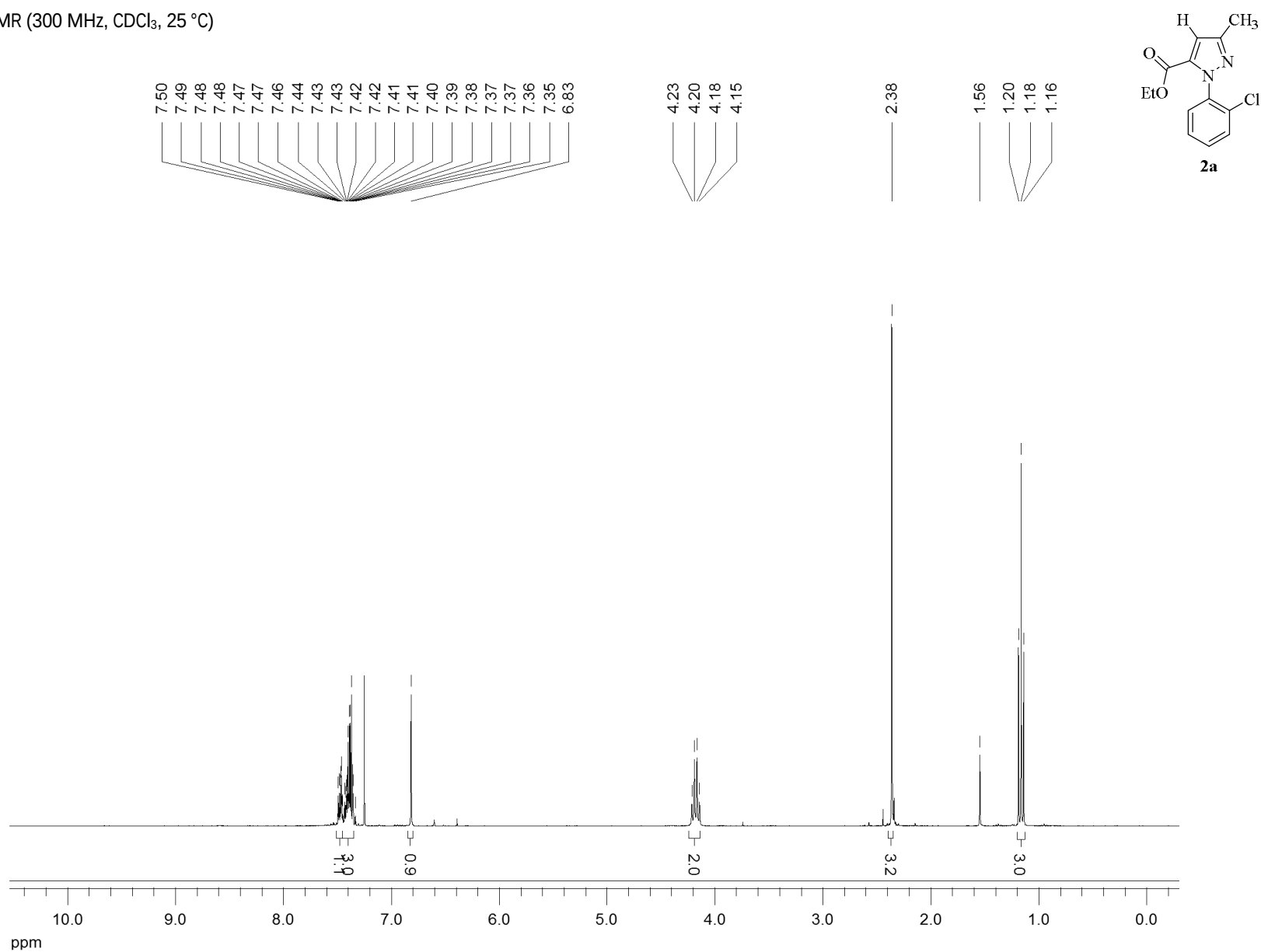
Carson Wiethan,^a Steffany Z. Franceschini,^a Helio G. Bonacorso ^{*a} and Mark Stradiotto^{*b}

^a Departamento de Química, Universidade Federal de Santa Maria, 97105-900 Santa Maria, Brazil

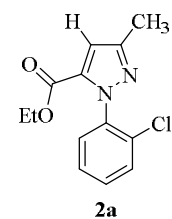
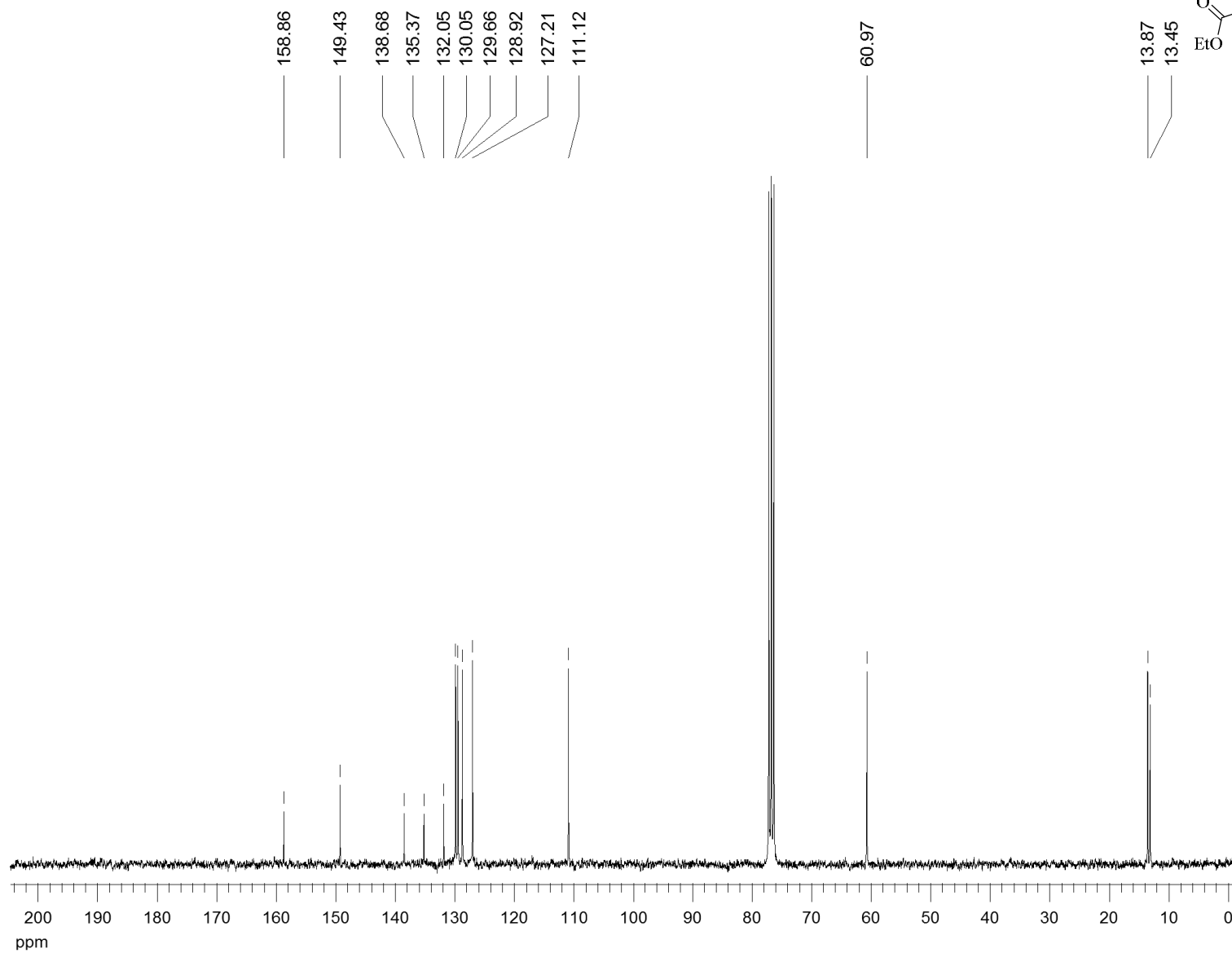
^b Department of Chemistry, Dalhousie University Halifax, NS, B3H 4R2 Canada

Contents: NMR spectral data.

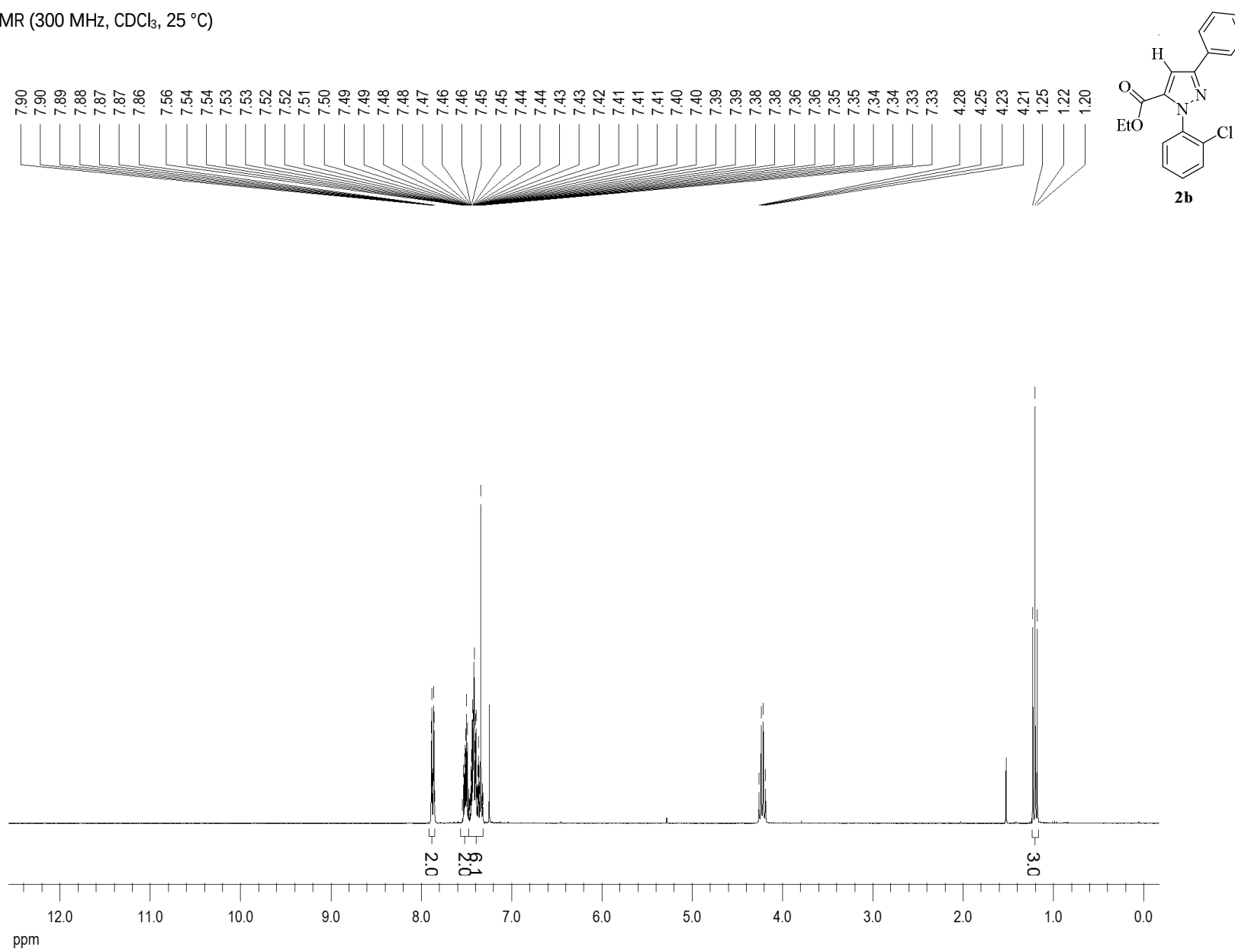
2a – ^1H NMR (300 MHz, CDCl_3 , 25 °C)



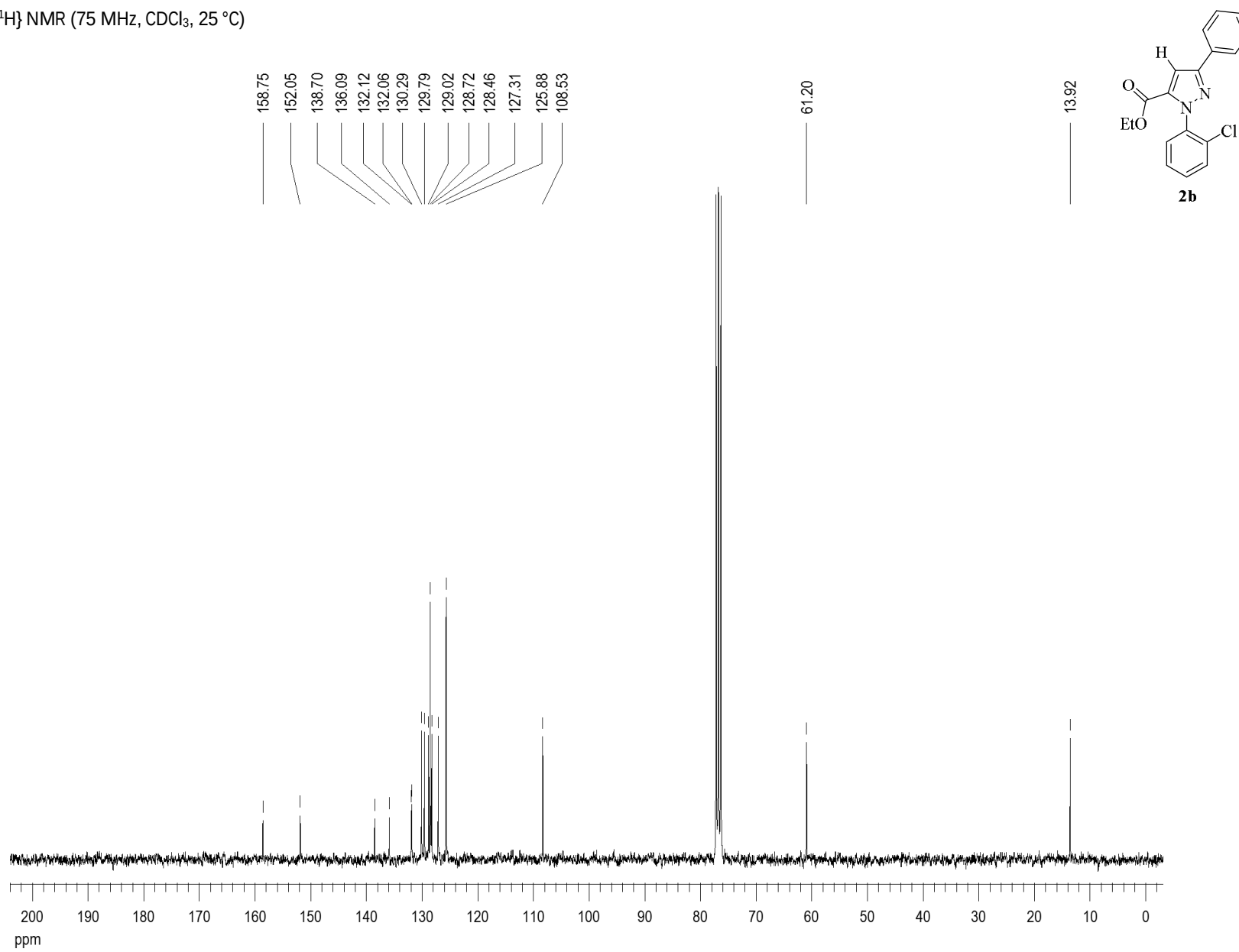
2a – ^{13}C { ^1H } NMR (75 MHz, CDCl_3 , 25 °C)



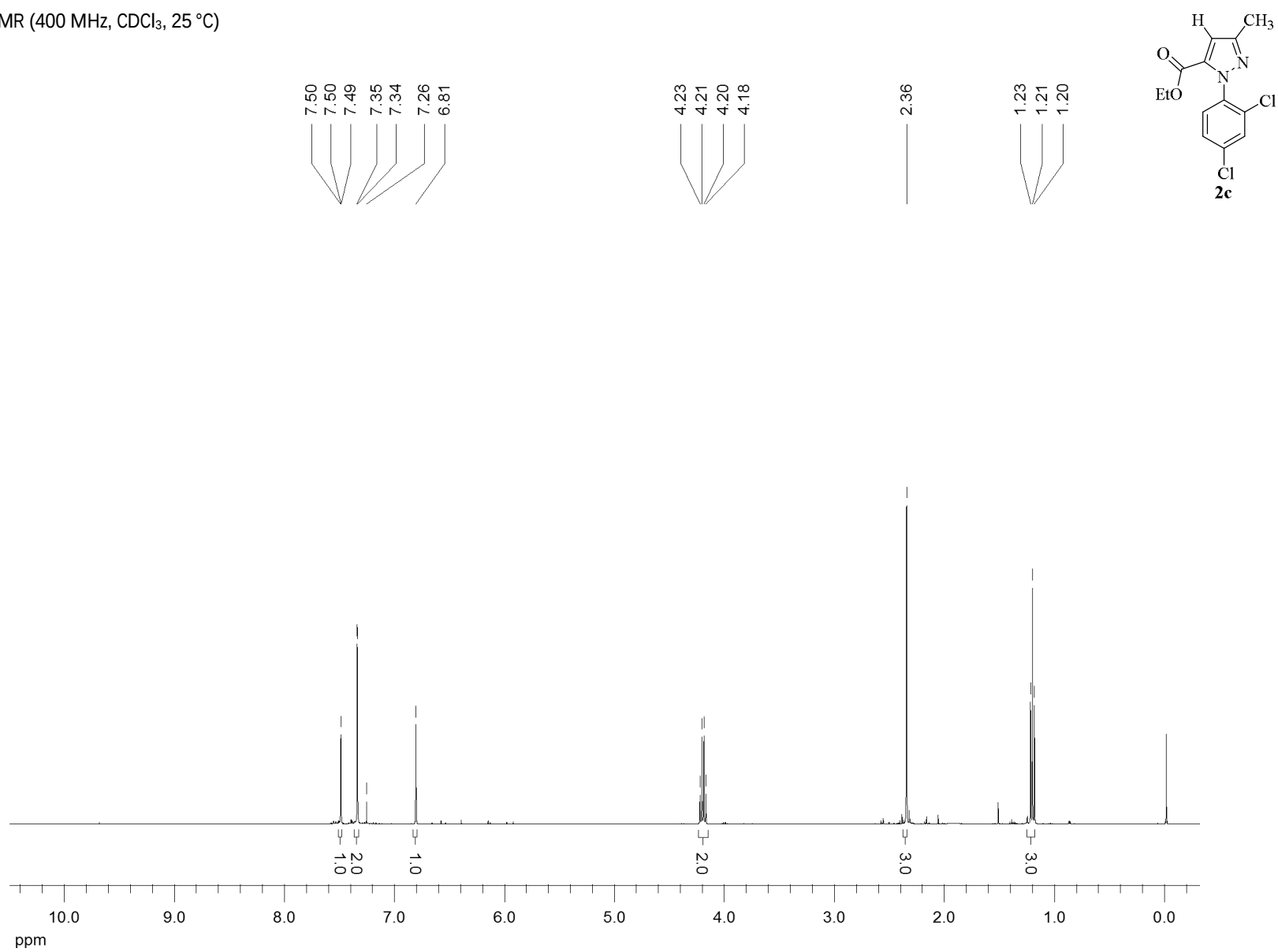
2b – ^1H NMR (300 MHz, CDCl_3 , 25 $^\circ\text{C}$)



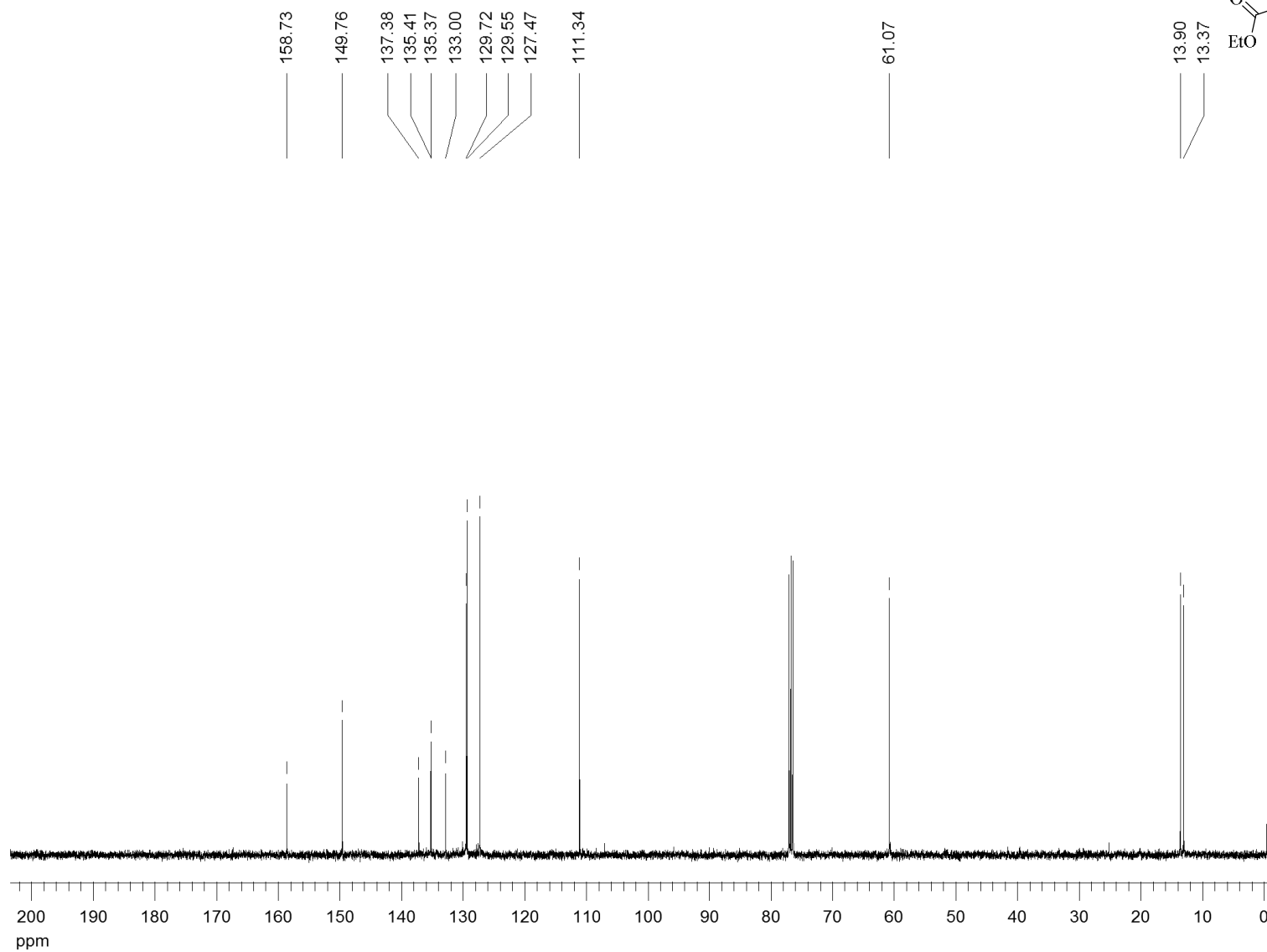
2b – ^{13}C { ^1H } NMR (75 MHz, CDCl_3 , 25 °C)



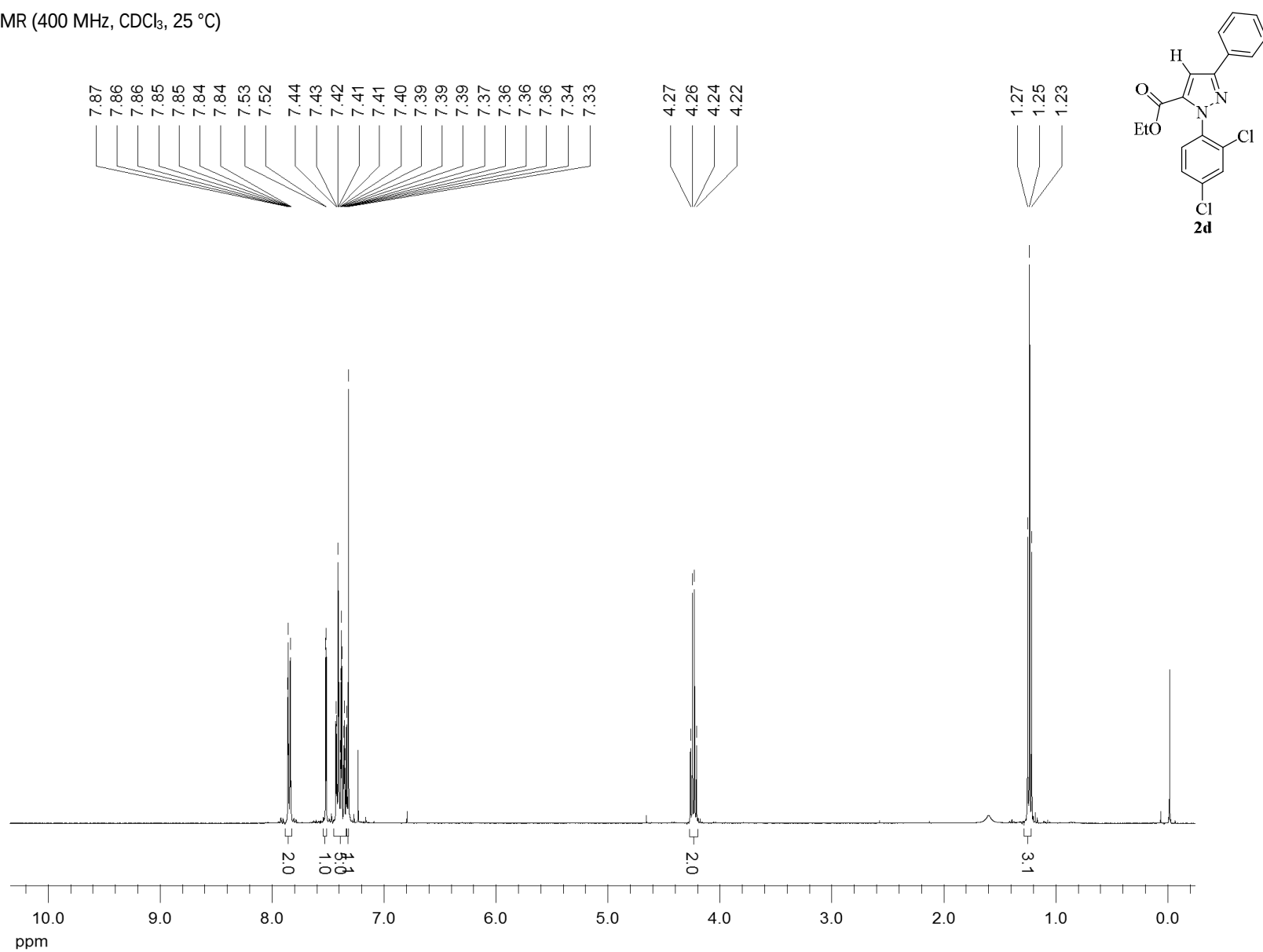
2c – ^1H NMR (400 MHz, CDCl_3 , 25 °C)



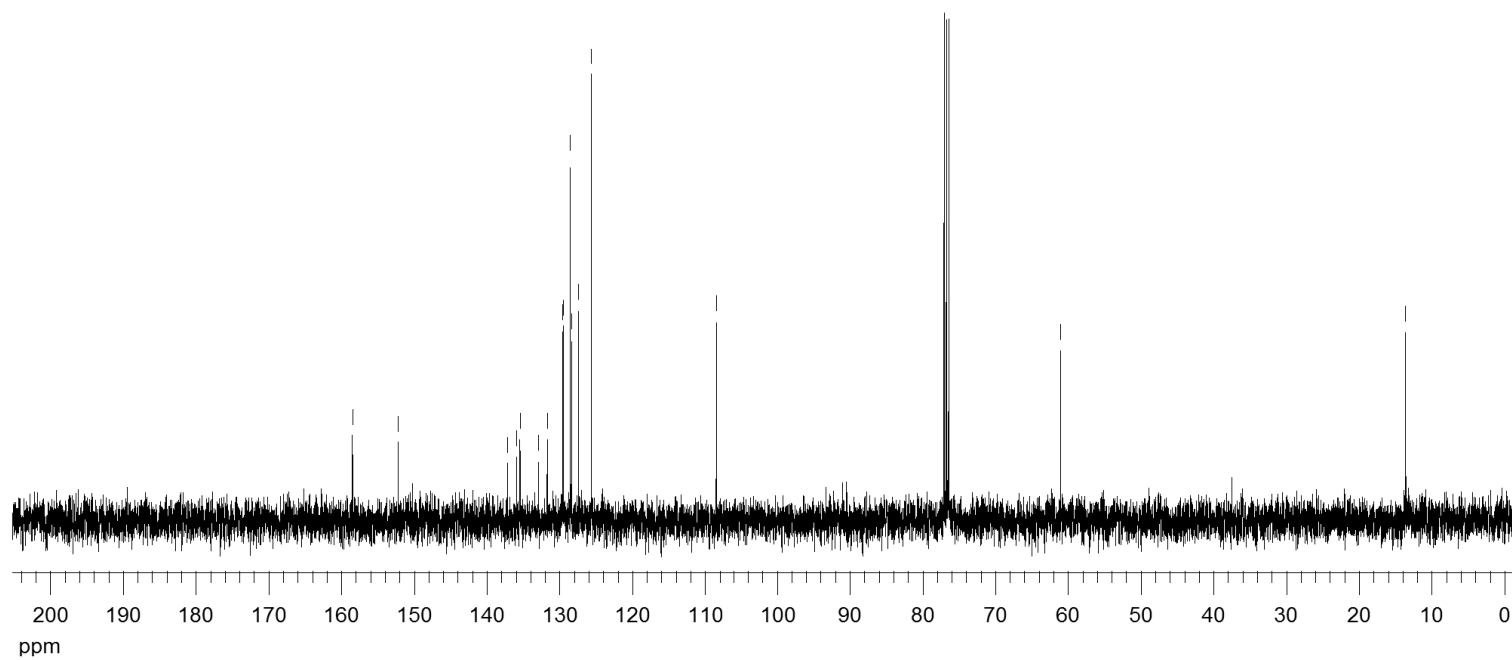
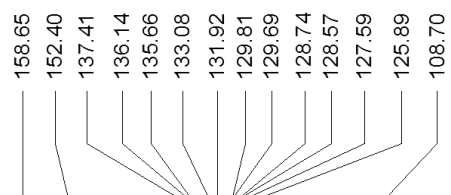
2c – ^{13}C { ^1H } NMR (100 MHz, CDCl_3 , 25 °C)



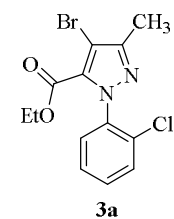
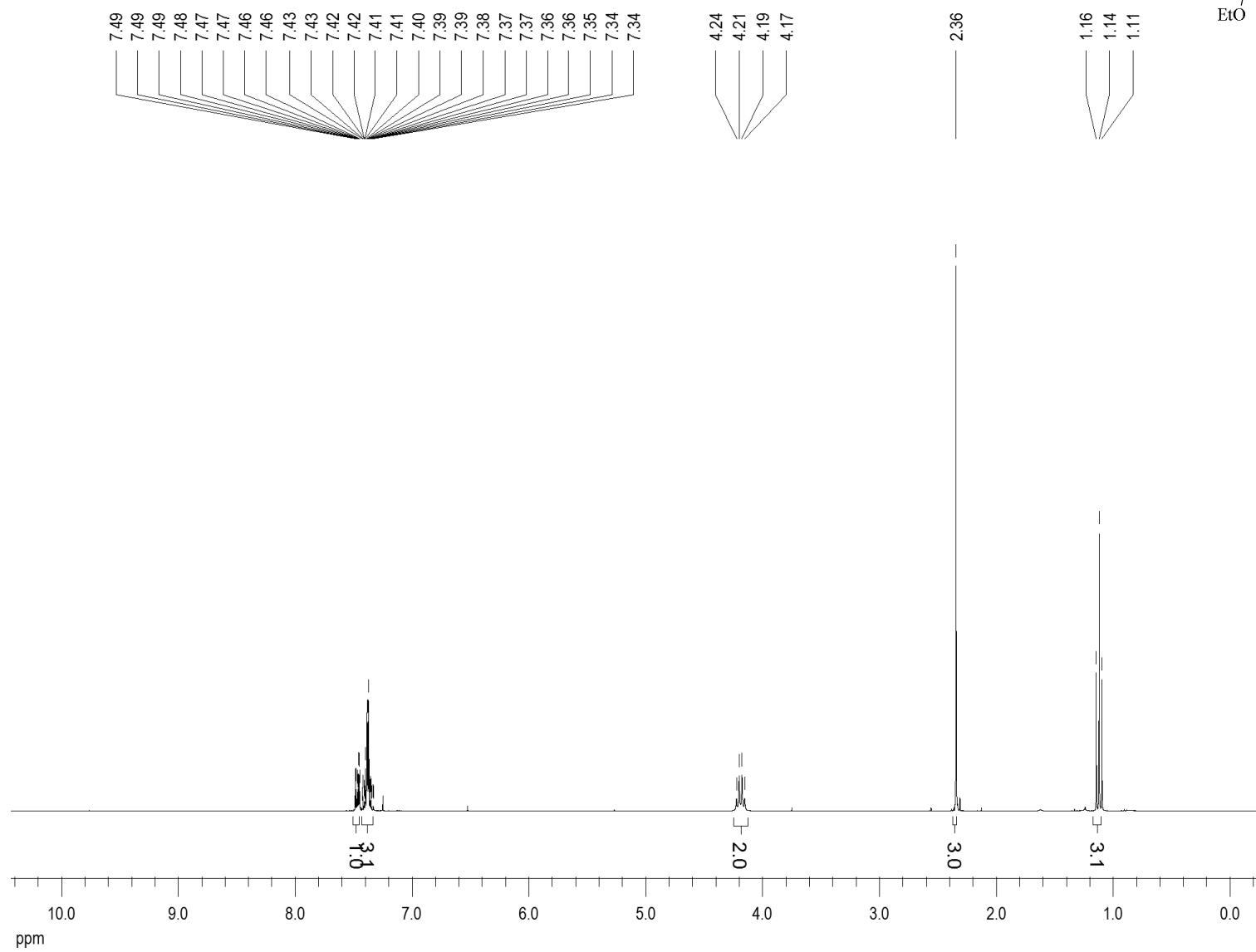
2d – ^1H NMR (400 MHz, CDCl_3 , 25 $^\circ\text{C}$)



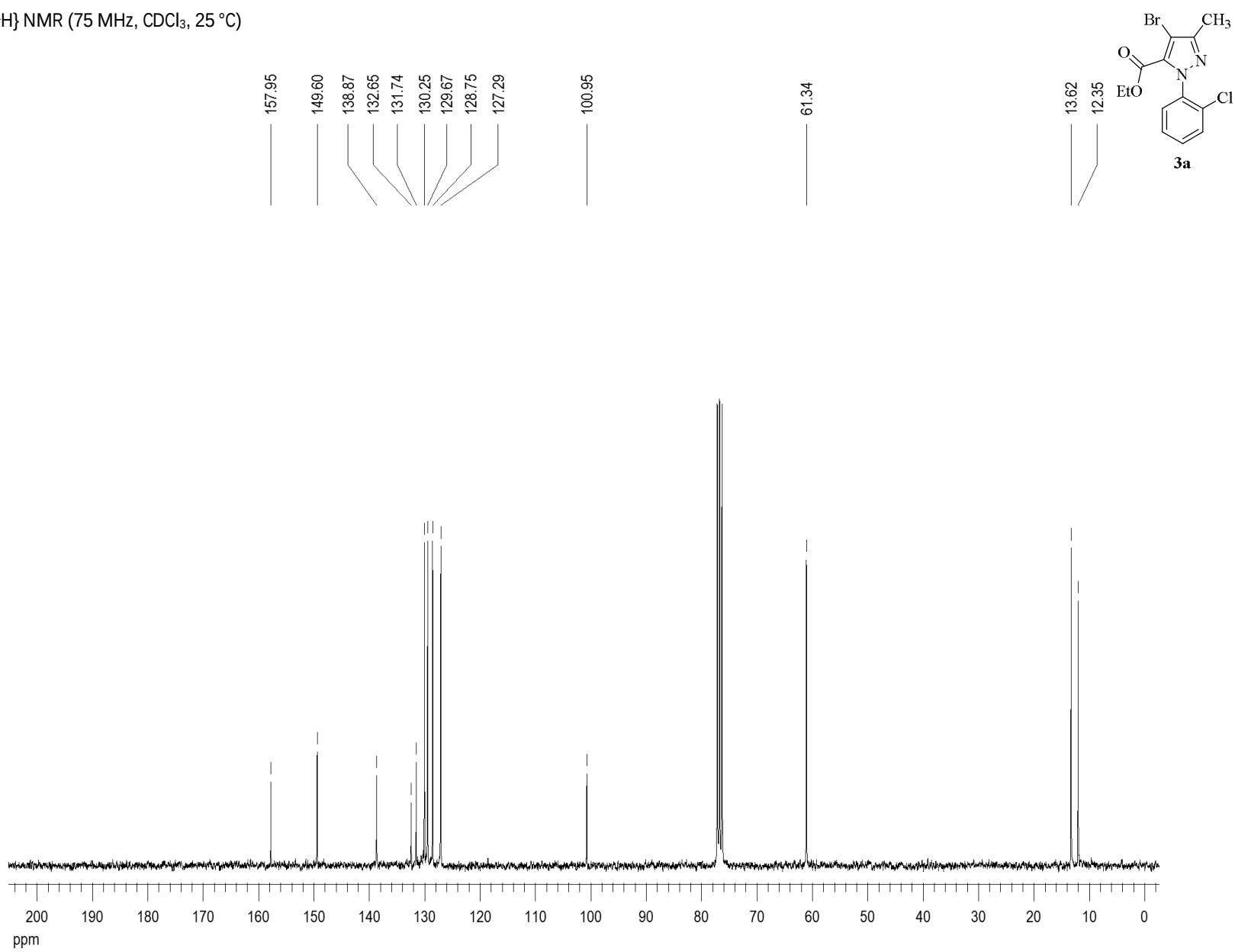
2d – ^{13}C { ^1H } NMR (100 MHz, CDCl_3 , 25 °C)



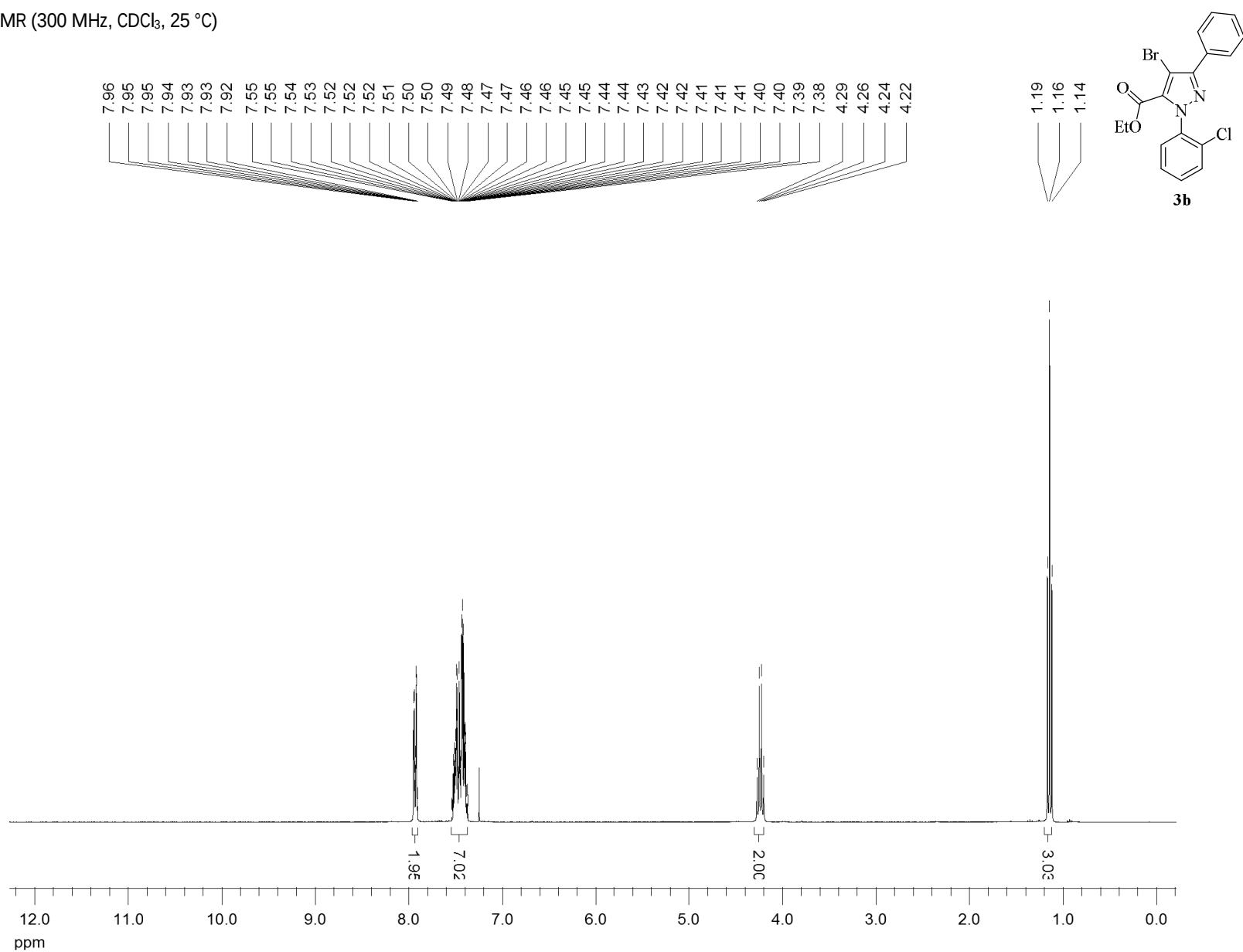
3a – ^1H NMR (300 MHz, CDCl_3 , 25 $^\circ\text{C}$)



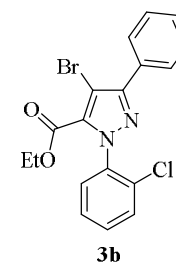
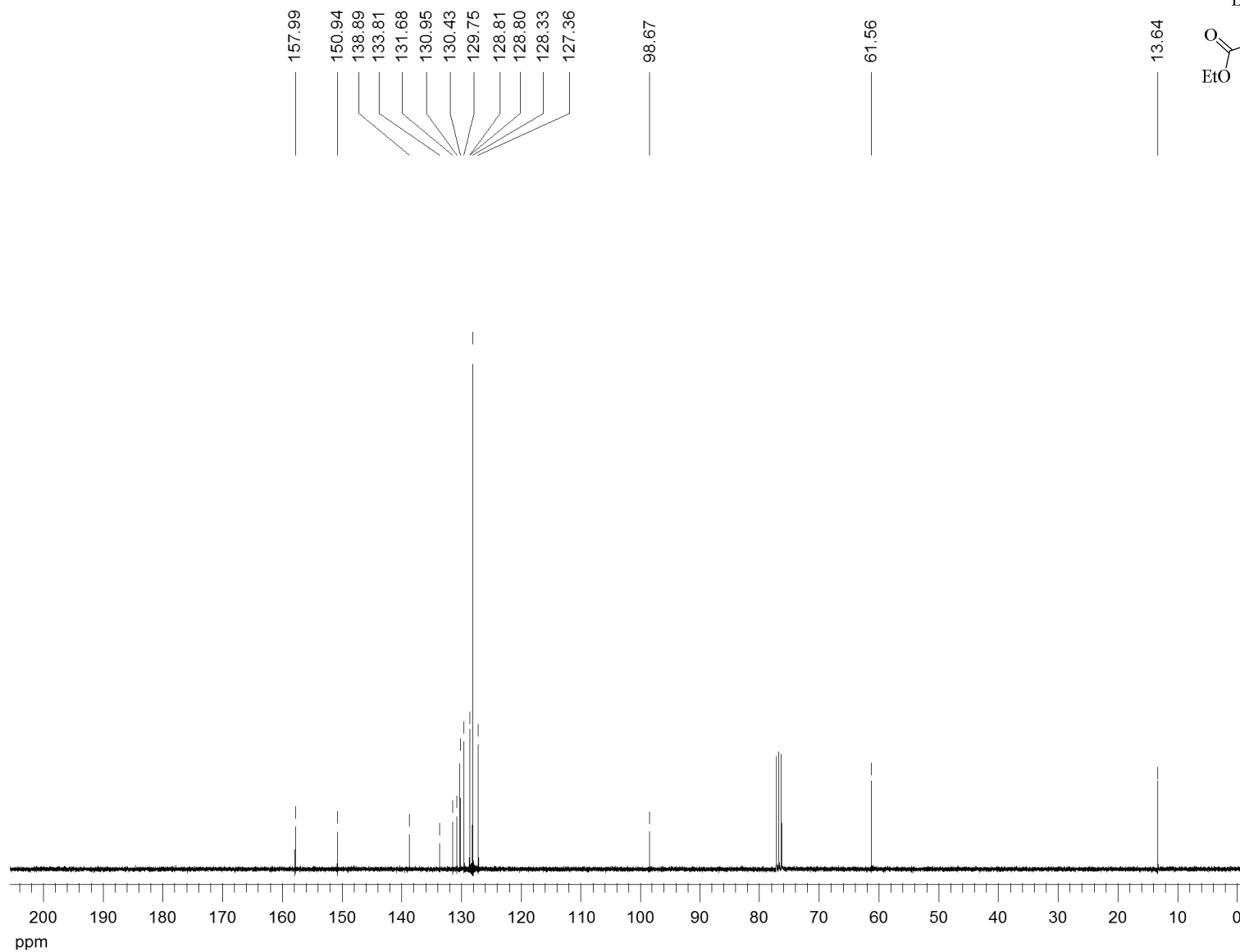
3a – ^{13}C { ^1H } NMR (75 MHz, CDCl_3 , 25 °C)



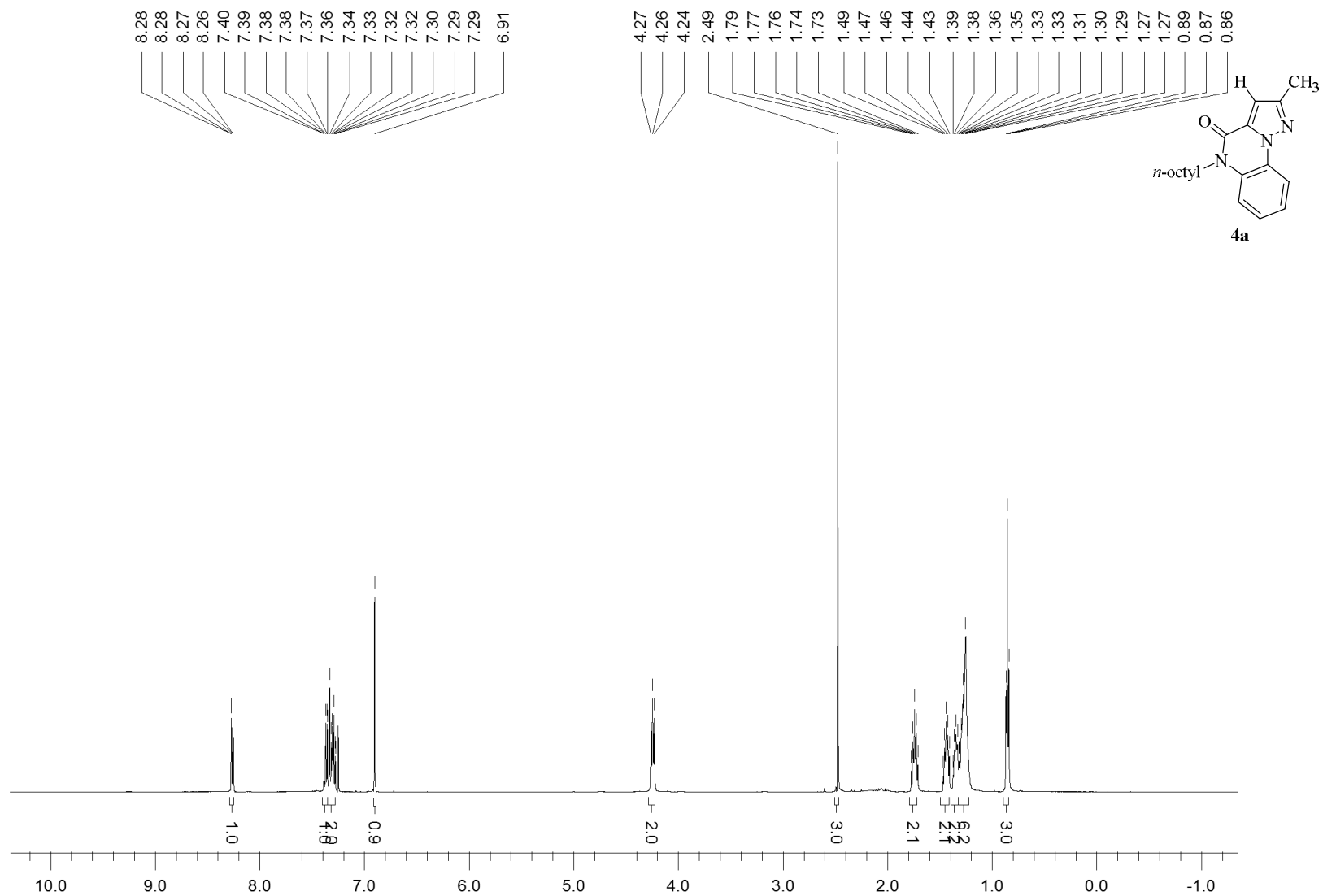
3b – ^1H NMR (300 MHz, CDCl_3 , 25 $^\circ\text{C}$)



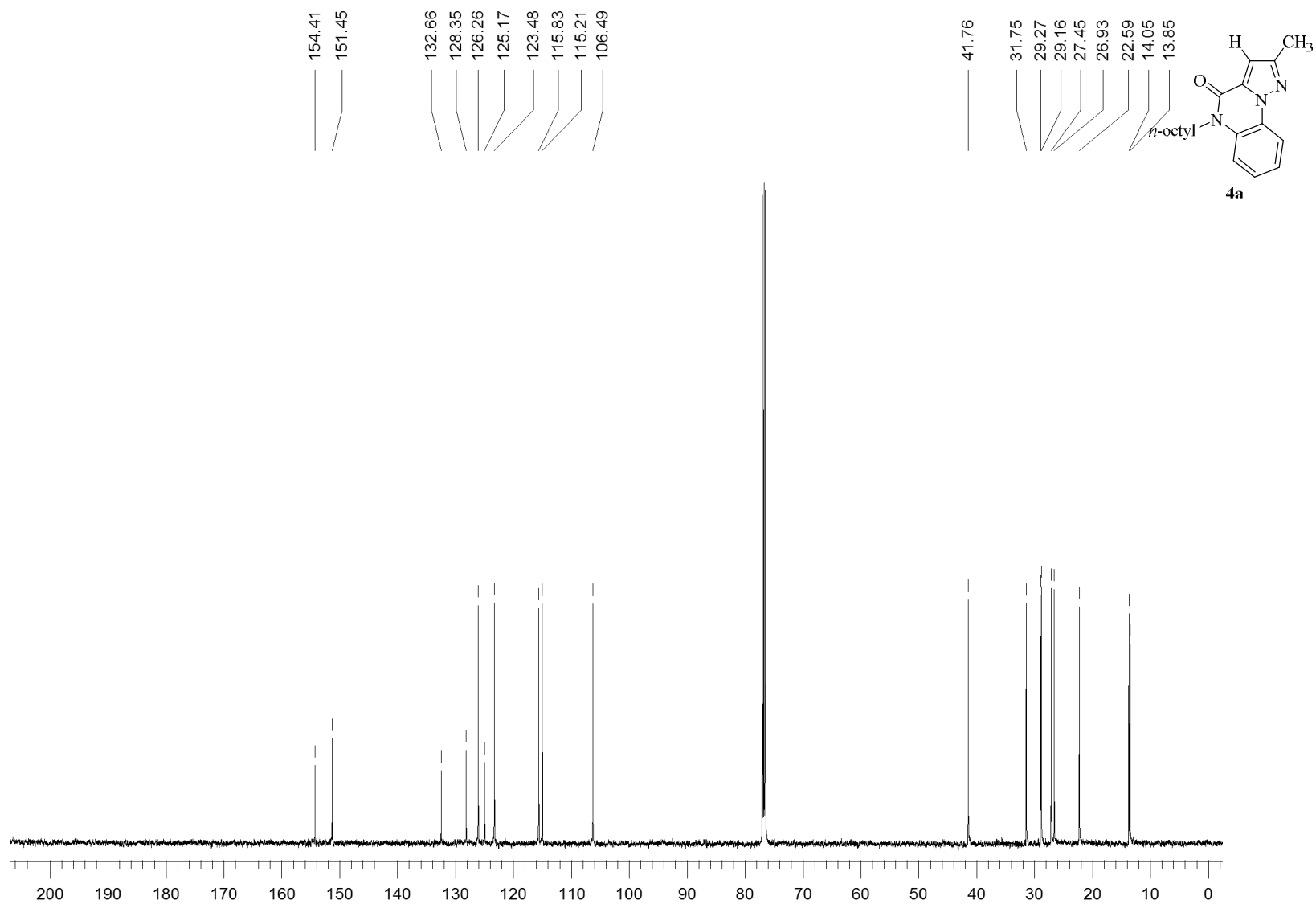
3b – ^{13}C { ^1H } NMR (75 MHz, CDCl_3 , 25 °C)



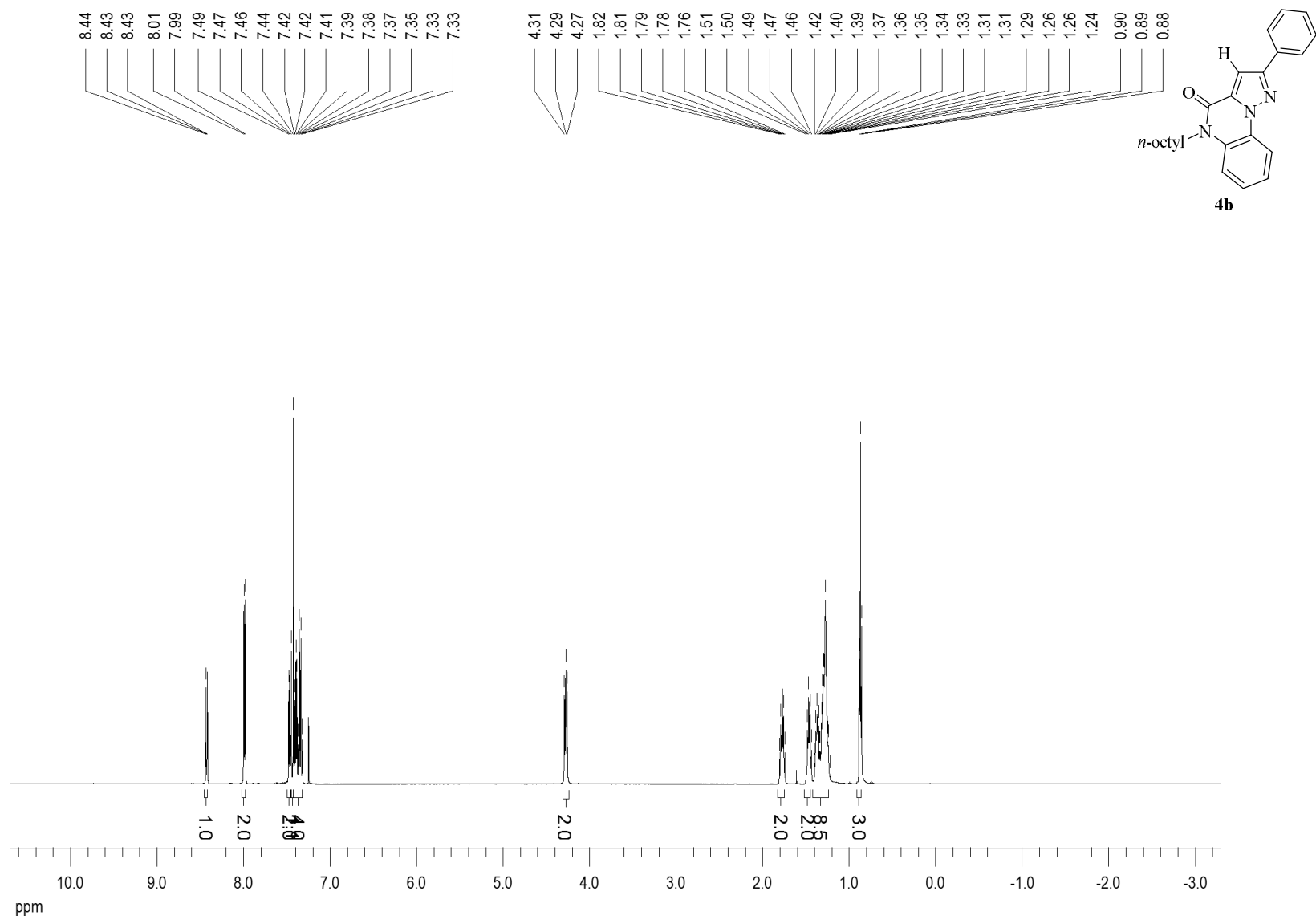
4a – ^1H NMR (500 MHz, CDCl_3 , 25 $^\circ\text{C}$)



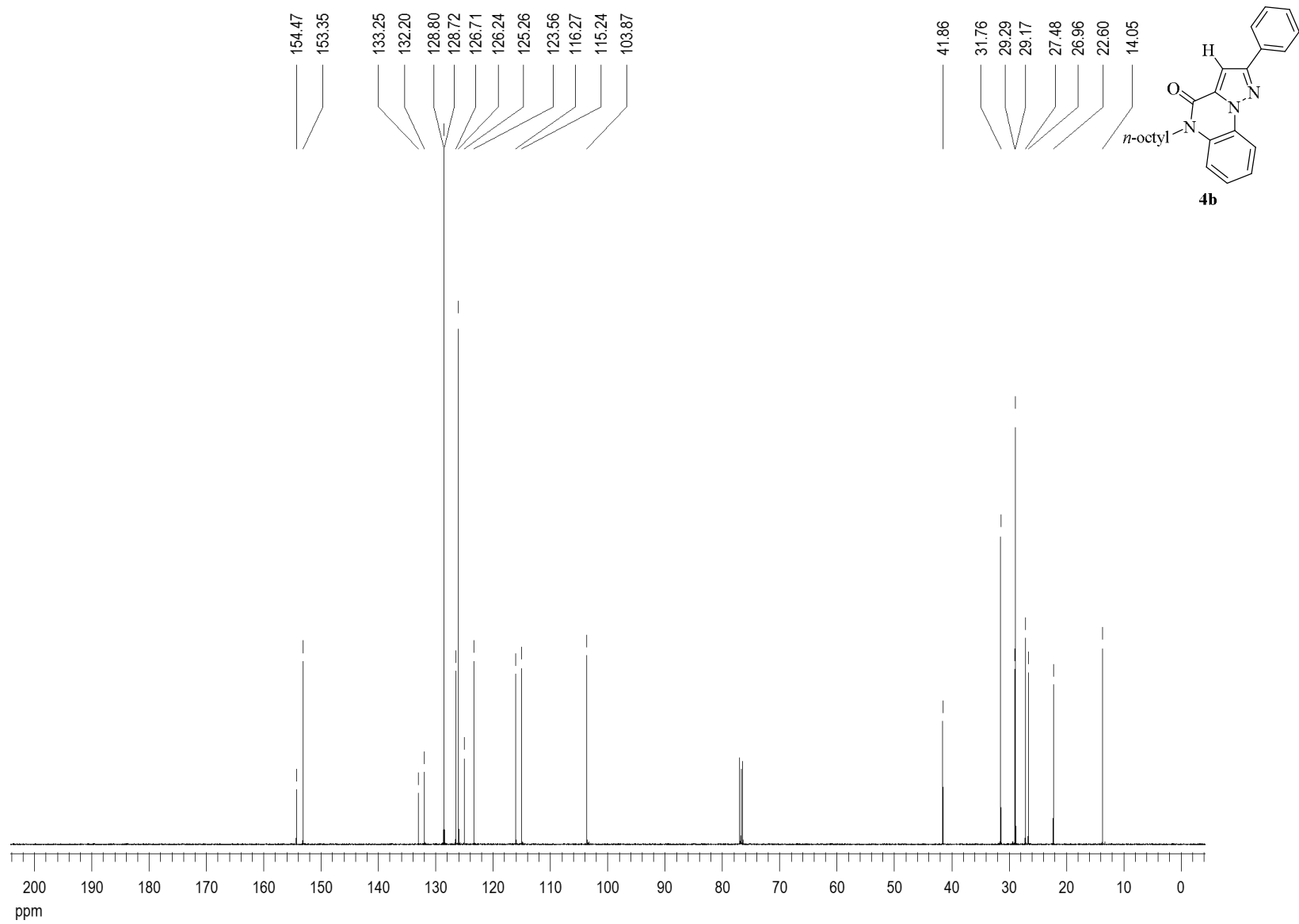
4a – ^{13}C { ^1H } NMR (125 MHz, CDCl_3 , 25 °C)



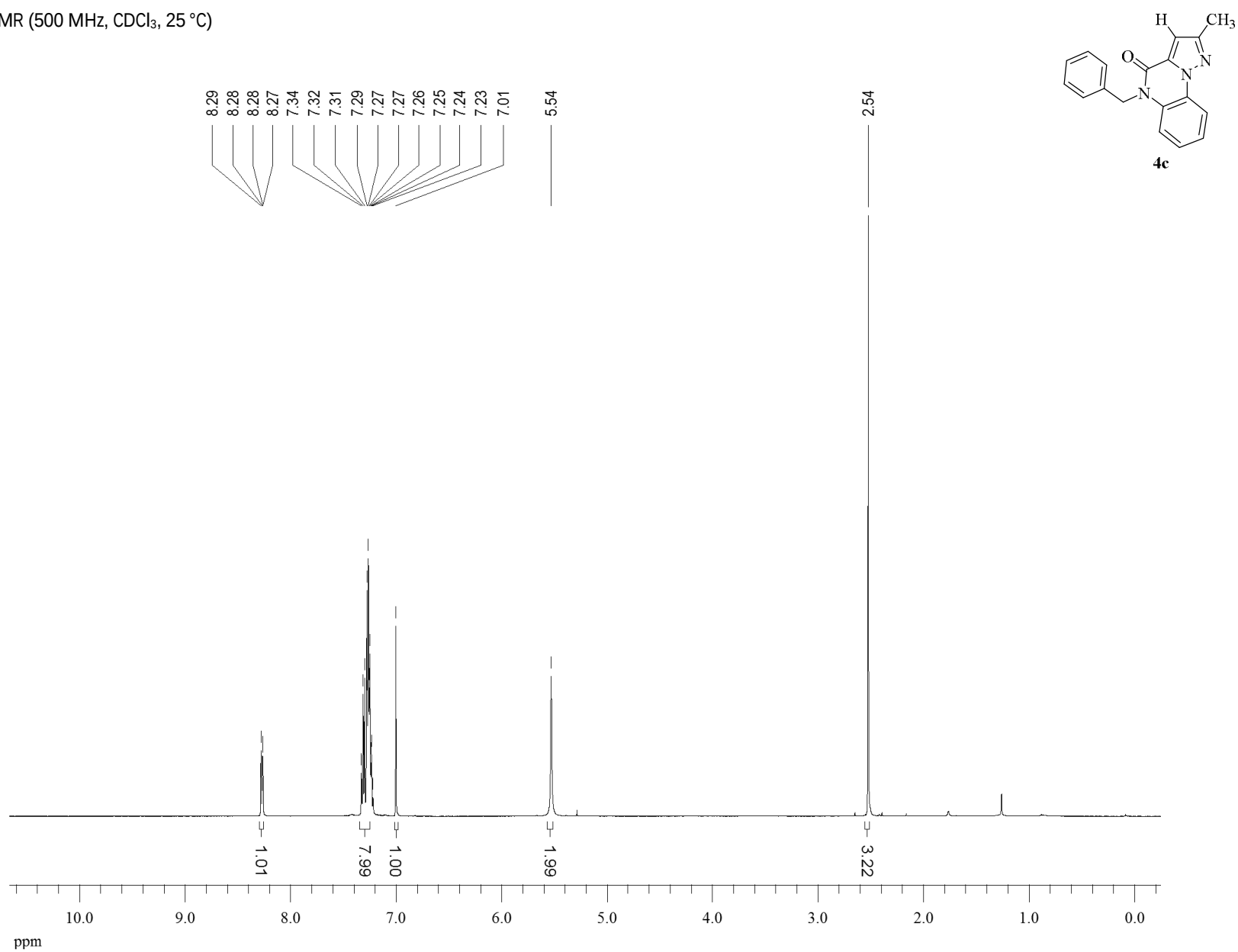
4b – ^1H NMR (500 MHz, CDCl_3 , 25 $^\circ\text{C}$)



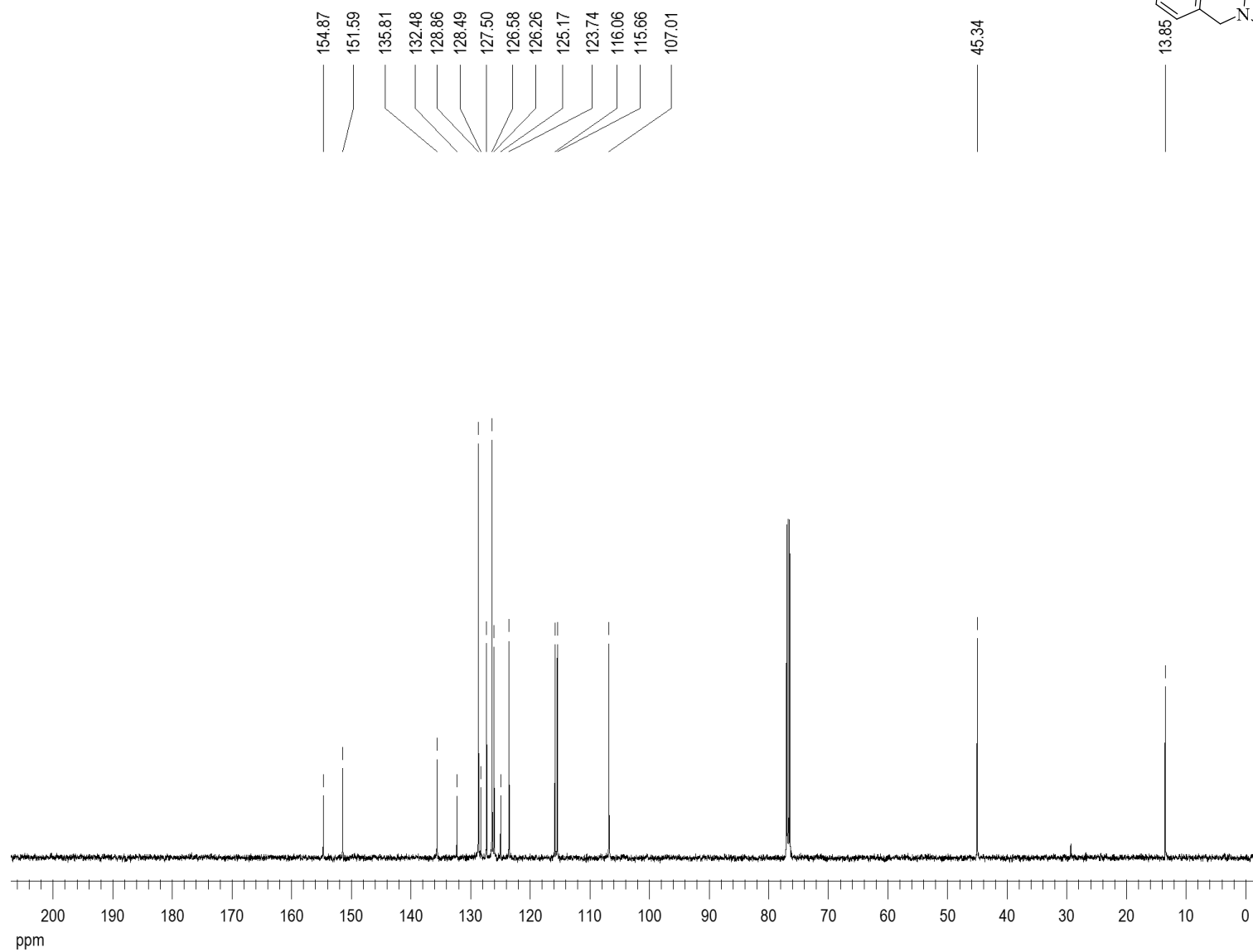
4b – ^{13}C { ^1H } NMR (125 MHz, CDCl_3 , 25 °C)



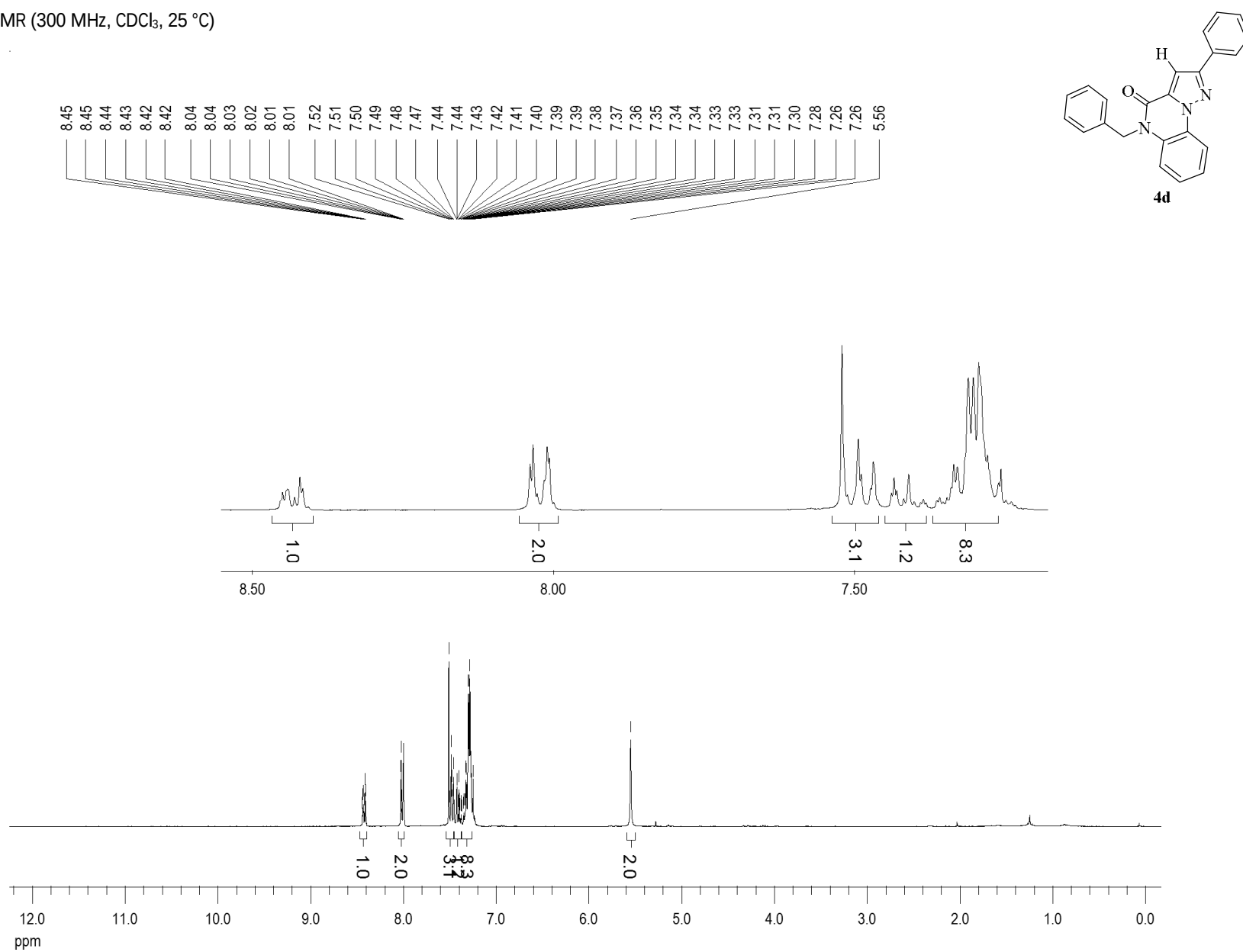
4c – ^1H NMR (500 MHz, CDCl_3 , 25 °C)



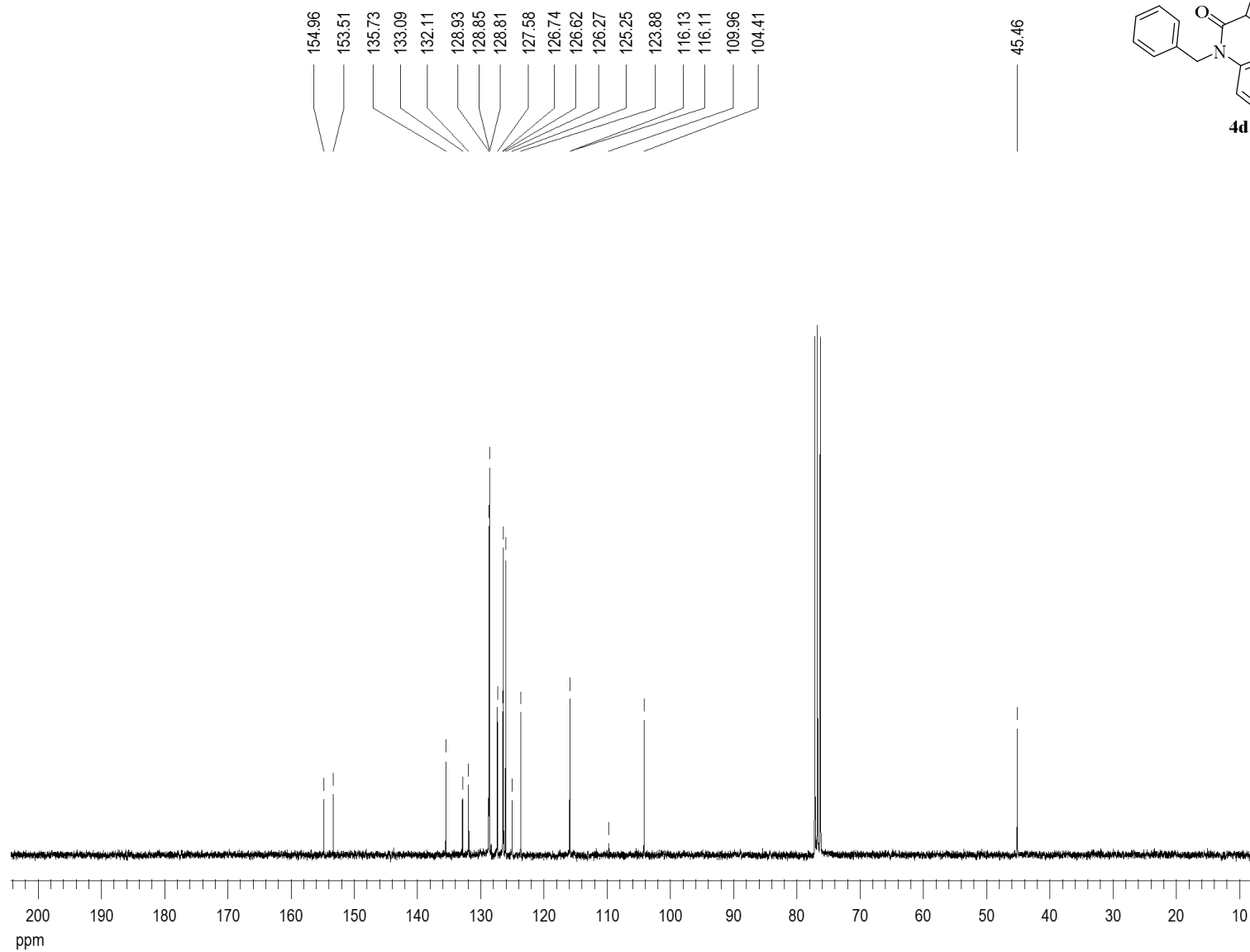
4c – ^{13}C { ^1H } NMR (125 MHz, CDCl_3 , 25 °C)



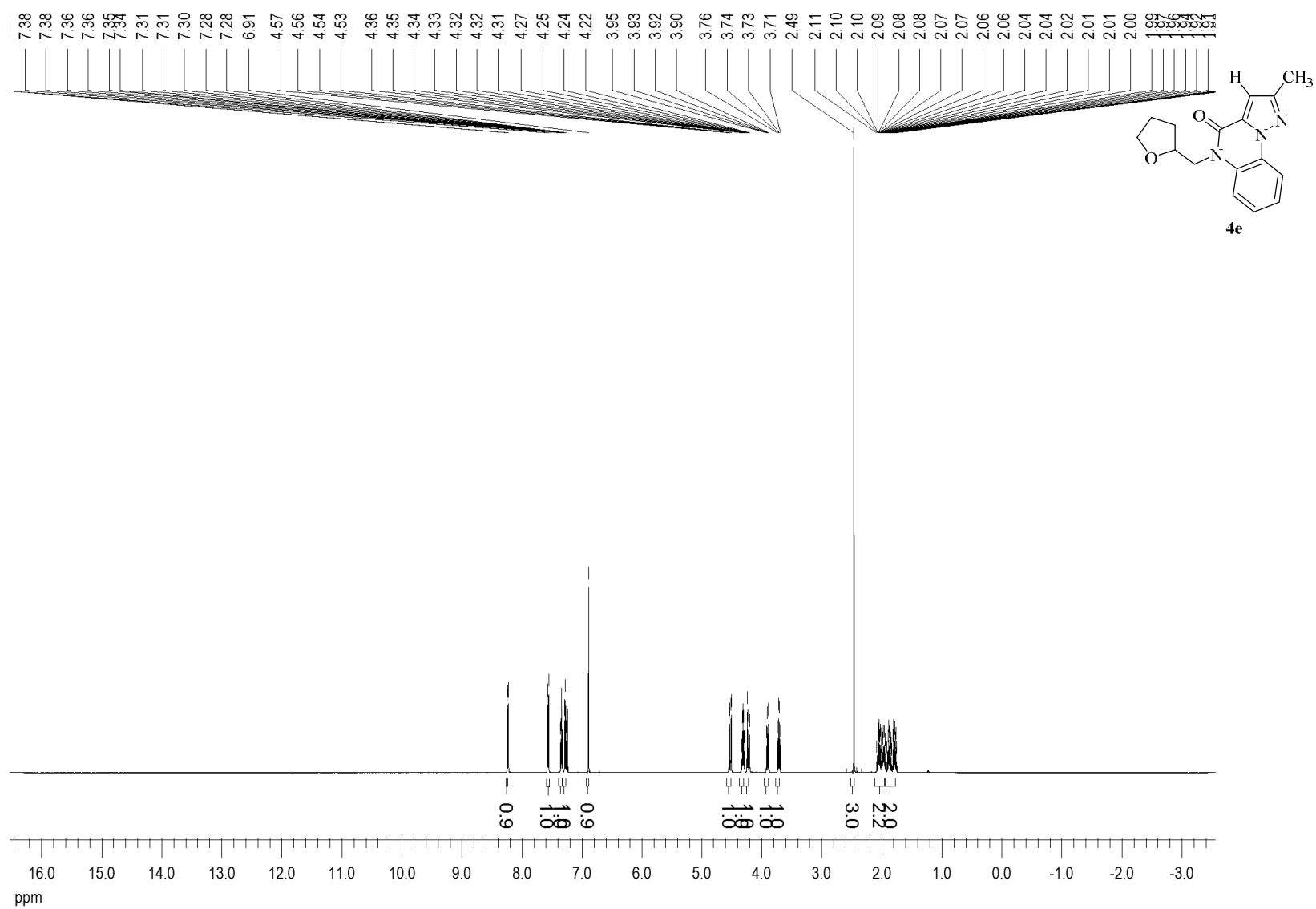
4d – ^1H NMR (300 MHz, CDCl_3 , 25 °C)



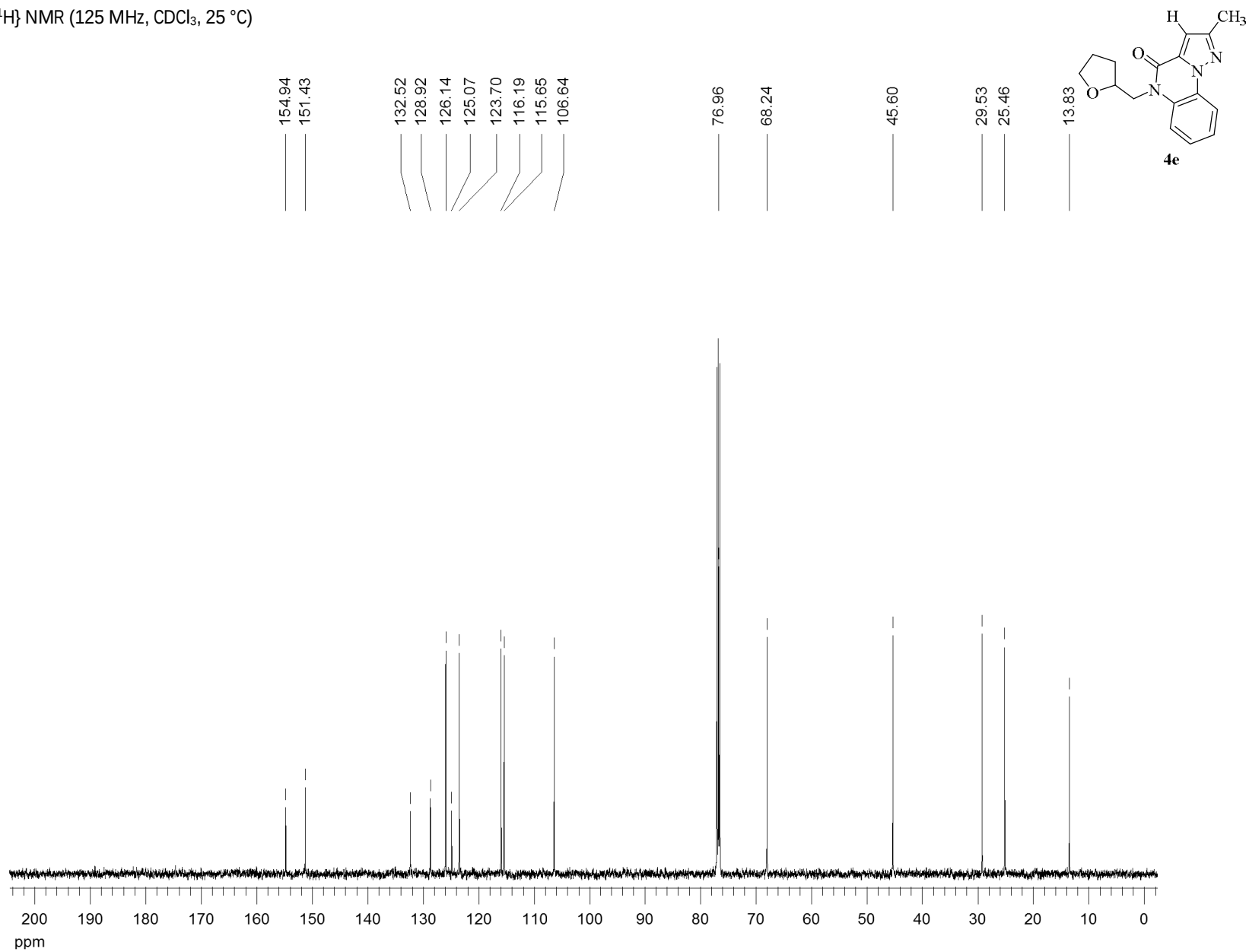
4d – ^{13}C { ^1H } NMR (75 MHz, CDCl_3 , 25 °C)



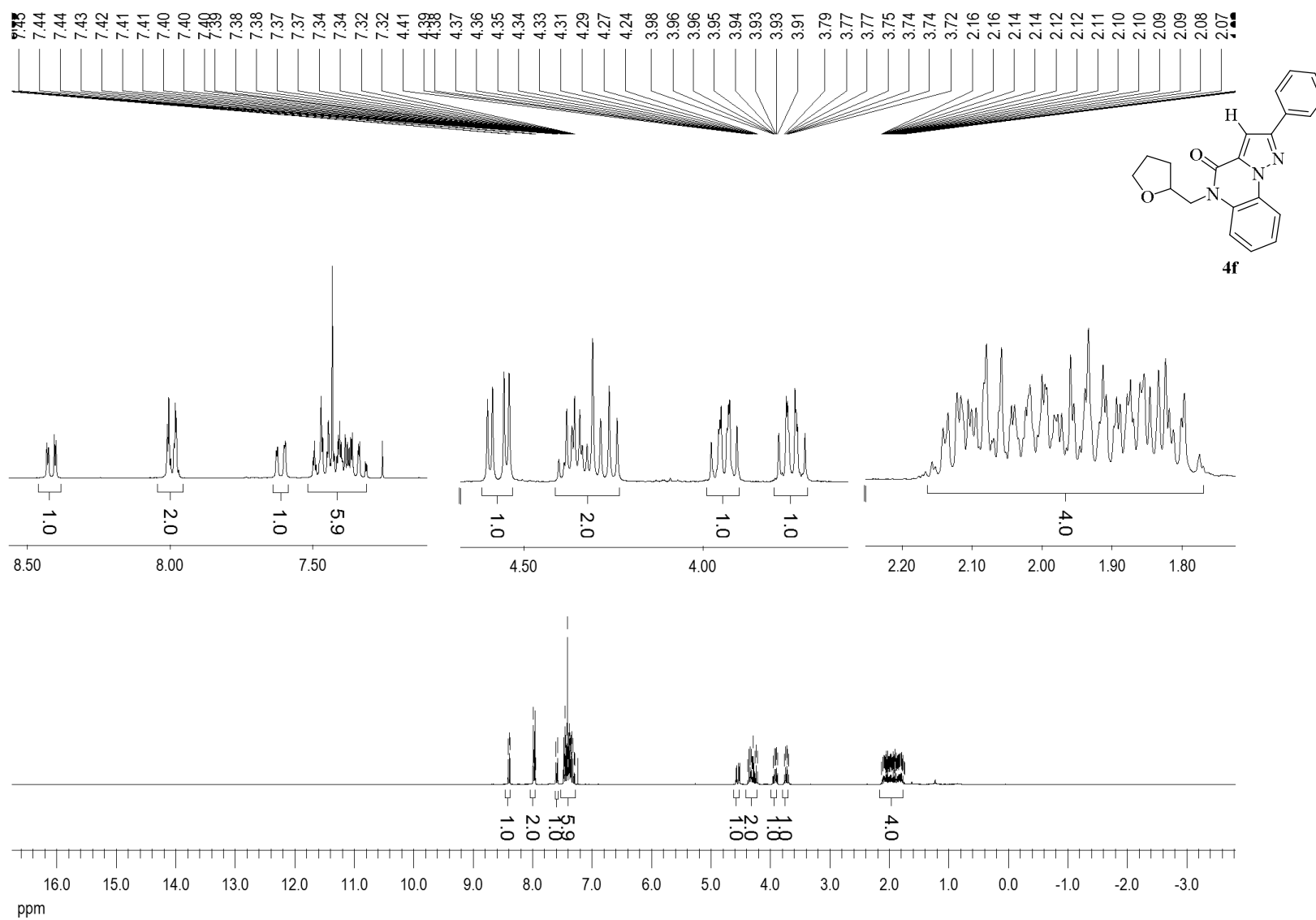
4e – ^1H NMR (500 MHz, CDCl_3 , 25 $^\circ\text{C}$)



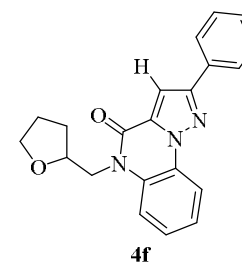
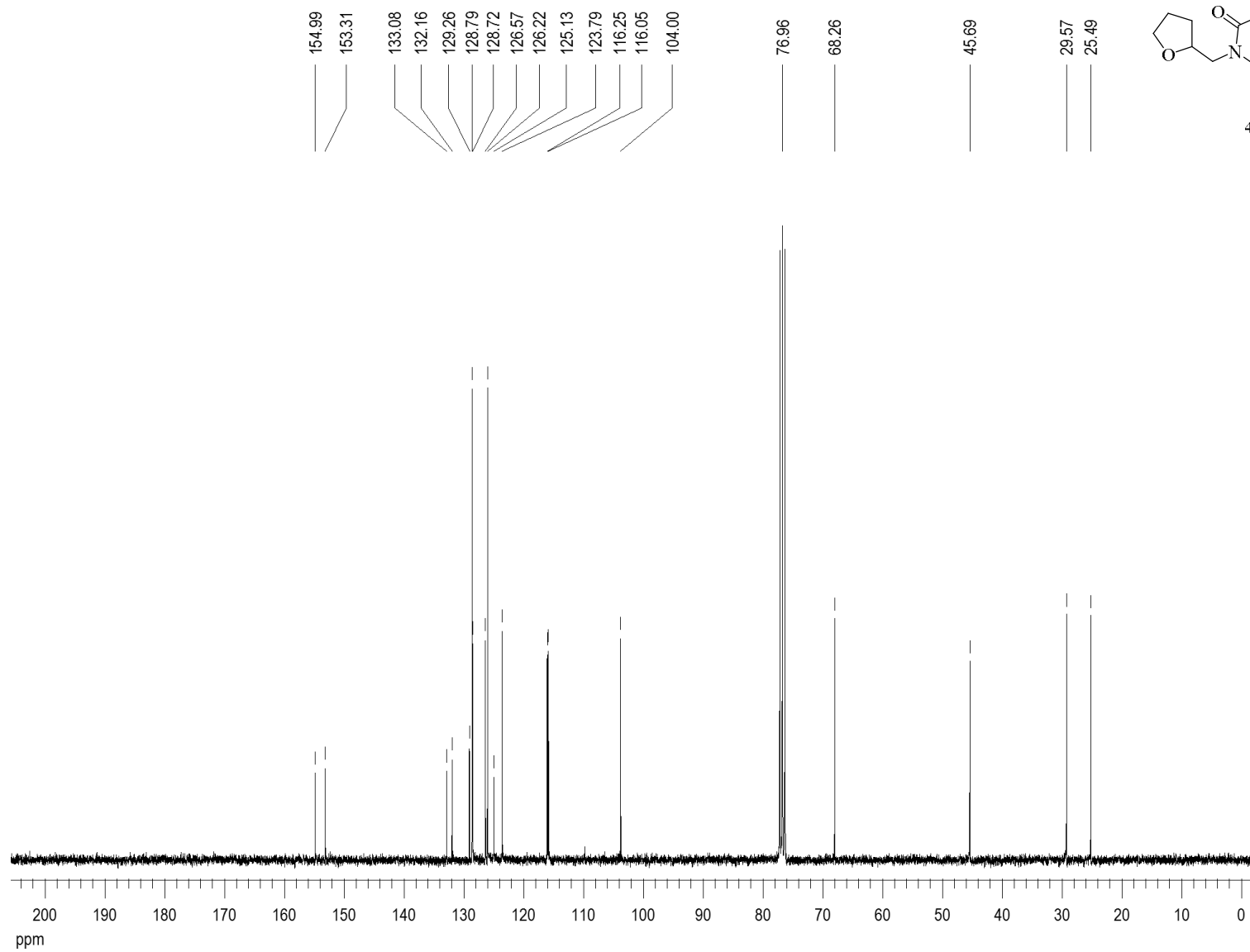
4e – ^{13}C { ^1H } NMR (125 MHz, CDCl_3 , 25 °C)



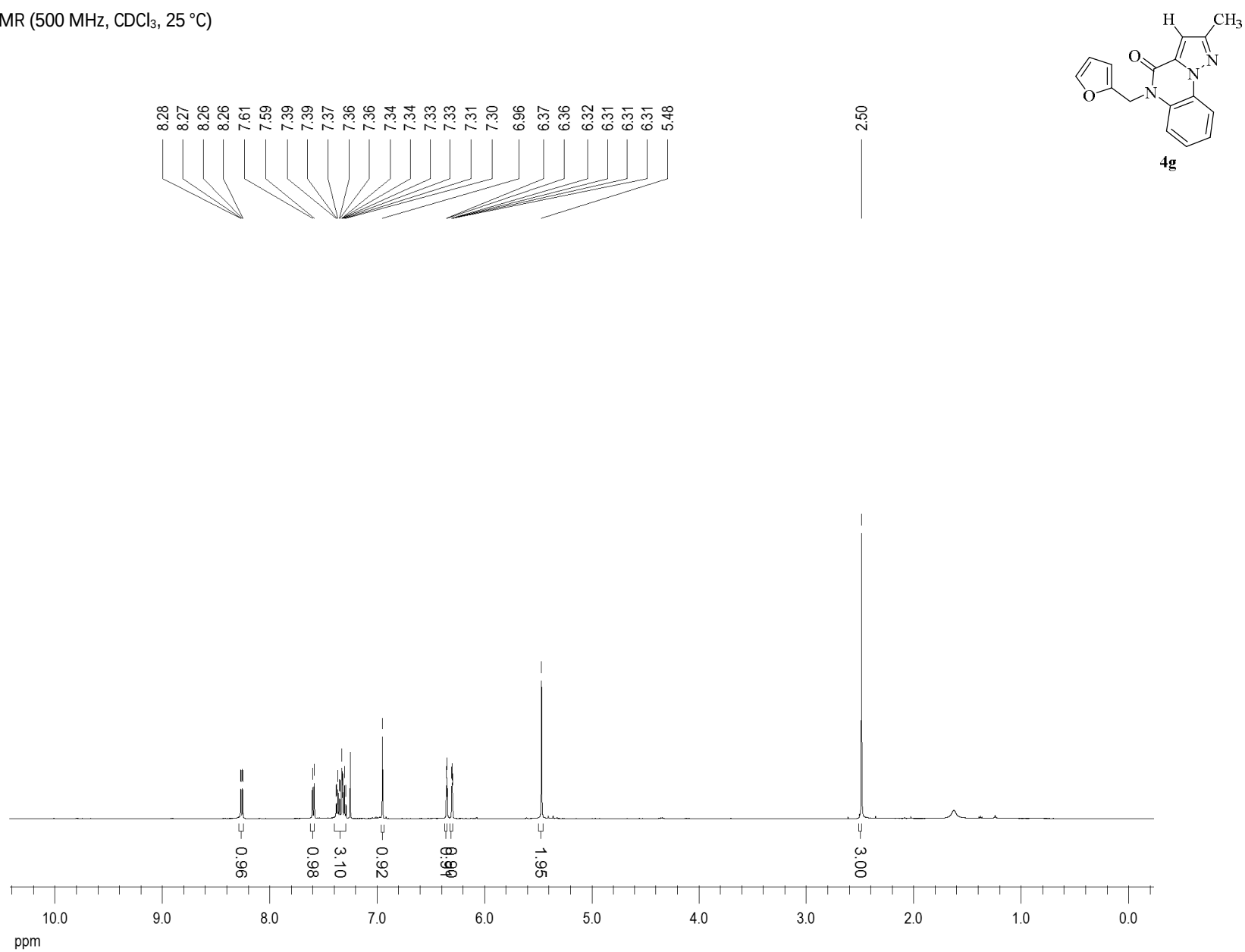
4f – ^1H NMR (500 MHz, CDCl_3 , 25 $^\circ\text{C}$)



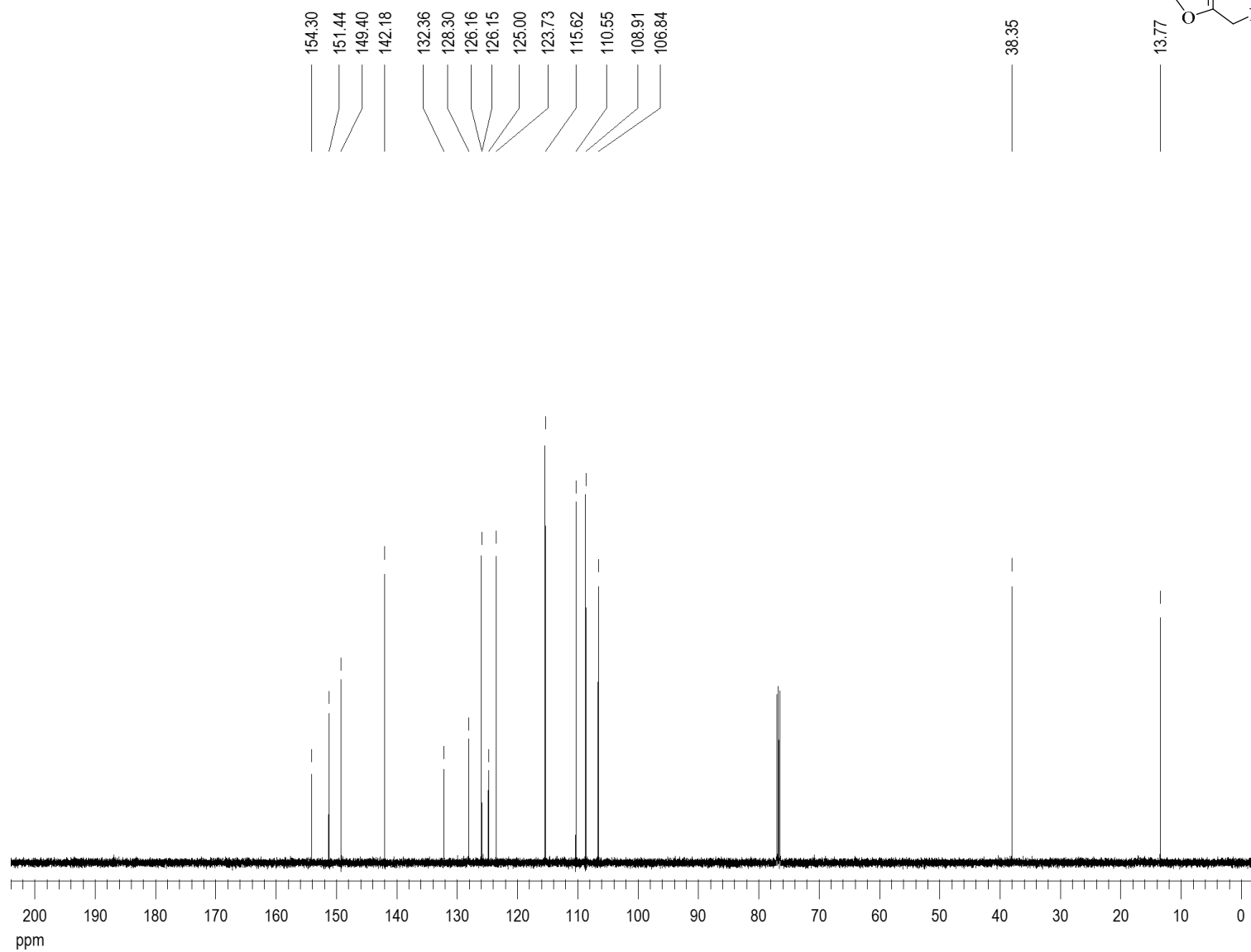
4f – ^{13}C { ^1H } NMR (75 MHz, CDCl_3 , 25 °C)



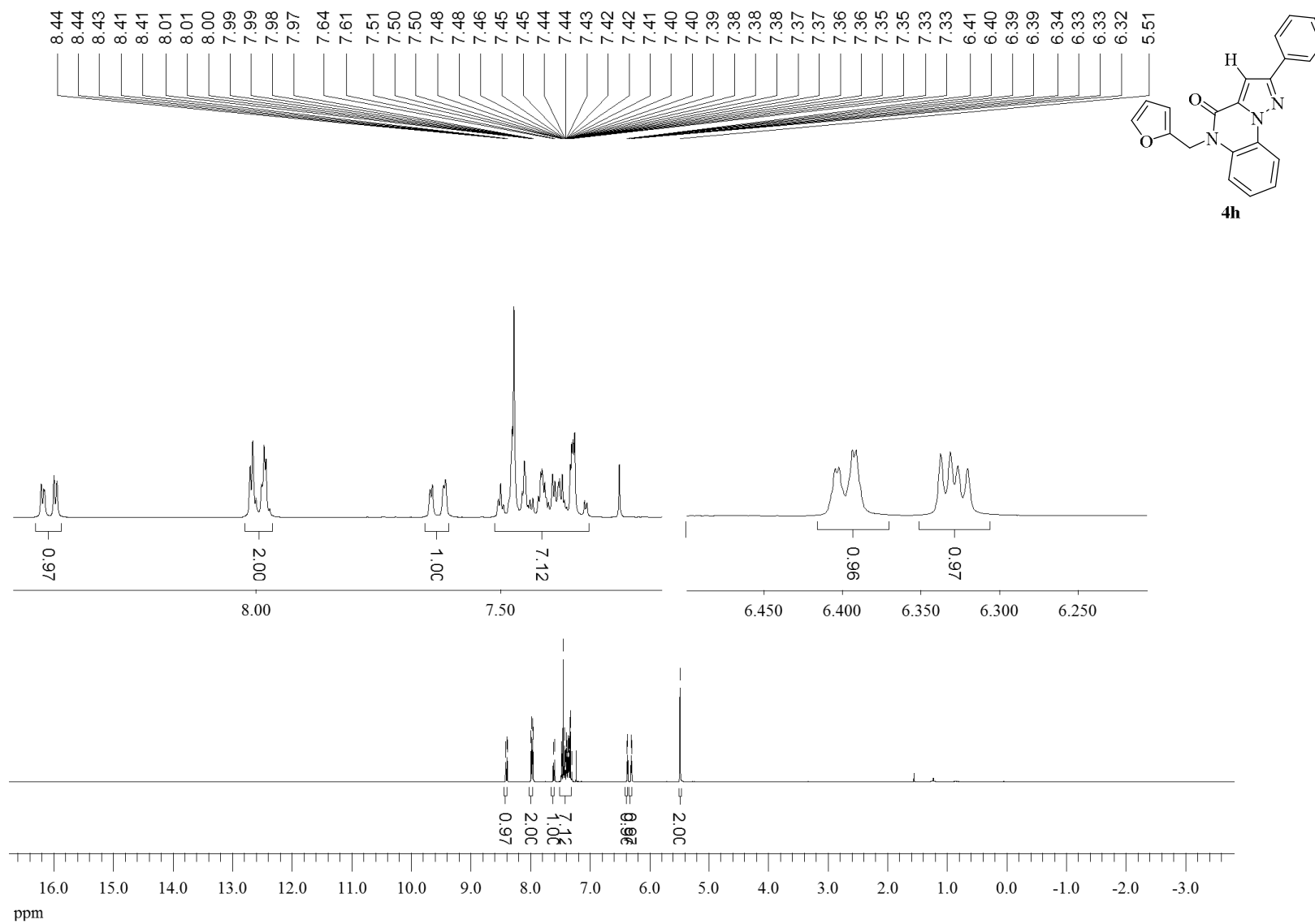
4g – ^1H NMR (500 MHz, CDCl_3 , 25 °C)



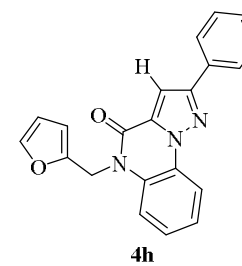
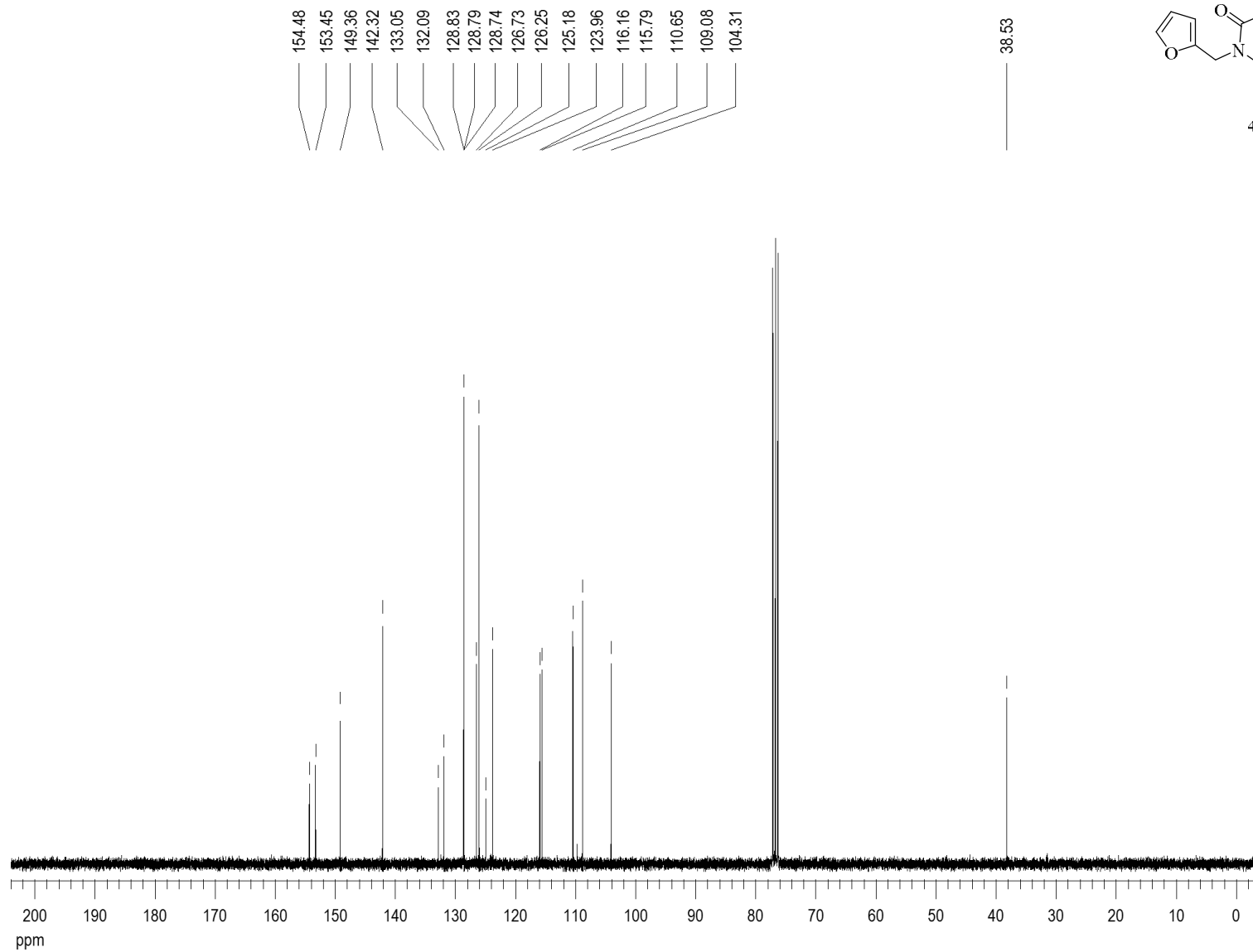
4g – ^{13}C { ^1H } NMR (125 MHz, CDCl_3 , 25 °C)



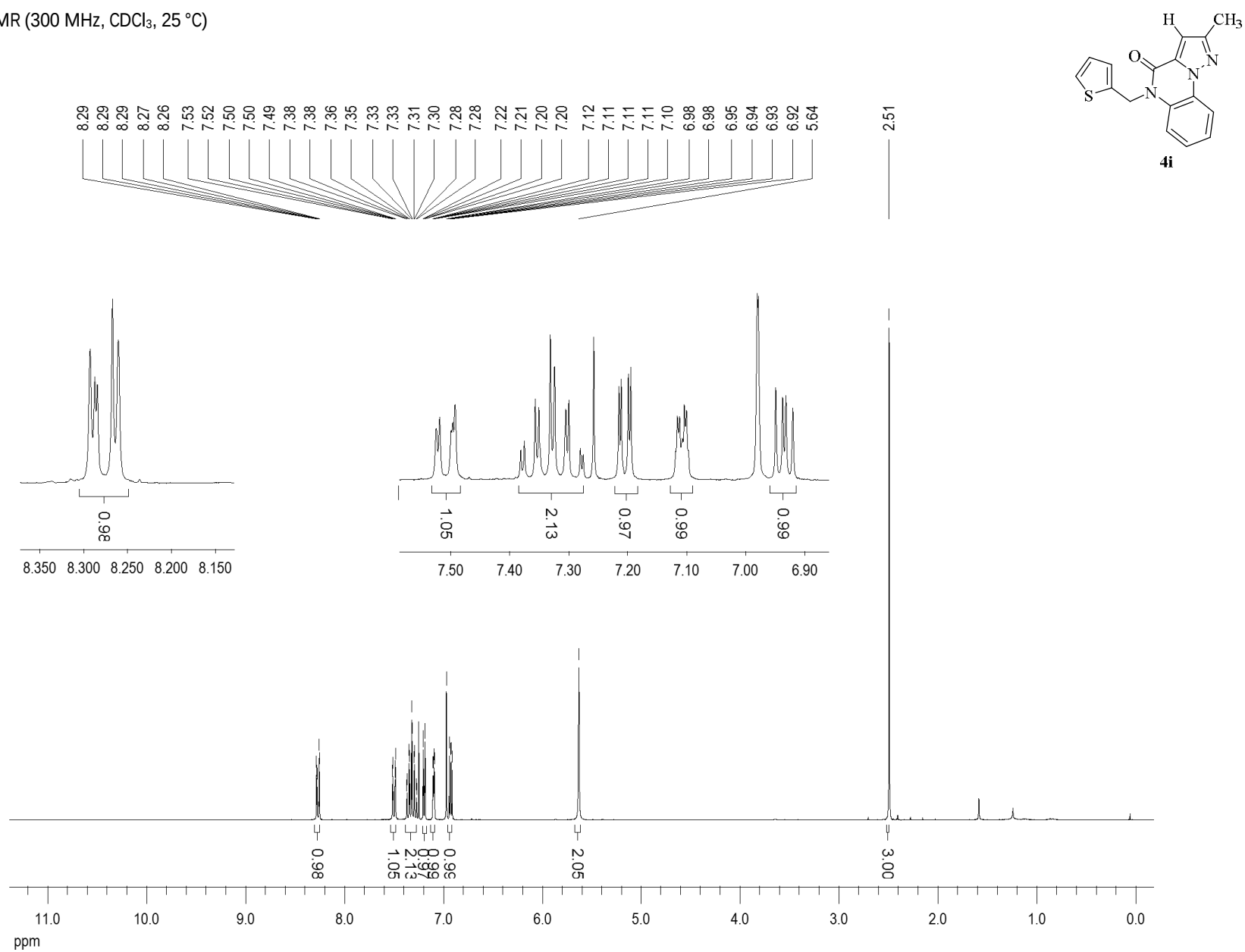
4h – ^1H NMR (300 MHz, CDCl_3 , 25 $^\circ\text{C}$)



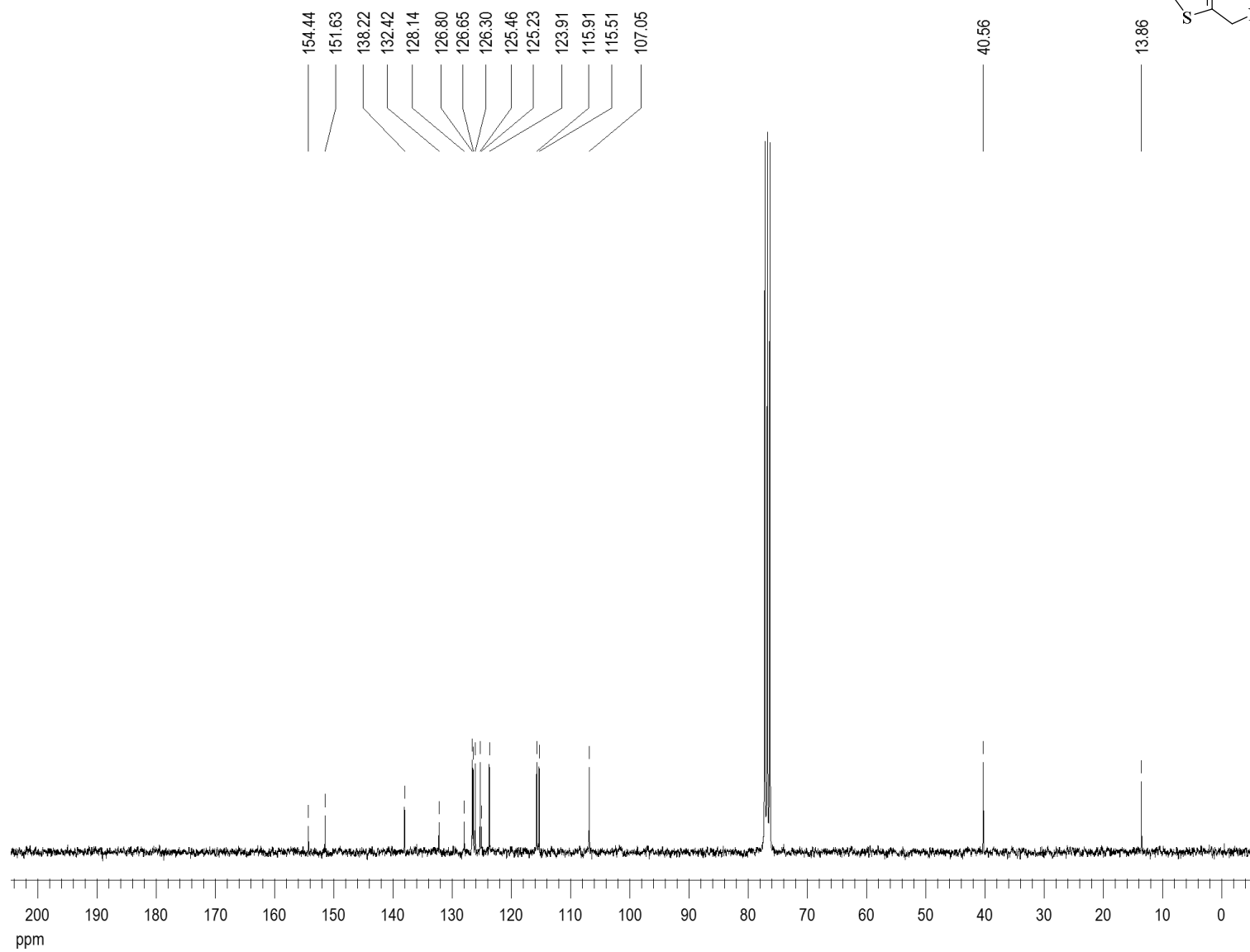
4h – ^{13}C $\{^1\text{H}\}$ NMR (75 MHz, CDCl_3 , 25 °C)



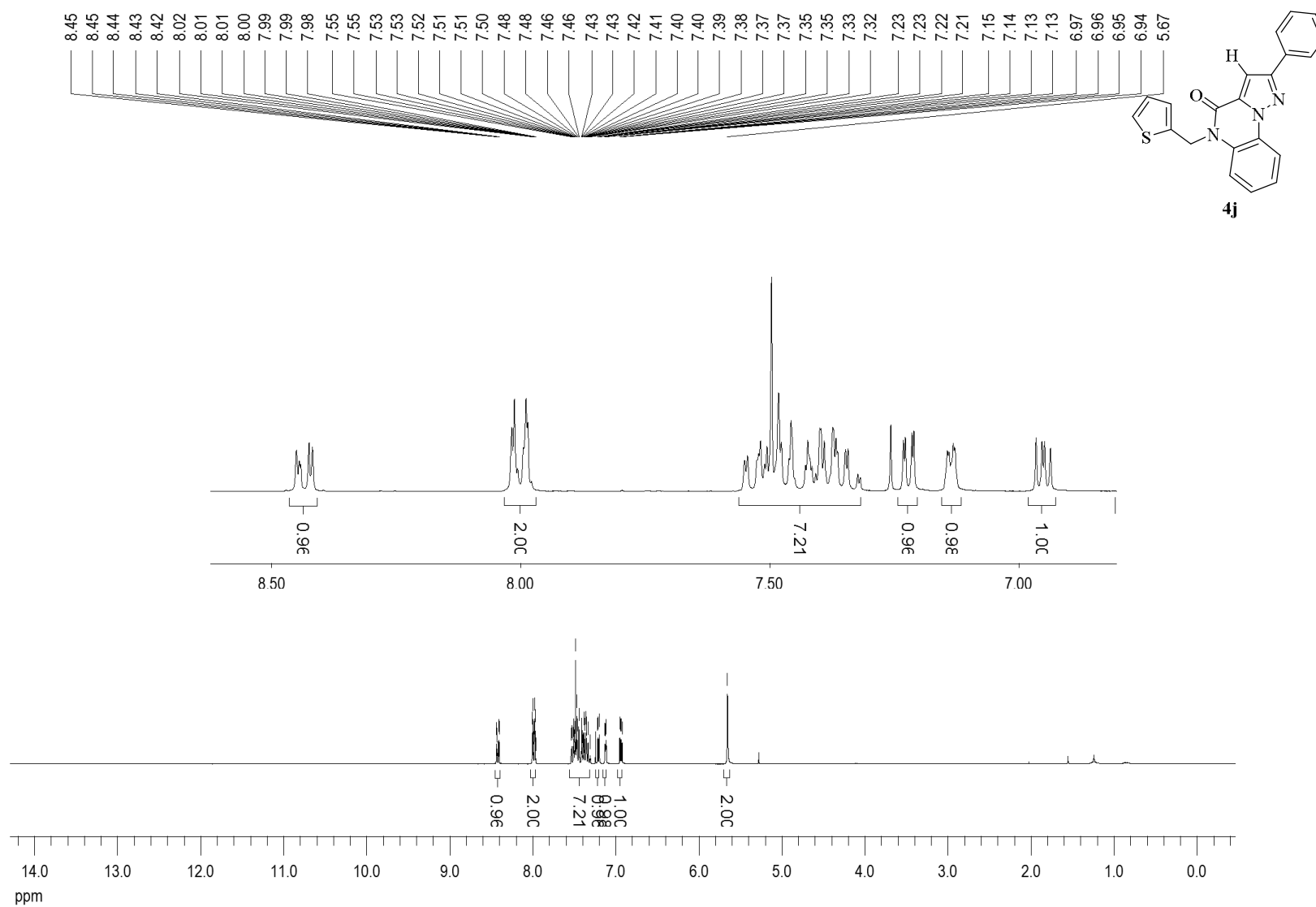
4i – ^1H NMR (300 MHz, CDCl_3 , 25 $^\circ\text{C}$)



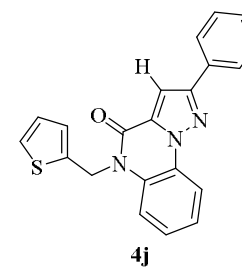
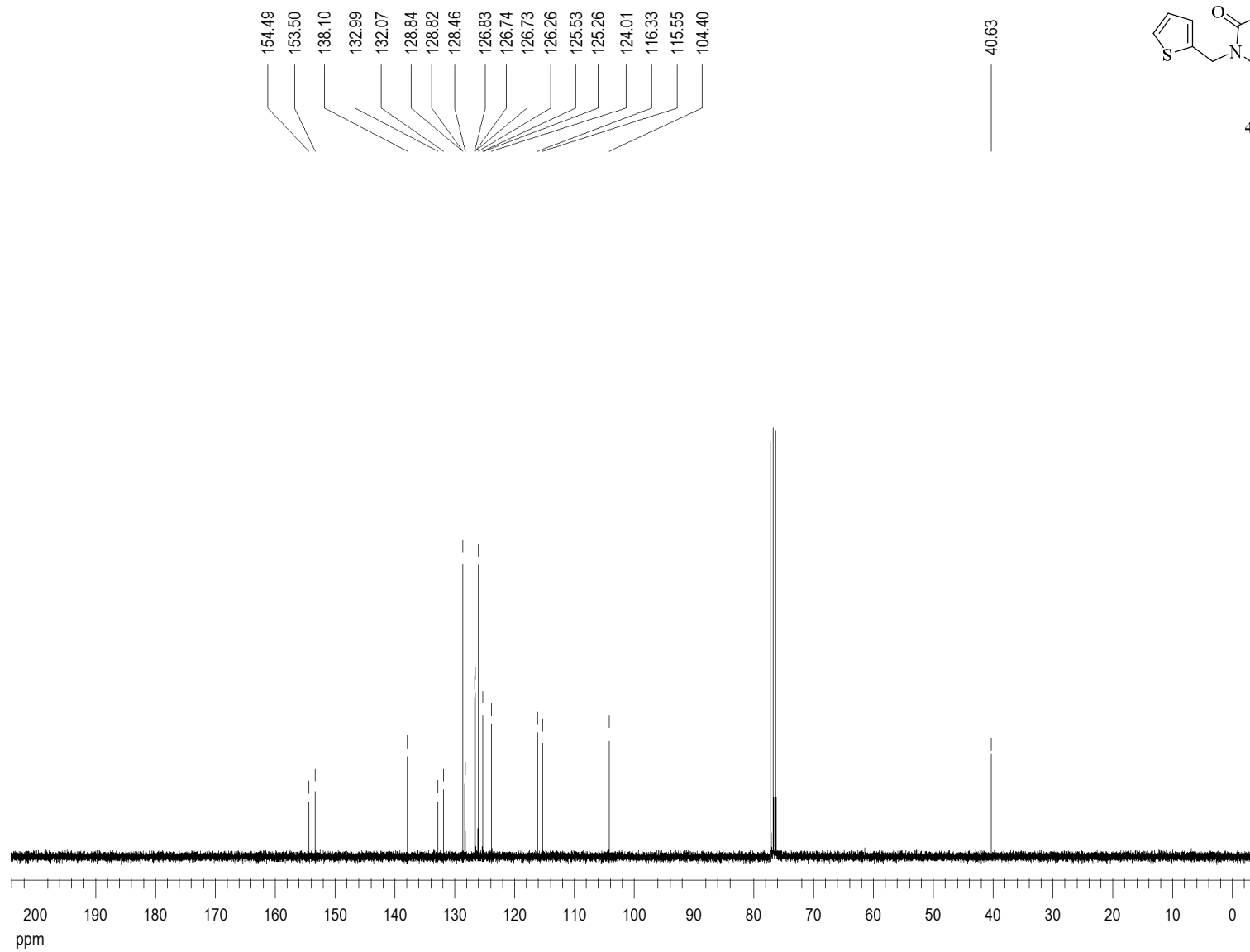
4i – ^{13}C { ^1H } NMR (75 MHz, CDCl_3 , 25 °C)



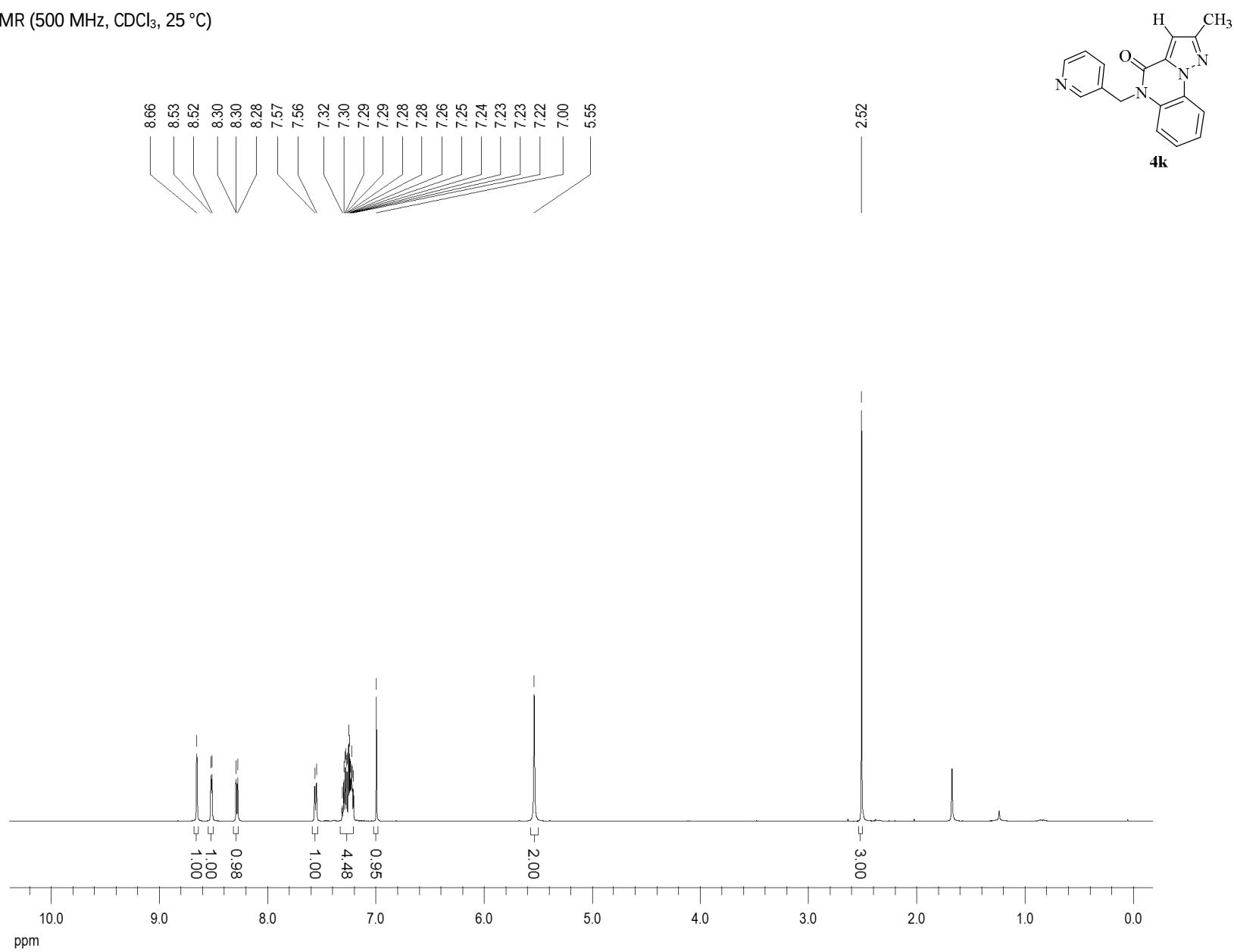
4j – ^1H NMR (300 MHz, CDCl_3 , 25 $^\circ\text{C}$)



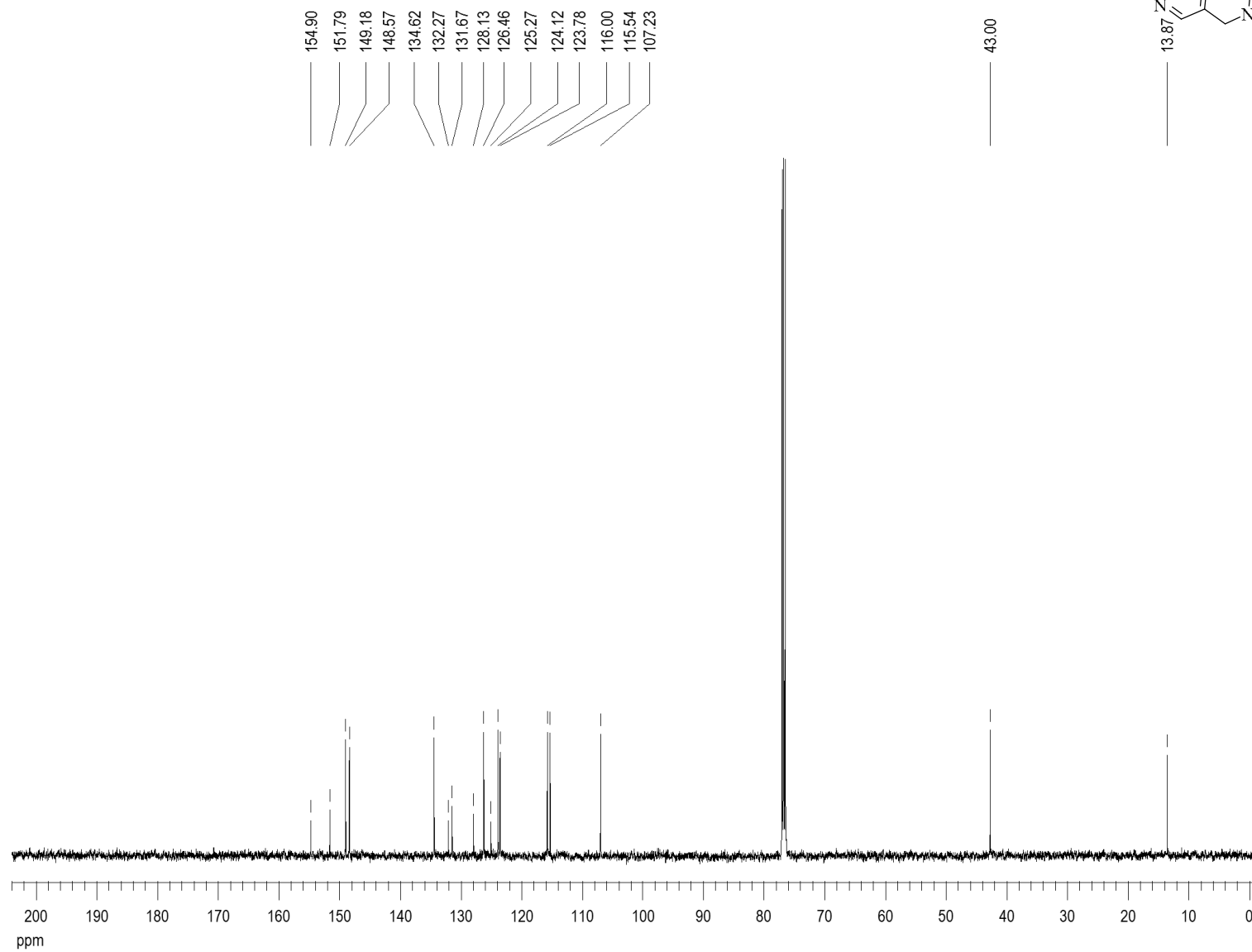
4j – ^{13}C { ^1H } NMR (75 MHz, CDCl_3 , 25 °C)



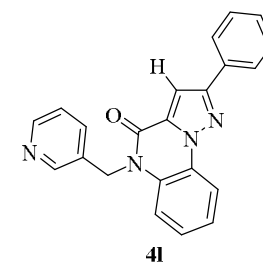
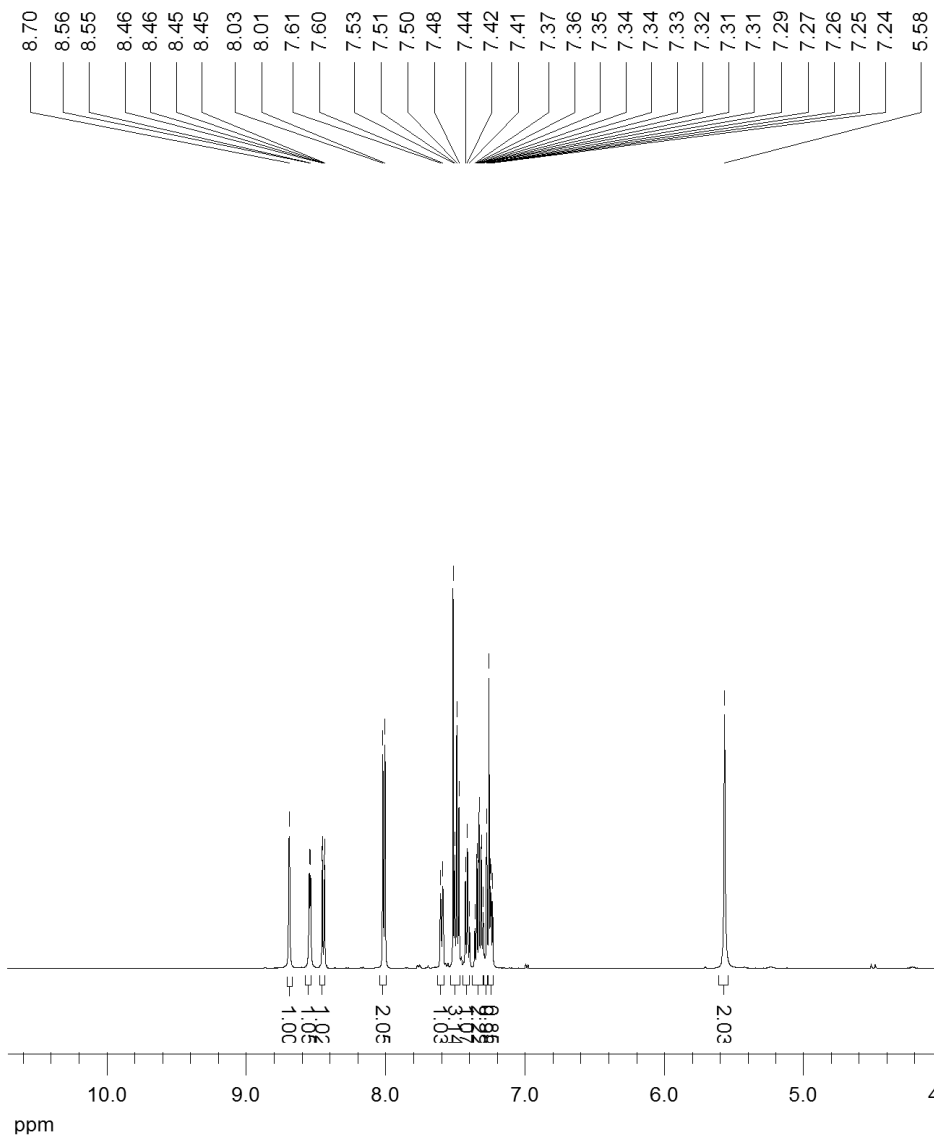
4k – ^1H NMR (500 MHz, CDCl_3 , 25 $^\circ\text{C}$)



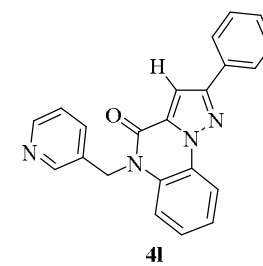
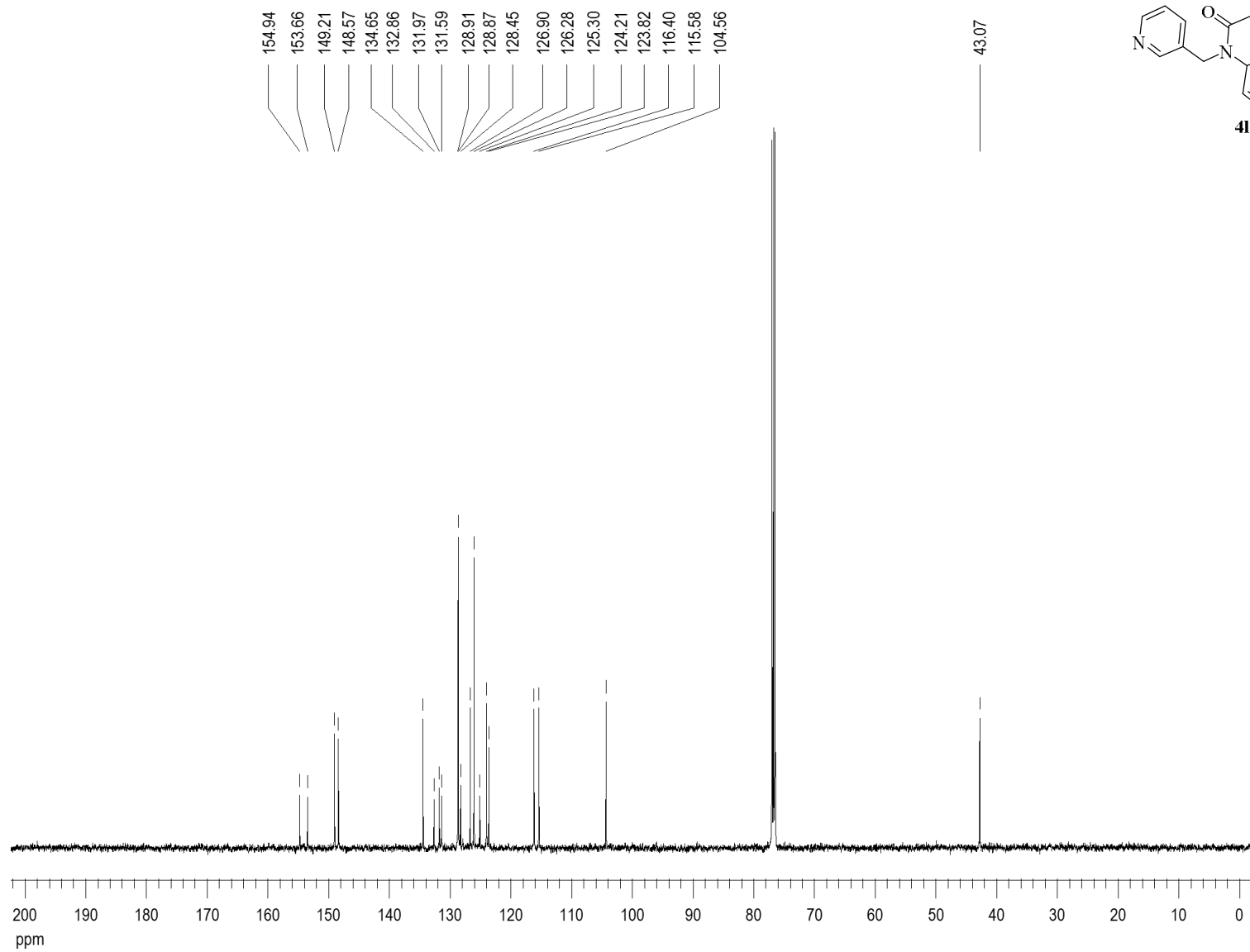
4k – ^{13}C { ^1H } NMR (125 MHz, CDCl_3 , 25 °C)



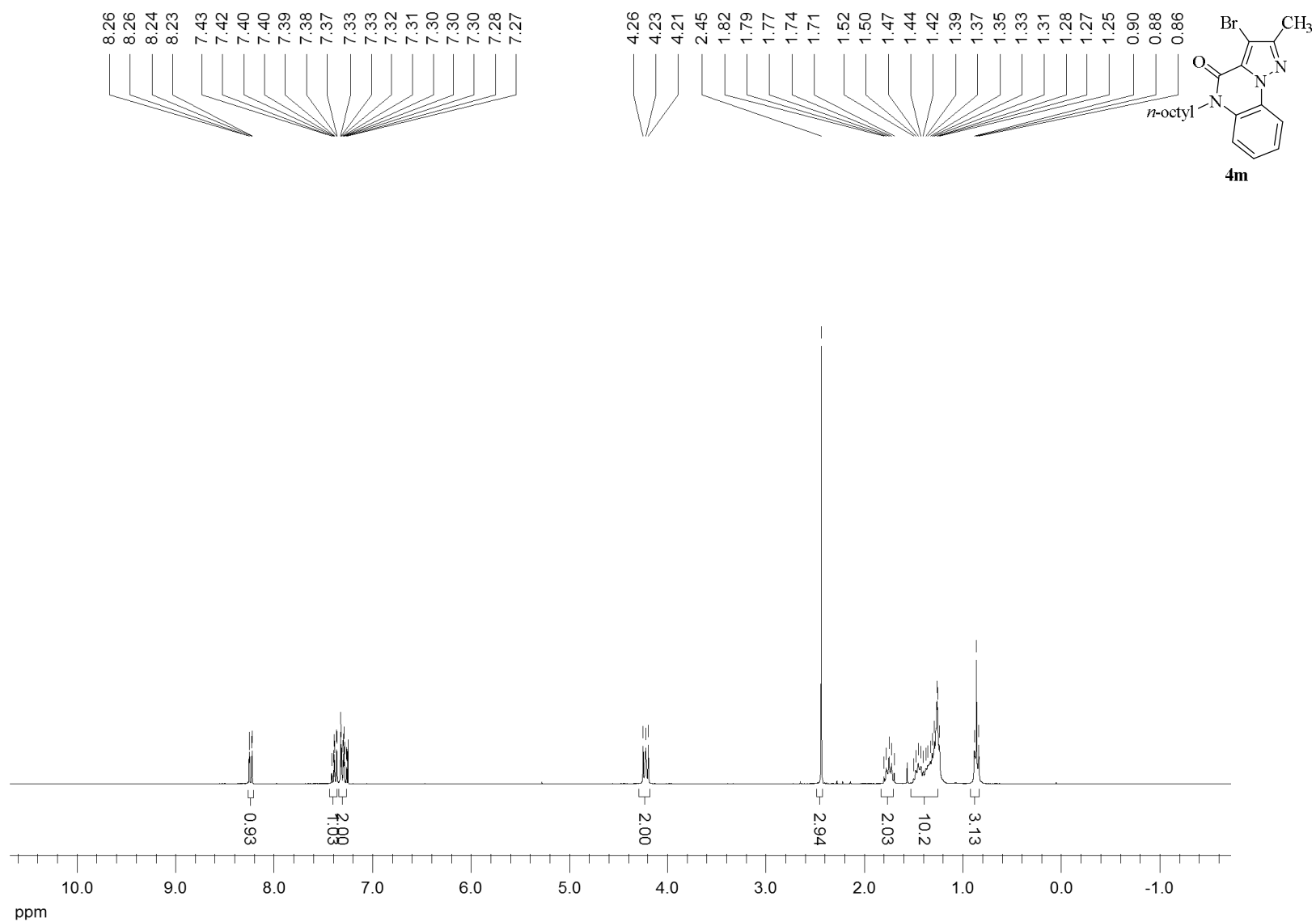
4l – ^1H NMR (500 MHz, CDCl_3 , 25 $^\circ\text{C}$)



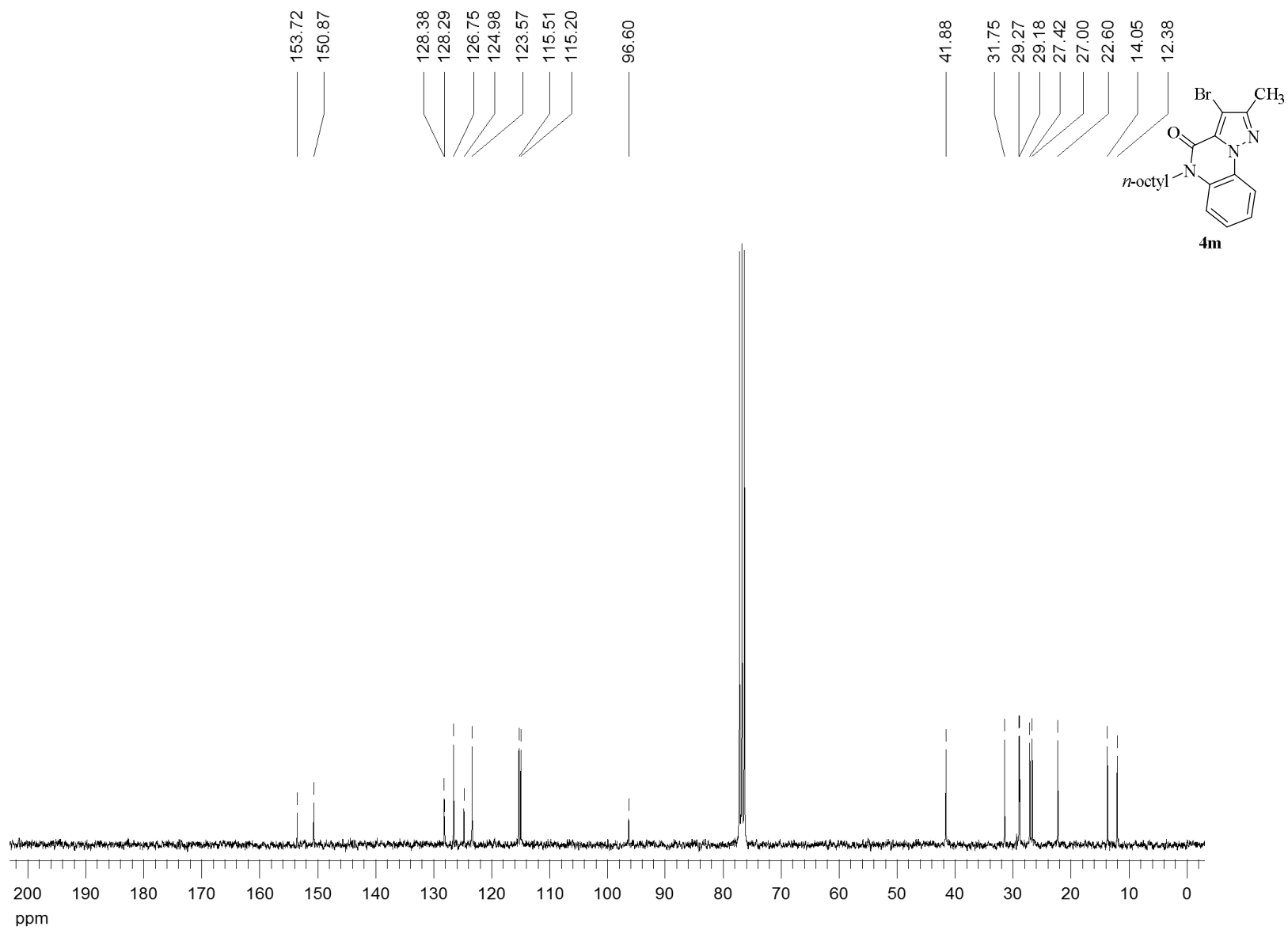
4l – ^{13}C { ^1H } NMR (125 MHz, CDCl_3 , 25 °C)



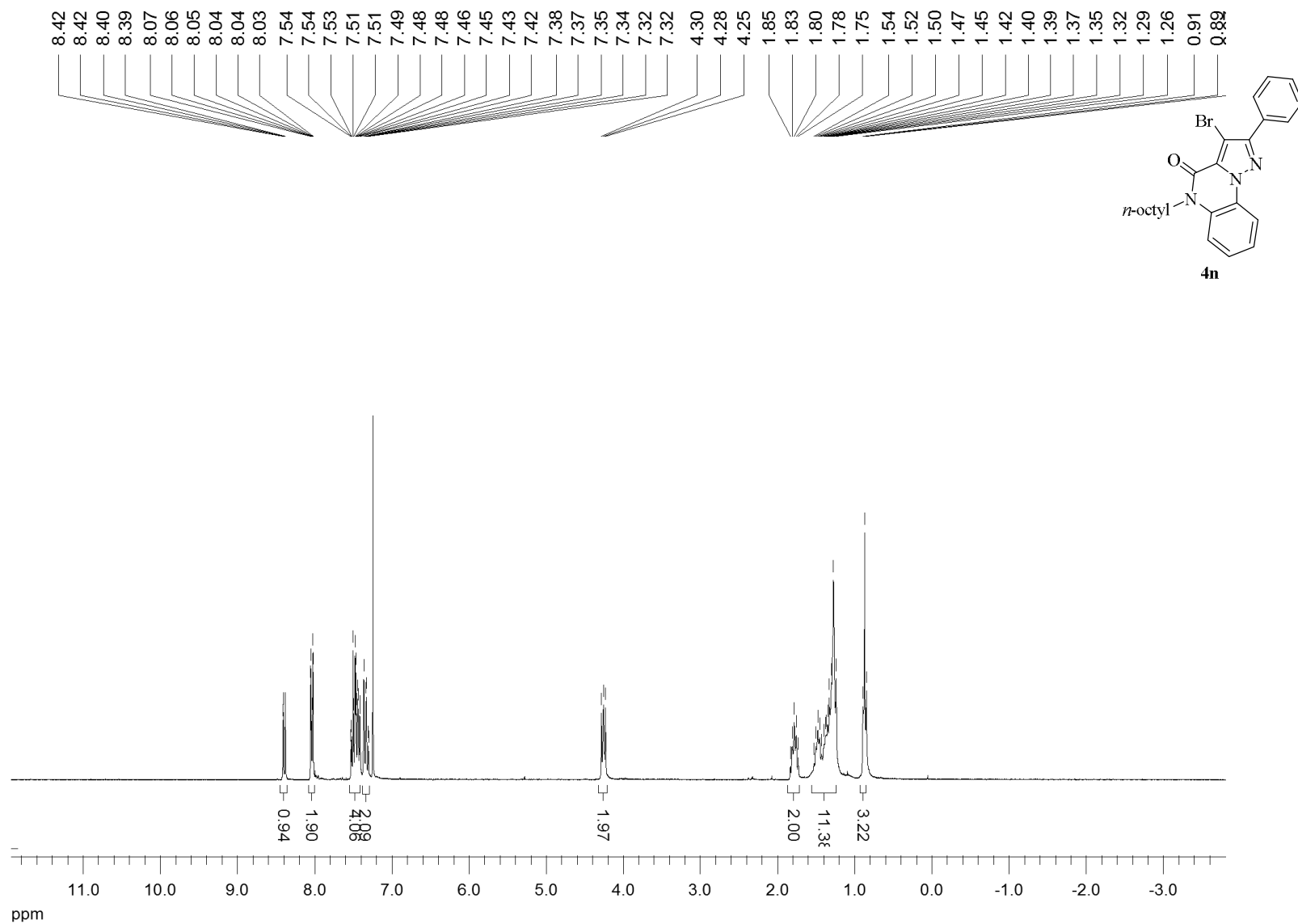
4m – ^1H NMR (300 MHz, CDCl_3 , 25 °C)



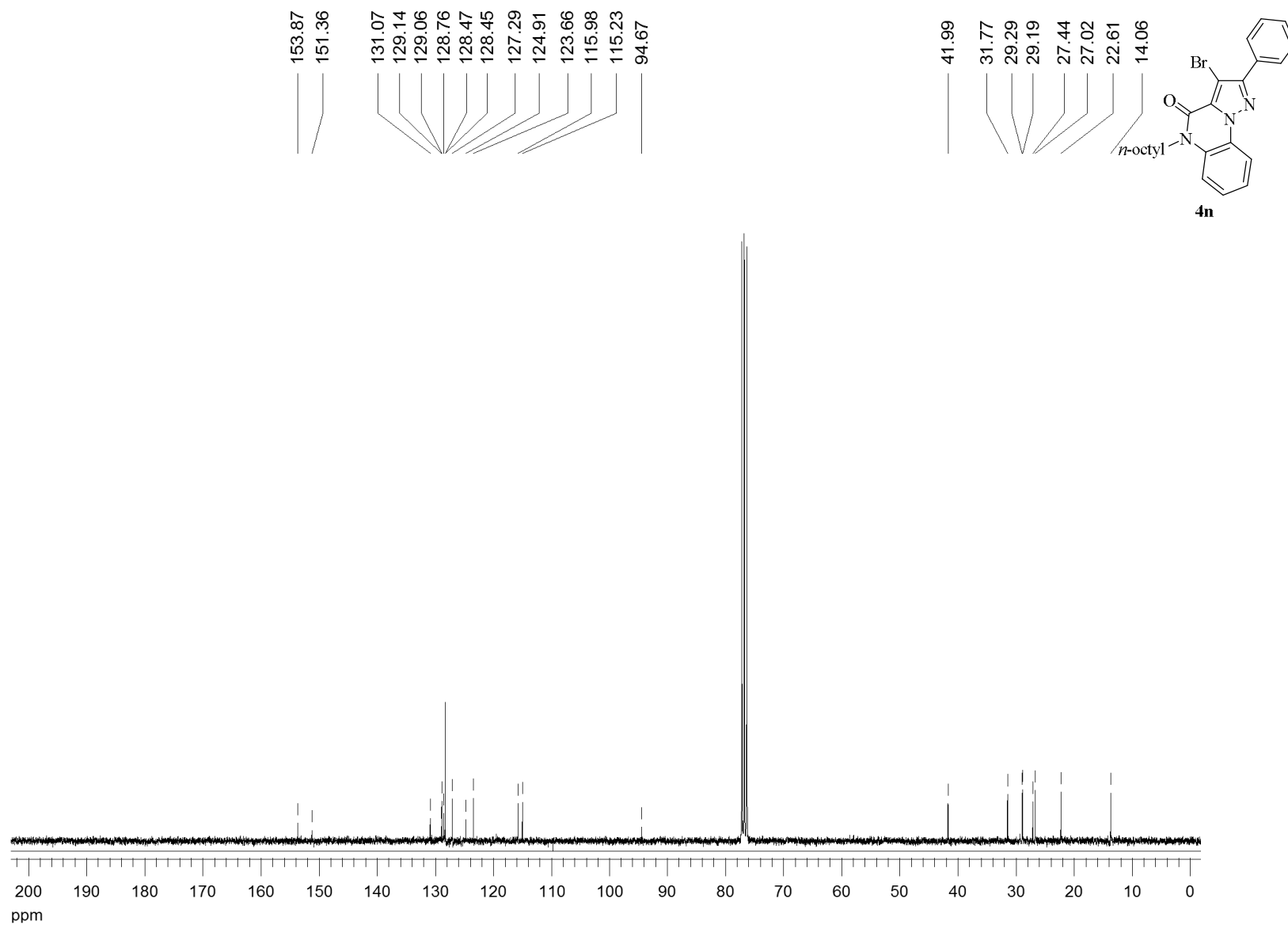
4m – ^{13}C { ^1H } NMR (75 MHz, CDCl_3 , 25 °C)



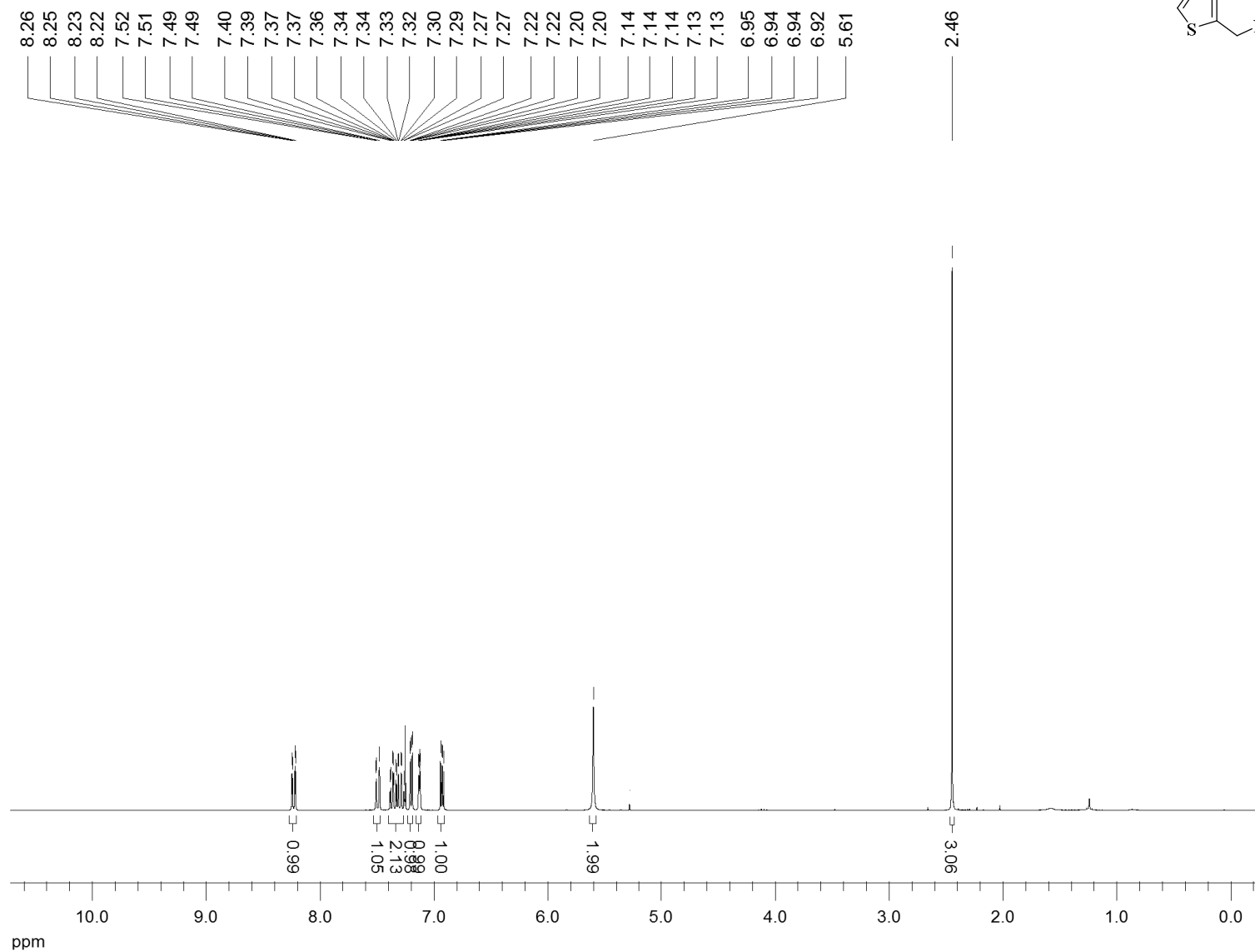
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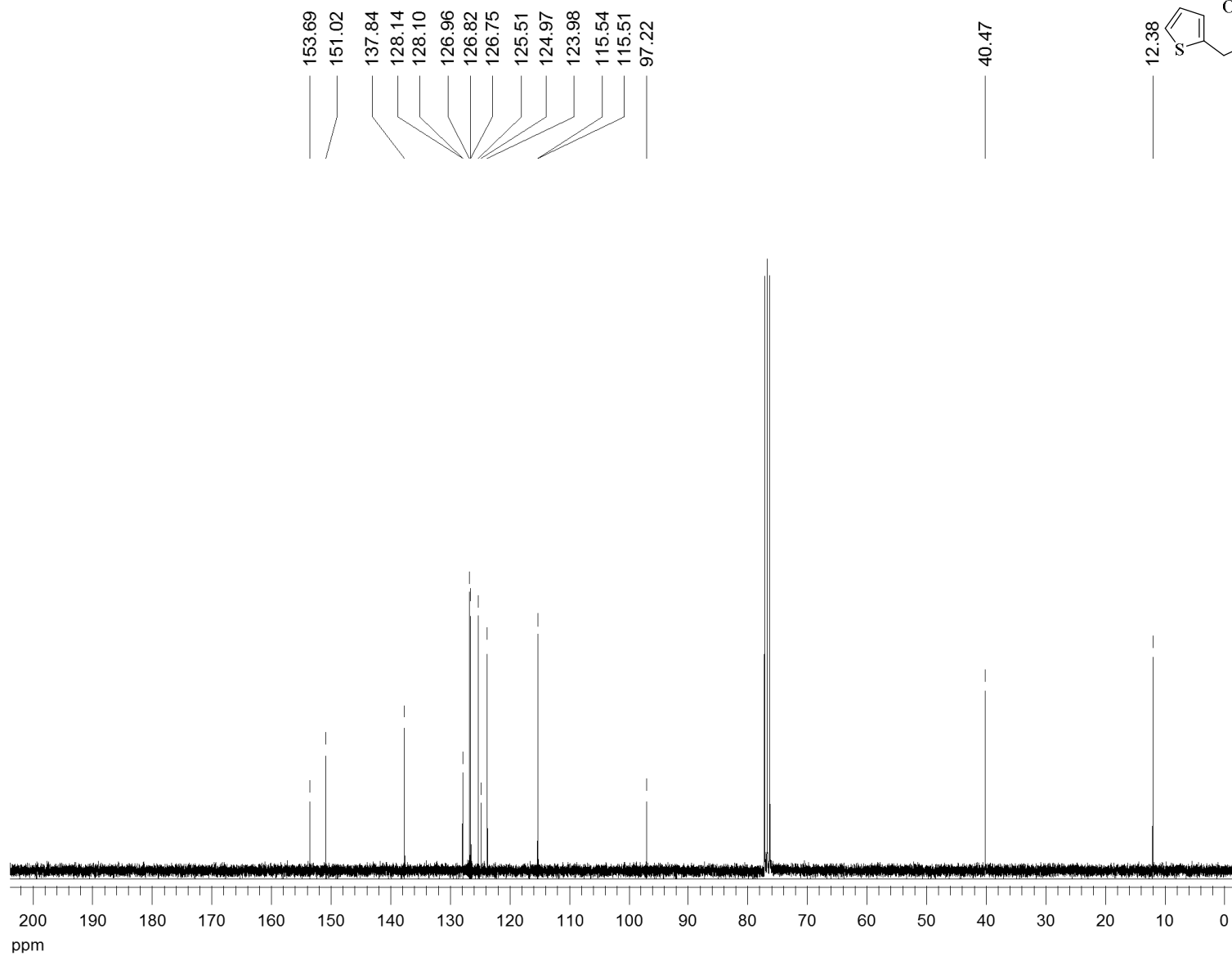
4n – ^{13}C { ^1H } NMR (75 MHz, CDCl_3 , 25 °C)



4o – ^1H NMR (300 MHz, CDCl_3 , 25 $^\circ\text{C}$)

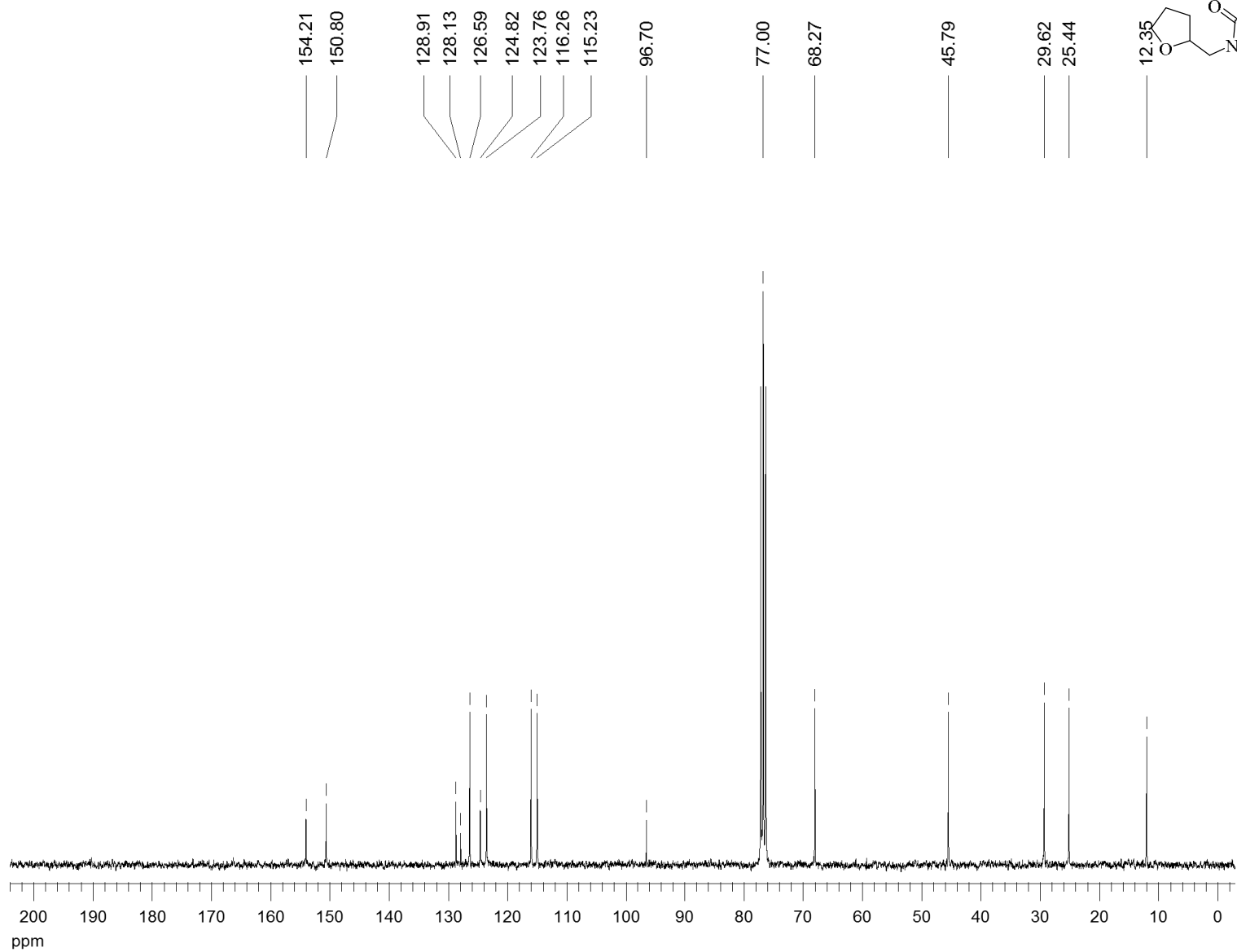


4o – ^{13}C { ^1H } NMR (75 MHz, CDCl_3 , 25 °C)



[illegible]

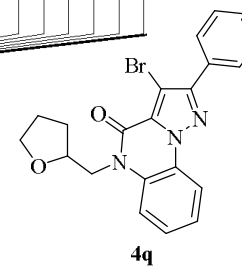
4p – ^{13}C { ^1H } NMR (75 MHz, CDCl_3 , 25 °C)



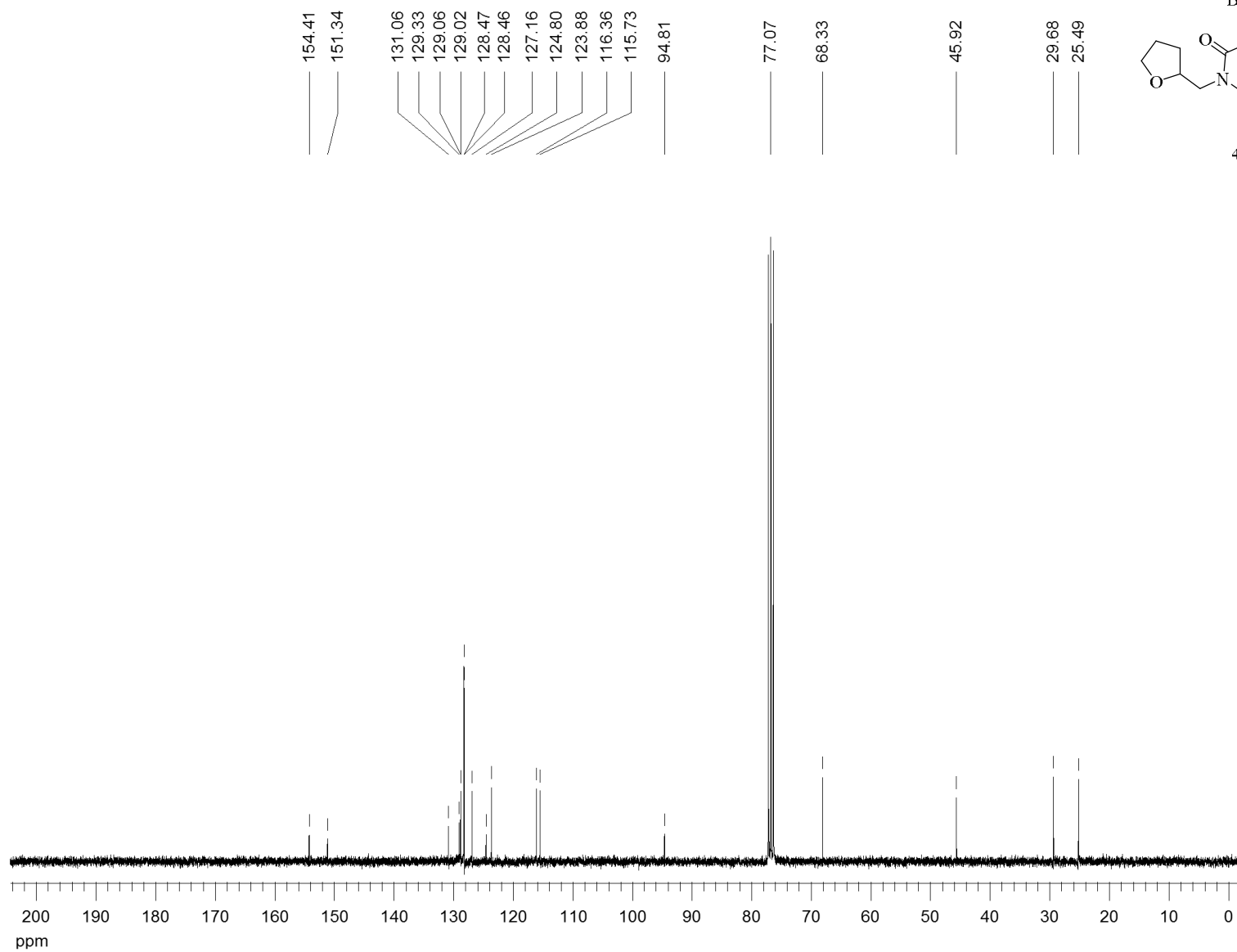
Chemical structure of **4q** is shown in the top right corner. The structure is a substituted cyclopentane ring with a bromine atom (Br) and a carbonyl group (C=O) attached to the ring. The carbonyl group is part of a larger functional group, possibly a ketone or an amide, which is further substituted with a phenyl ring and a methyl group.

The ¹H NMR spectrum (CDCl₃) shows the following peaks and integrations:

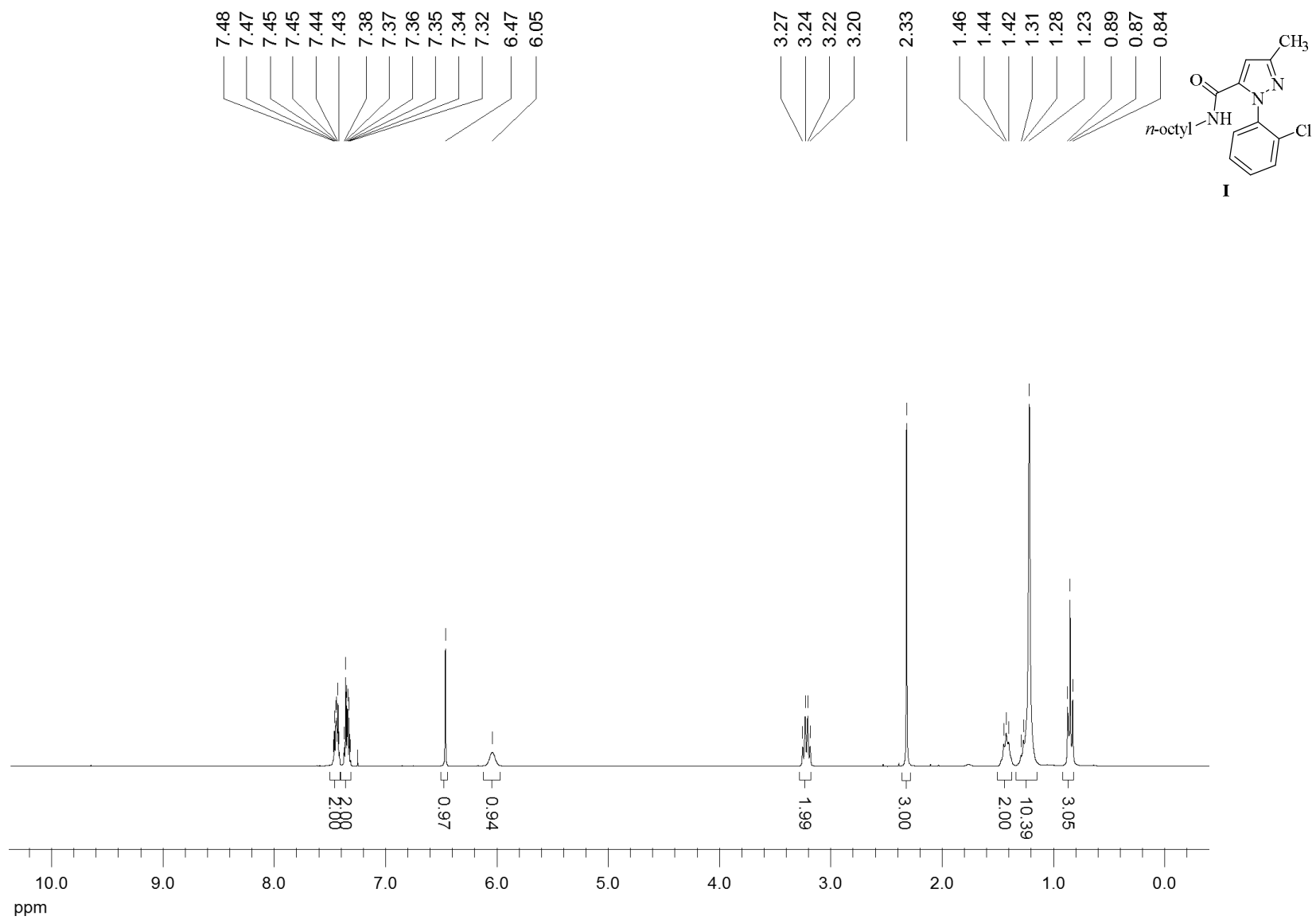
Chemical Shift (ppm)	Integration
~7.5	0.93
~7.2	1.65
~7.1	1.99
~4.5	1.00
~4.2	1.09
~4.0	1.00
~3.8	1.03
~2.1	4.26



4q – ^{13}C { ^1H } NMR (75 MHz, CDCl_3 , 25 °C)



I – ^1H NMR (300 MHz, CDCl_3 , 25 °C)



I - ^{13}C { ^1H } NMR (75 MHz, CDCl_3 , 25 °C)

