

## Supplementary materials

### The construction of polycyclic pyridones *via* ring-opening transformations of 3-hydroxy-3,4-dihydropyrido[2,1-*c*][1,4]oxazine-1,8-diones

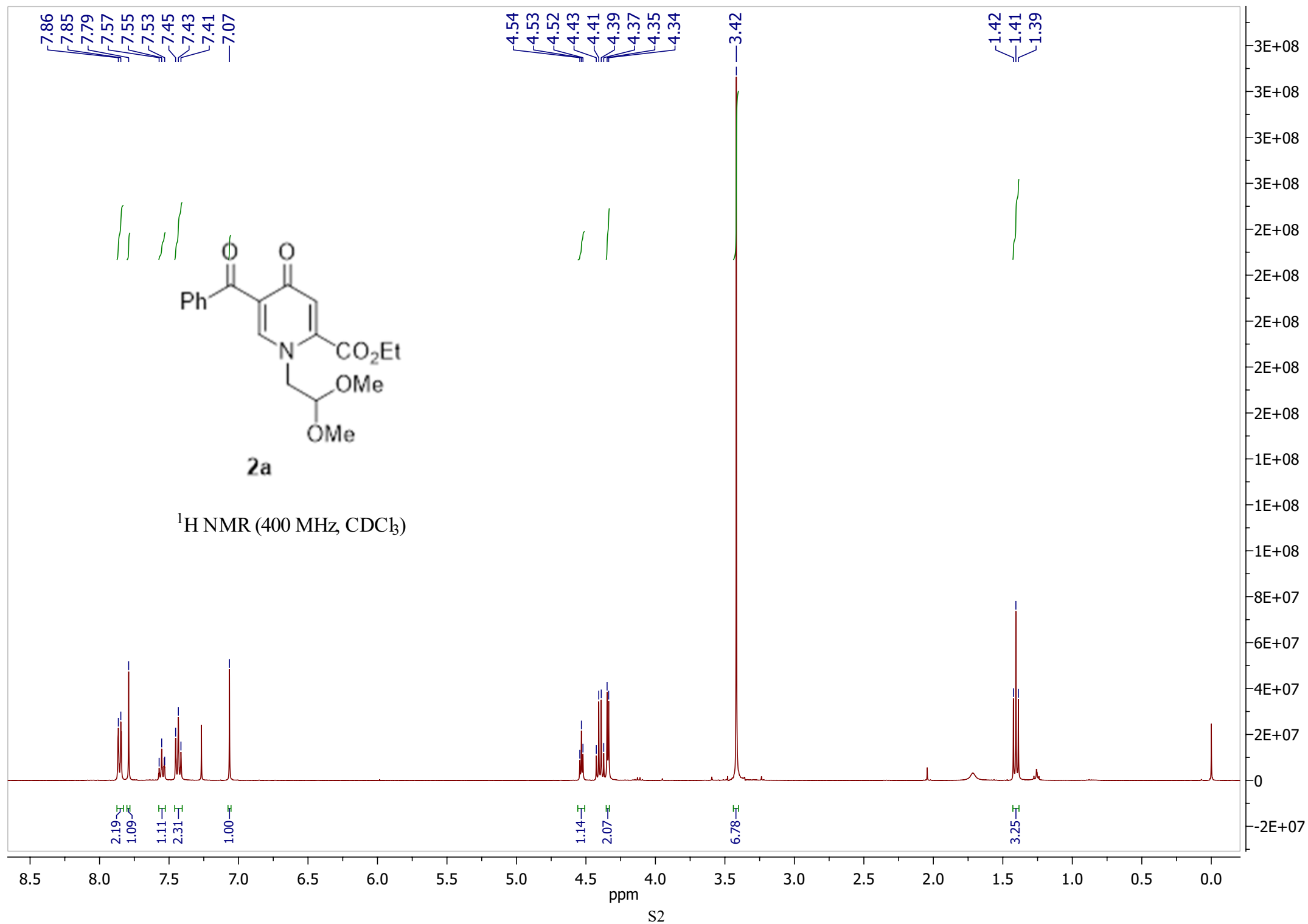
Viktoriya V. Viktorova, Elena V. Steparuk, Dmitrii L. Obydenov,\* and Vyacheslav Y. Sosnovskikh\*

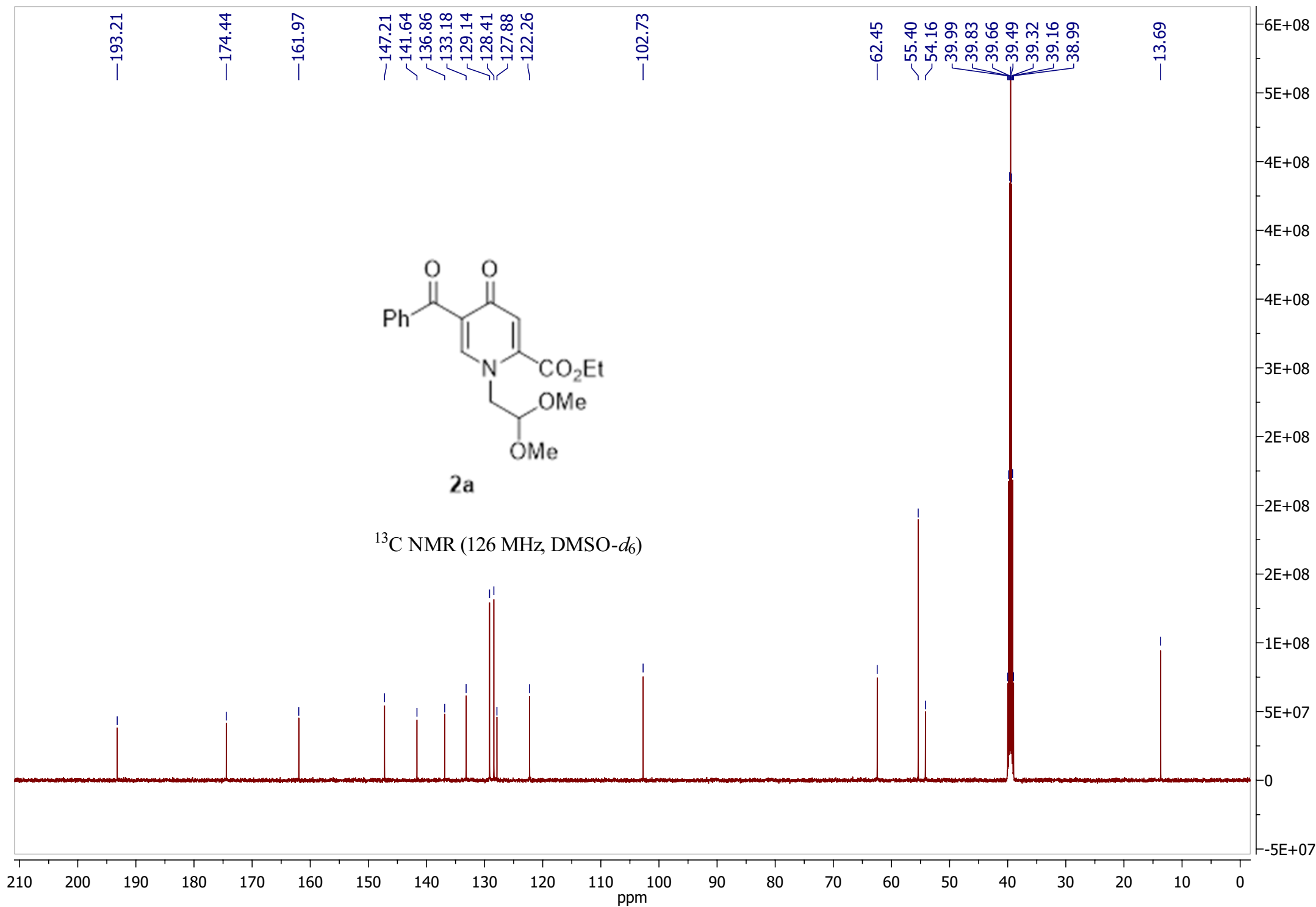
Institute of Natural Sciences and Mathematics, Ural Federal University, 51 Lenina Ave., 620000 Ekaterinburg, Russia

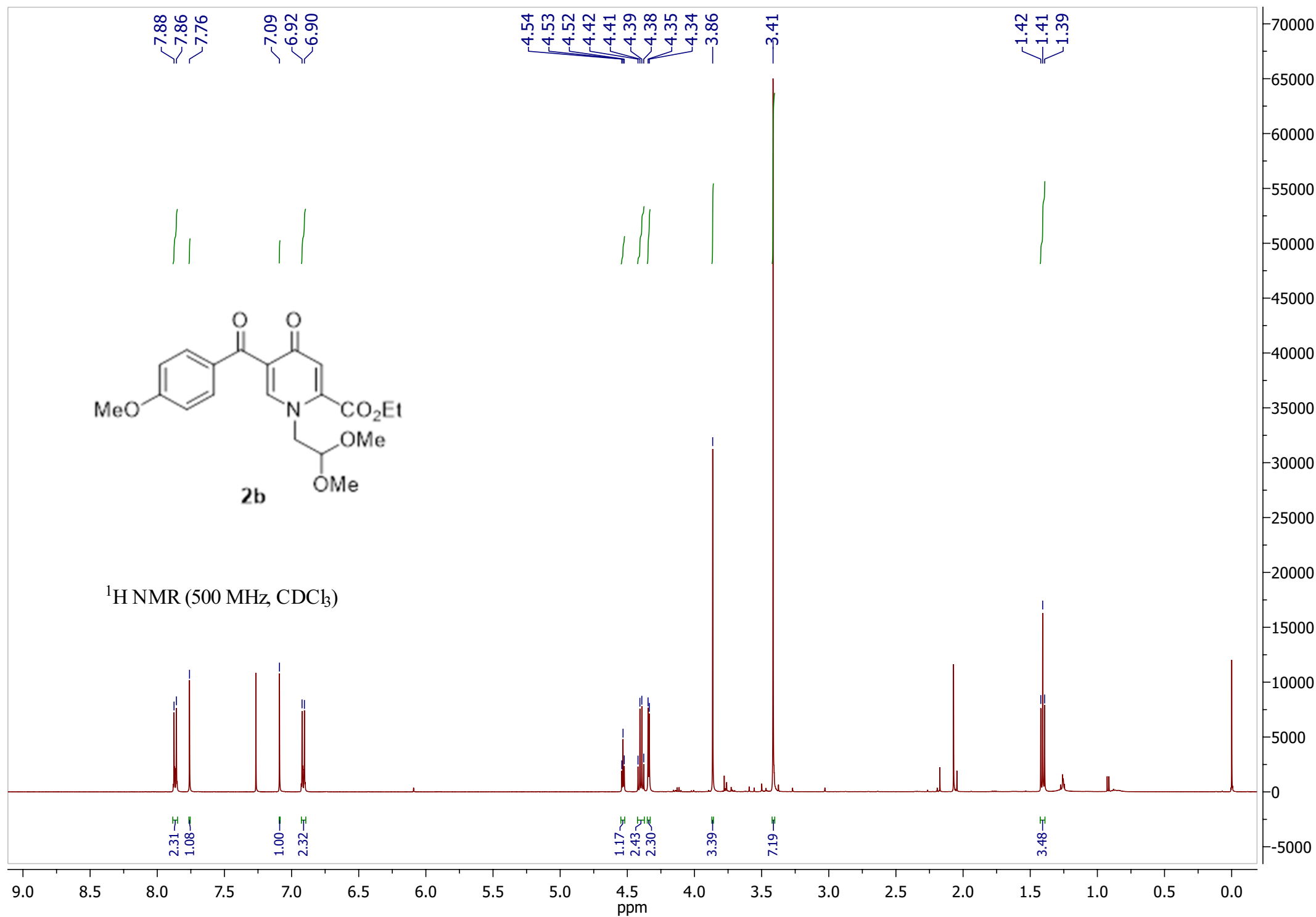
\* Correspondence: vy.sosnovskikh@urfu.ru; dobydenov@mail.ru; Tel.: +7-343-3899597

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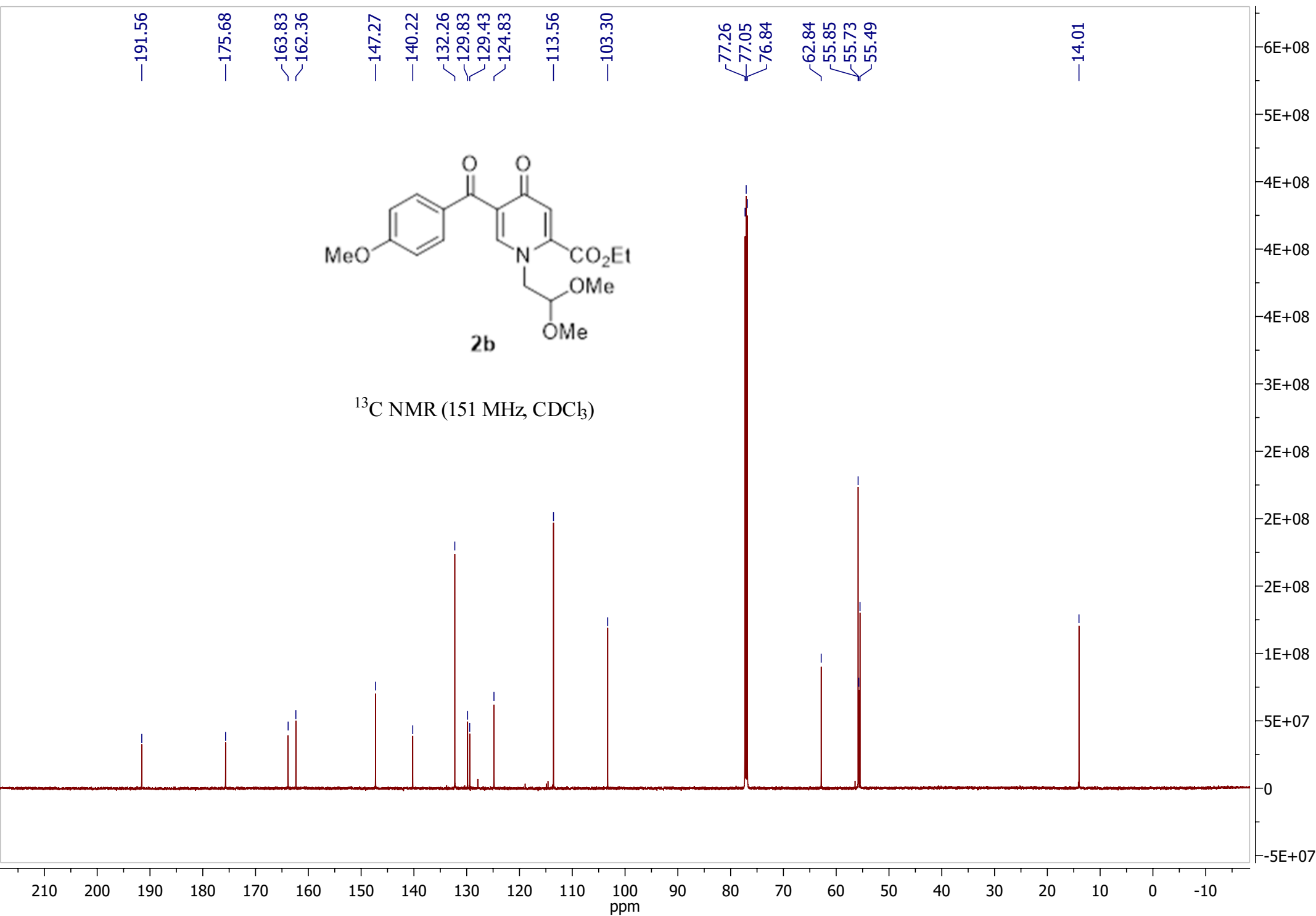
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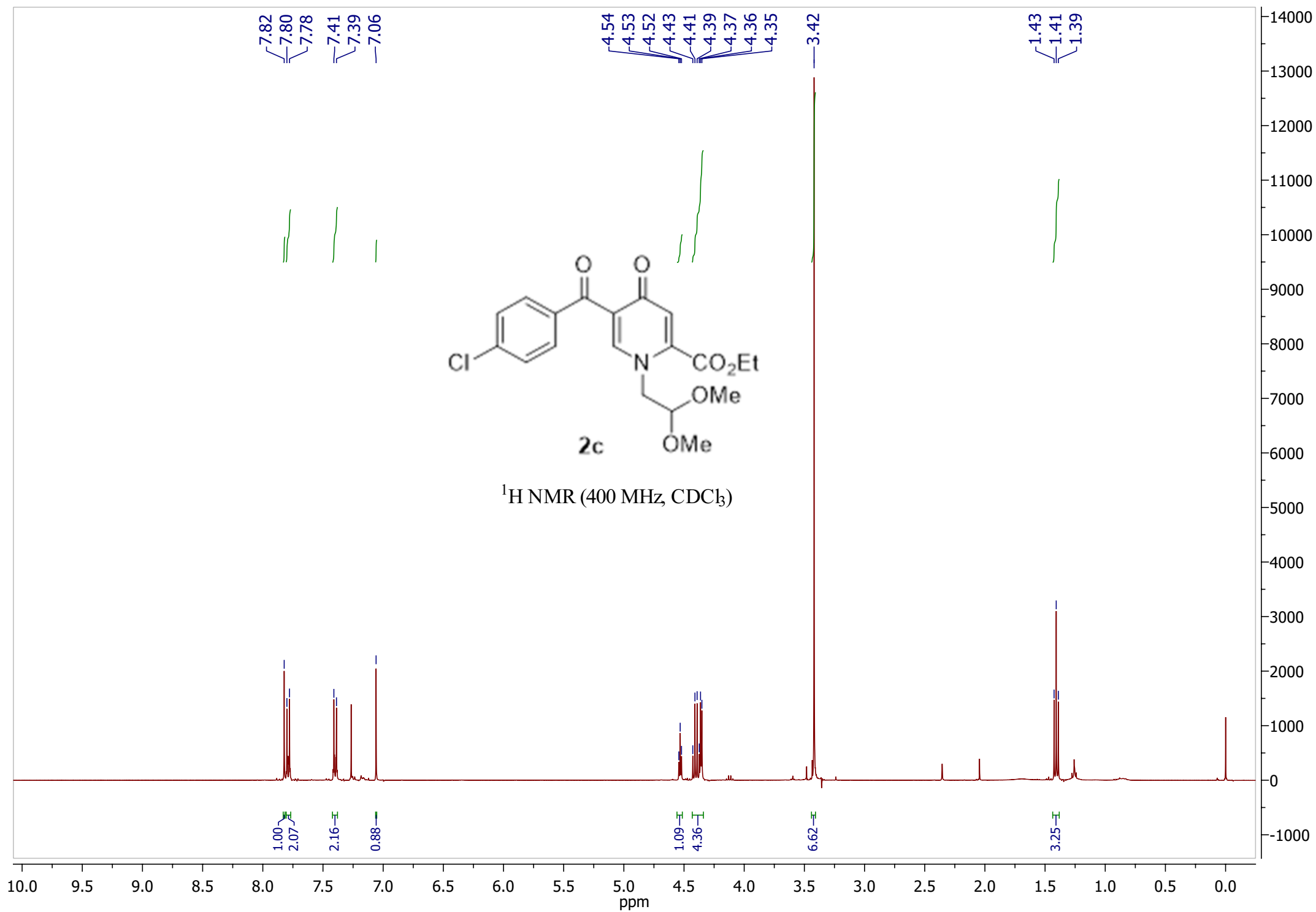


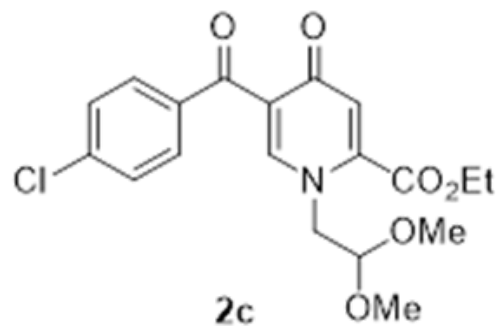




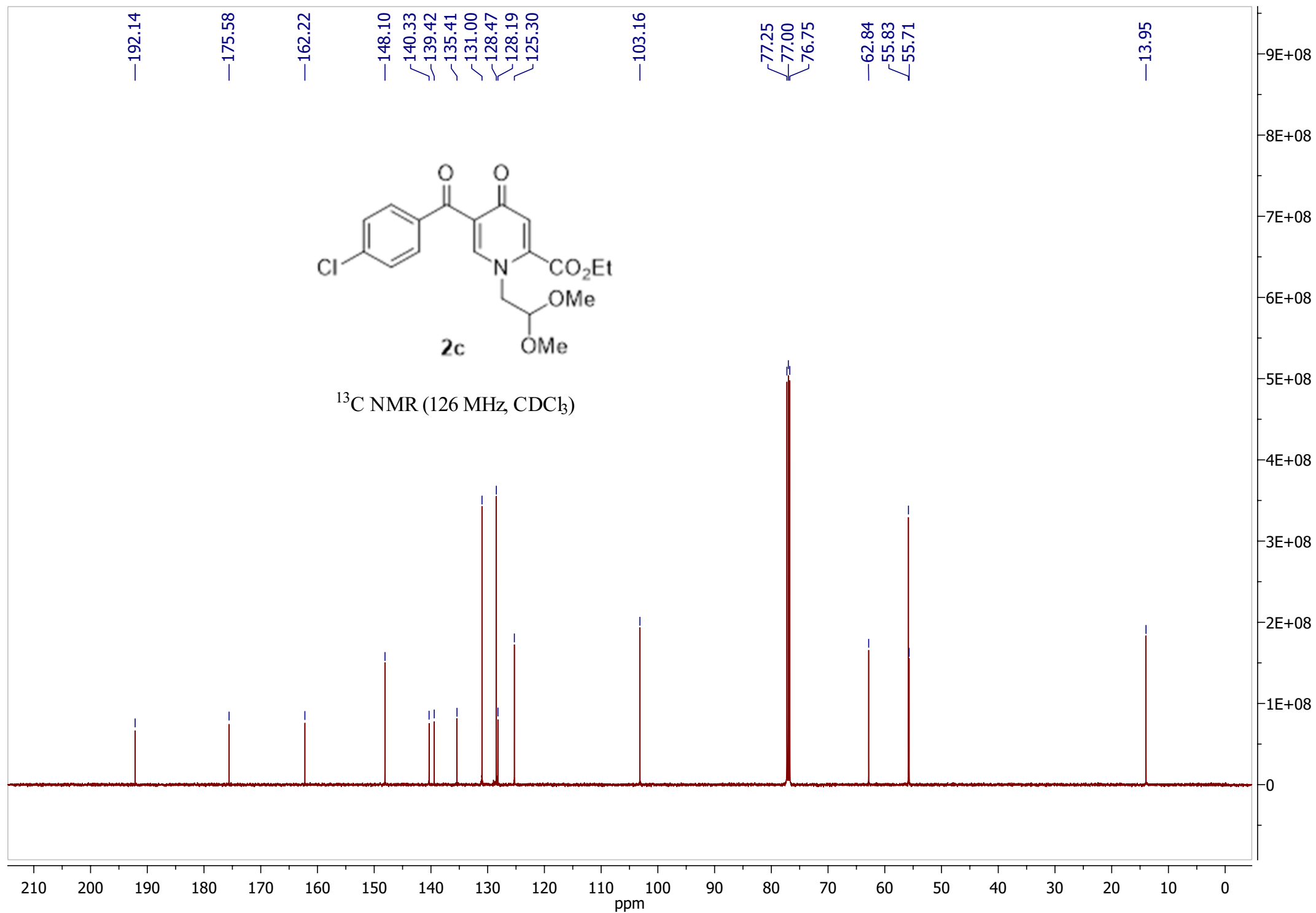


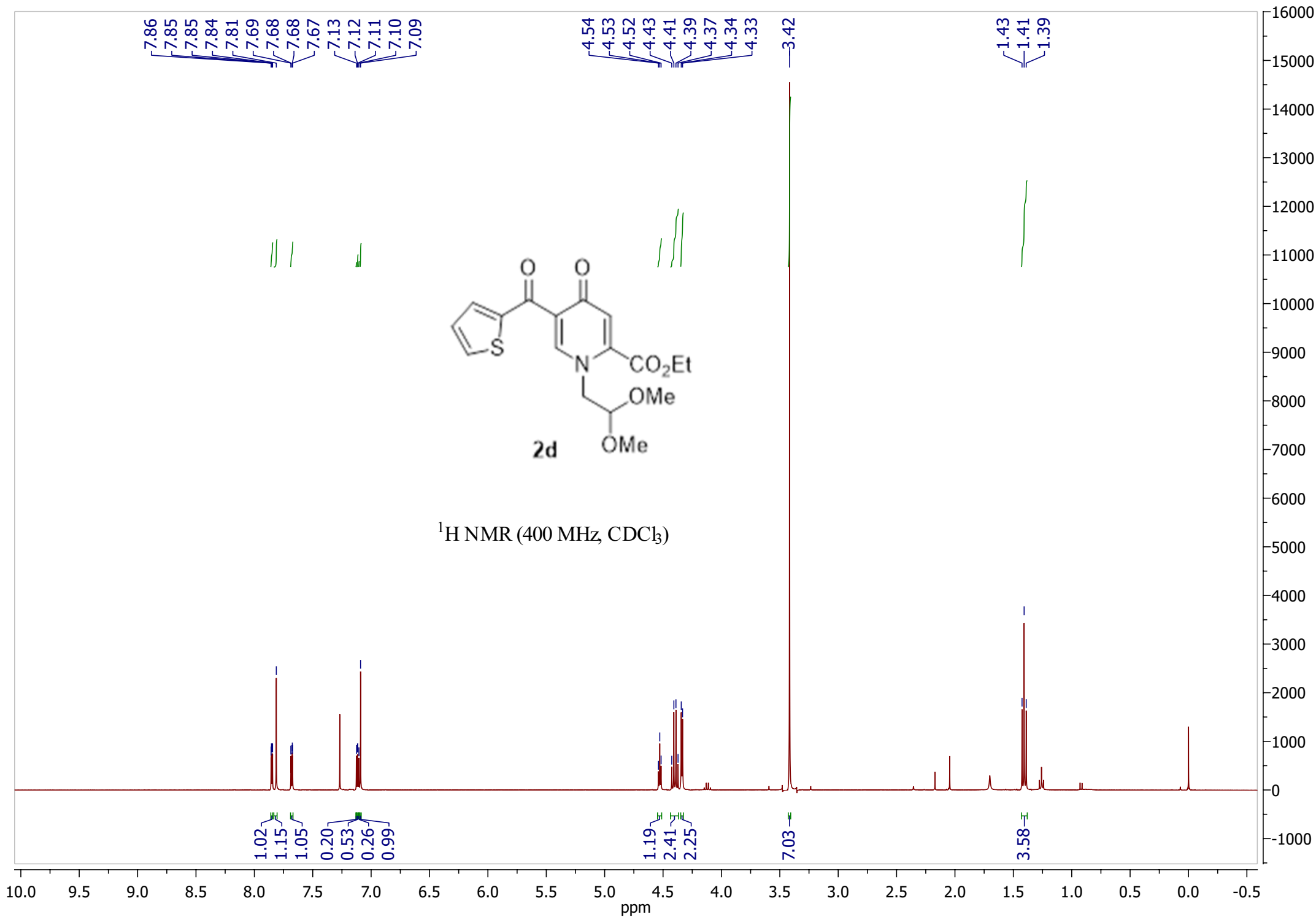


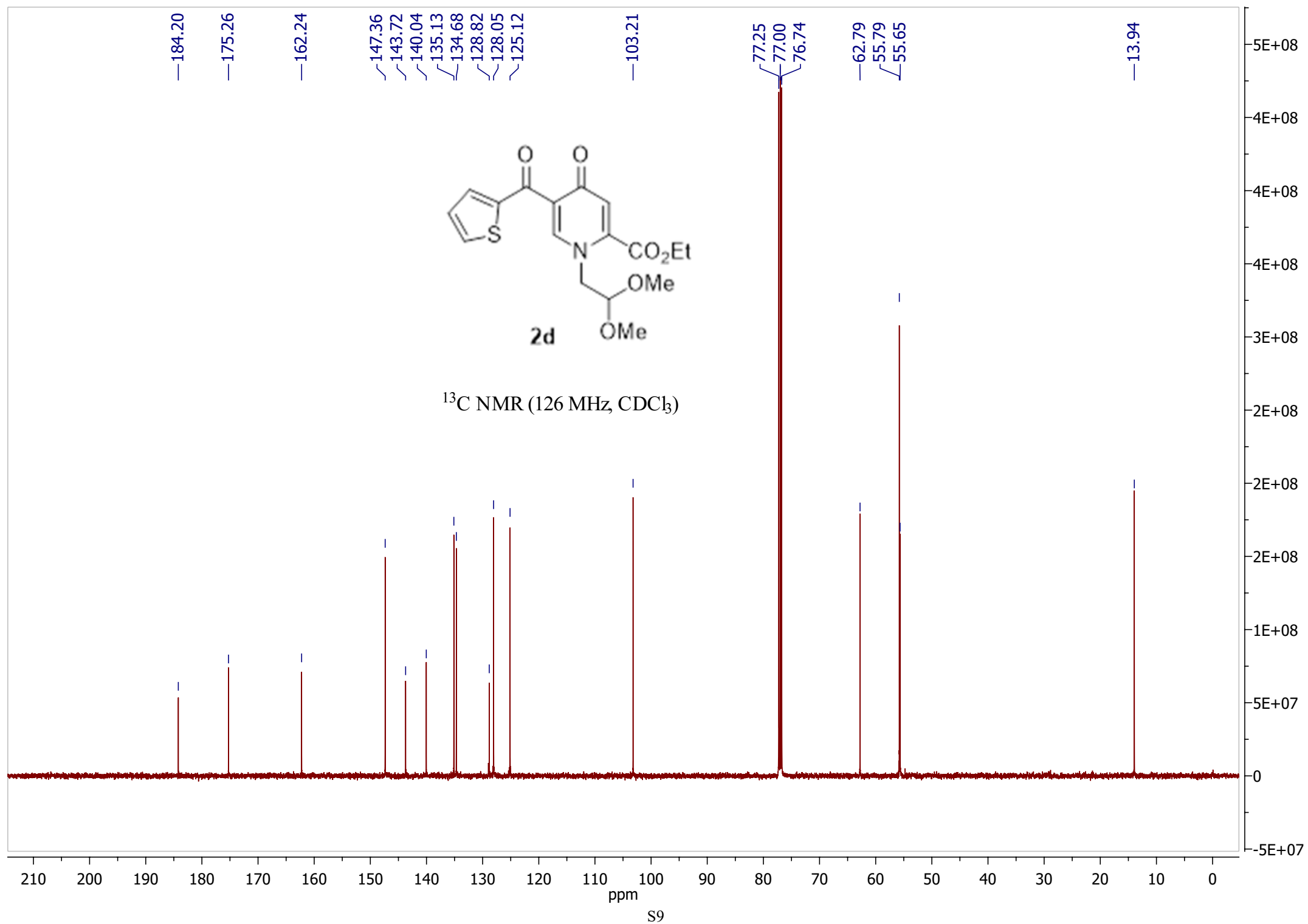


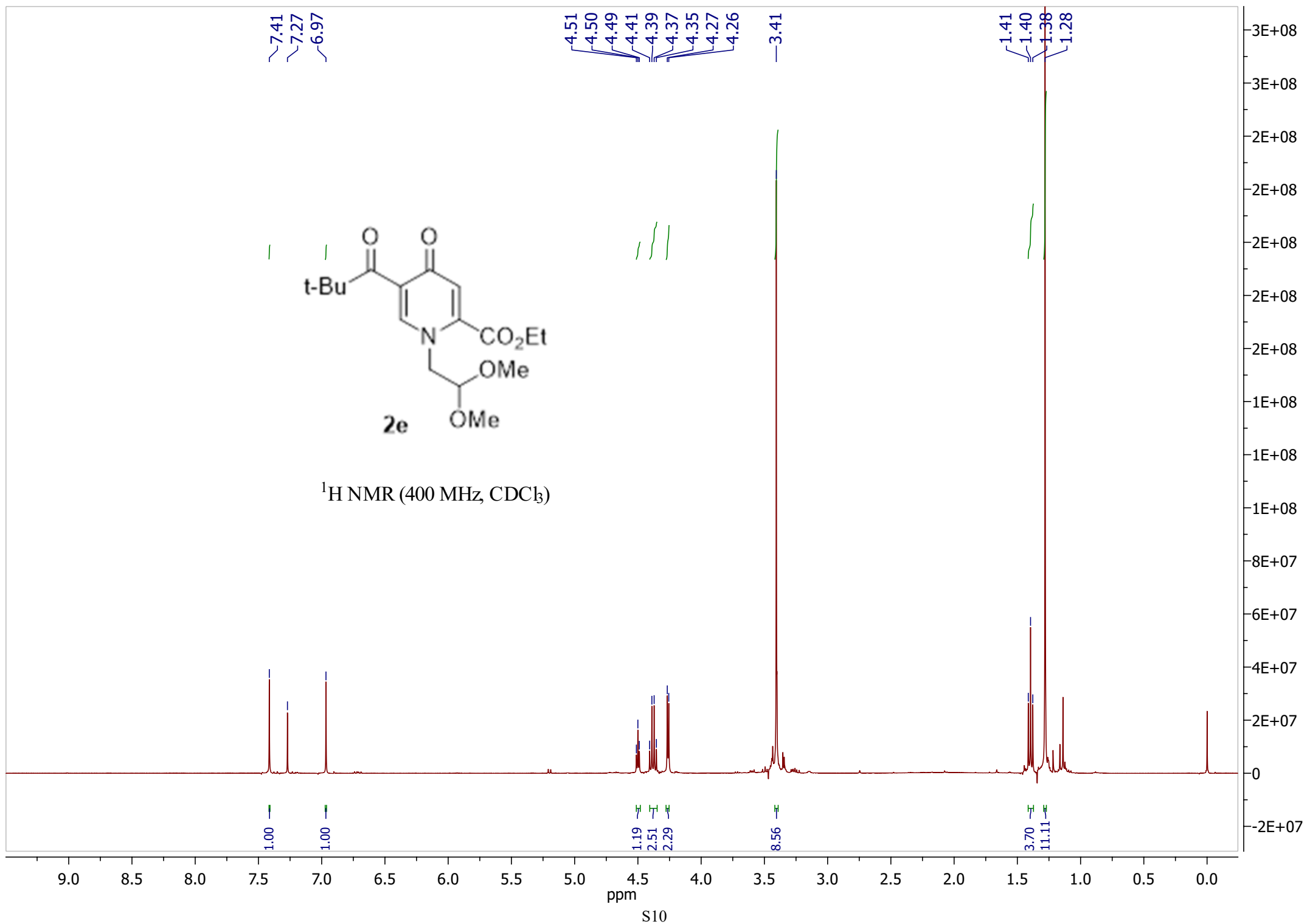


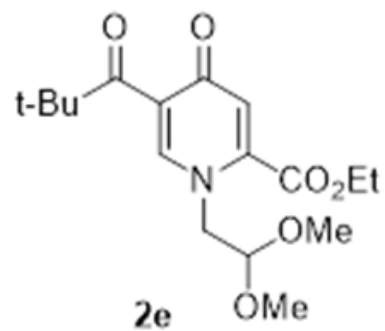
$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )



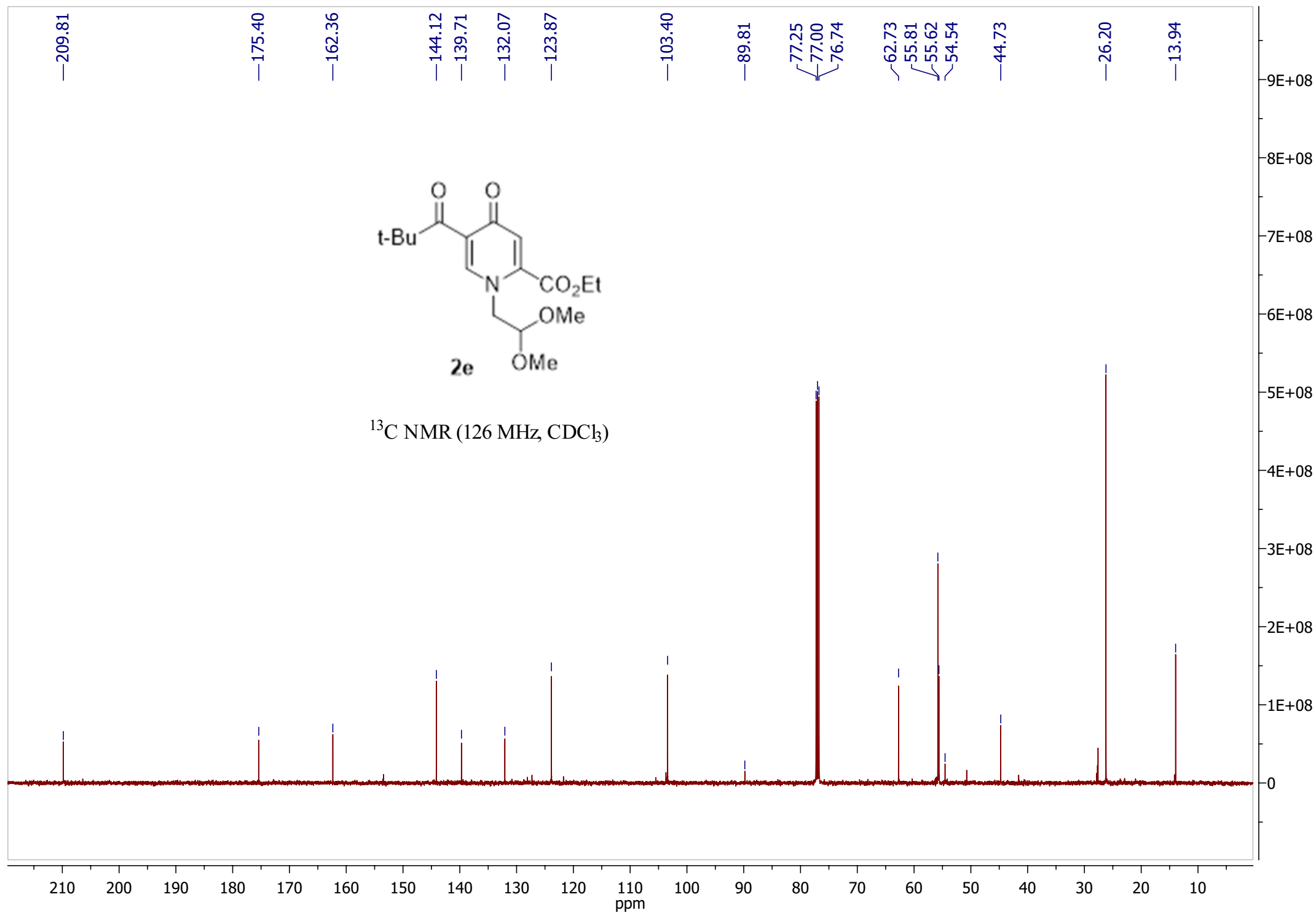


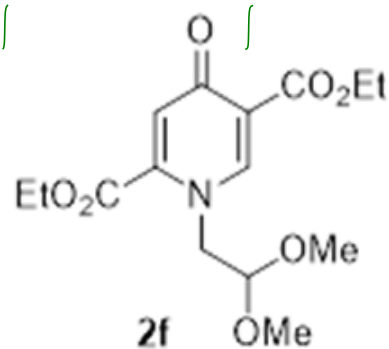




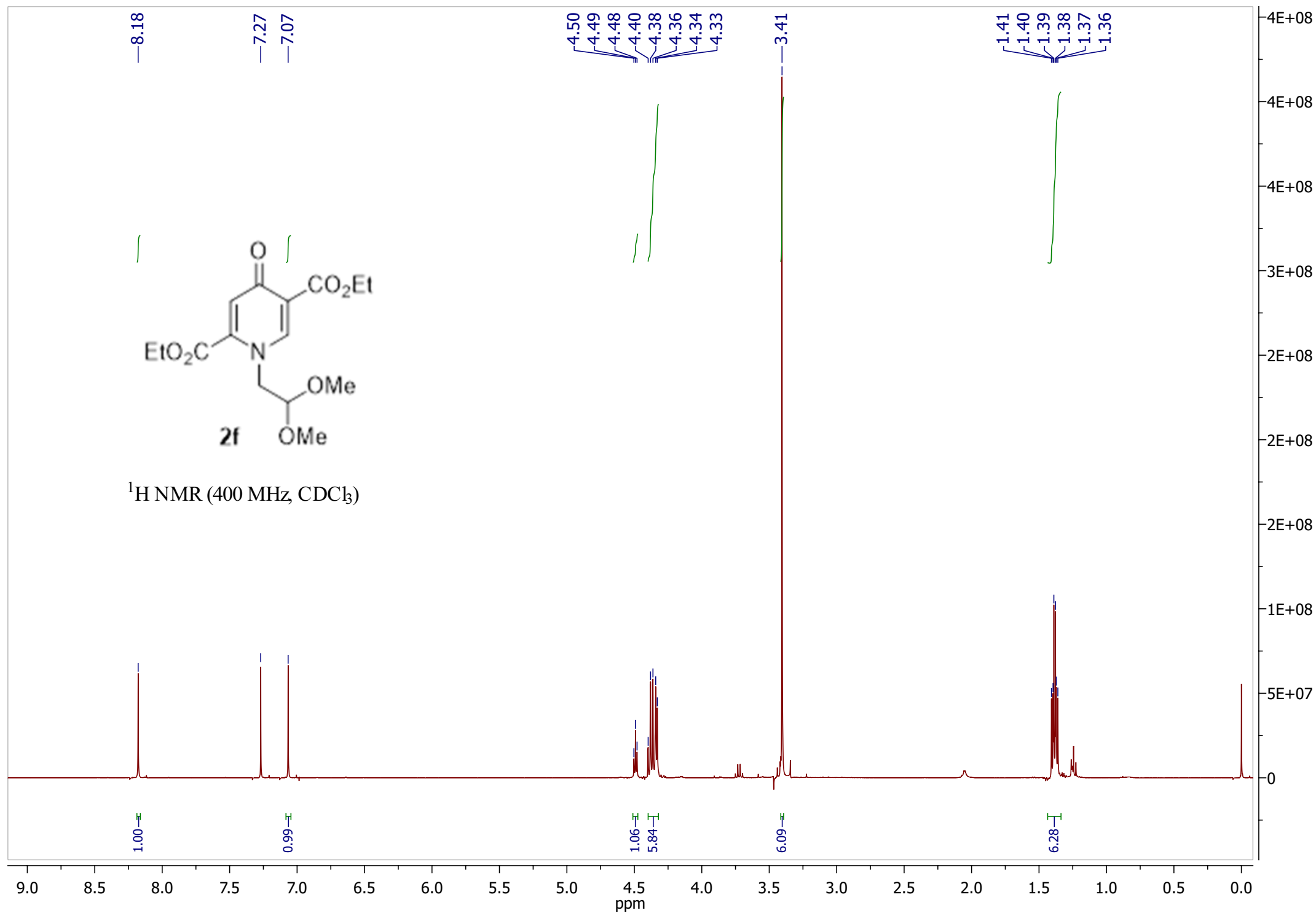


$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )

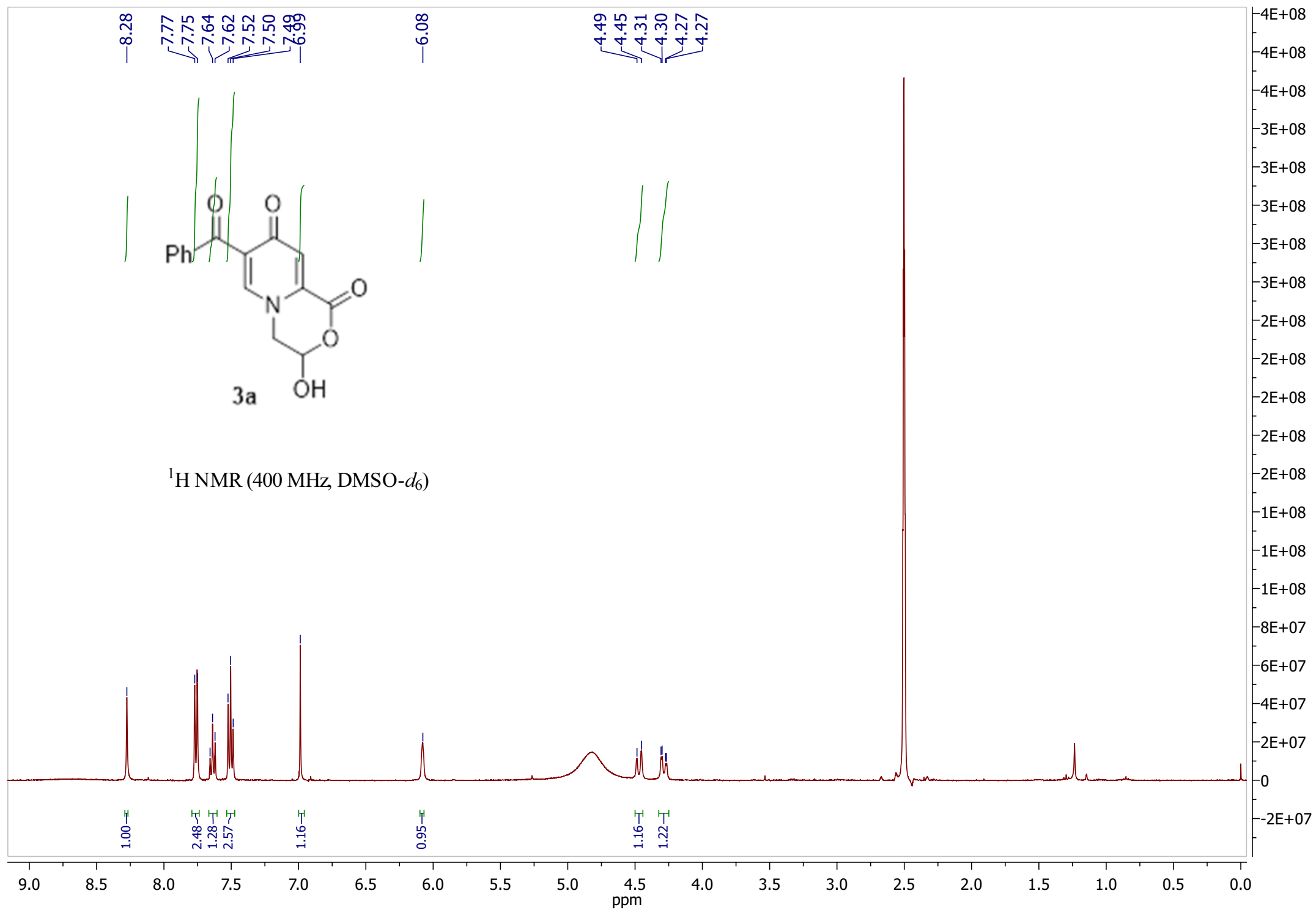


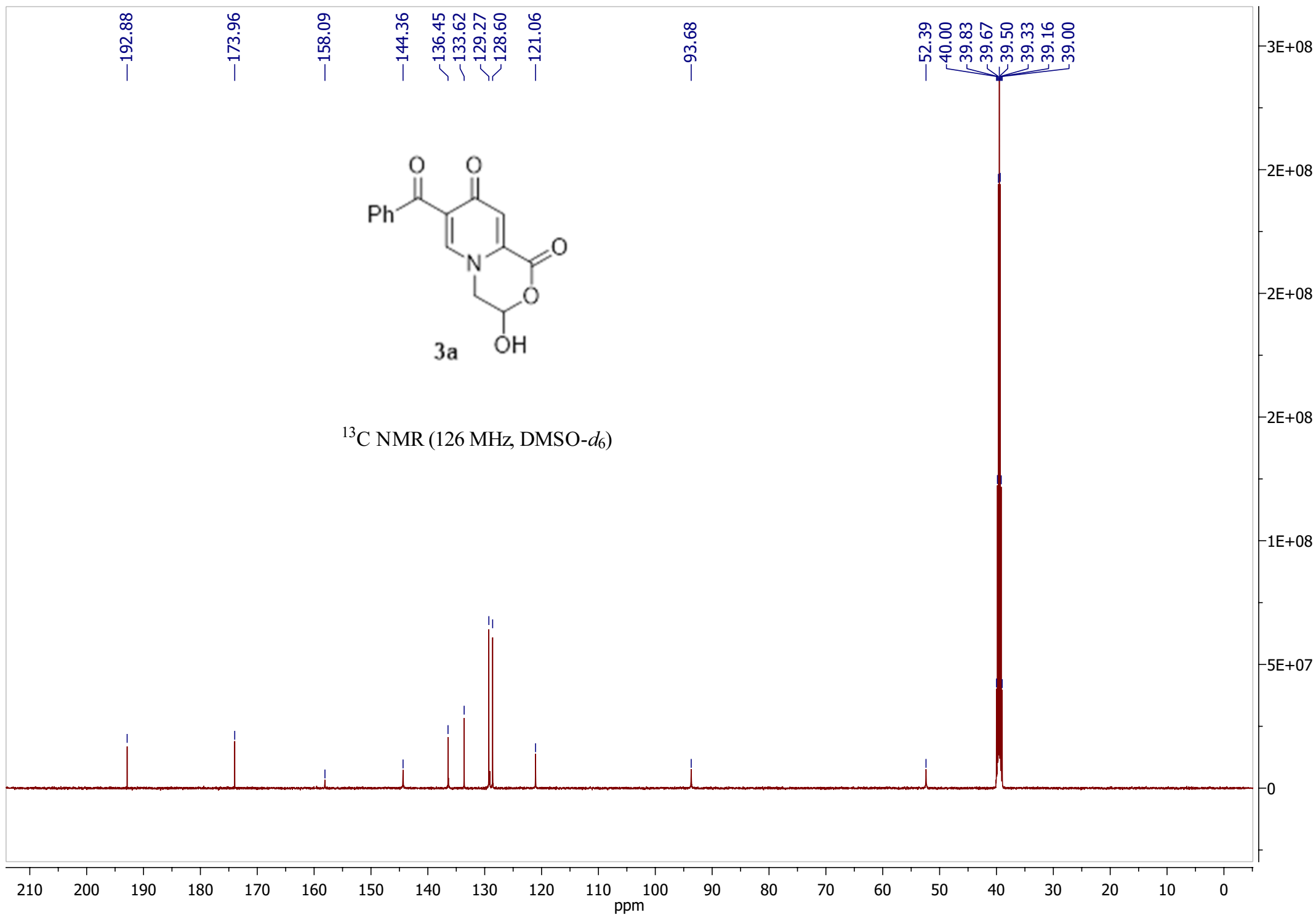


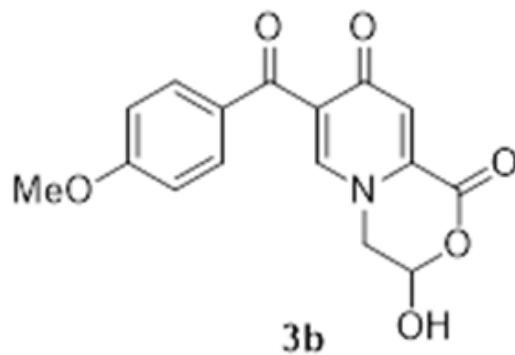
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )



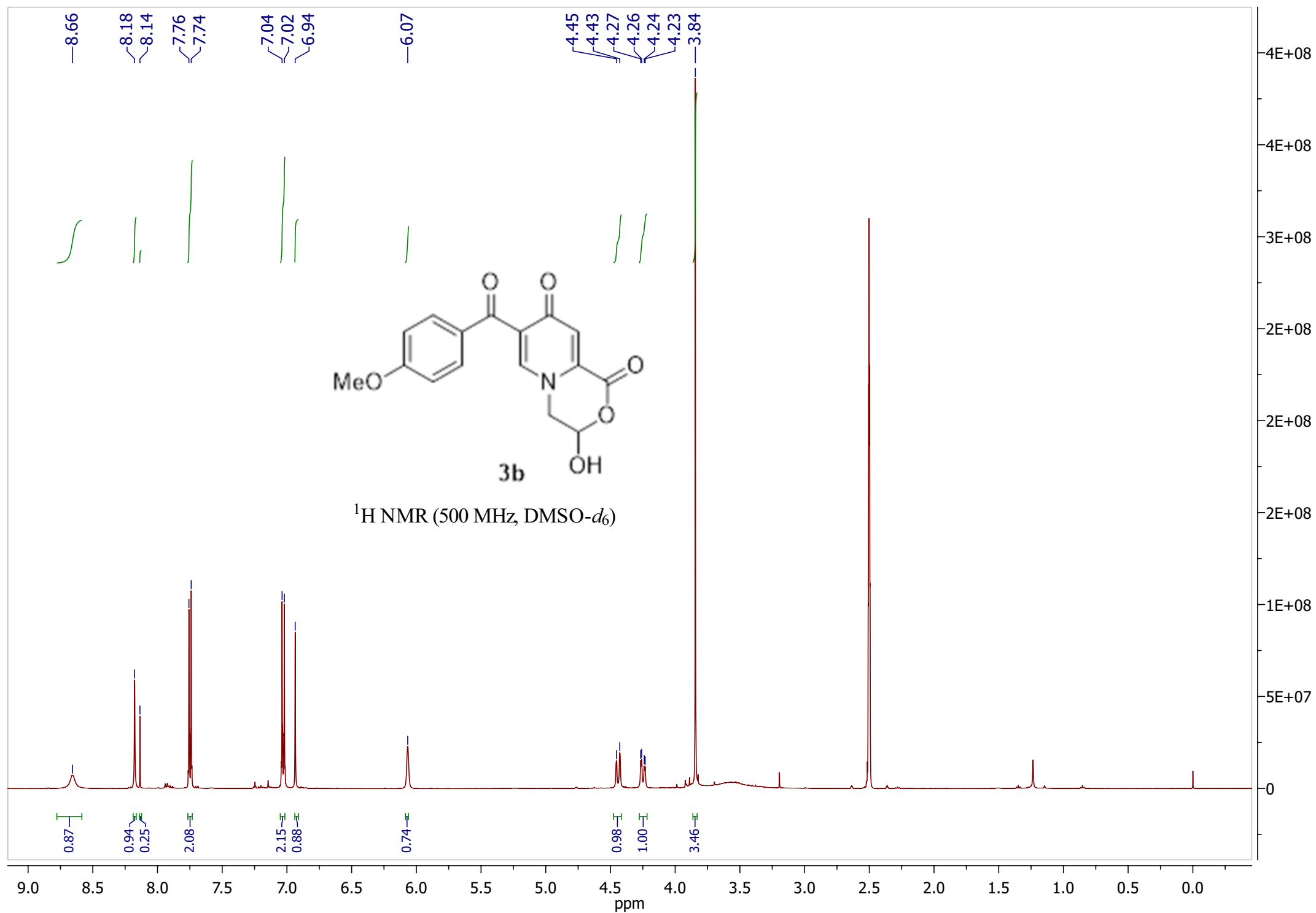


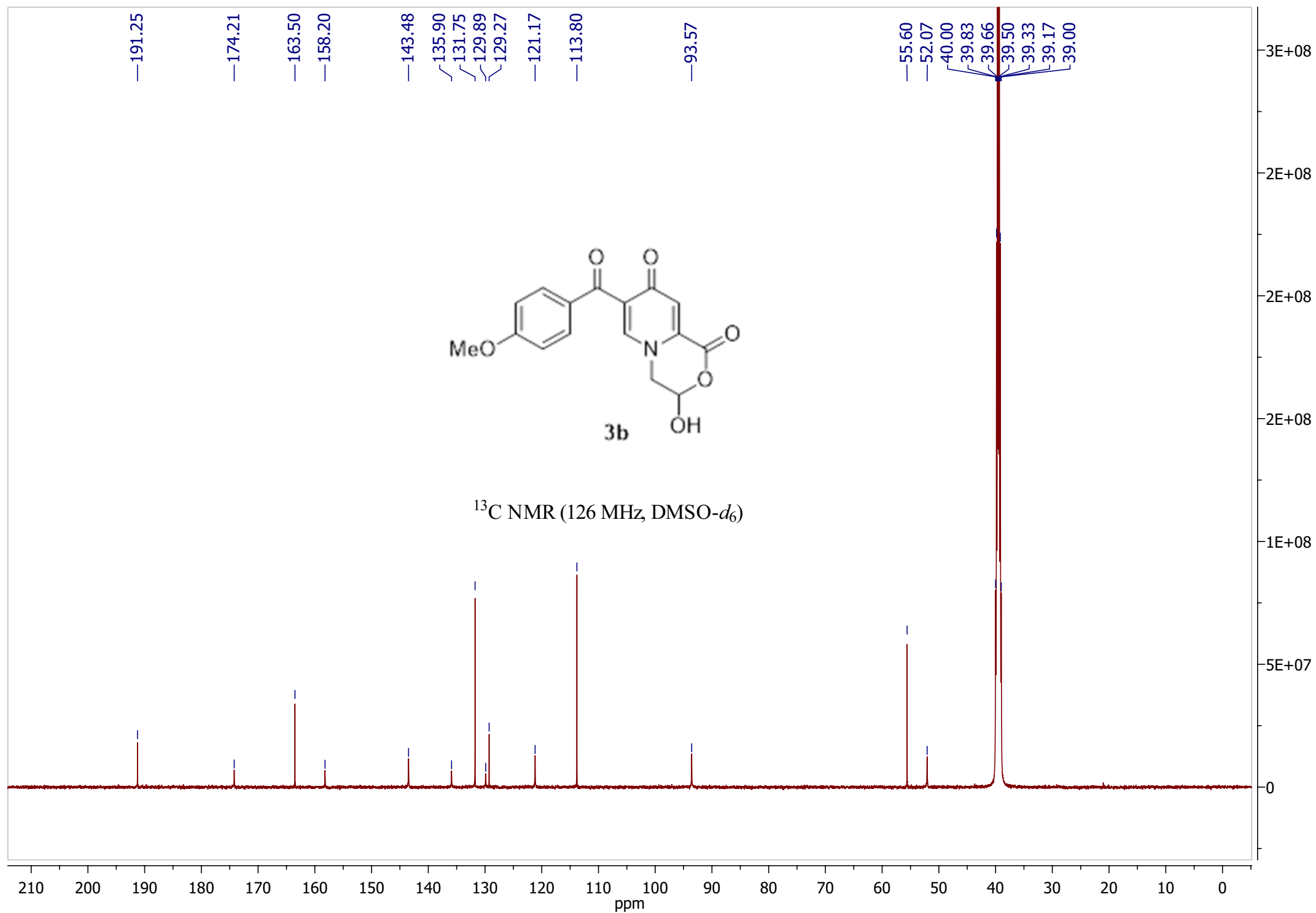


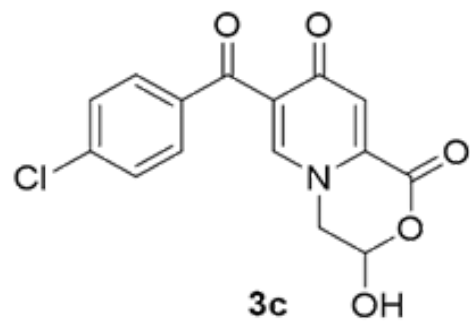




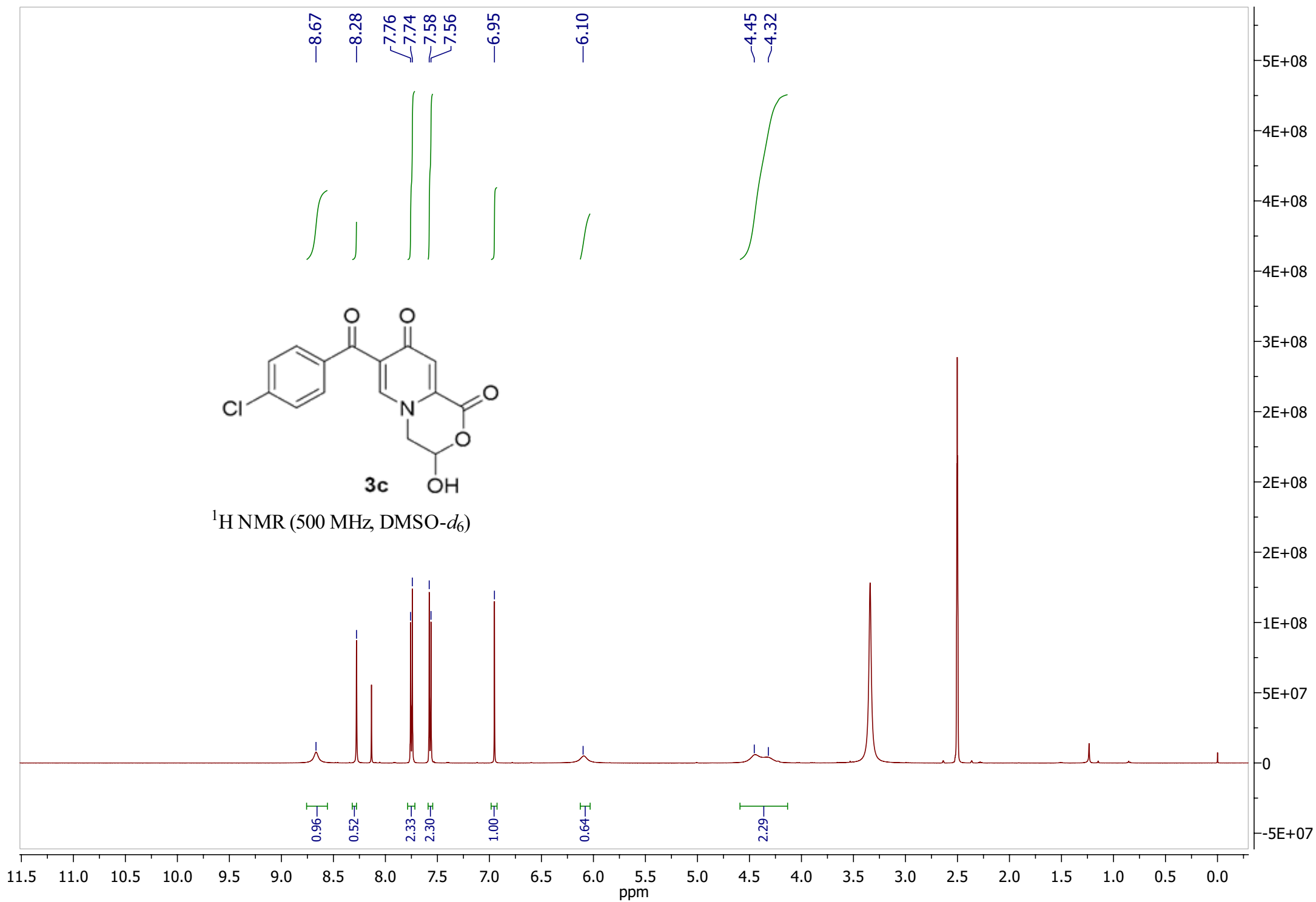
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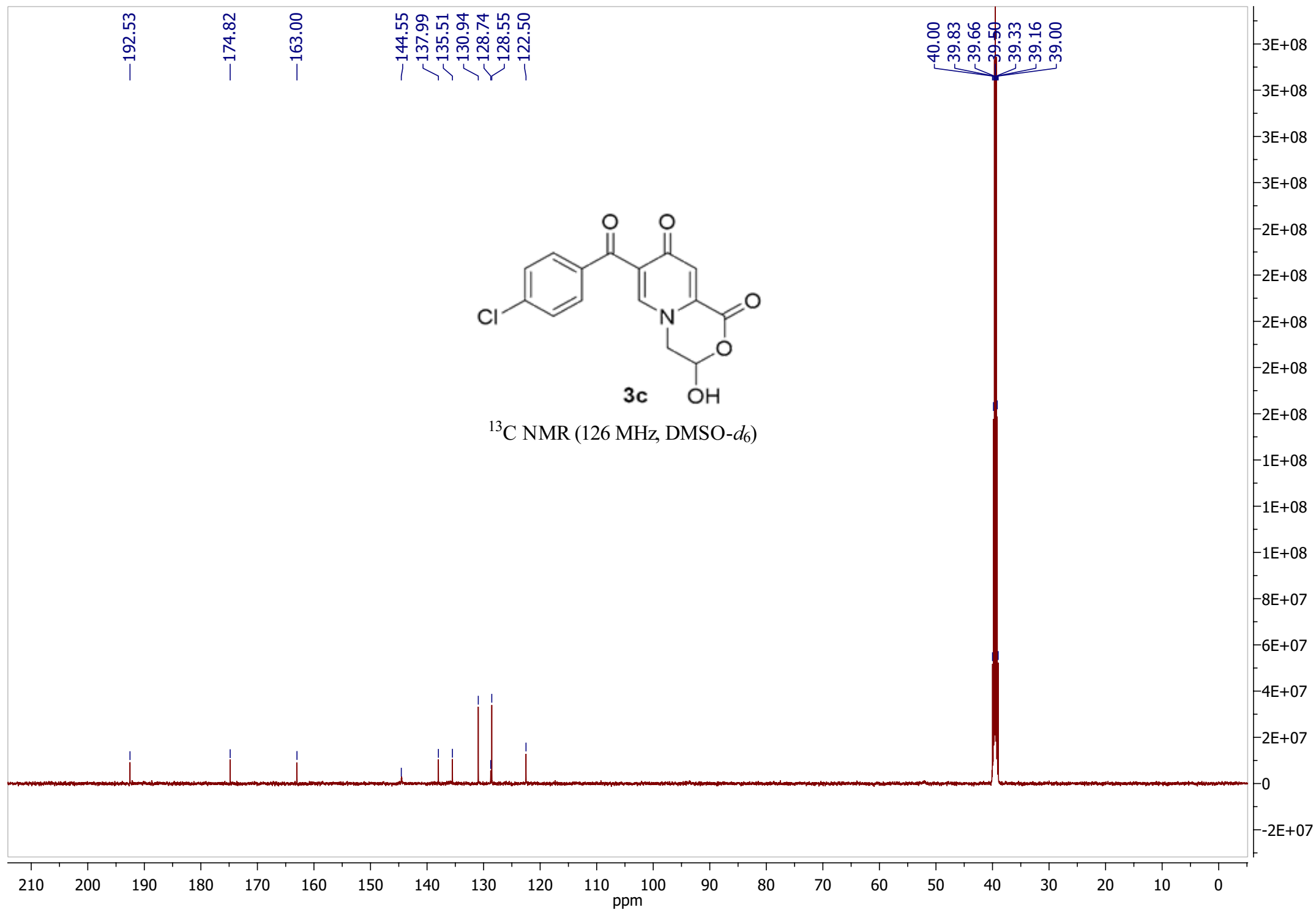


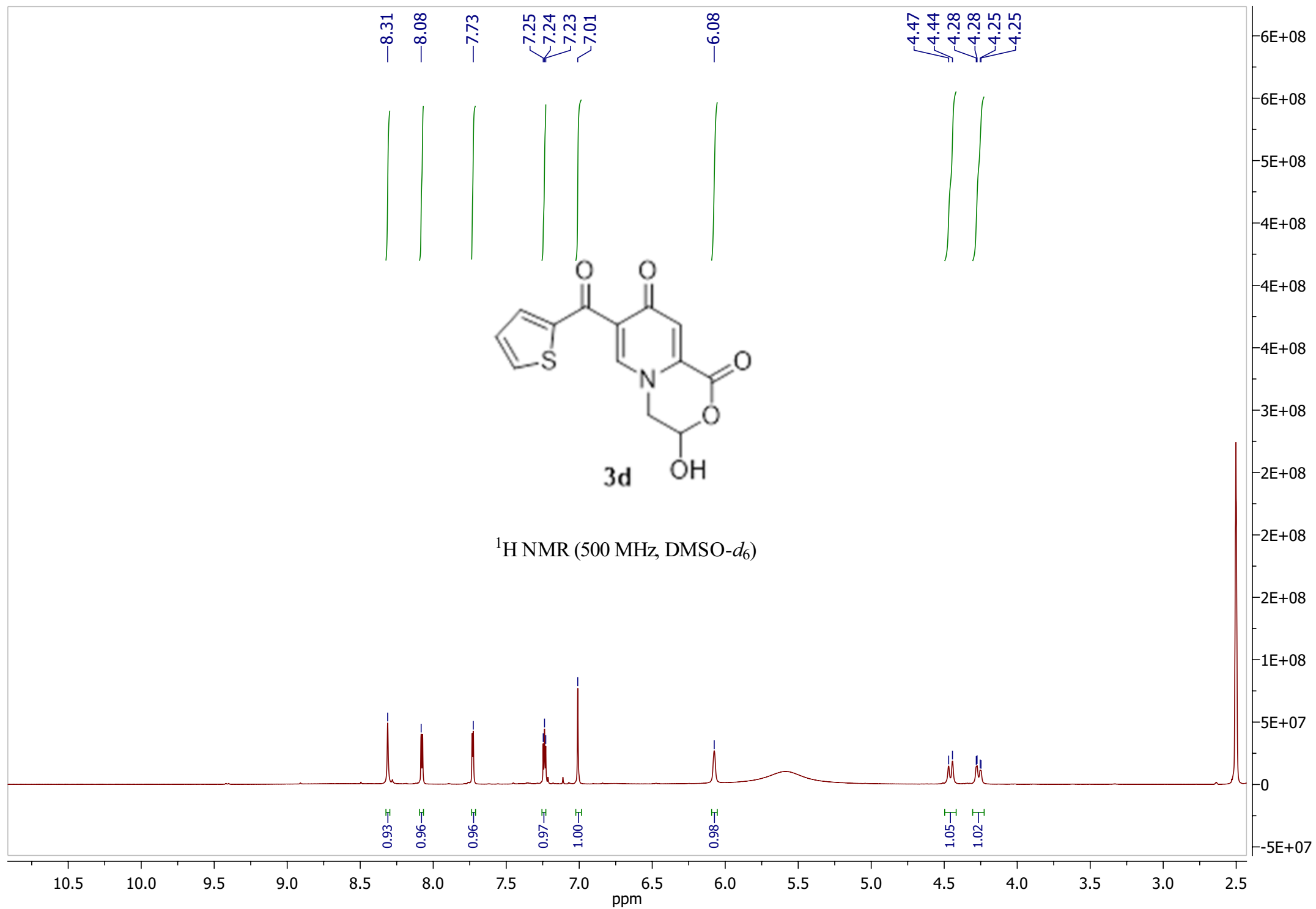


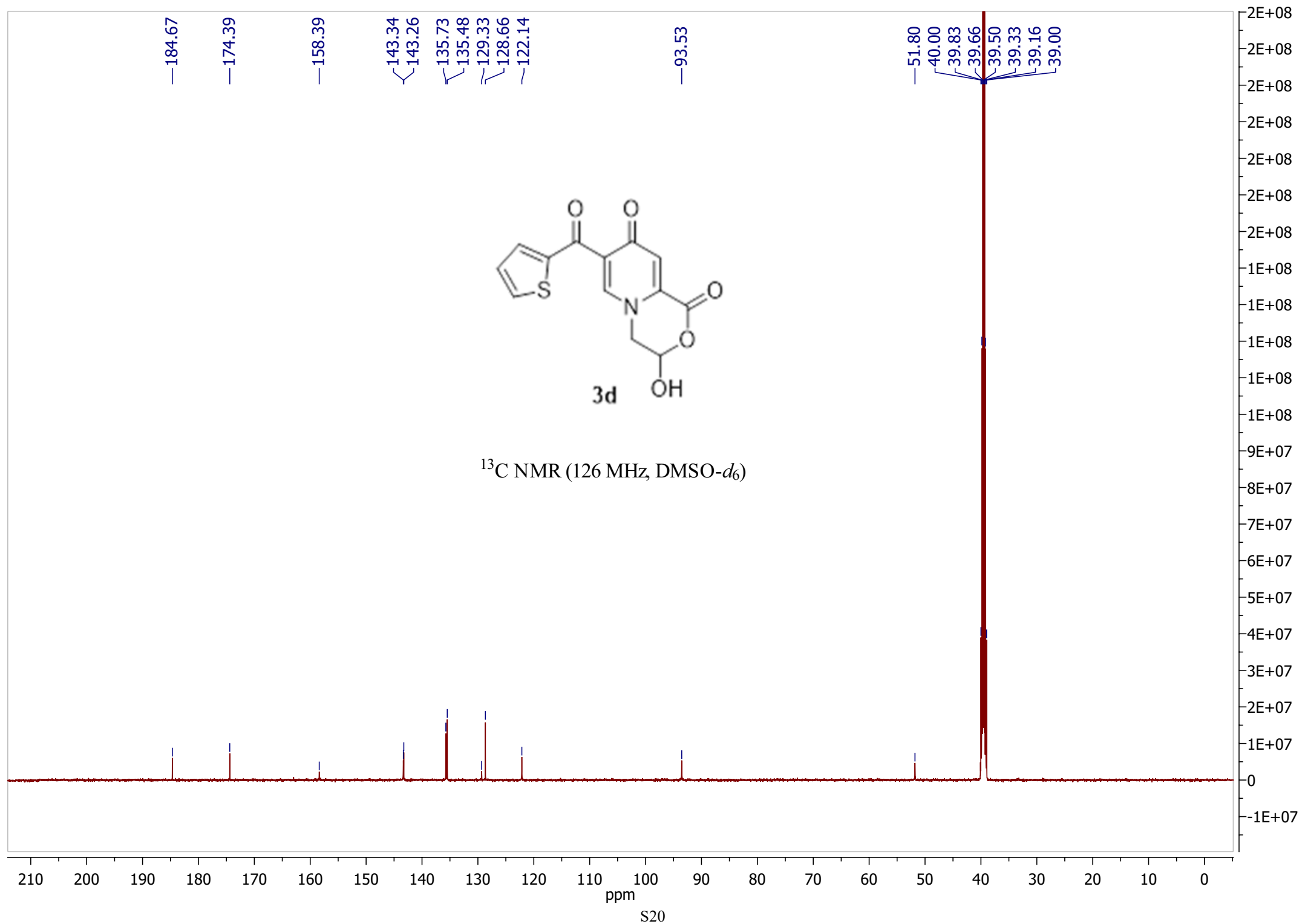


$^1\text{H}$  NMR (500 MHz,  $\text{DMSO}-d_6$ )

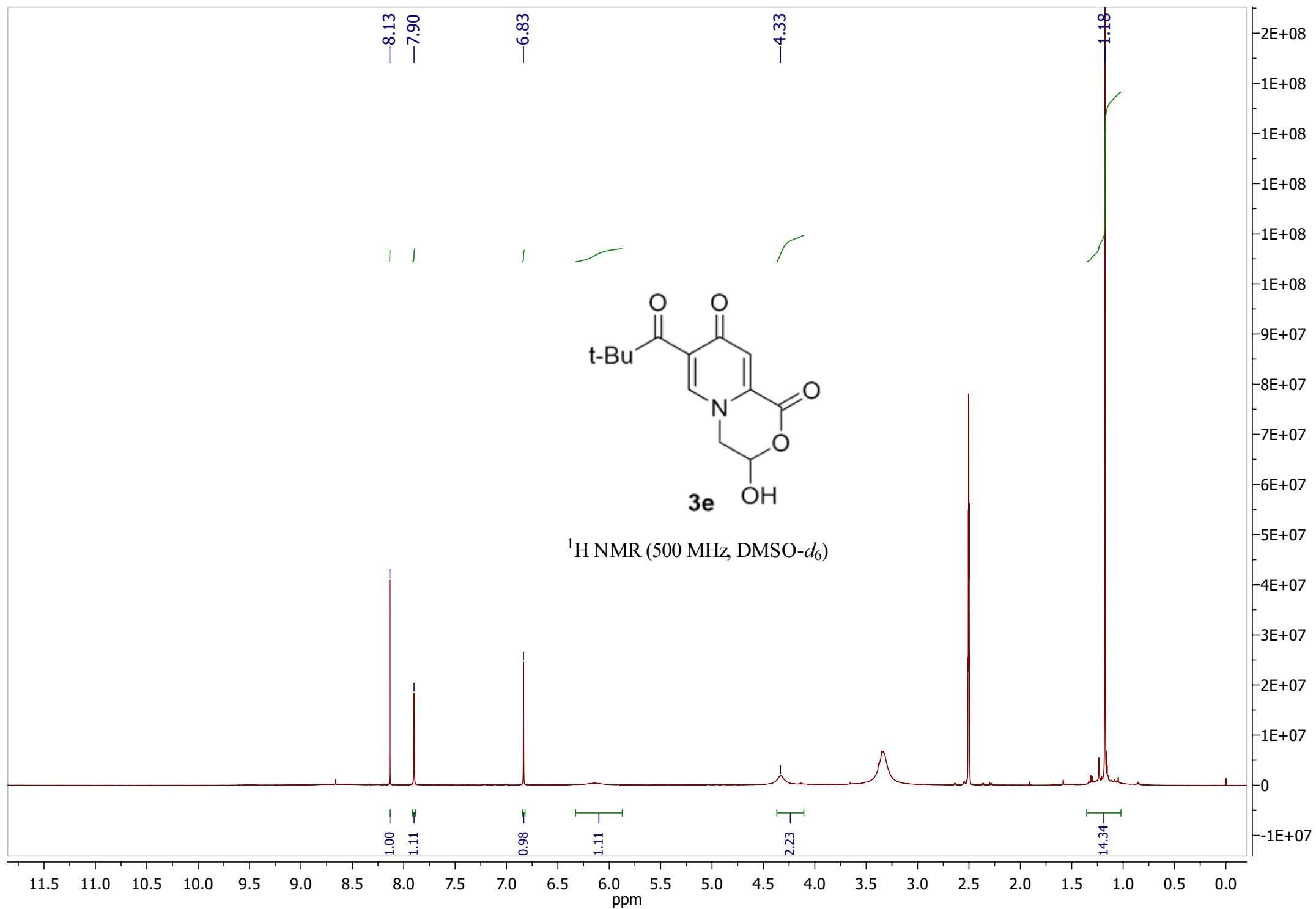


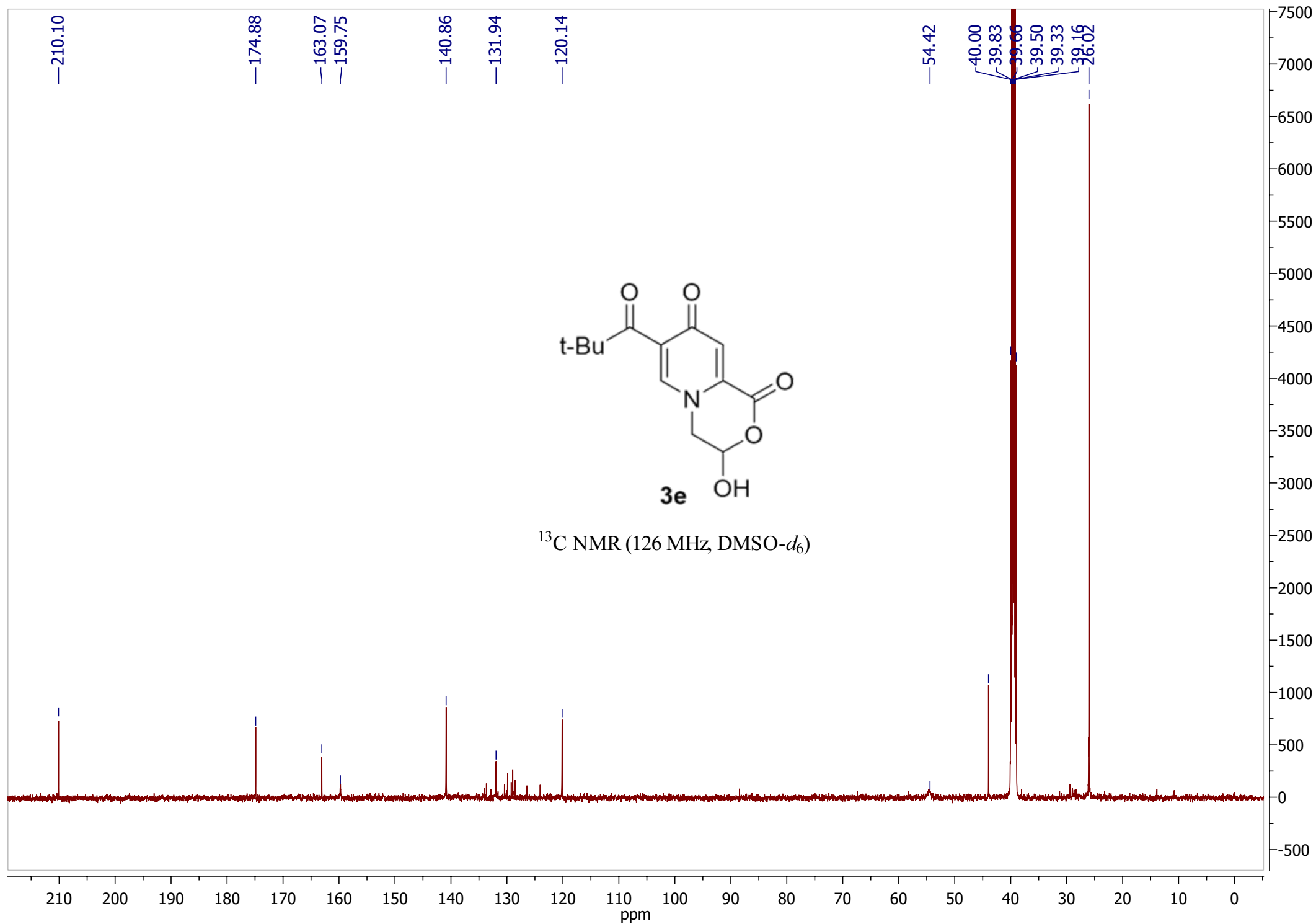


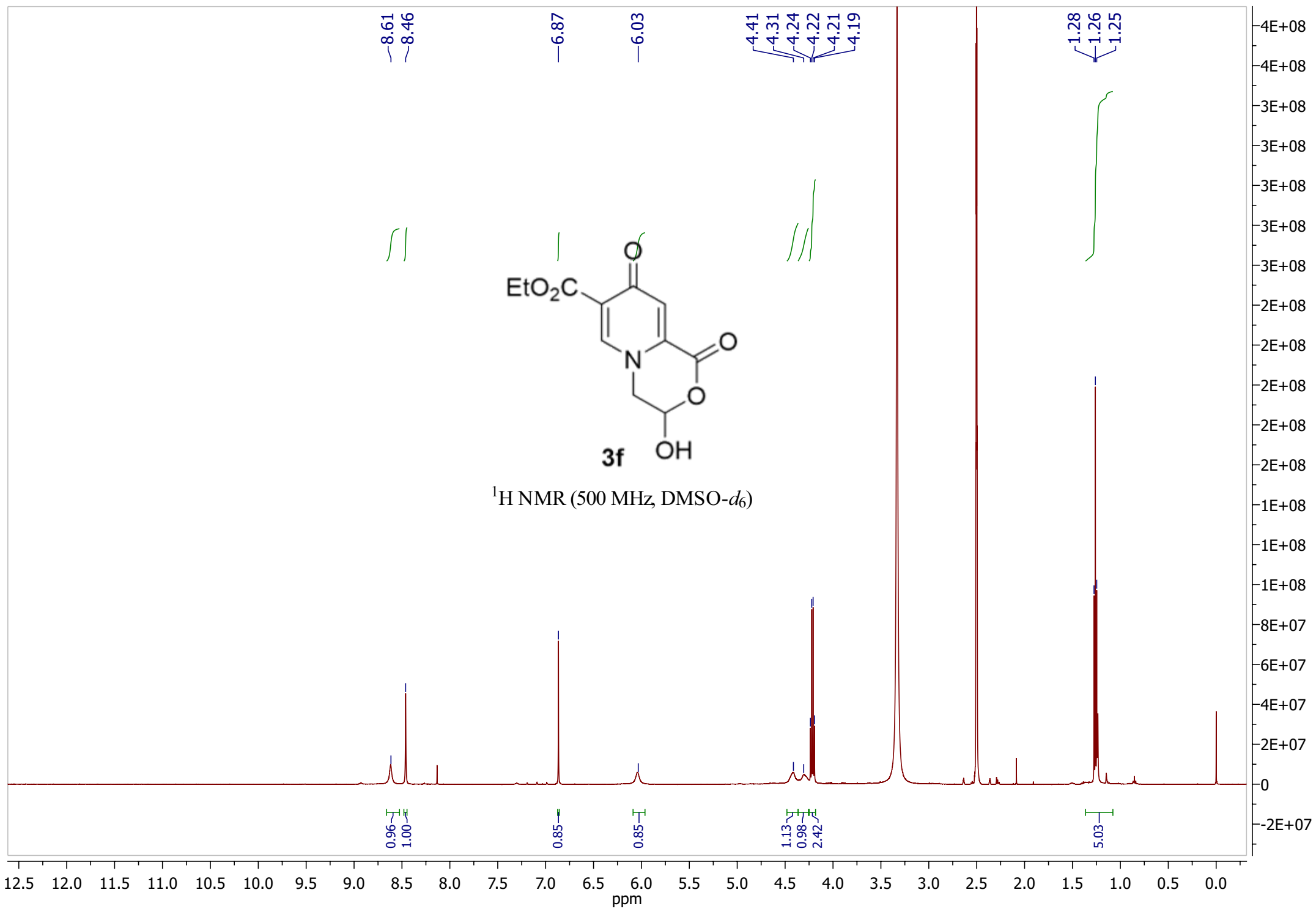


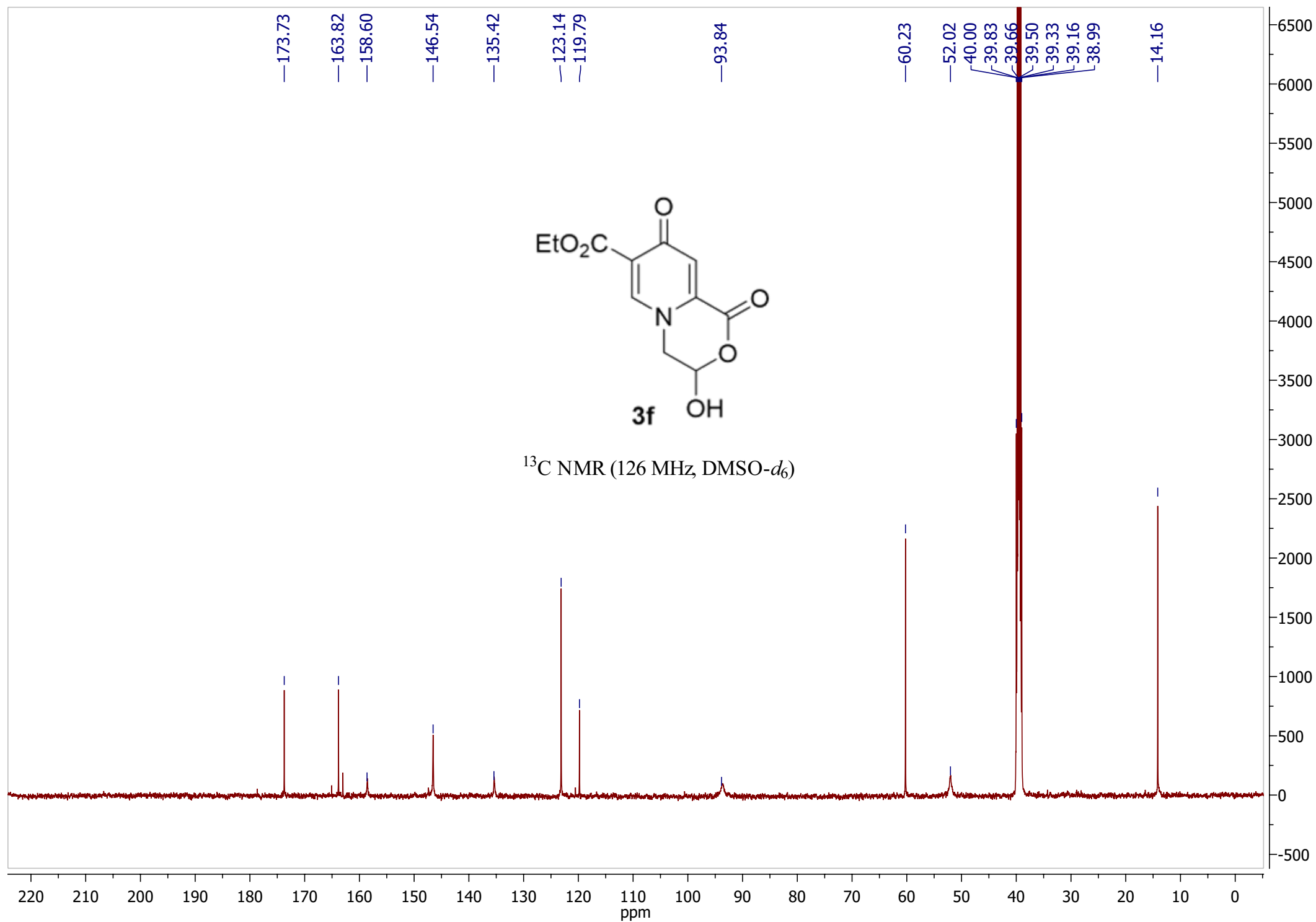


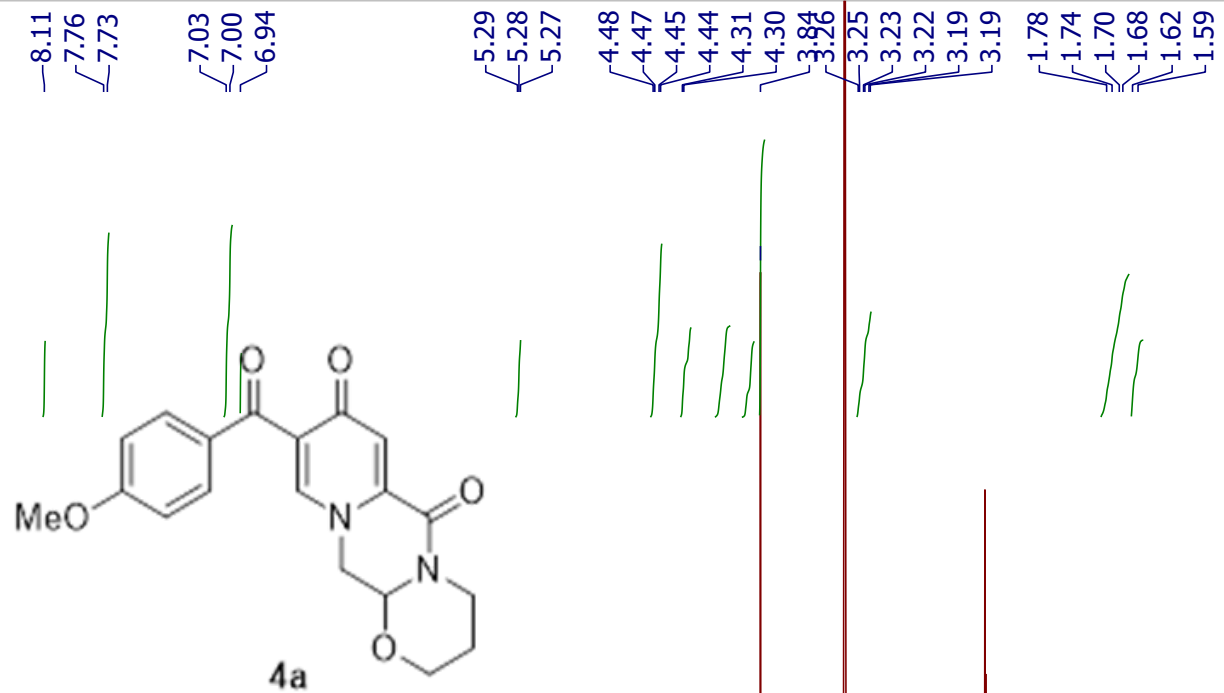




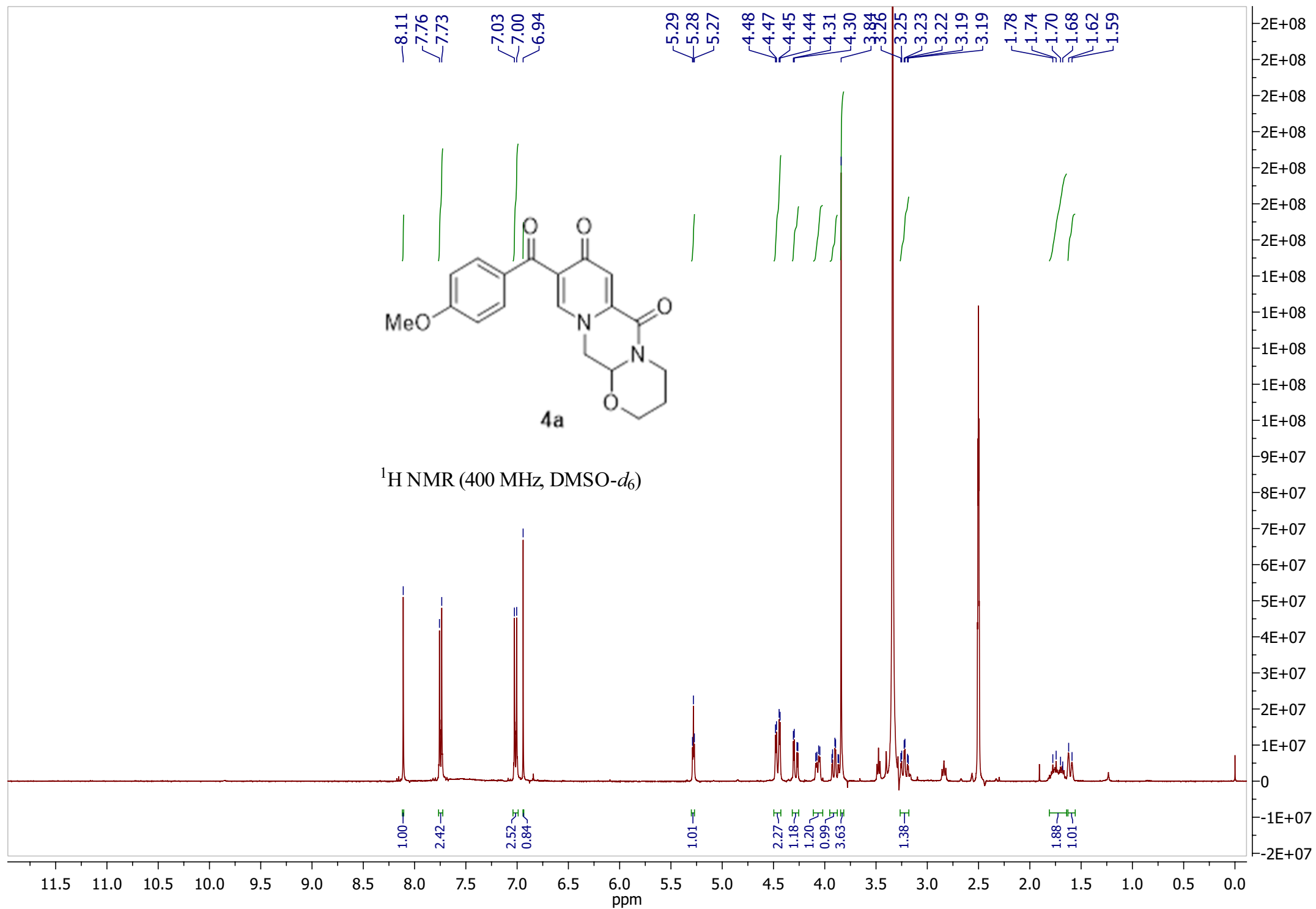


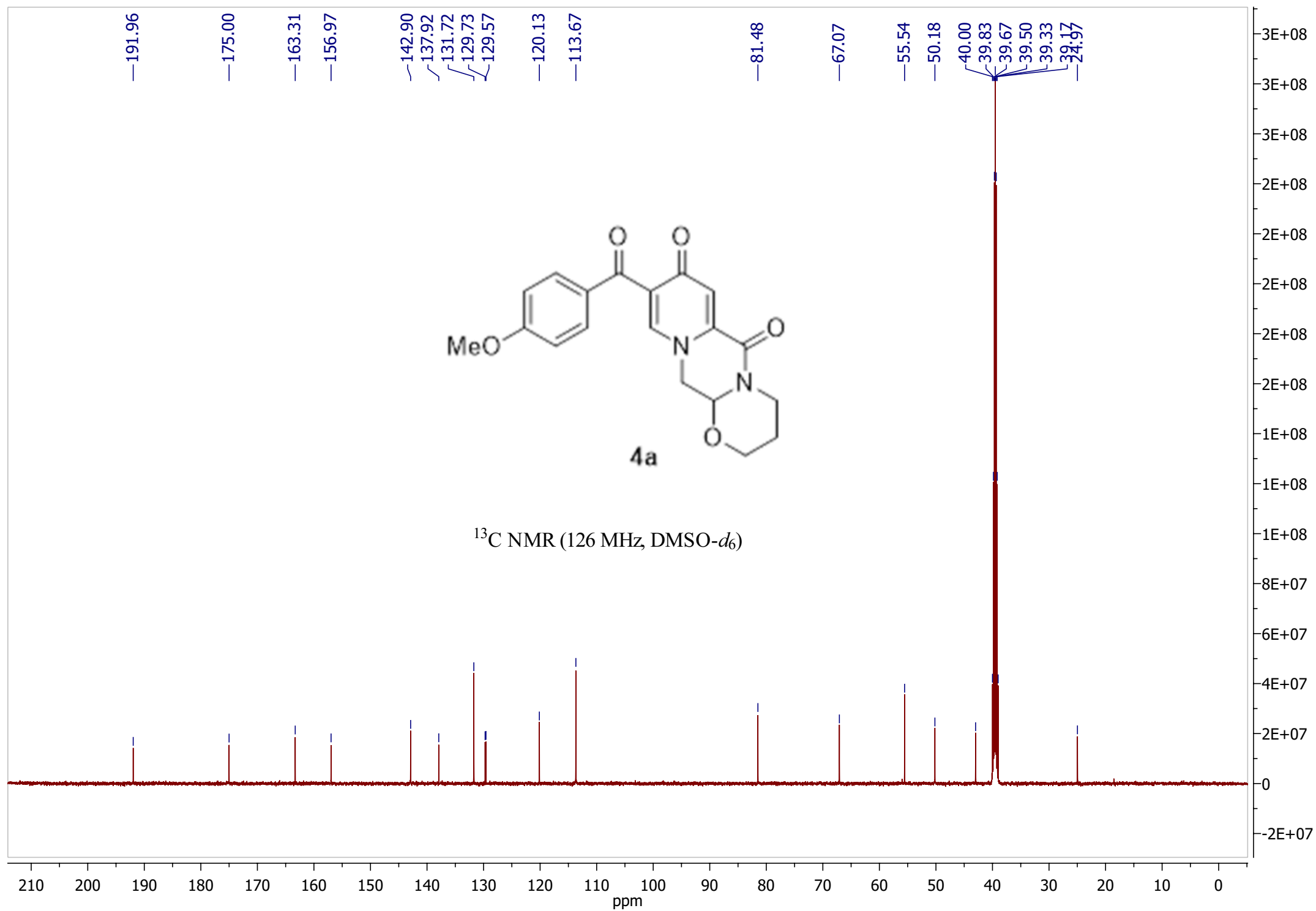




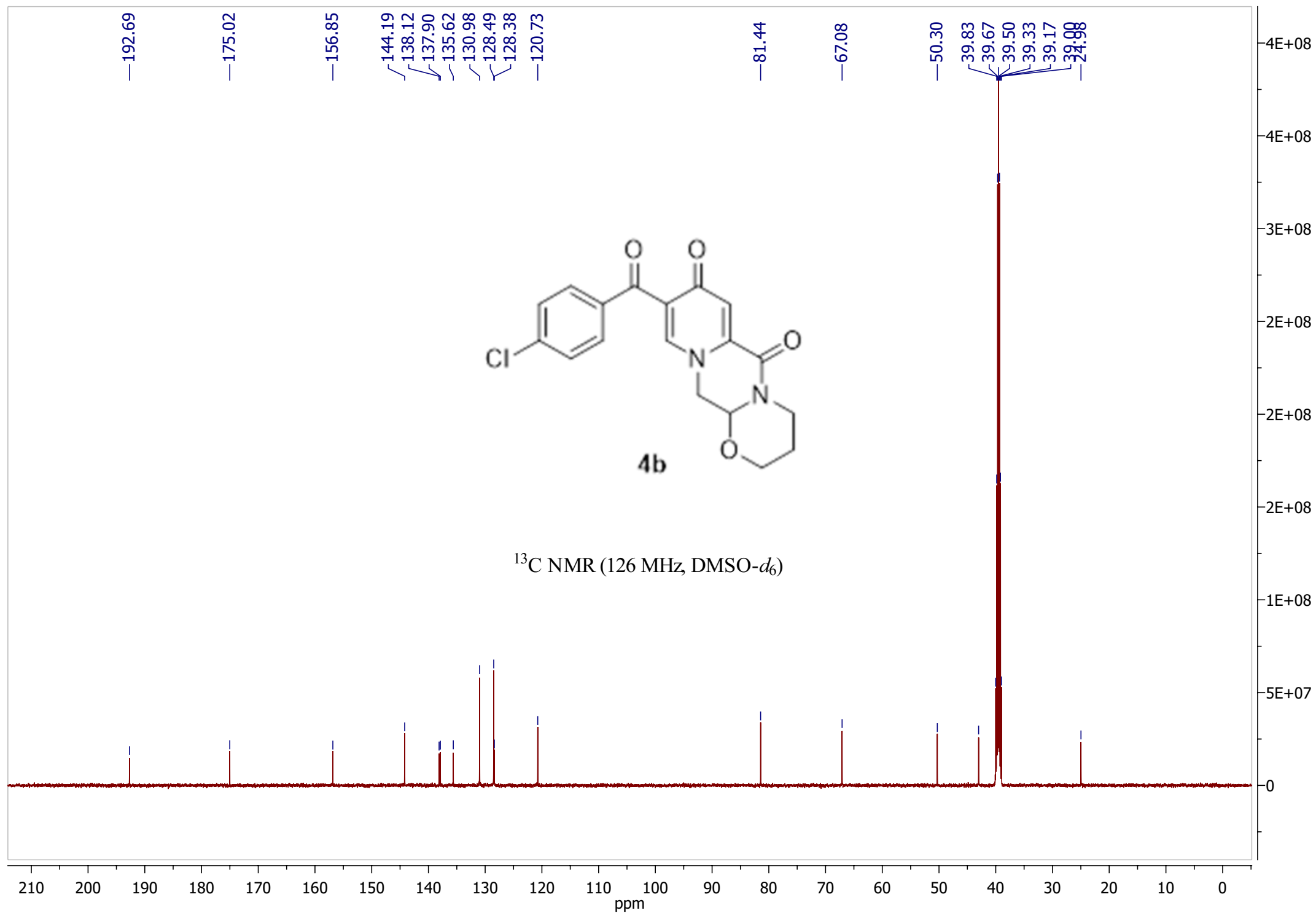


$^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ )

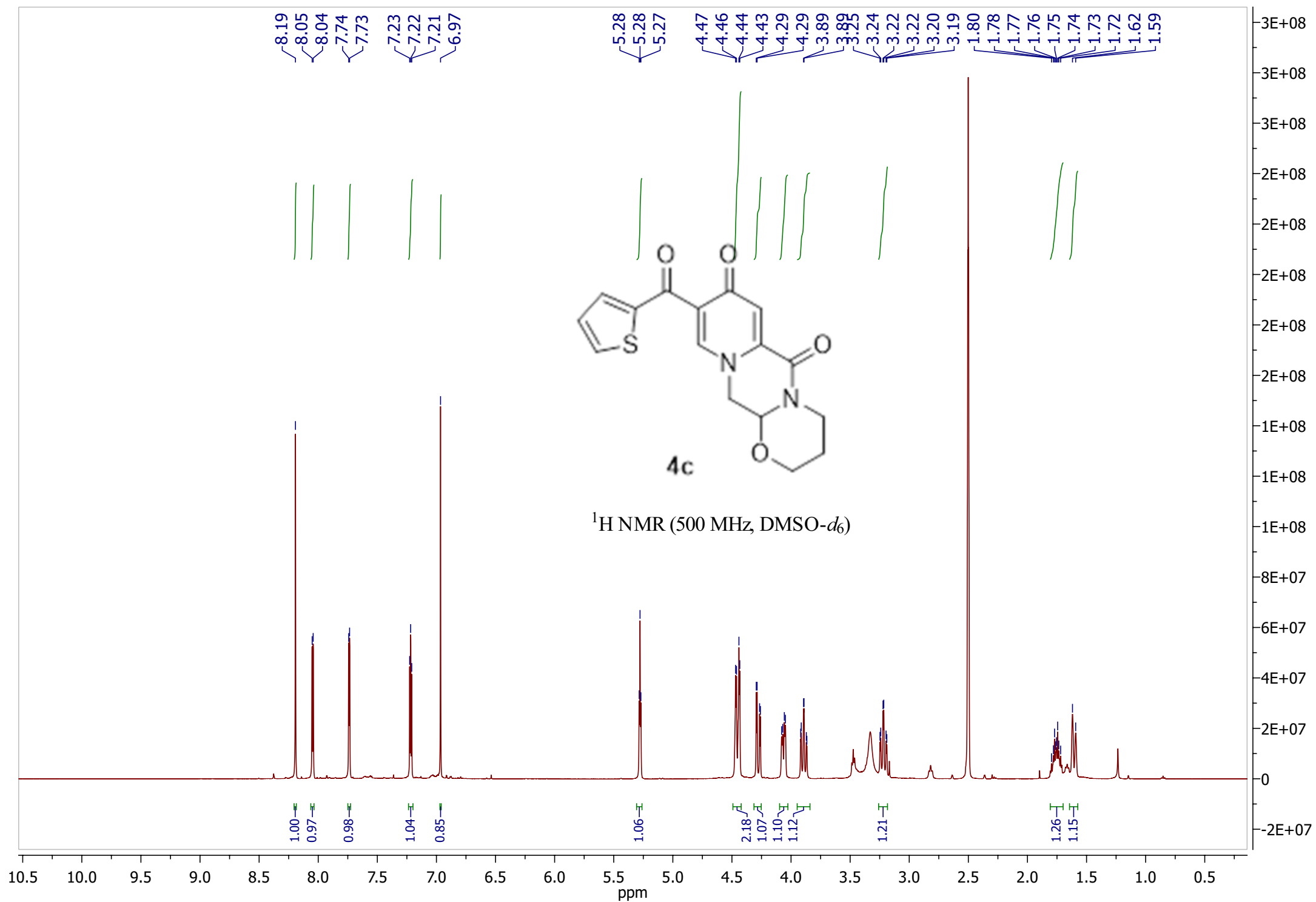


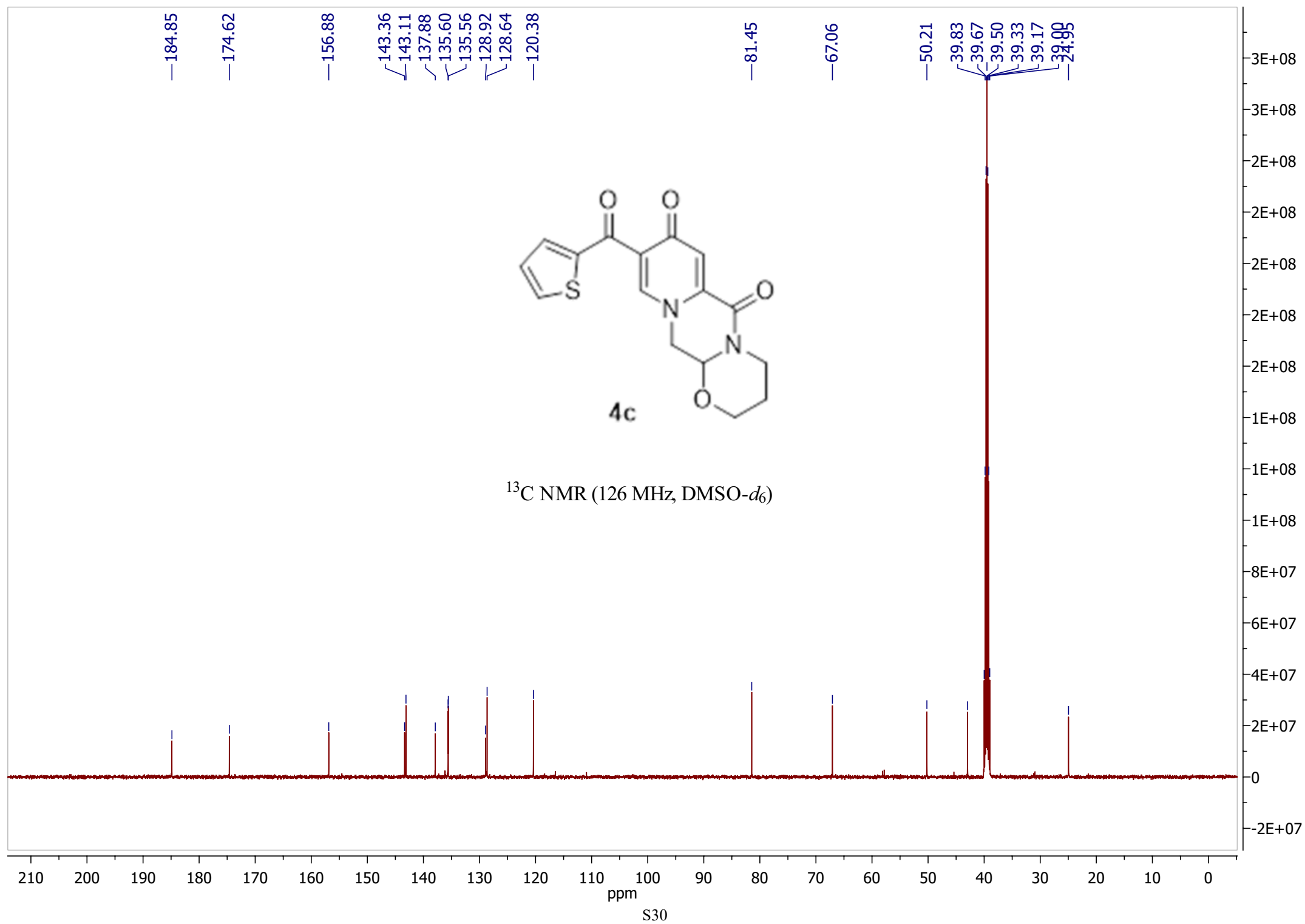


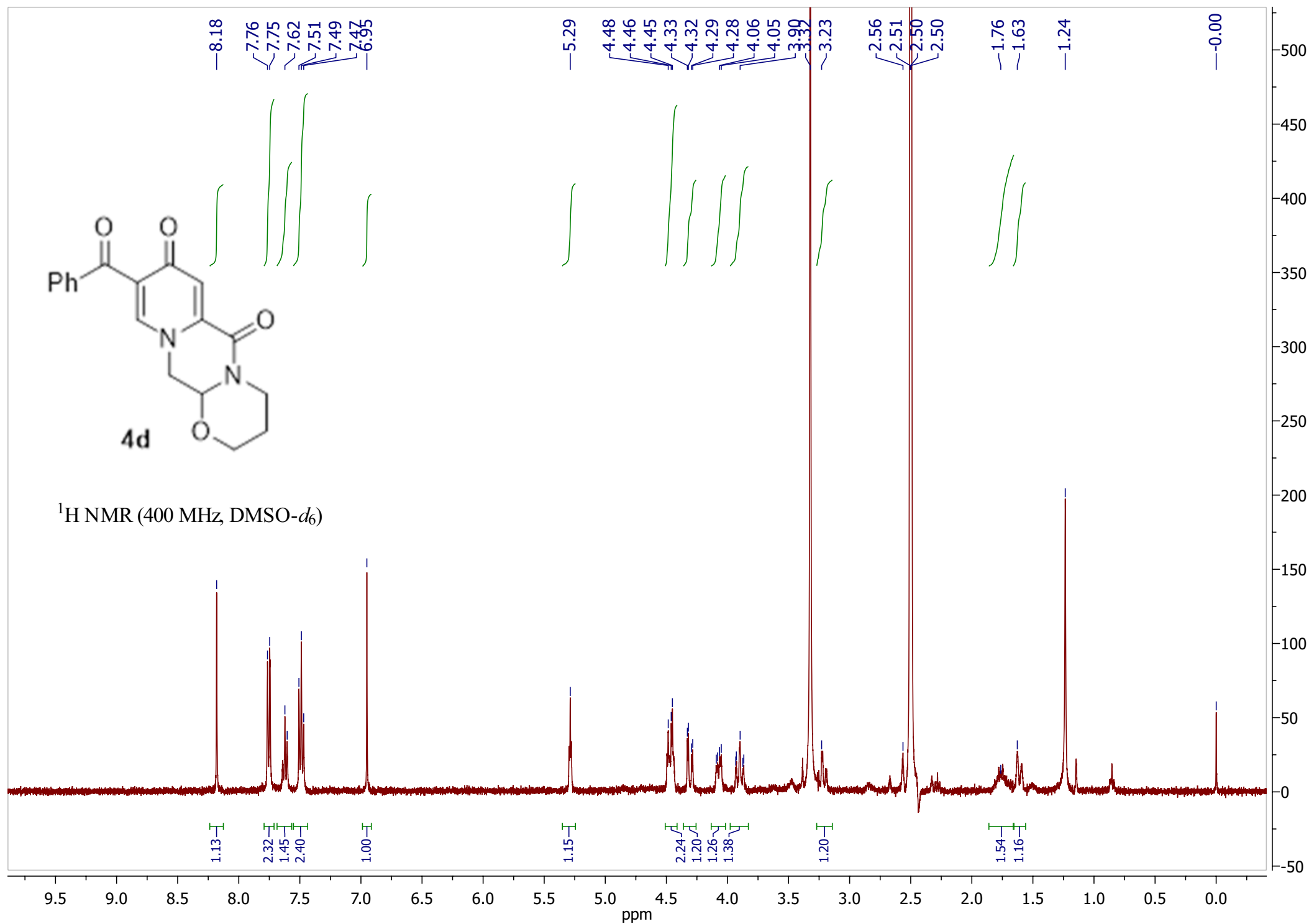


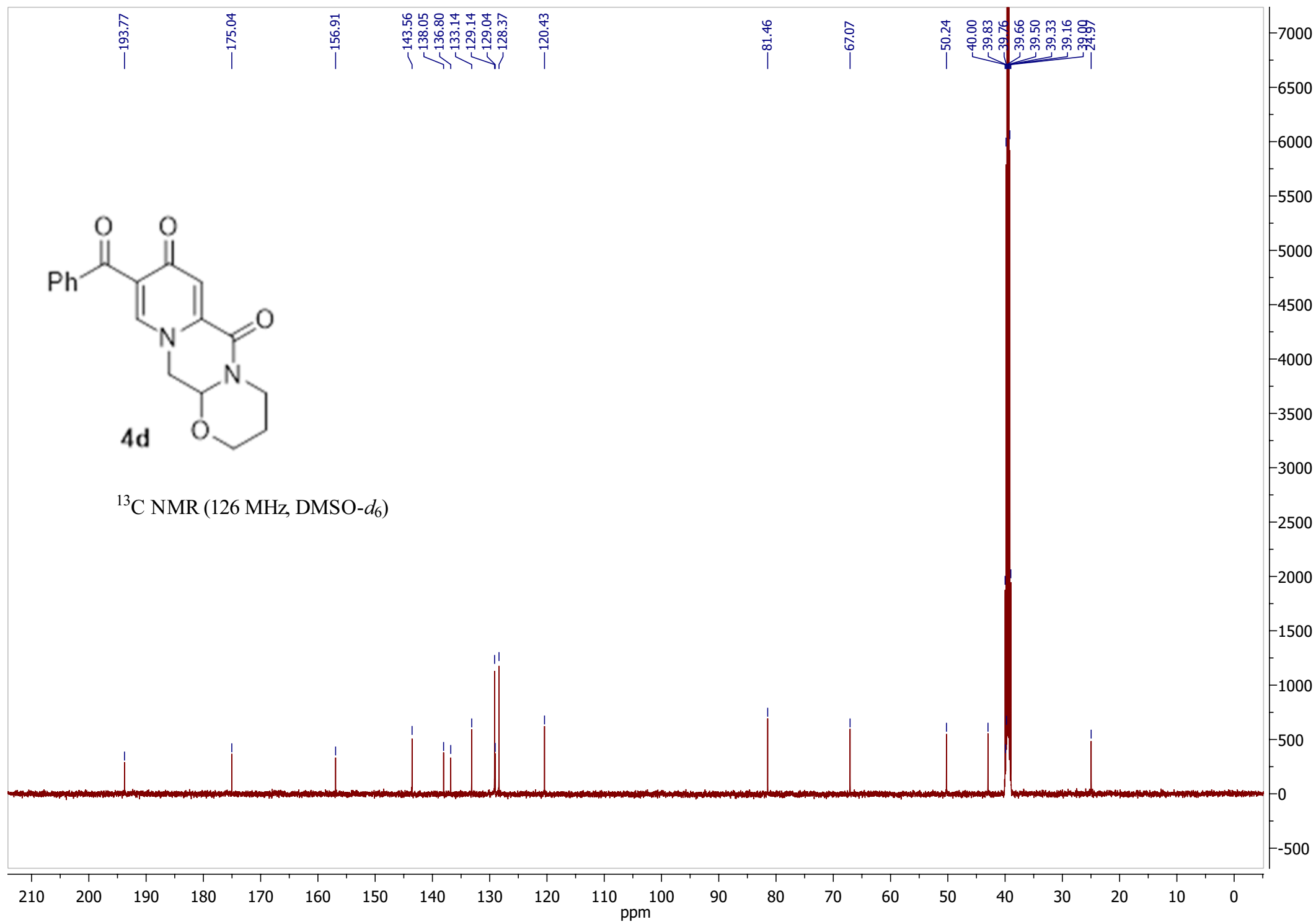


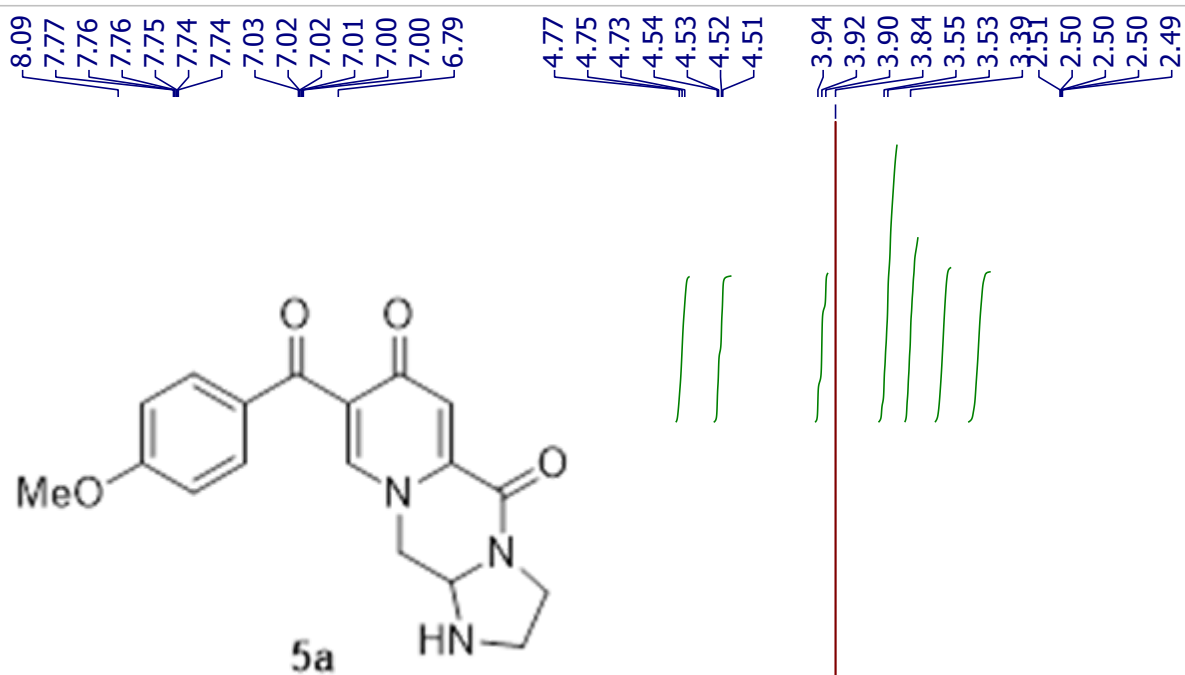




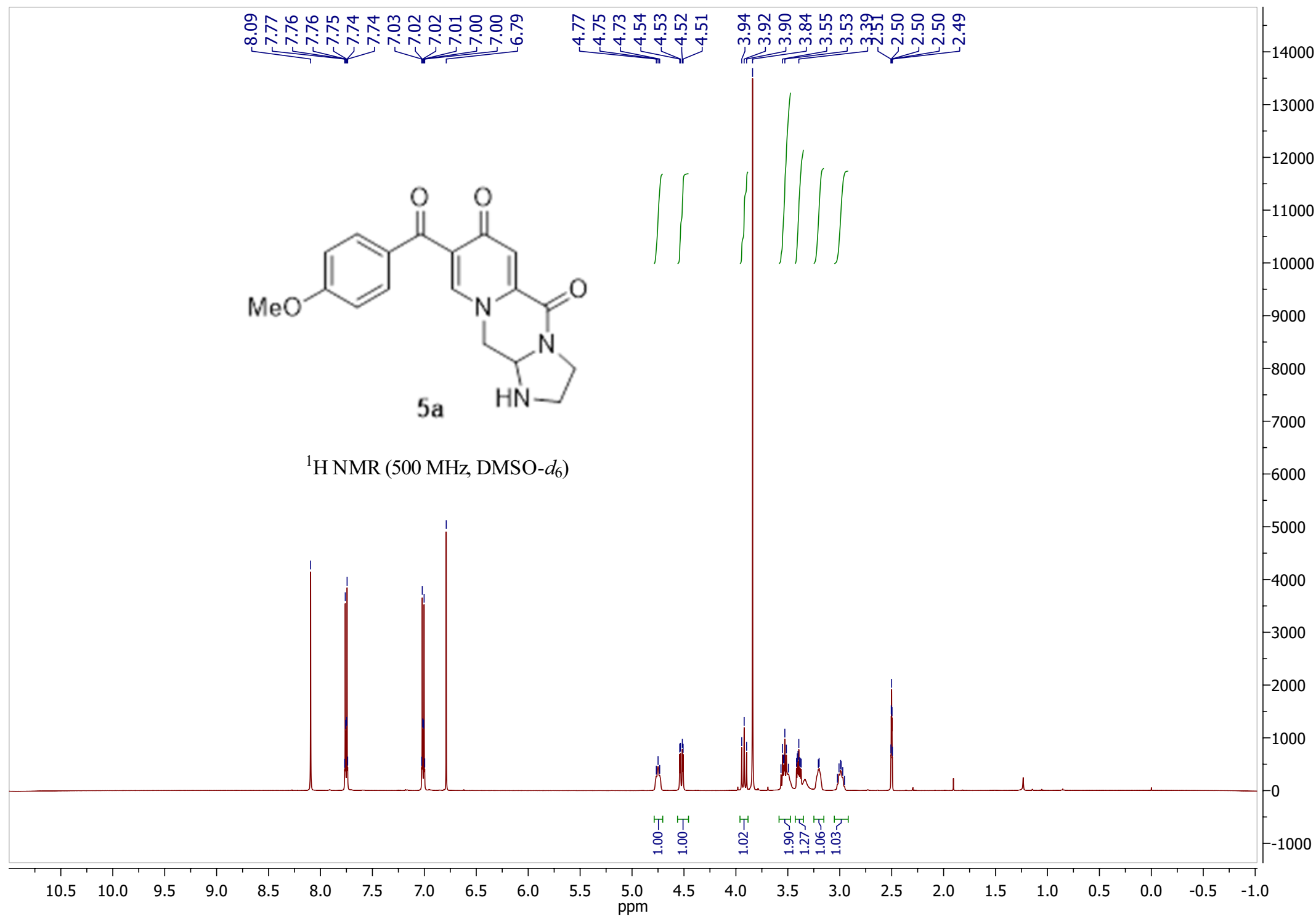


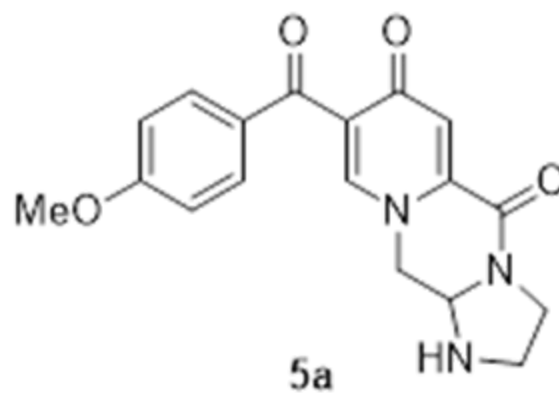




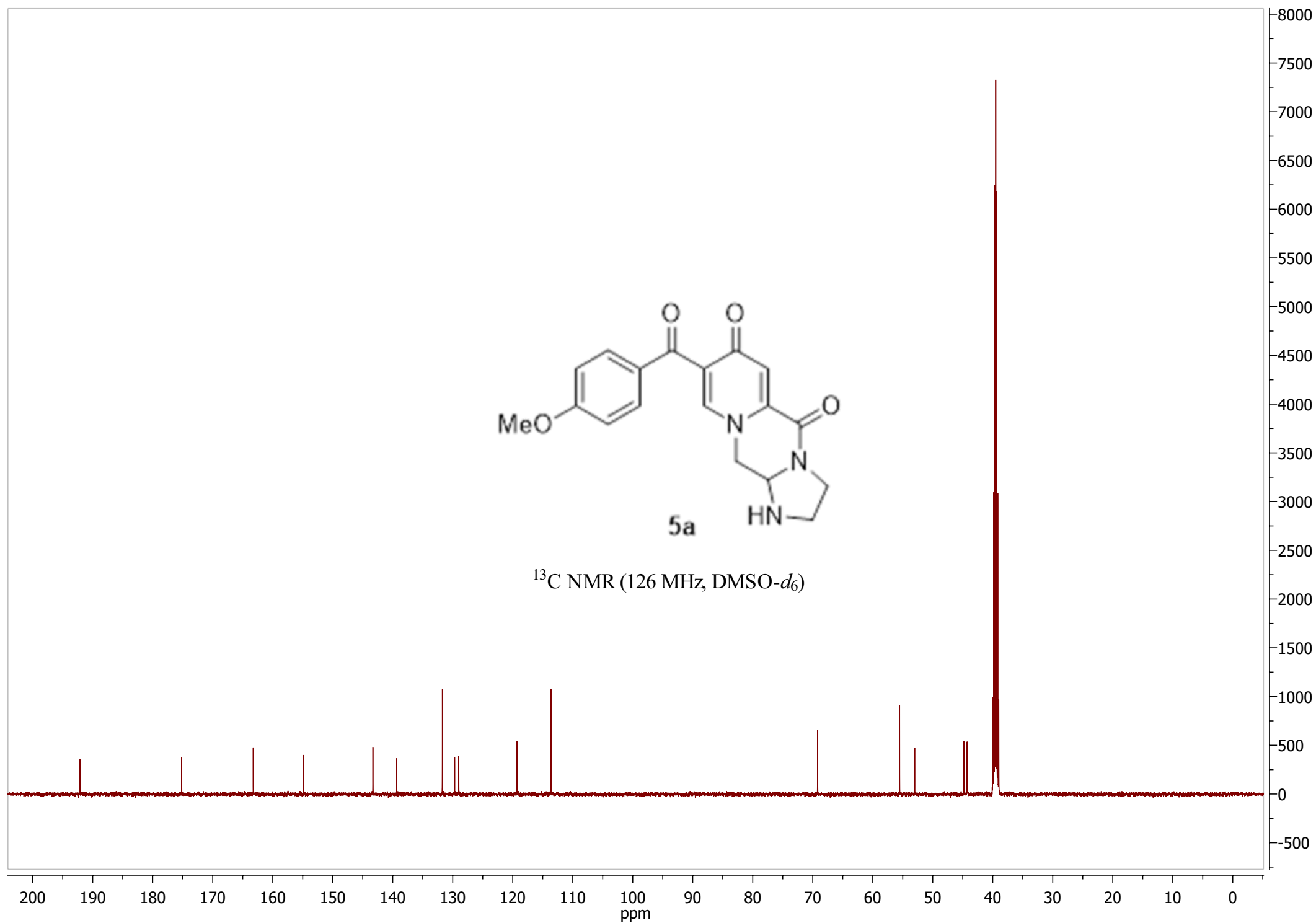


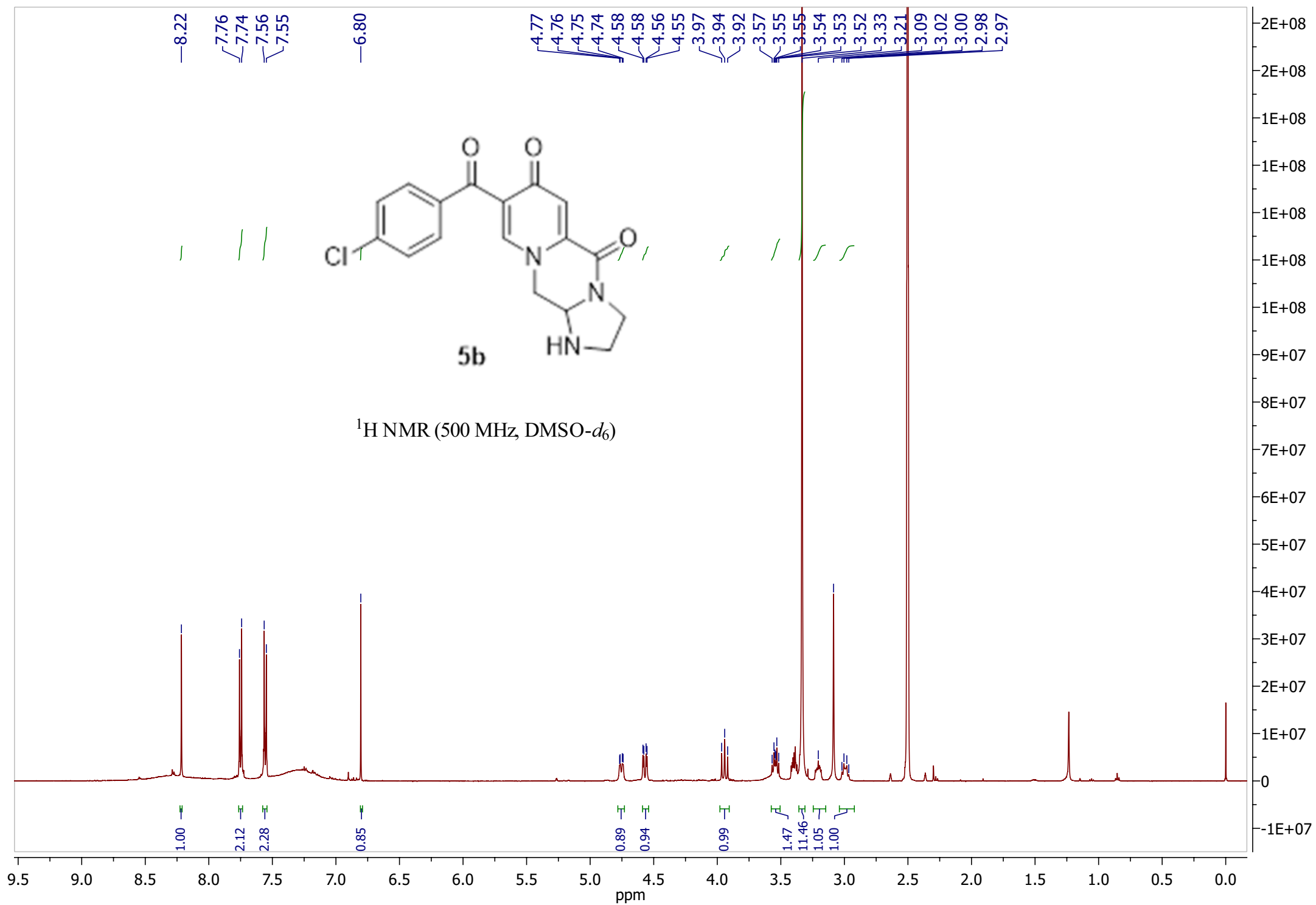
$^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ )

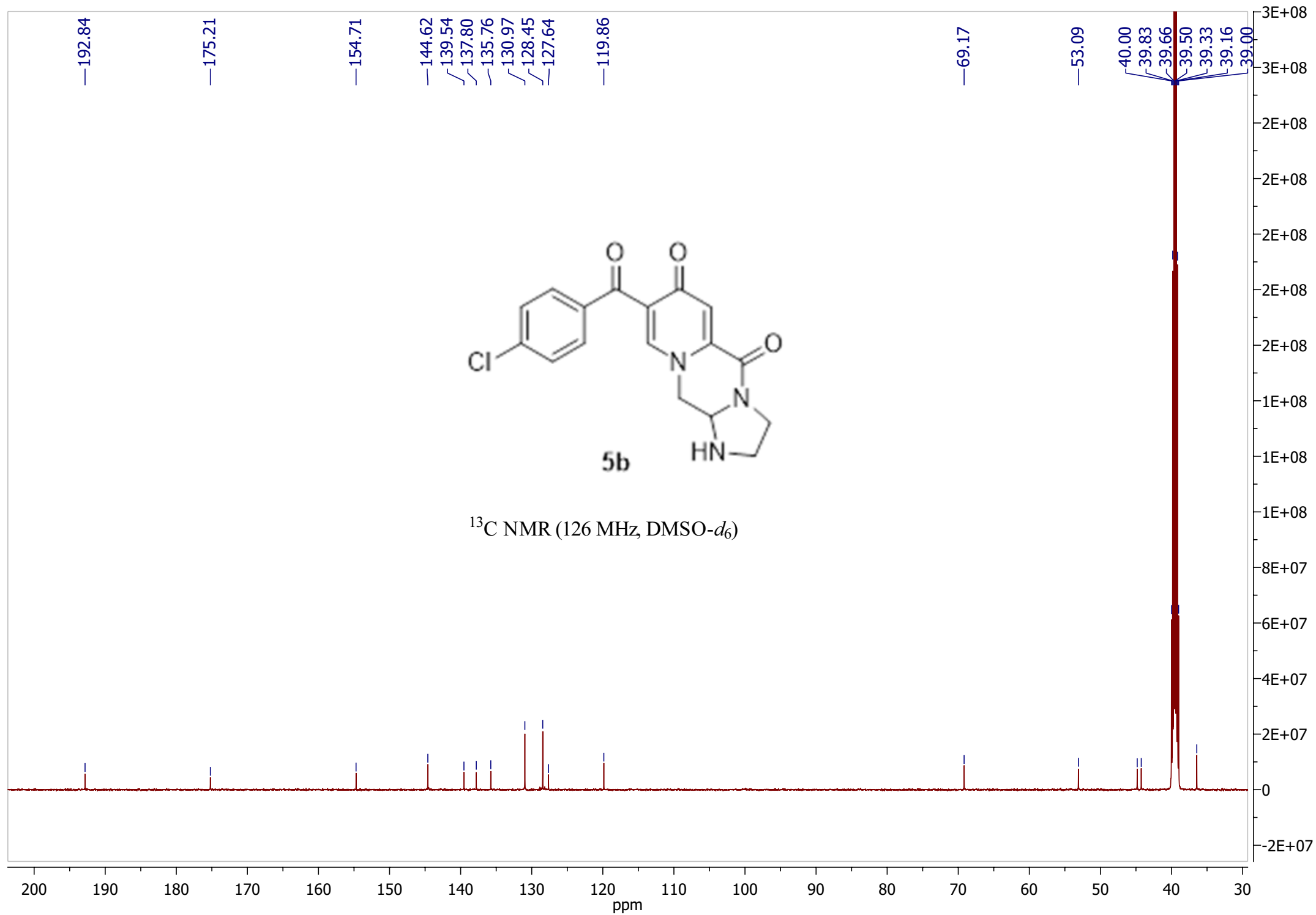




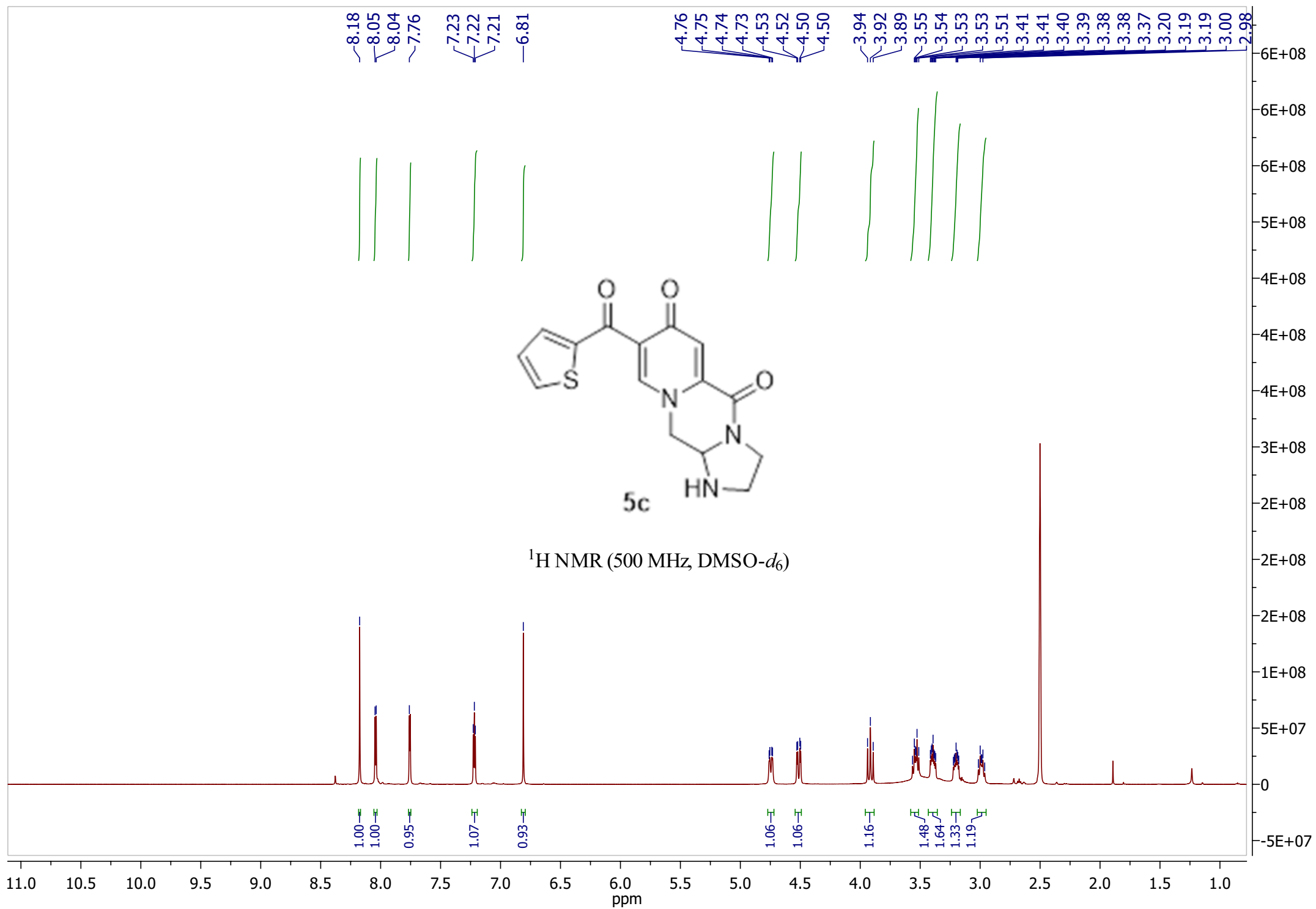
$^{13}\text{C}$  NMR (126 MHz, DMSO- $d_6$ )

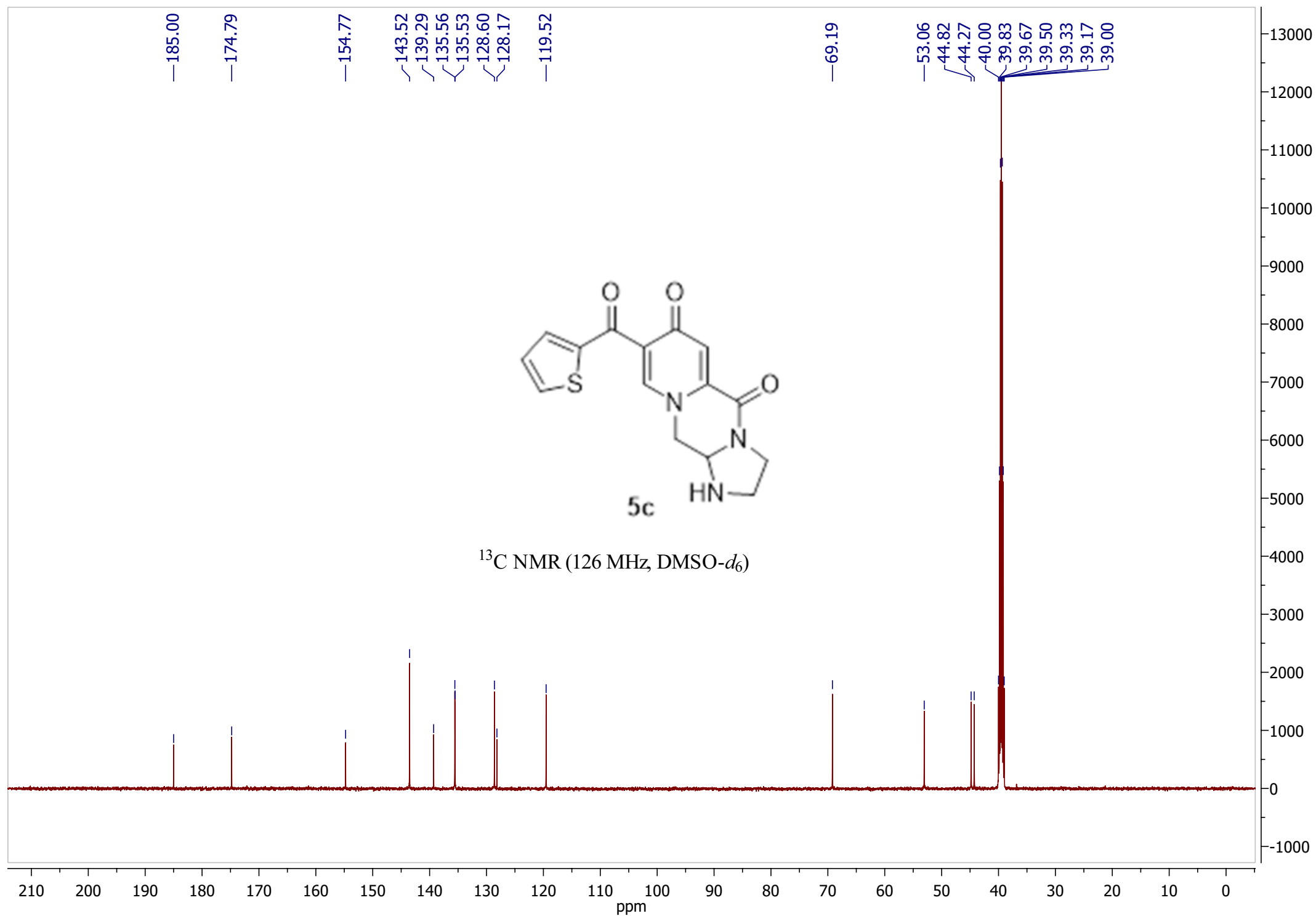


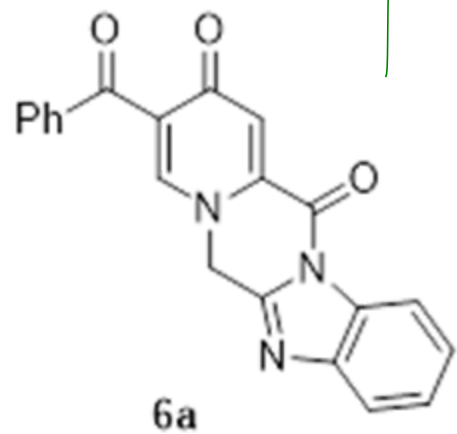




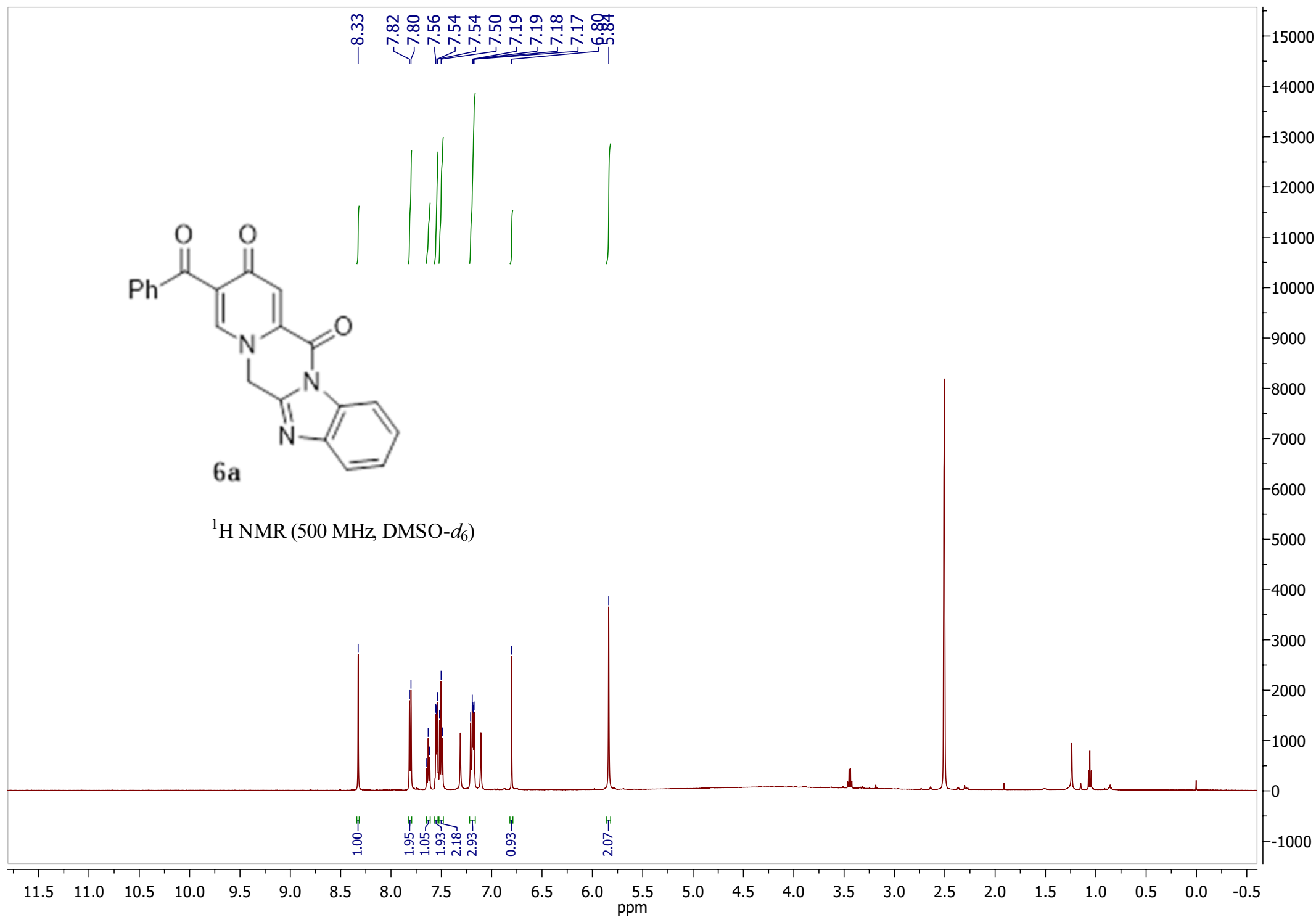


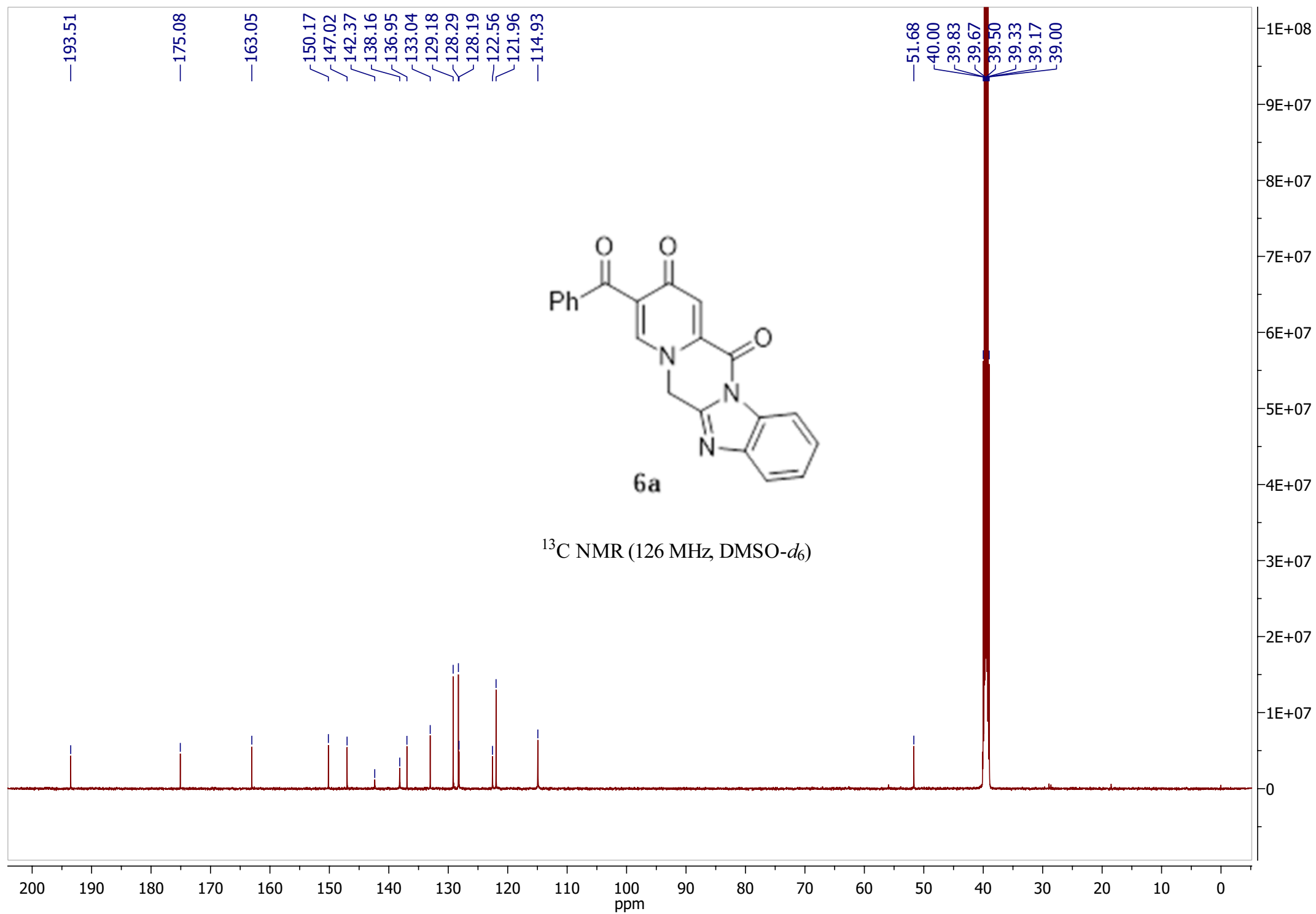


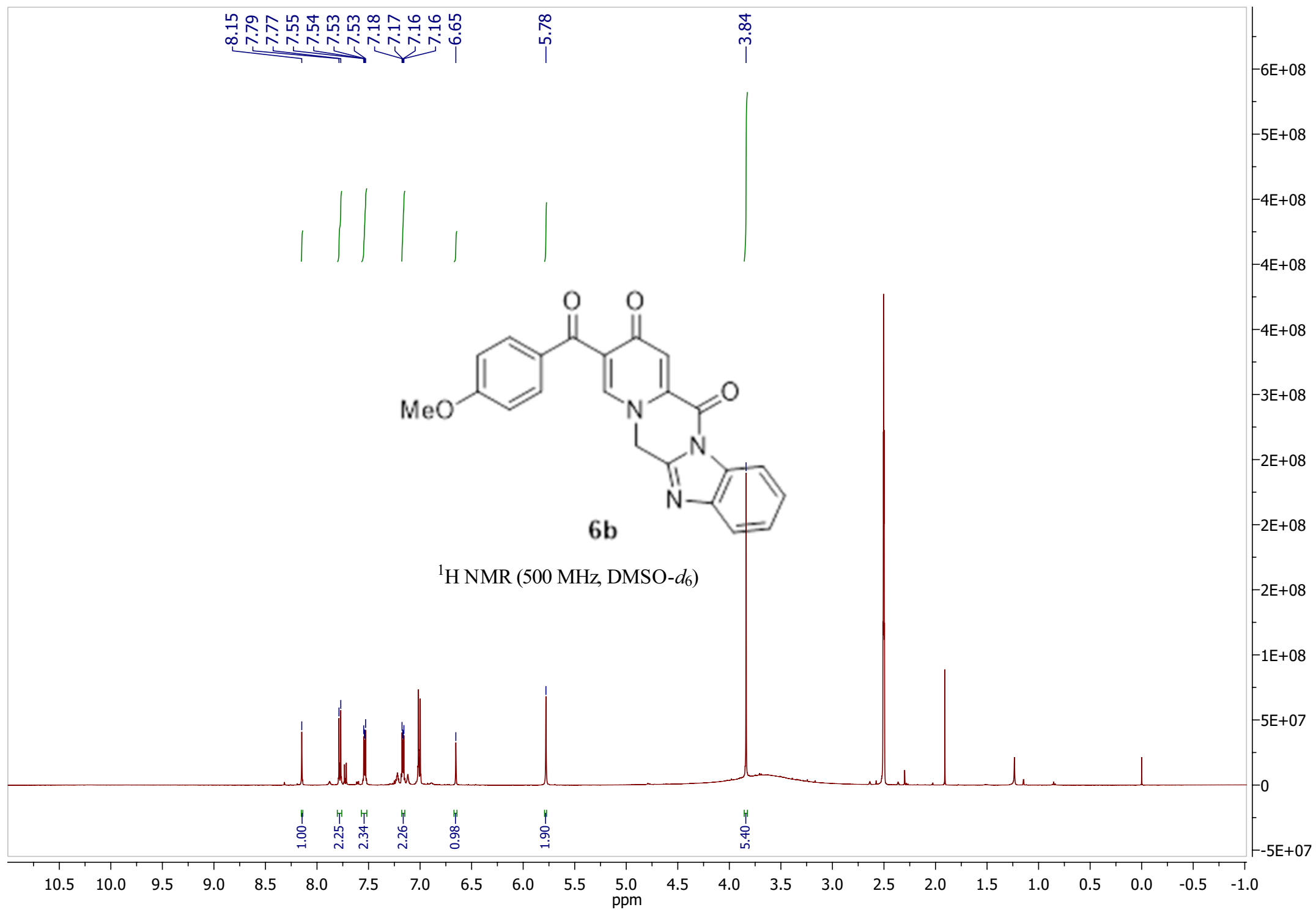


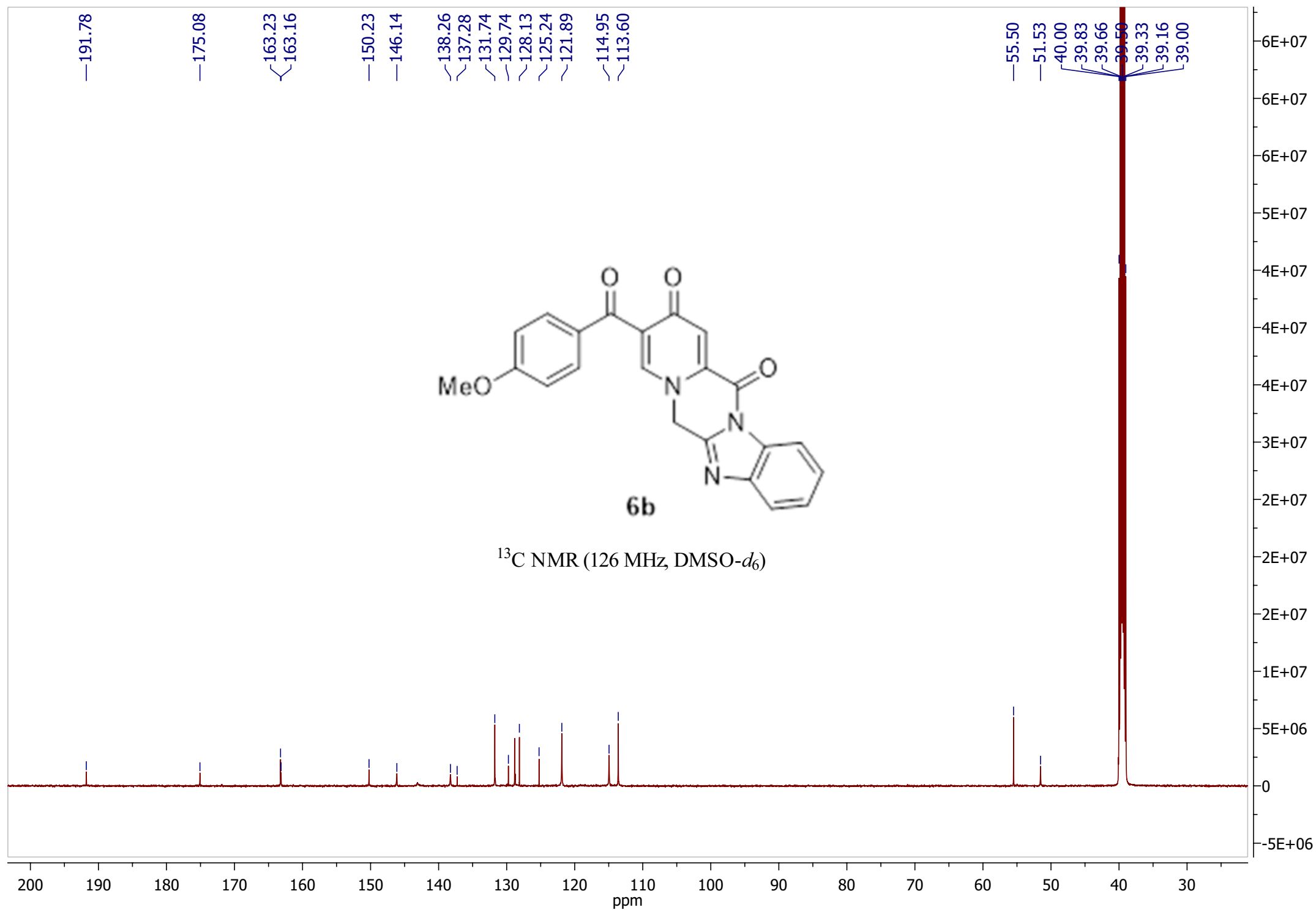


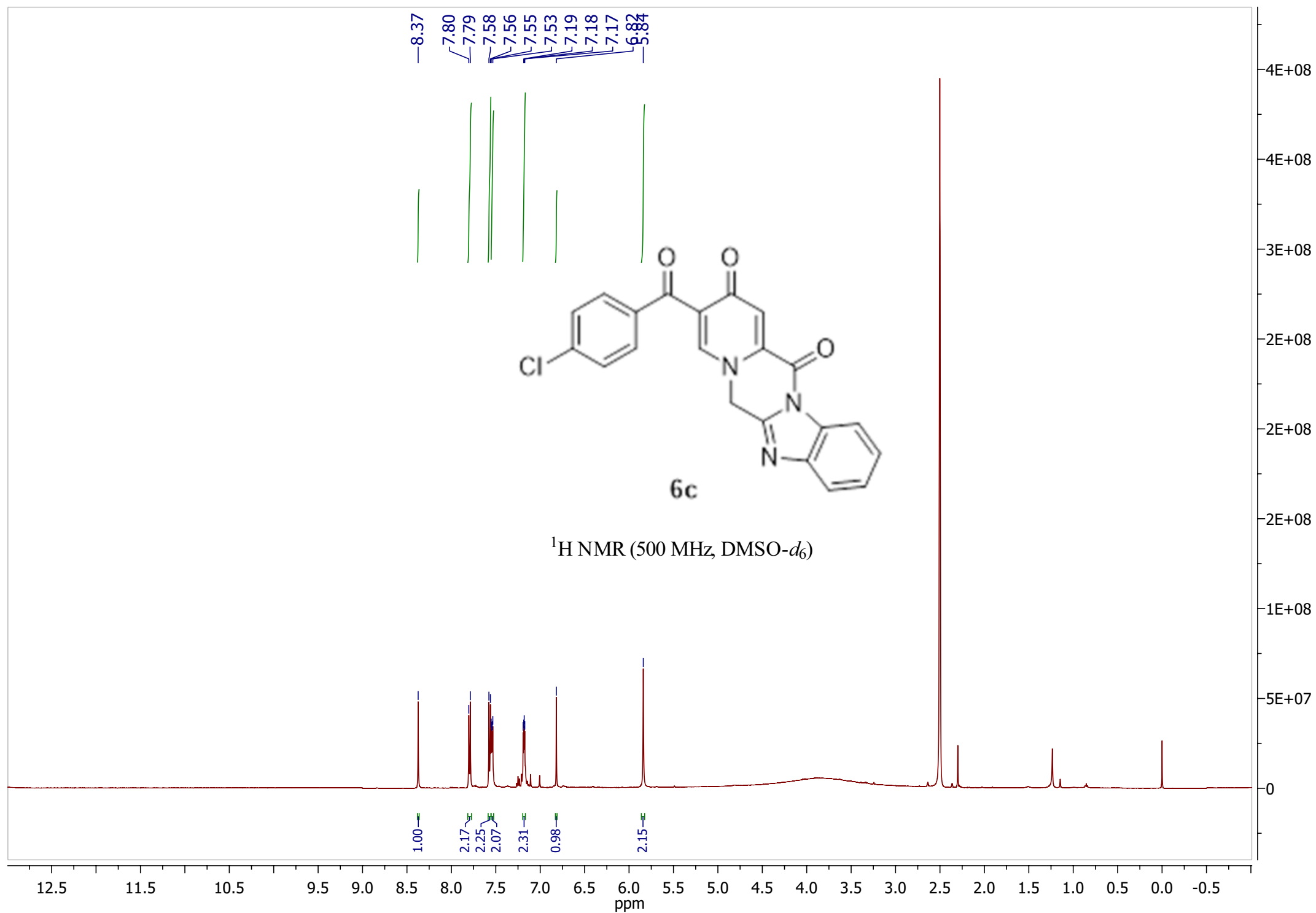
$^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ )

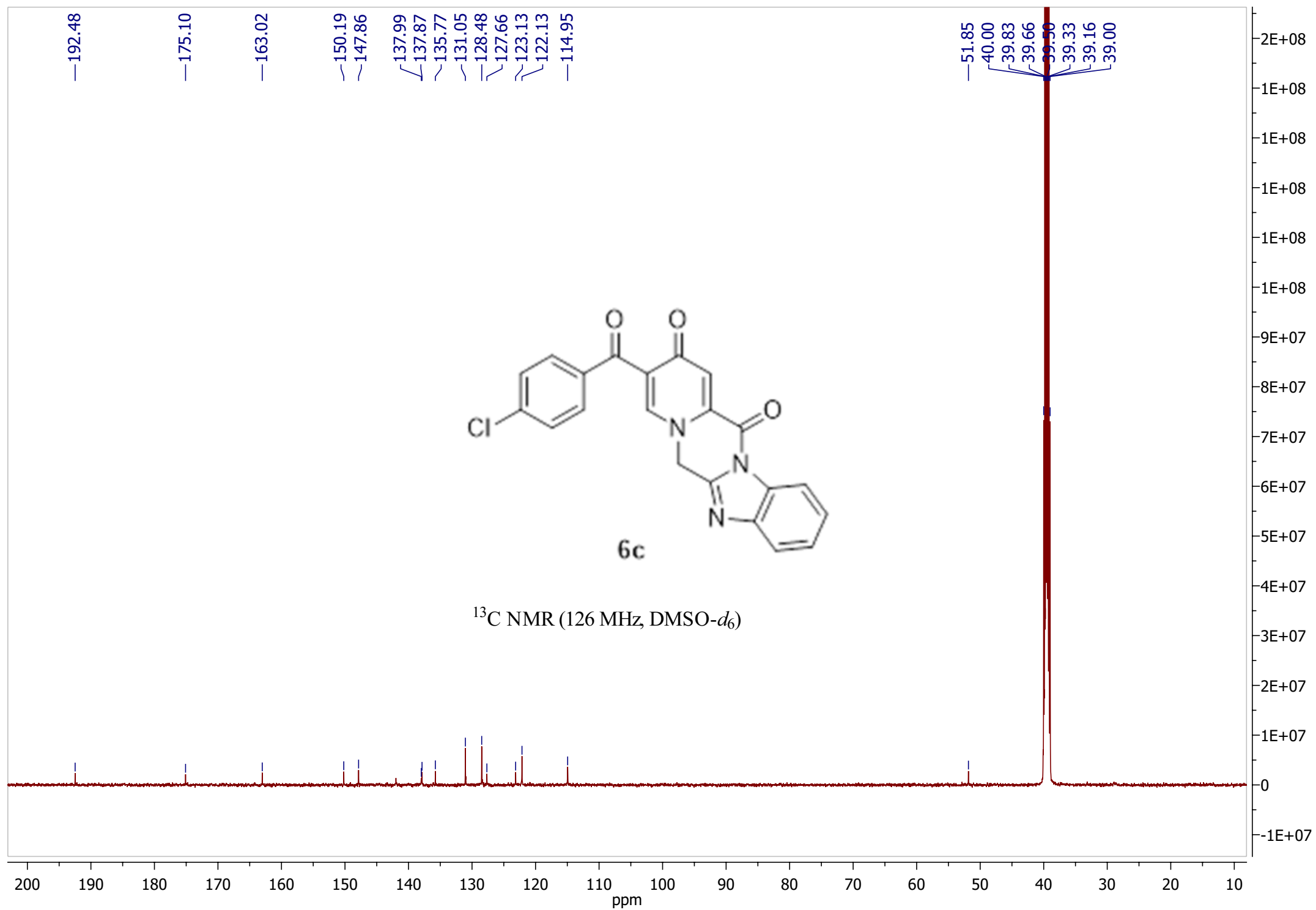




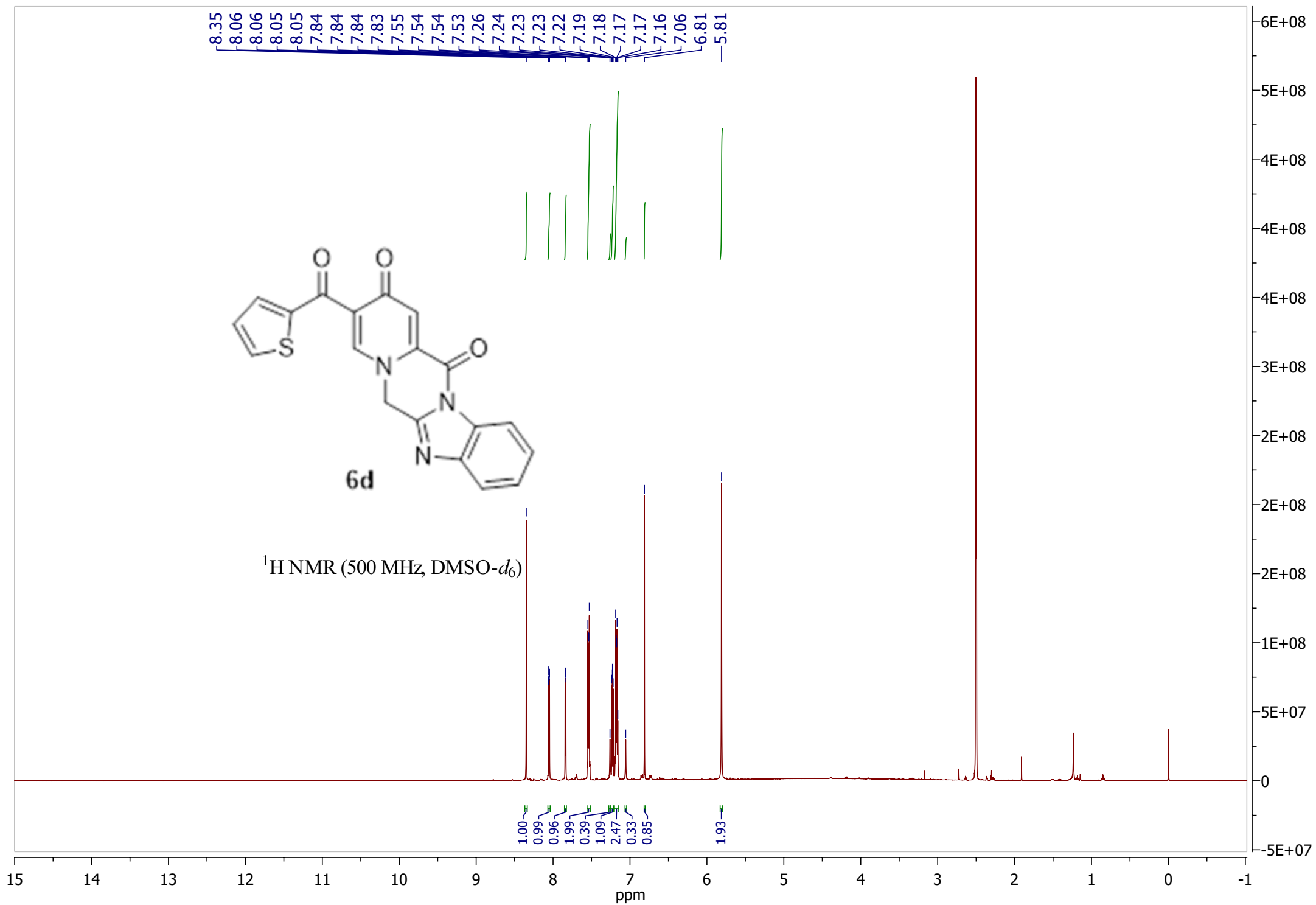


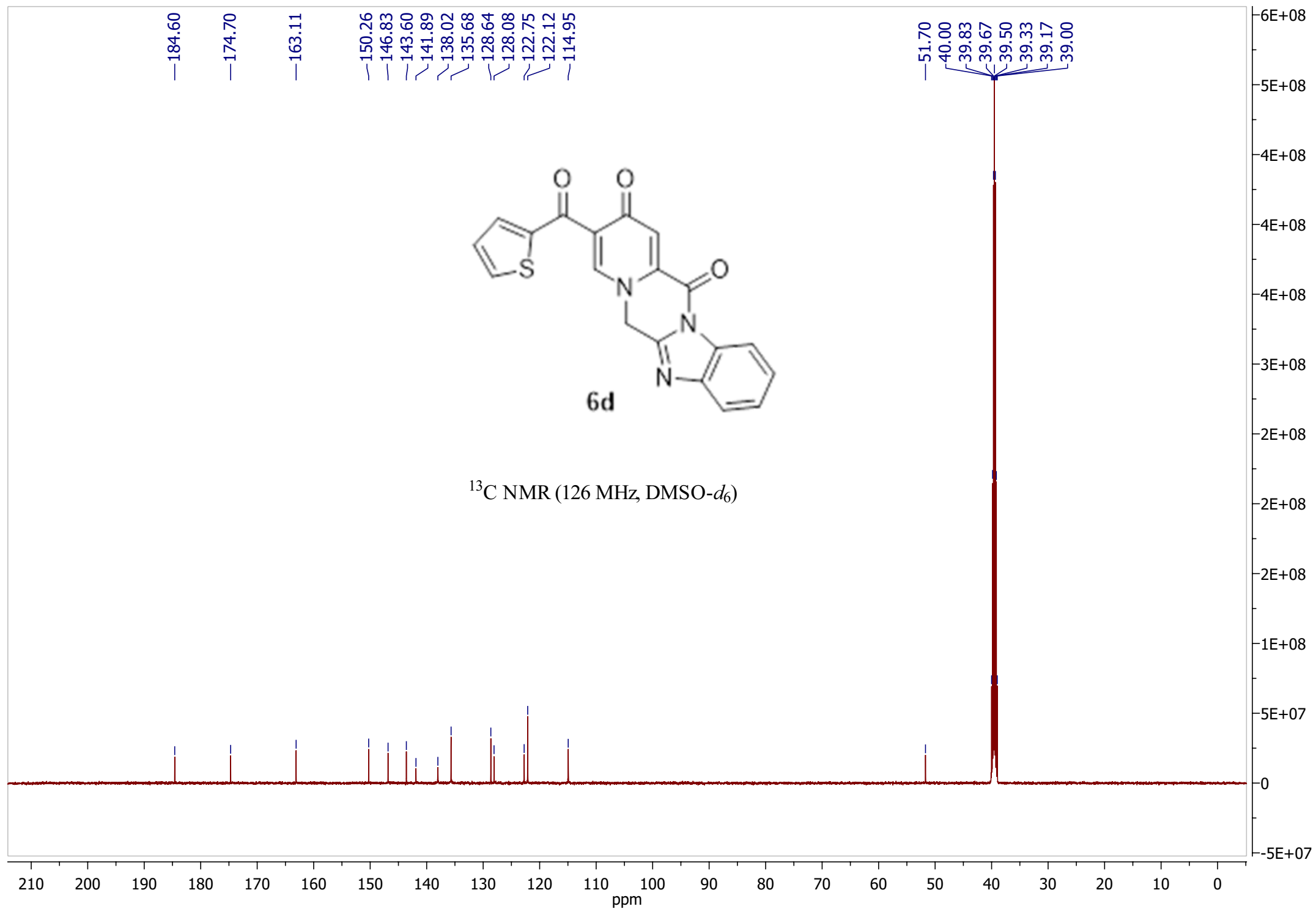


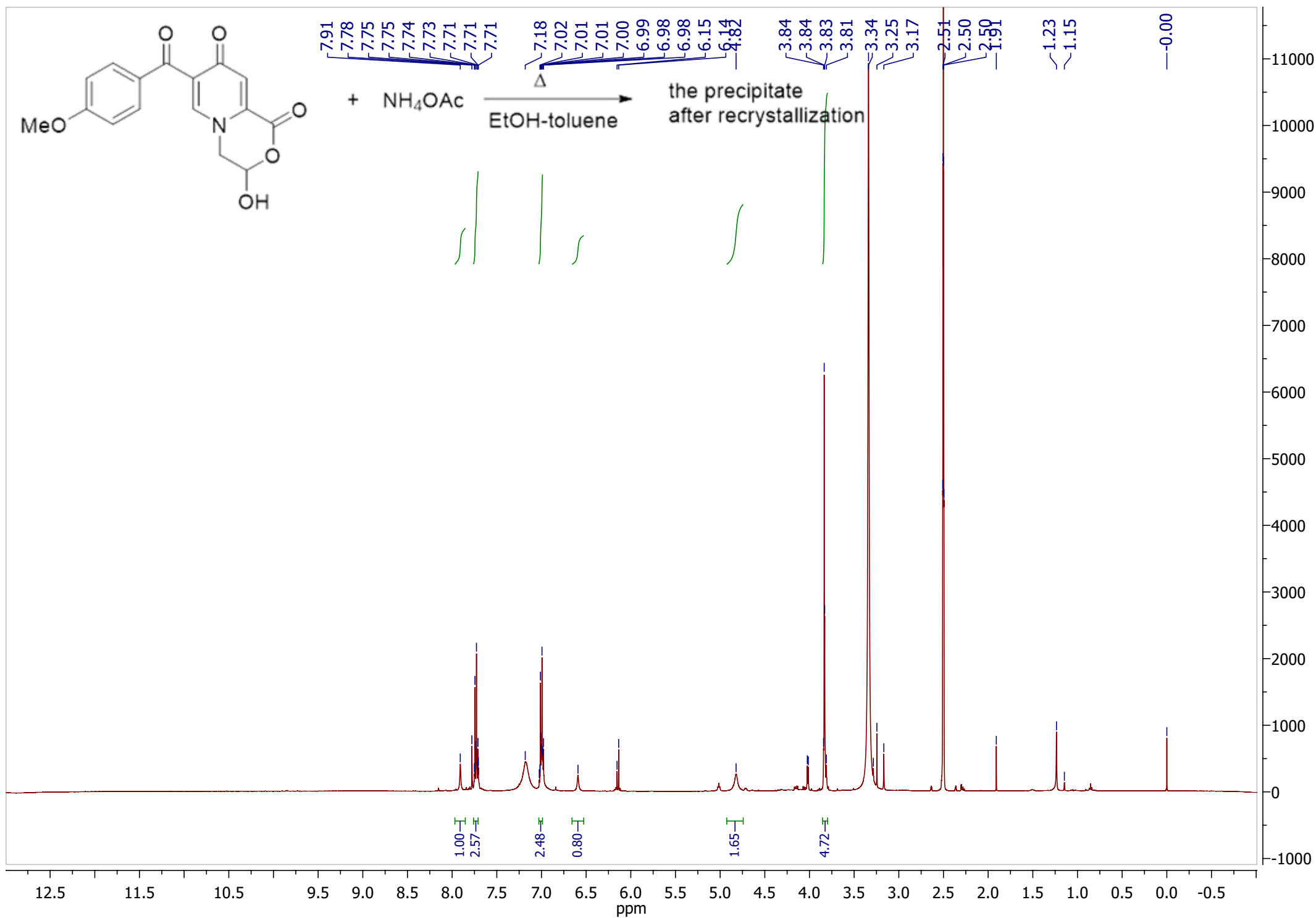












Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

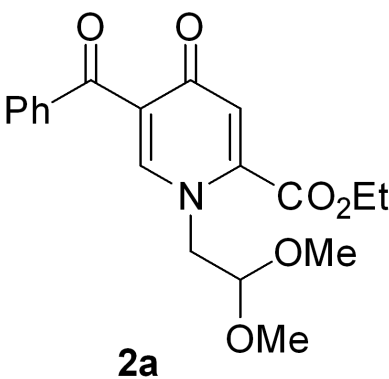
476 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

Elements Used:

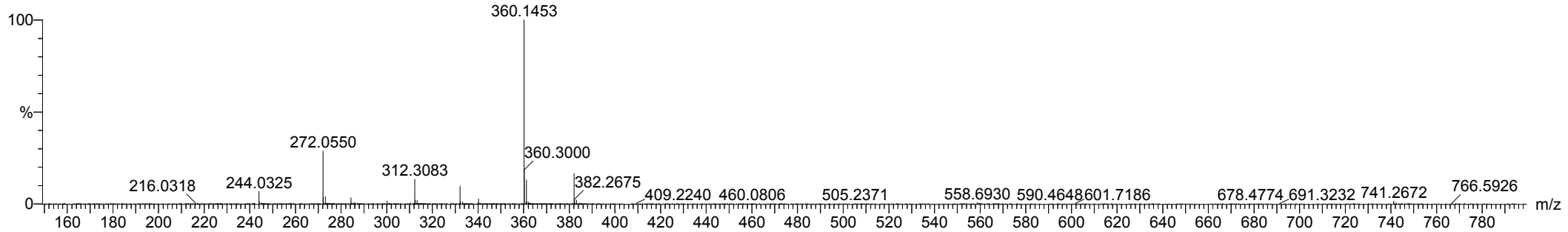
C: 1-500 H: 1-1000 N: 1-10 O: 1-200

OD 25.10.2022

HRMS-CB-273 29 (0.136)



25-Oct-2022 12:42:53  
TOF MS ES+  
1.10e+004



Minimum: -1.5  
Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula			
360.1453	360.1447	0.6	1.7	9.5	94.1	0.6	C19	H22	N	O6
	360.1461	-0.8	-2.2	14.5	94.2	0.7	C20	H18	N5	O2

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

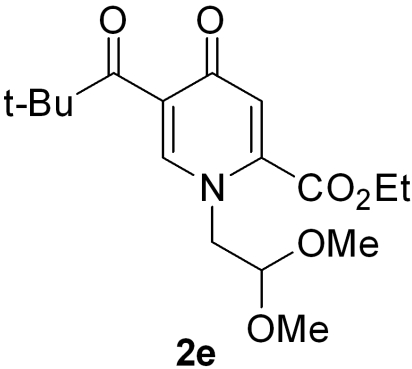
Element prediction: Off

Number of isotope peaks used for i-FIT = 3

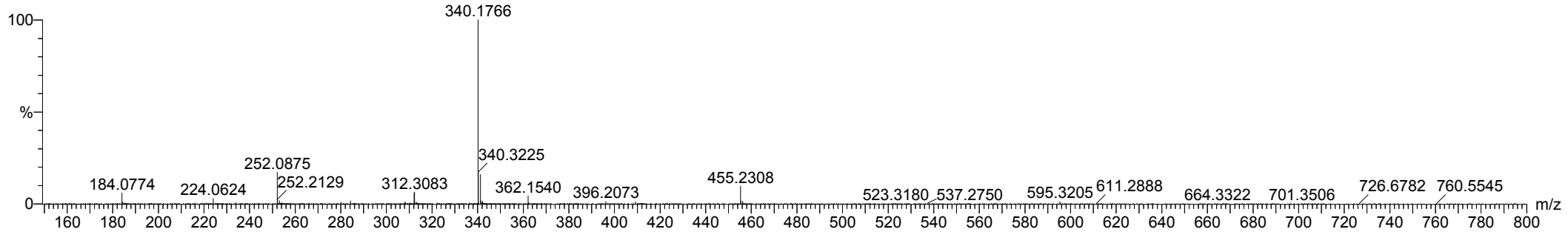
Monoisotopic Mass, Even Electron Ions  
421 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

Elements Used:  
C: 1-500 H: 1-1000 N: 1-10 O: 1-200

OD 25.10.2022  
HRMS-CB-274 29 (0.136)



25-Oct-2022 12:47:40  
TOF MS ES+  
1.17e+004



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula	
340.1766	340.1760	0.6	1.8	5.5	92.5	0.5	C17	H26 N O6
	340.1774	-0.8	-2.4	10.5	92.8	0.9	C18	H22 N5 O2

## Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

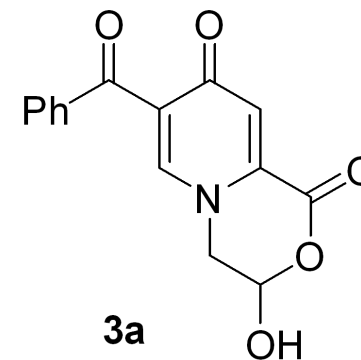
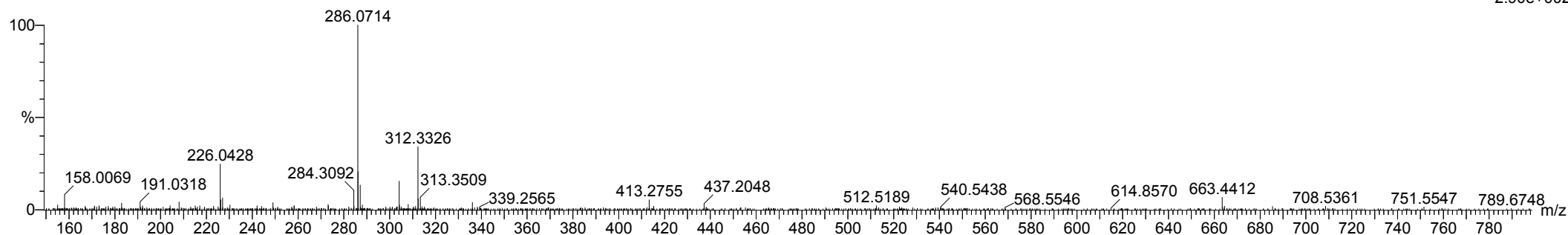
297 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 1-500 H: 1-1000 N: 1-10 O: 1-200

OD 28.07.2022

HRMS-CB-262 39 (0.177)

28-Jul-2022 11:55:27  
TOF MS ES+  
2.90e+002

Minimum: -1.5  
Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
286.0714	286.0715	-0.1	-0.3	10.5	32.4	0.0	C15 H12 N O5

## Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

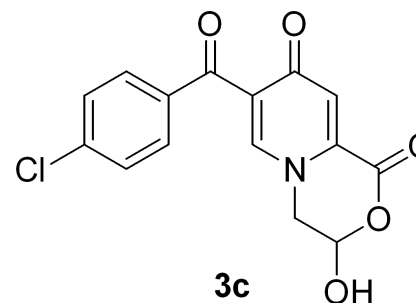
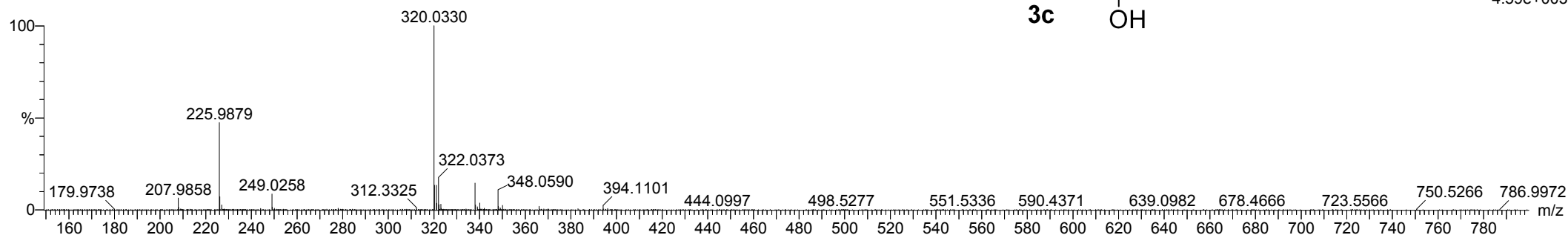
296 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 1-500 H: 1-1000 N: 1-10 O: 1-200 Cl: 1-1

OD 25.10.2022

HRMS-CB-282 24 (0.115)

25-Oct-2022 13:08:07  
TOF MS ES+  
4.59e+003

Minimum: -1.5  
Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
320.0330	320.0326	0.4	1.2	10.5	67.1	0.7	C15 H11 N O5 Cl
	320.0339	-0.9	-2.8	15.5	67.0	0.7	C16 H7 N5 O Cl

## Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

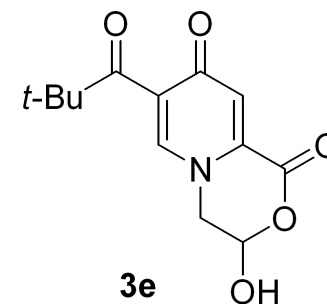
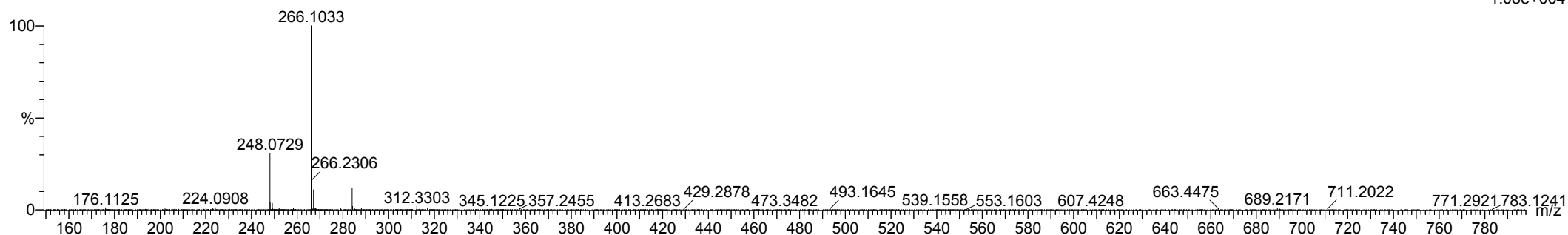
248 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 1-500 H: 1-1000 N: 1-10 O: 1-200

OD 28.07.2022

HRMS-CB-261 26 (0.123)

28-Jul-2022 11:53:00  
TOF MS ES+  
1.08e+004

Minimum: -1.5  
Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
266.1033	266.1028	0.5	1.9	6.5	101.3	0.5	C13 H16 N O5
	266.1042	-0.9	-3.4	11.5	101.7	0.9	C14 H12 N5 O



Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

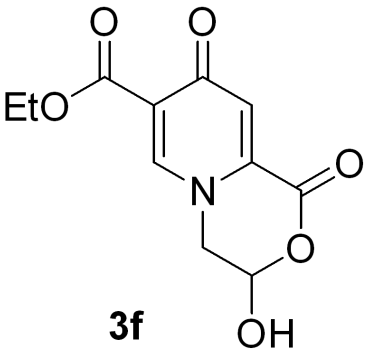
229 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

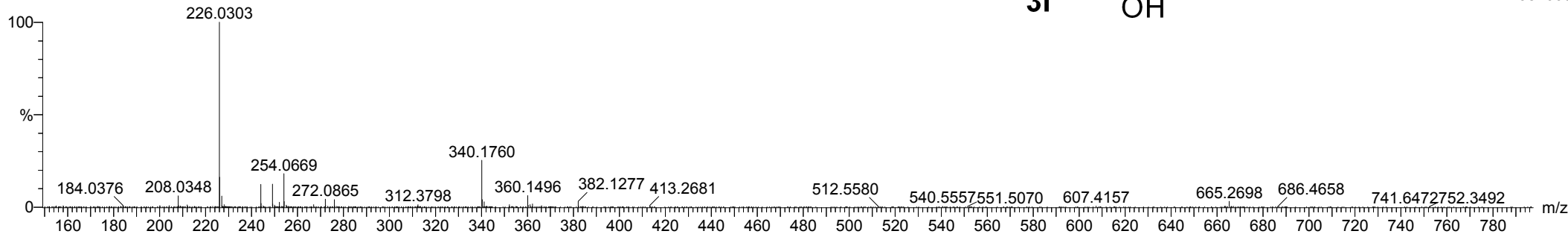
C: 1-500 H: 1-1000 N: 1-10 O: 1-200

OD 11.07.2022

HRMS-CB-242 49 (0.219)



11-Jul-2022 14:57:25  
TOF MS ES+  
1.13e+003



Minimum: -1.5  
Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
254.0669	254.0665	0.4	1.6	6.5	31.7	0.3	C11 H12 N O6
	254.0678	-0.9	-3.5	11.5	32.7	1.3	C12 H8 N5 O2

# Elemental Composition Report

Page 1

## Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

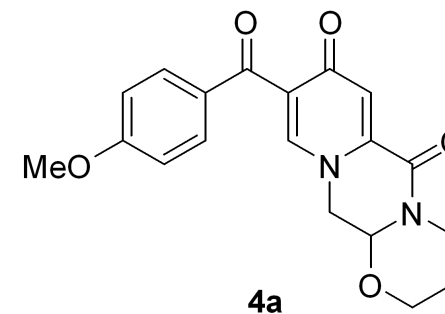
476 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

Elements Used:

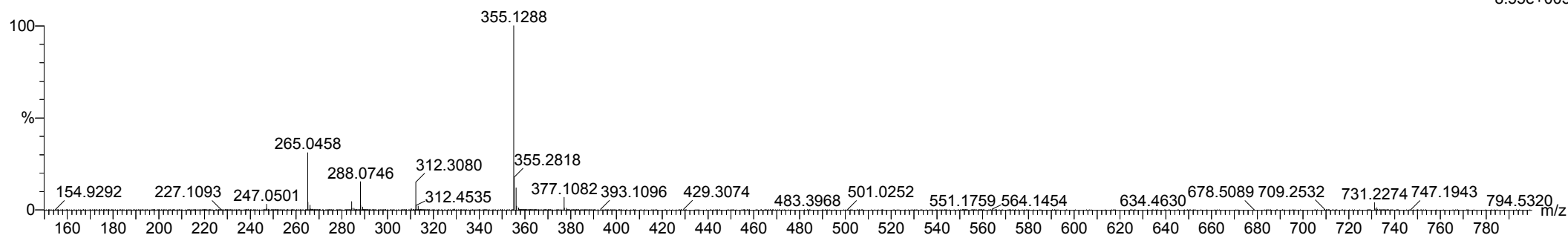
C: 1-500 H: 1-1000 N: 1-10 O: 1-200

OD 25.10.2022

HRMS-CB-276 27 (0.128)



25-Oct-2022 12:52:17  
TOF MS ES+  
8.55e+003



Minimum: -1.5  
Maximum: 5.0 5.0 50.0

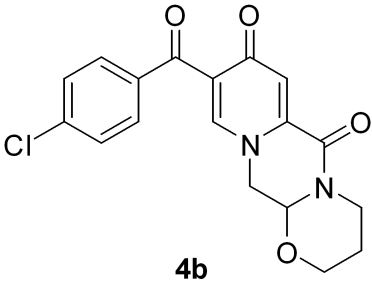
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
355.1288	355.1286	0.2	0.6	-0.5	62.5	0.2	C3 H19 N10 O10
	355.1294	-0.6	-1.7	11.5	63.9	1.6	C19 H19 N2 O5

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3



Monoisotopic Mass, Even Electron Ions

370 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 1-500 H: 1-1000 N: 1-10 O: 1-200 Cl: 1-1

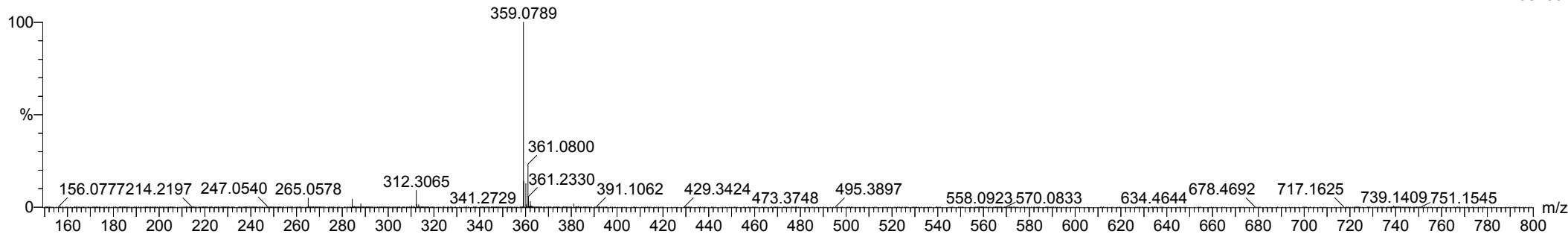
OD 25.10.2022

HRMS-CB-278 20 (0.098)

25-Oct-2022 12:56:53

TOF MS ES+

1.75e+004



Minimum: -1.5  
Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
359.0789	359.0790	-0.1	-0.3	-0.5	106.4	2.3	C2 H16 N10 O9 Cl
	359.0799	-1.0	-2.8	11.5	104.9	0.8	C18 H16 N2 O4 Cl
	359.0772	1.7	4.7	12.5	104.9	0.8	C14 H12 N8 O2 Cl

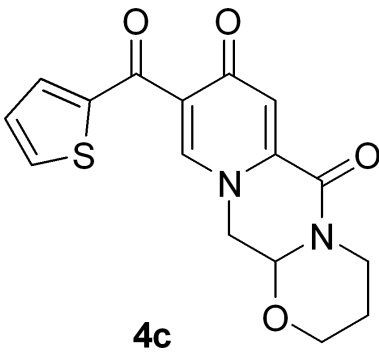
Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

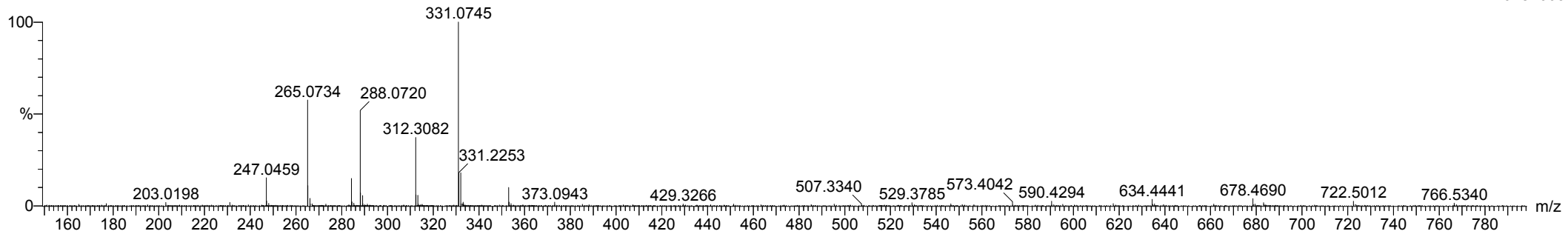
Element prediction: Off

Number of isotope peaks used for i-FIT = 3



Monoisotopic Mass, Even Electron Ions  
336 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)  
Elements Used:  
C: 1-500 H: 1-1000 N: 1-10 O: 1-200 S: 1-1  
OD 25.10.2022  
HRMS-CB-280 22 (0.107)

25-Oct-2022 13:03:30  
TOF MS ES+  
4.07e+003



Minimum: -1.5  
Maximum: 50.0

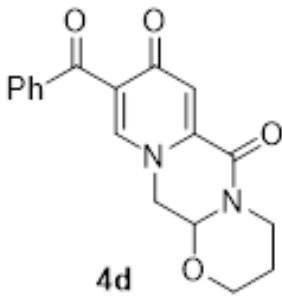
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
331.0745	331.0753	-0.8	-2.4	10.5	69.0	0.0	C16 H15 N2 O4 S

Single Mass Analysis

Tolerance = 15.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3



Monoisotopic Mass, Even Electron Ions

145 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 1-500 H: 1-1000 N: 1-3 O: 1-200

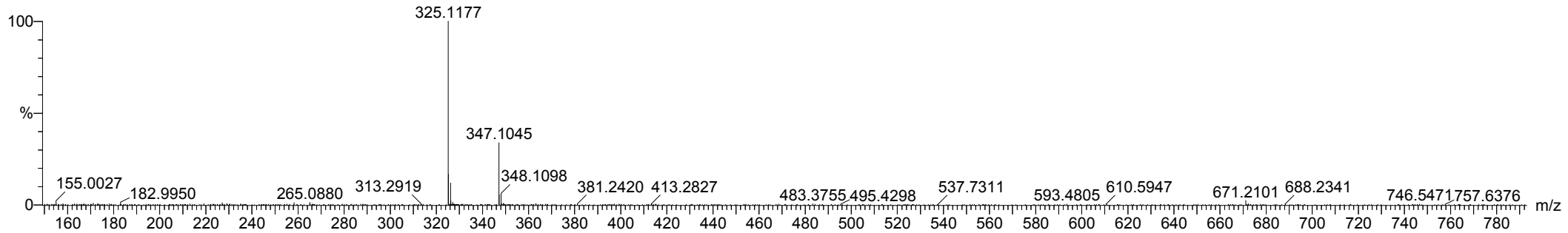
OD 26.12.2022

CB-305 53 (0.236)

26-Dec-2022 17:15:36

TOF MS ES+

8.16e+002



Minimum: -1.5  
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
325.1177	325.1188	-1.1	-3.4	11.5	50.6	0.0	C18 H17 N2 O4

## Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

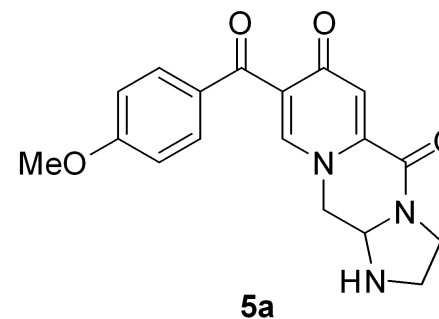
421 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 1-500 H: 1-1000 N: 1-10 O: 1-200

OD 25.10.2022

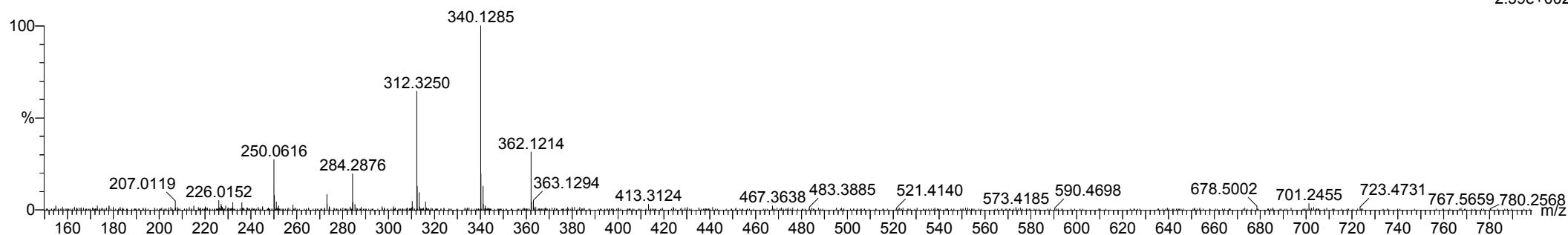
HRMS-CB-279 31 (0.144)



25-Oct-2022 13:01:11

TOF MS ES+

2.39e+002



Minimum: -1.5  
Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula			
340.1285	340.1297	-1.2	-3.5	11.5	31.4	0.6	C18	H18	N3	O4
	340.1270	1.5	4.4	12.5	31.6	0.8	C14	H14	N9	O2

## Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

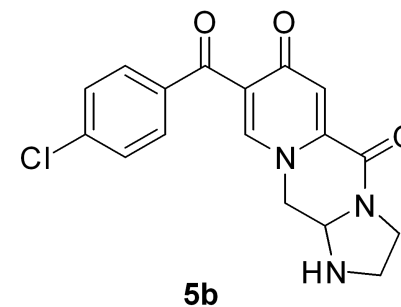
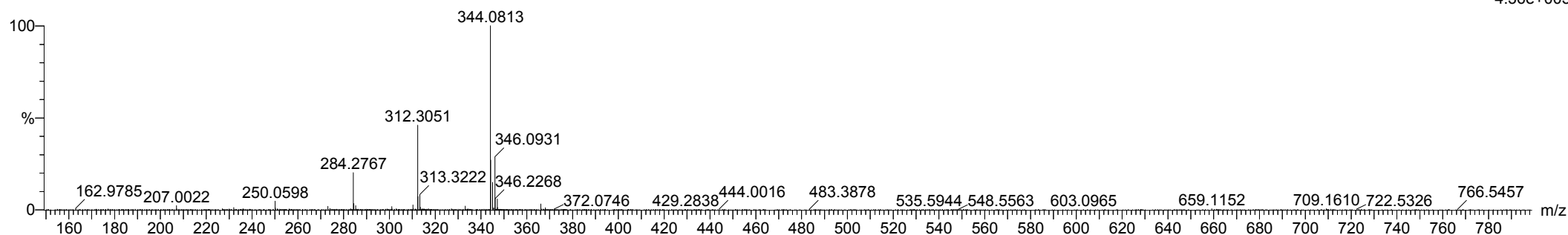
344 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 1-500 H: 1-1000 N: 1-10 O: 1-200 Cl: 1-1

OD 25.10.2022

HRMS-CB-281 24 (0.115)

25-Oct-2022 13:05:50  
TOF MS ES+  
4.36e+003

Minimum: -1.5  
Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
344.0813	344.0820	-0.7	-2.0	-1.5	72.5	1.6	C5 H19 N5 O10 Cl
	344.0802	1.1	3.2	11.5	71.2	0.2	C17 H15 N3 O3 Cl

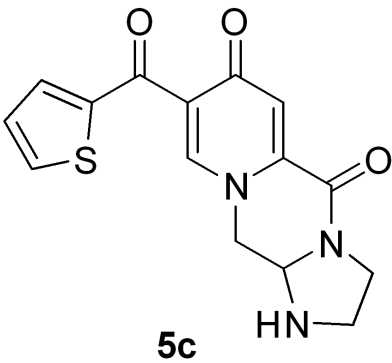
Single Mass Analysis

Tolerance = 15.0 PPM / DBE: min = -1.5, max = 50.0

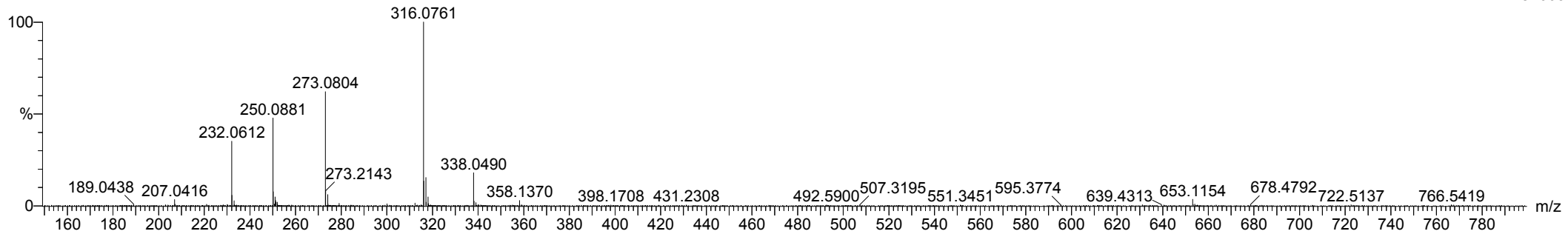
Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions  
113 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)  
Elements Used:  
C: 1-500 H: 1-1000 N: 1-3 O: 1-200 S: 1-1  
OD 27.12.2022  
CB-312 23 (0.111)



27-Dec-2022 13:32:08  
TOF MS ES+  
4.24e+003



Minimum: -1.5  
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
316.0761	316.0756	0.5	1.6	10.5	61.5	0.1	C15 H14 N3 O3 S
	316.0796	-3.5	-11.1	14.5	64.1	2.6	C20 H14 N O S



Single Mass Analysis

Tolerance = 15.0 PPM / DBE: min = -1.5, max = 50.0

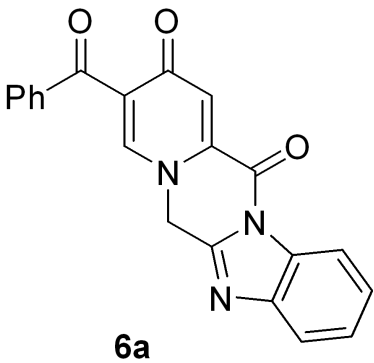
Element prediction: Off

Number of isotope peaks used for i-FIT = 3

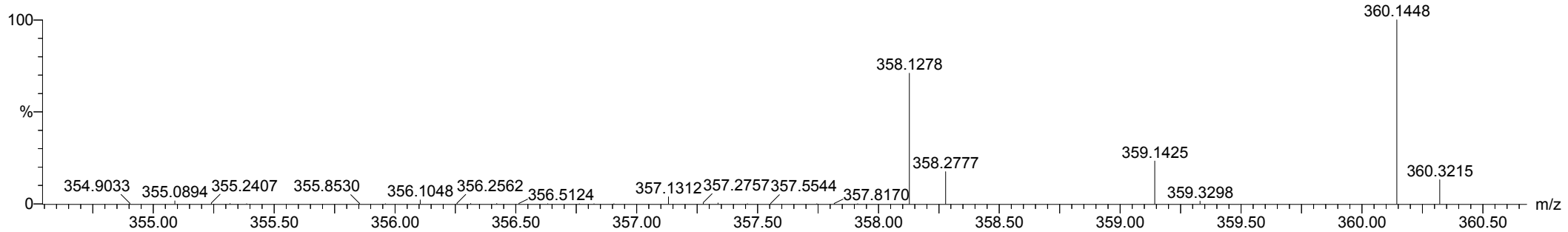
Monoisotopic Mass, Even Electron Ions  
168 formula(e) evaluated with 4 results within limits (up to 50 closest results for each mass)

Elements Used:  
C: 1-500 H: 1-1000 N: 1-3 O: 1-200

OD 27.12.2022  
CB-306\_2 22 (0.107)



27-Dec-2022 13:36:05  
TOF MS ES+  
2.80e+003



Minimum: -1.5  
Maximum: 5.0 15.0 50.0

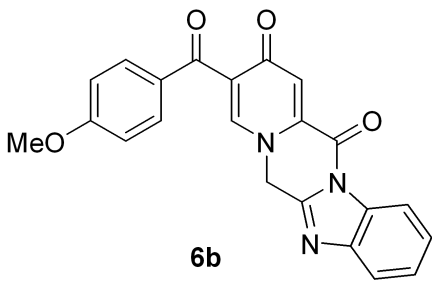
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
356.1048	356.1040	0.8	2.2	-1.5	73.4	2.0	C8 H22 N O14
	356.1035	1.3	3.7	16.5	73.1	1.8	C21 H14 N3 O3
	356.1075	-2.7	-7.6	20.5	72.4	1.0	C26 H14 N O
	356.1094	-4.6	-12.9	7.5	72.5	1.1	C14 H18 N3 O8

Single Mass Analysis

Tolerance = 15.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3



Monoisotopic Mass, Even Electron Ions  
194 formula(e) evaluated with 4 results within limits (up to 50 closest results for each mass)

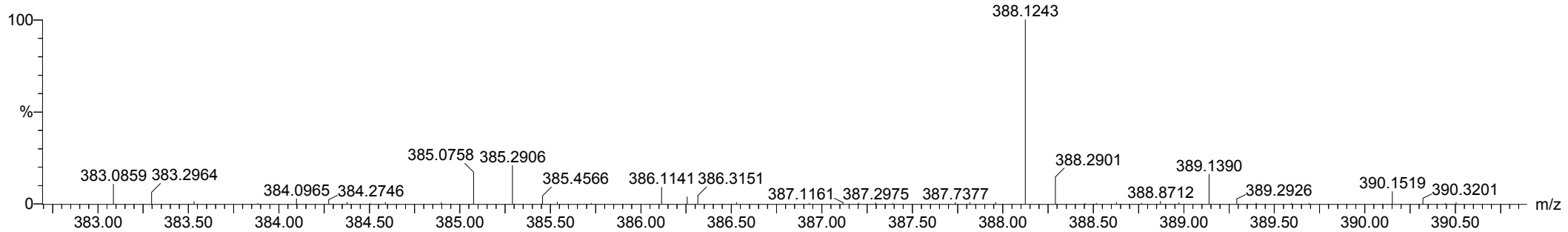
Elements Used:

C: 1-500 H: 1-1000 N: 1-3 O: 1-200

OD 27.12.2022

CB-309\_2 30 (0.140)

27-Dec-2022 13:54:26  
TOF MS ES+  
3.48e+002



Minimum: -1.5  
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
386.1141	386.1141	0.0	0.0	16.5	54.8	1.8	C22 H16 N3 O4
	386.1146	-0.5	-1.3	-1.5	55.2	2.2	C9 H24 N O15
	386.1181	-4.0	-10.4	20.5	53.3	0.3	C27 H16 N O2
	386.1087	5.4	14.0	7.5	57.7	4.7	C16 H20 N O10