

Supporting Information

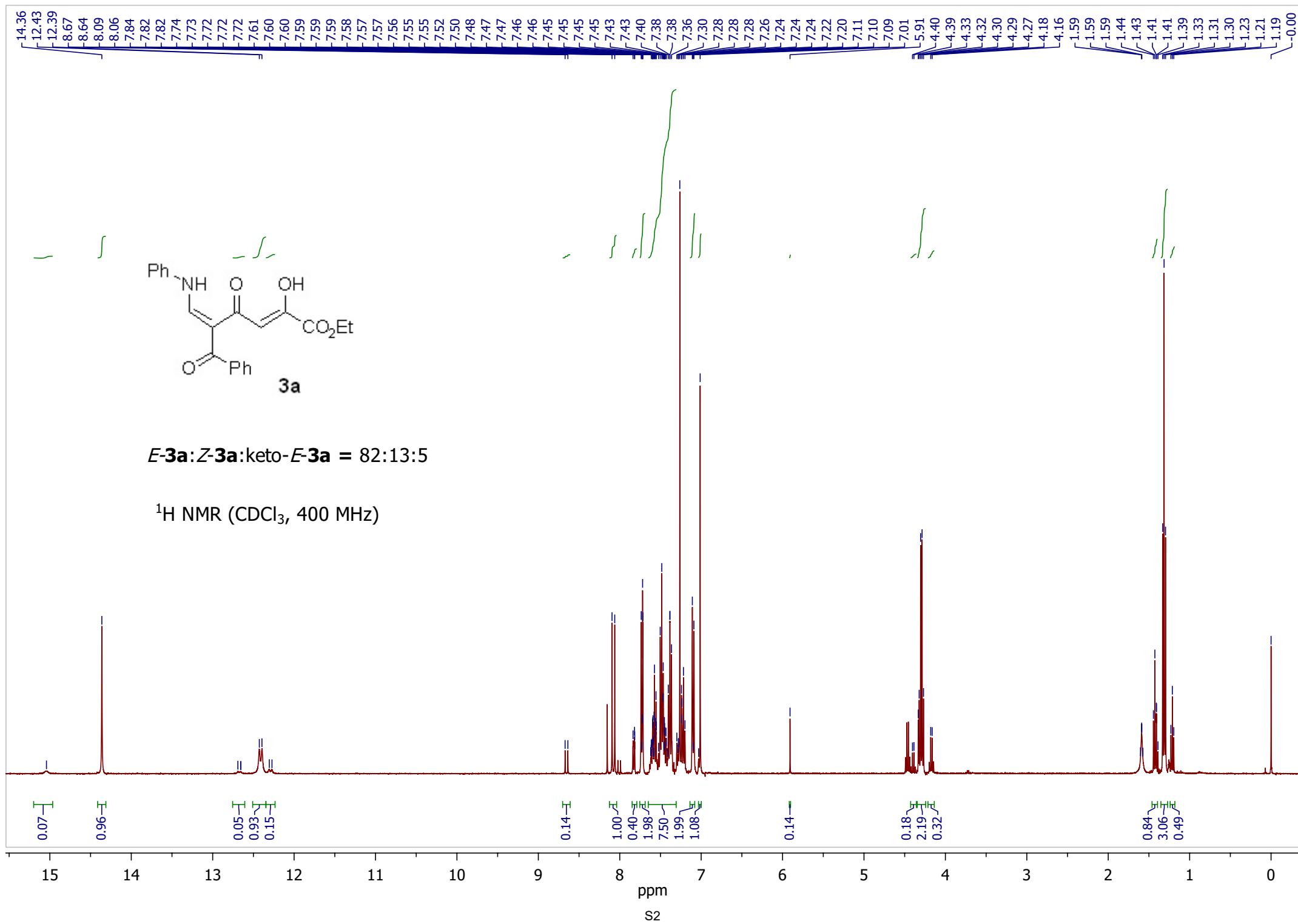
Synthesis of novel polycarbonyl Schiff bases by ring-opening reaction of ethyl 5-acyl-4-pyrone-2-carboxylates with primary mono- and diamines

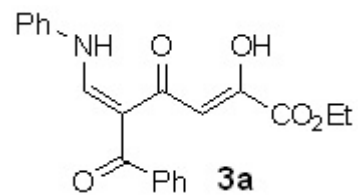
D. L. Obydenov,* L. R. Khammatova, V. D. Steben'kov and V. Y. Sosnovskikh

Institute of Natural Sciences and Mathematics, Ural Federal University, 51 Lenina Ave., 620000 Ekaterinburg,
Russian Federation. E-mail: dobydenov@mail.ru

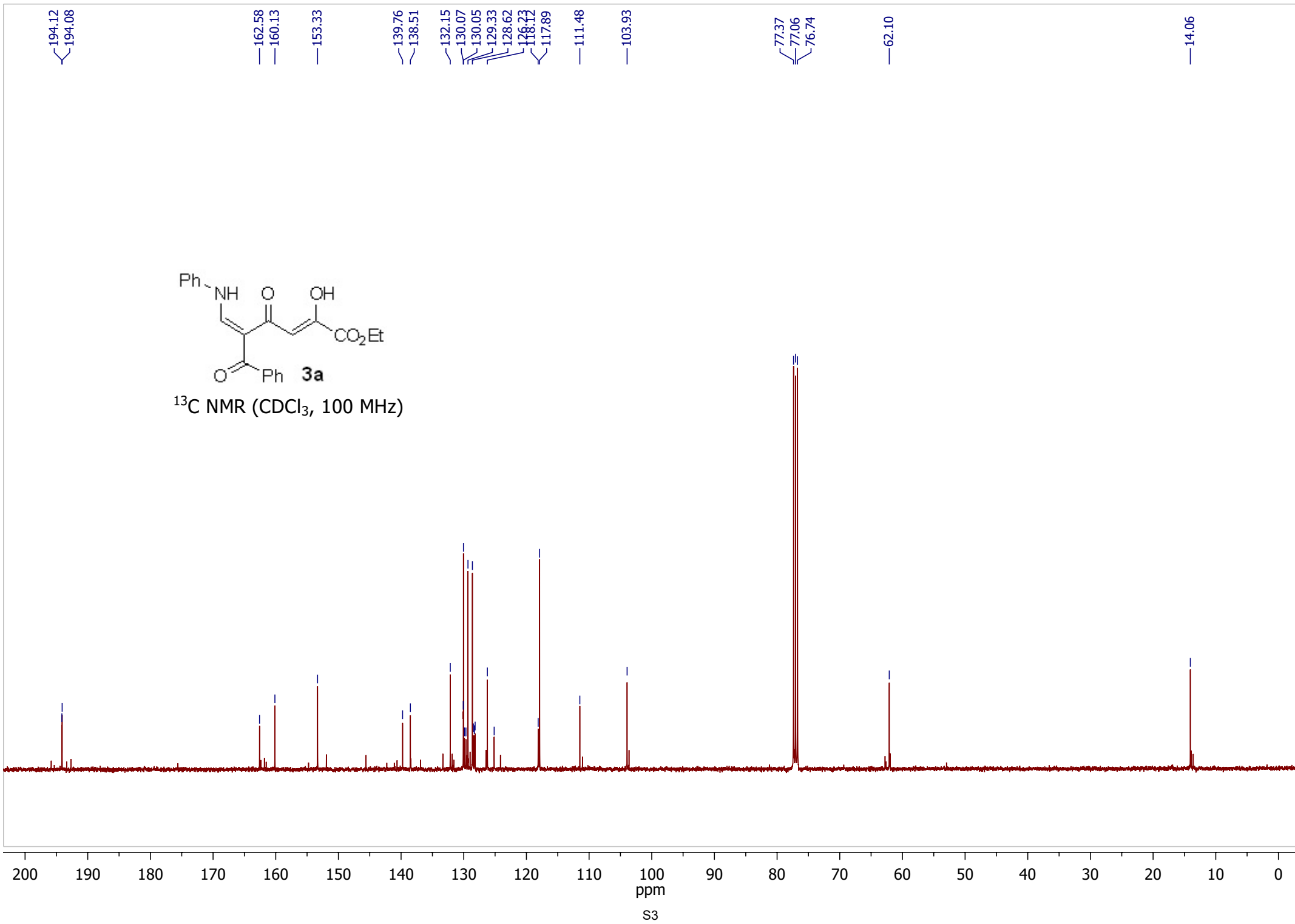
Table of Contents

1.	NMR spectra of compounds 3	S2
2.	NMR spectra of compounds 4	S22
3.	¹ H NMR spectrum of compound 5	S32
4.	ESI-MS data of compound 5	S33
5.	IR spectrum of compound 5	S34
6.	NMR spectrum of compound 6	S35
7.	NMR spectra of compounds 7	S36
8.	NMR spectra of compounds 8	S43
9.	NMR spectra of compounds 9	S50
10.	NMR spectrum of compound 10	S52
11.	NMR spectra of compound 11	S53
12.	NMR spectra of compound 12	S55
13.	2D ¹ H- ¹³ C HMBC spectrum of compound 3b	S57

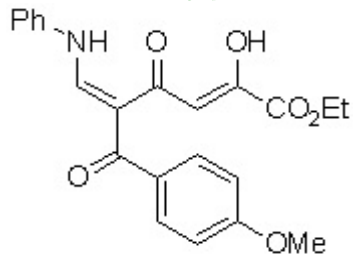




¹³C NMR (CDCl₃, 100 MHz)

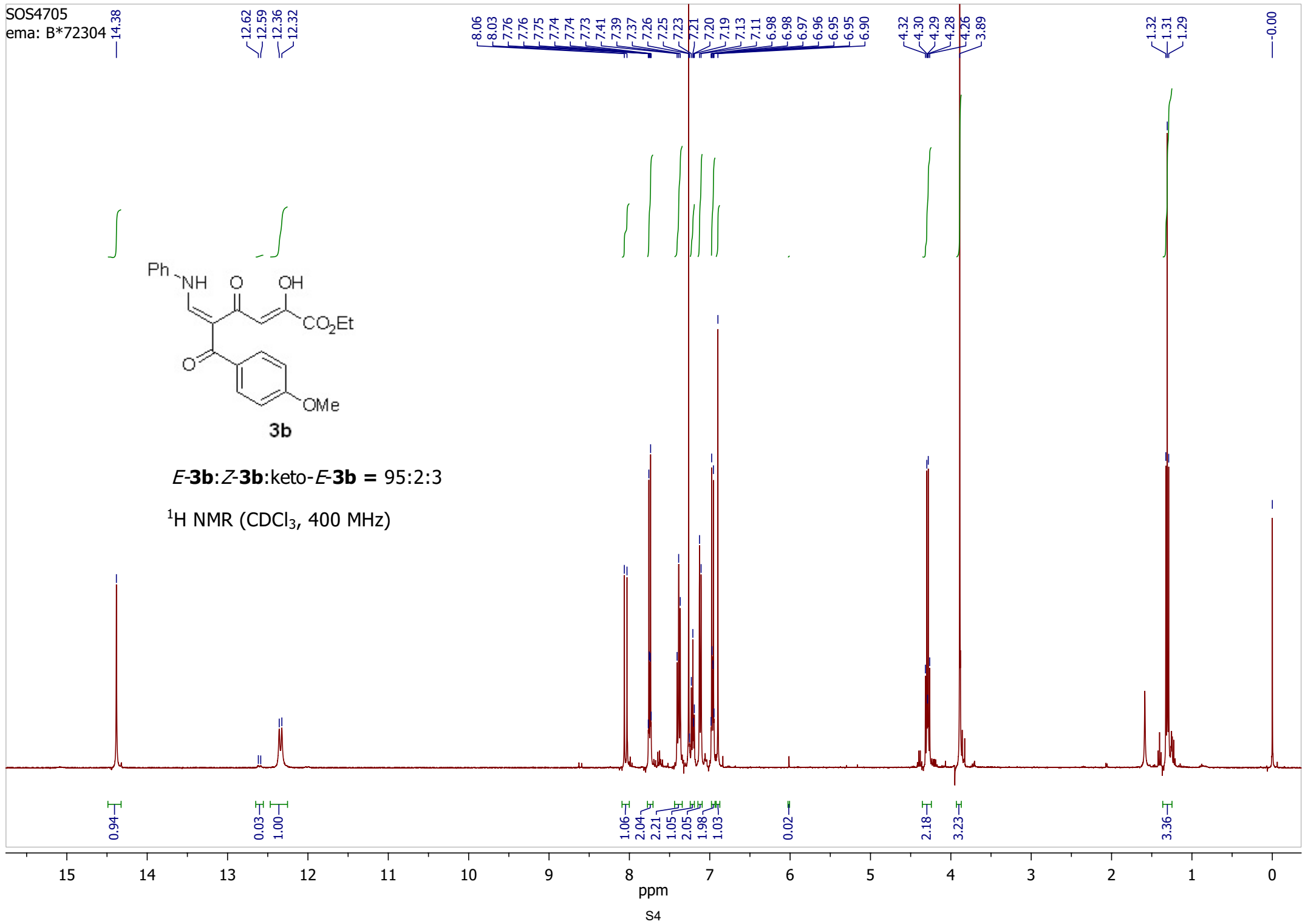


SOS4705
ema: B*72304



E-**3b**:*Z*-**3b**:keto-*E*-**3b** = 95:2:3

¹H NMR (CDCl₃, 400 MHz)



193.87
192.95

163.05
162.61
159.88

152.39

138.64

132.07
131.78
130.02

126.03

117.78
113.82
111.70

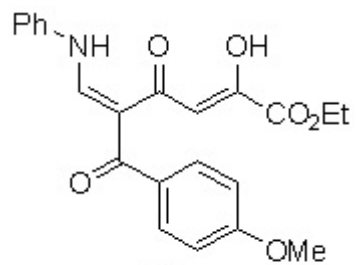
103.91

77.38
77.06
76.74

62.05

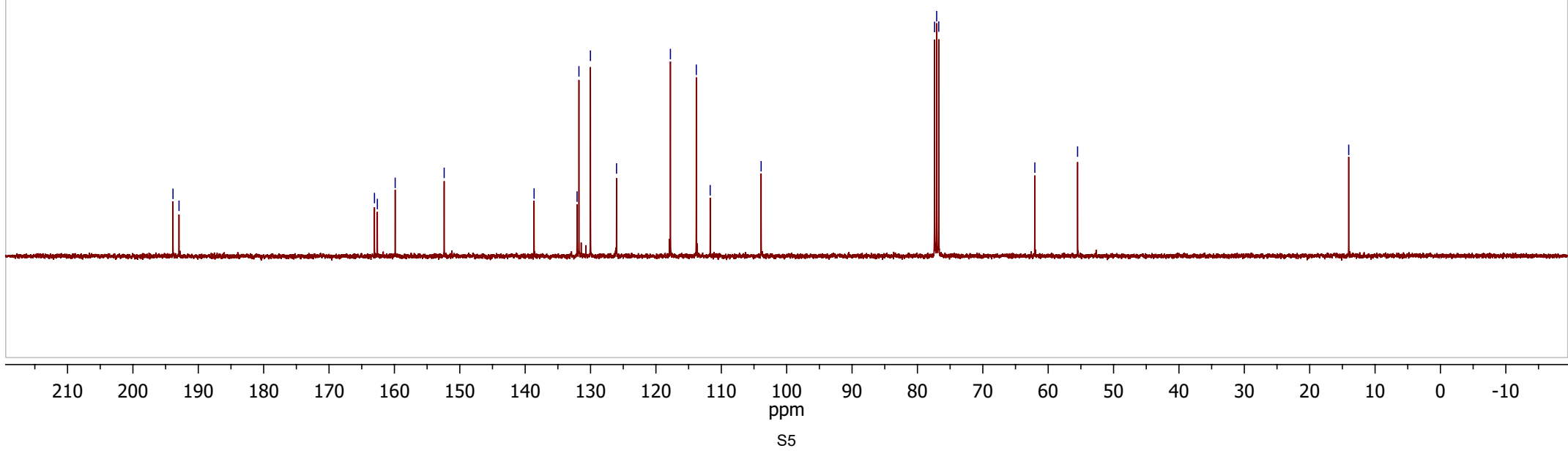
55.50

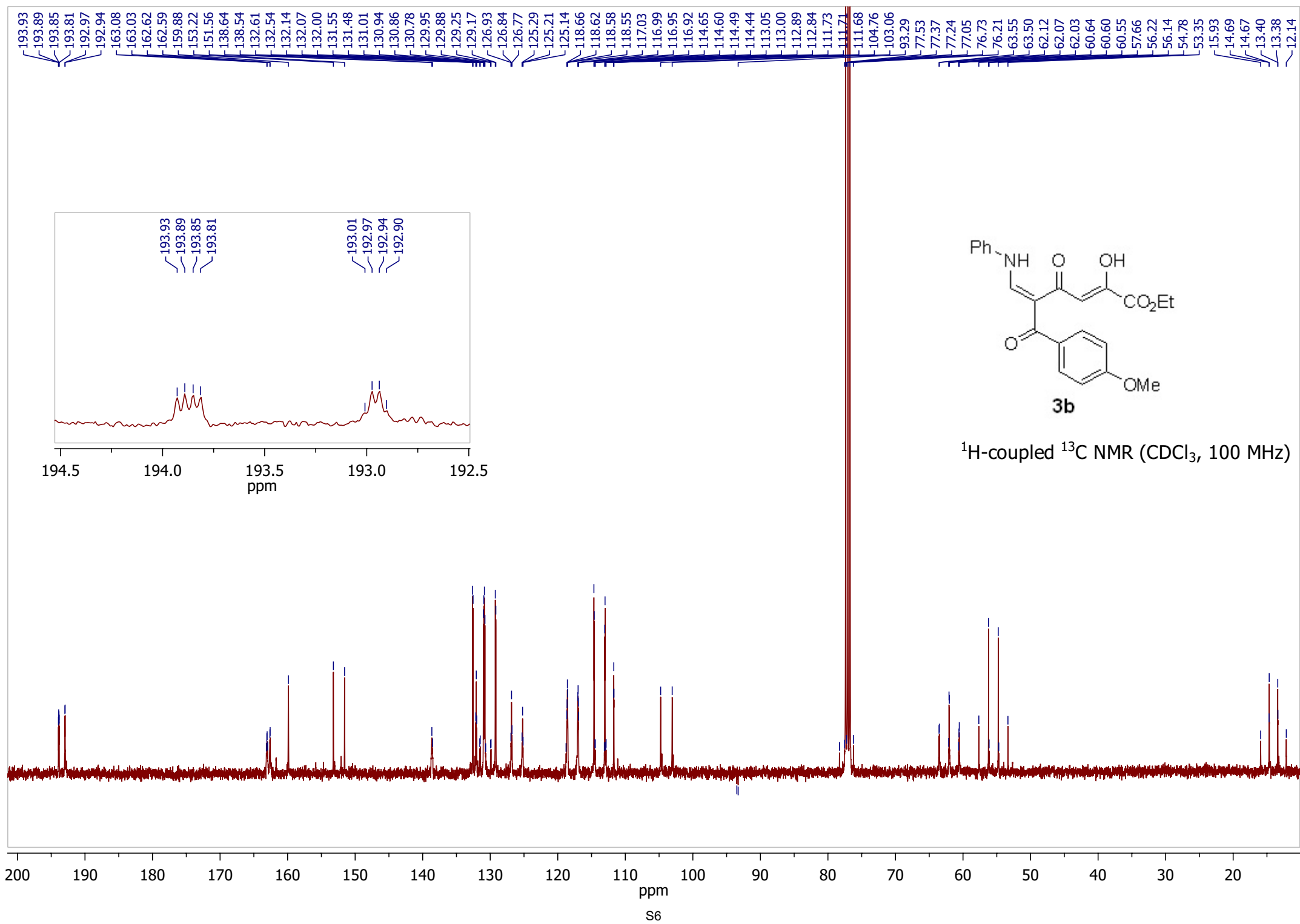
14.03

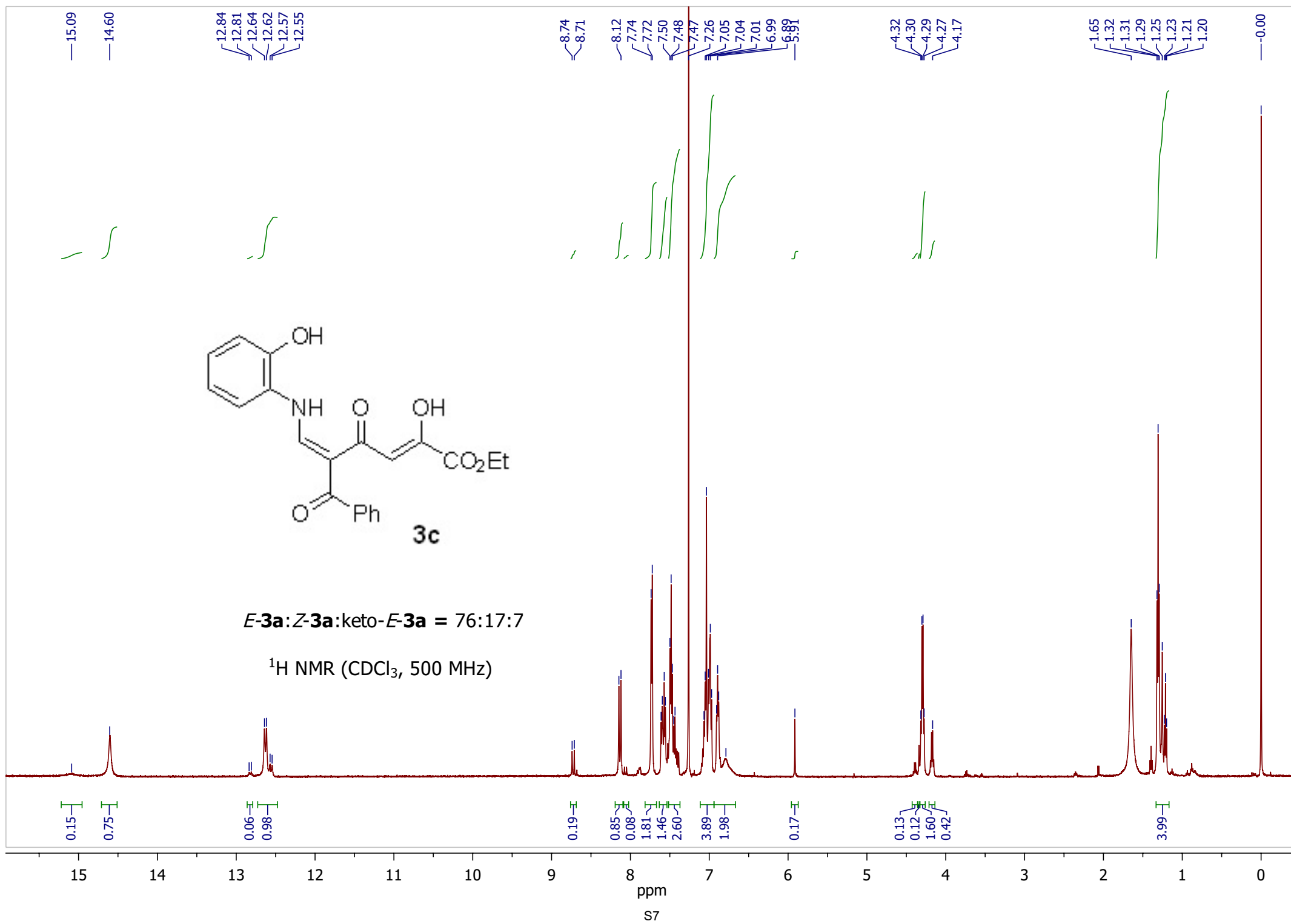


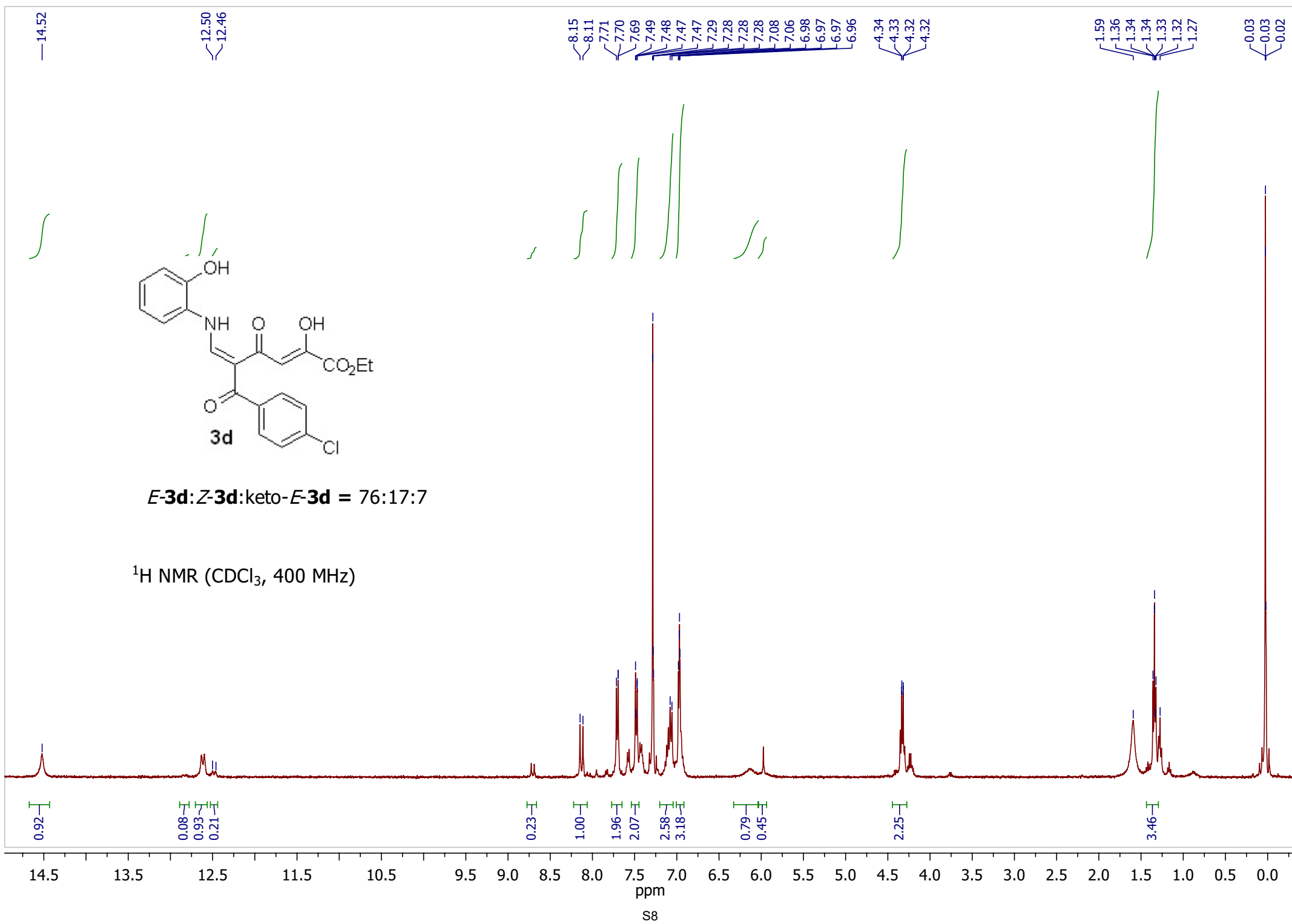
3b

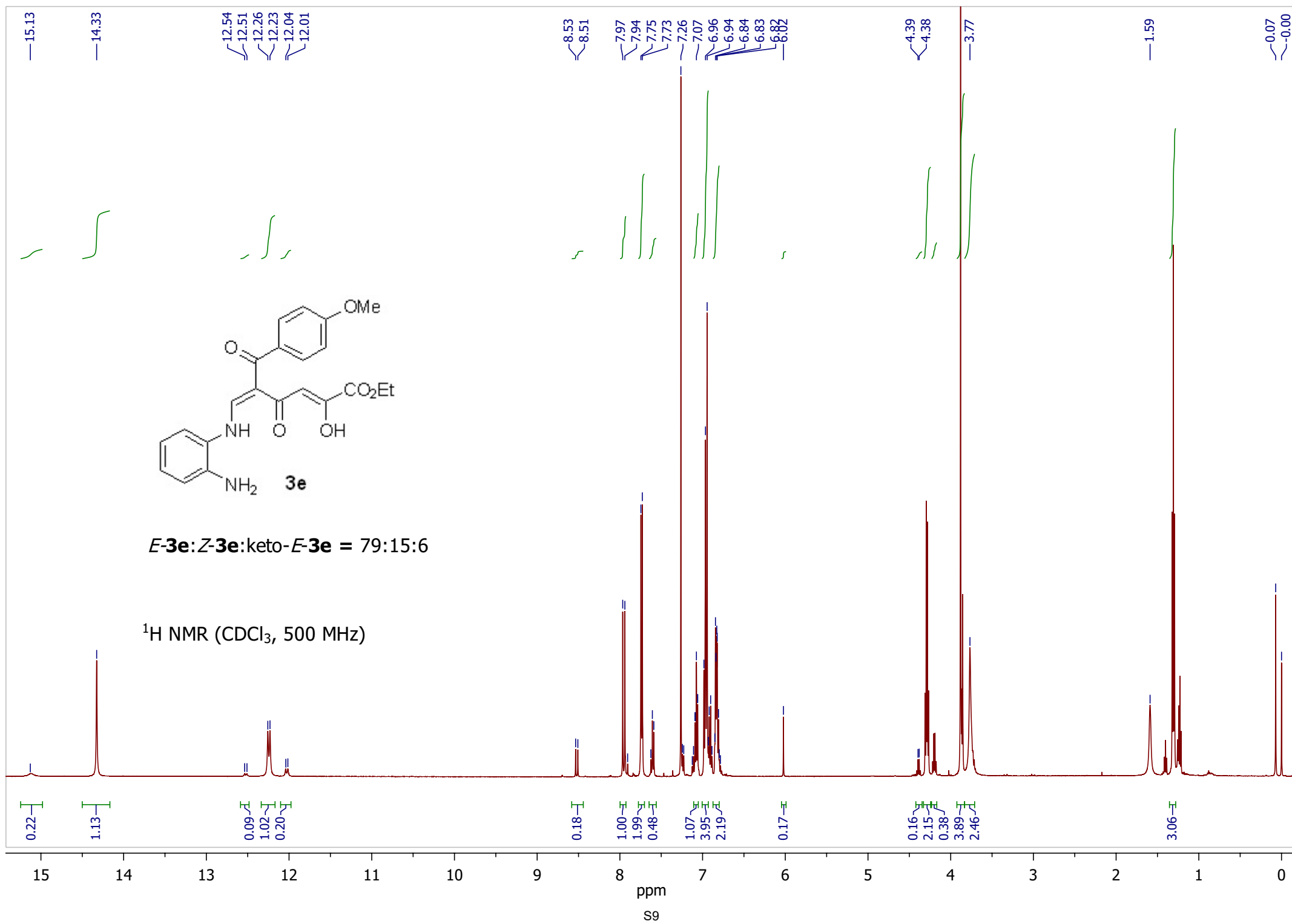
¹³C NMR (CDCl₃, 100 MHz)

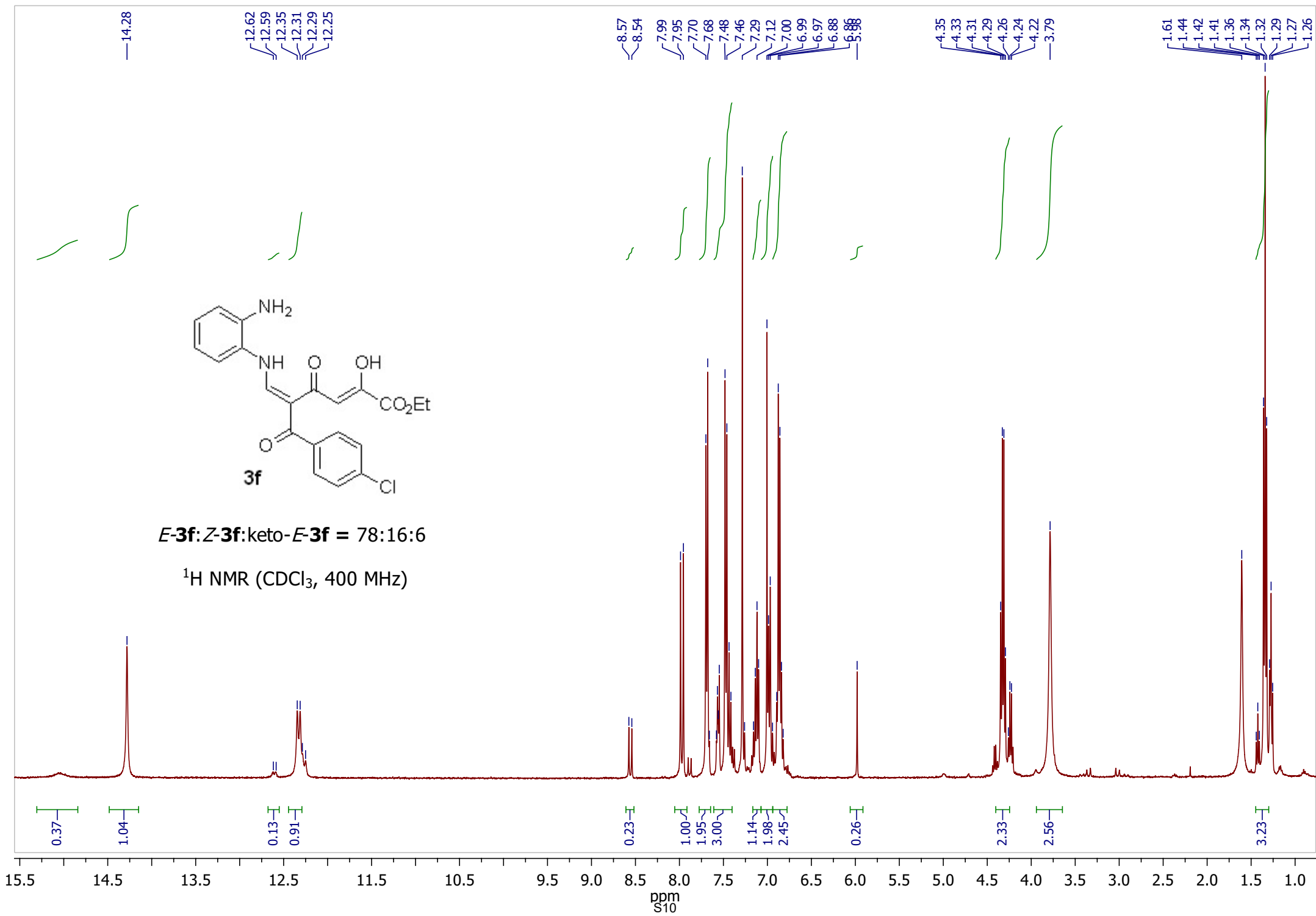


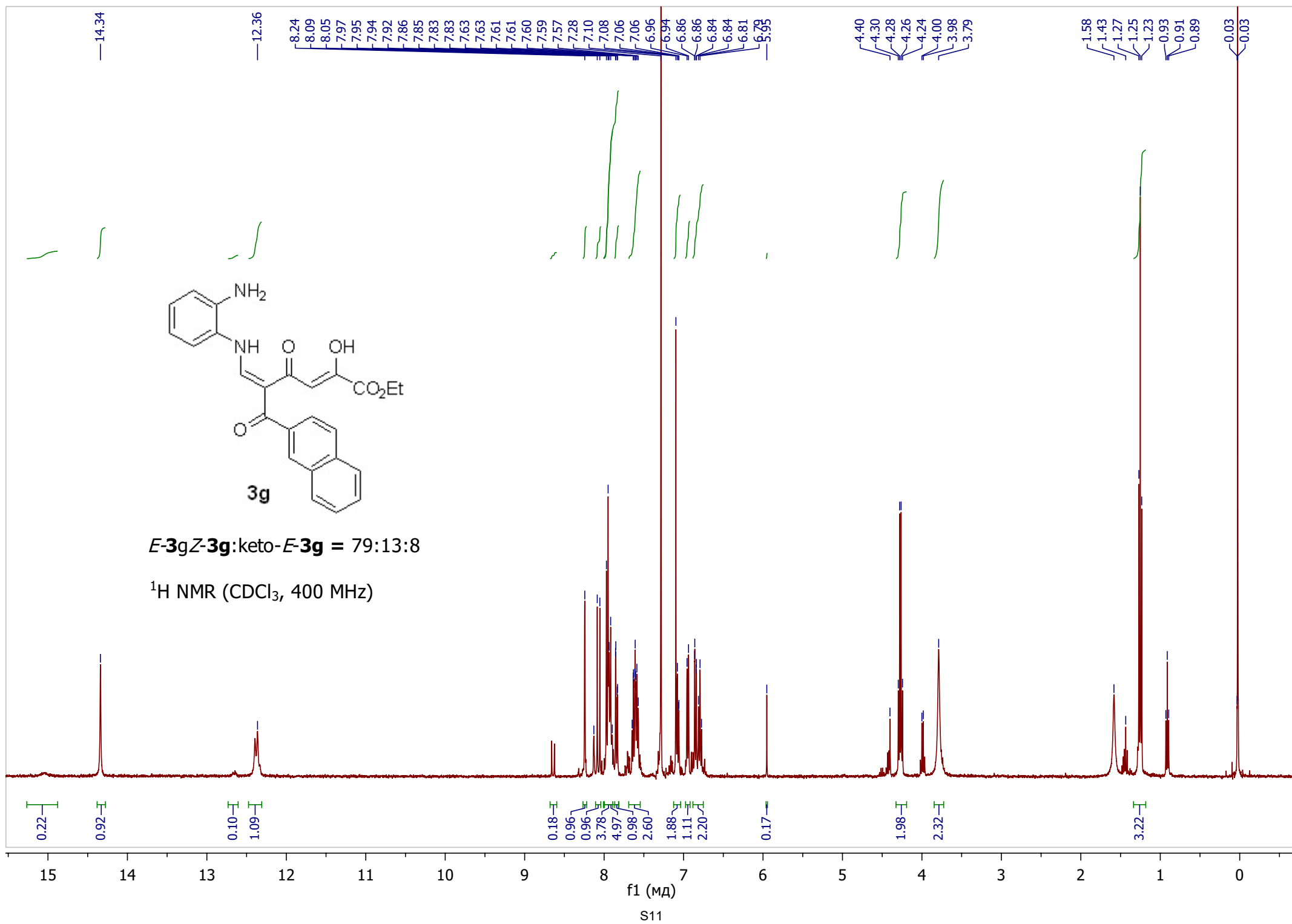


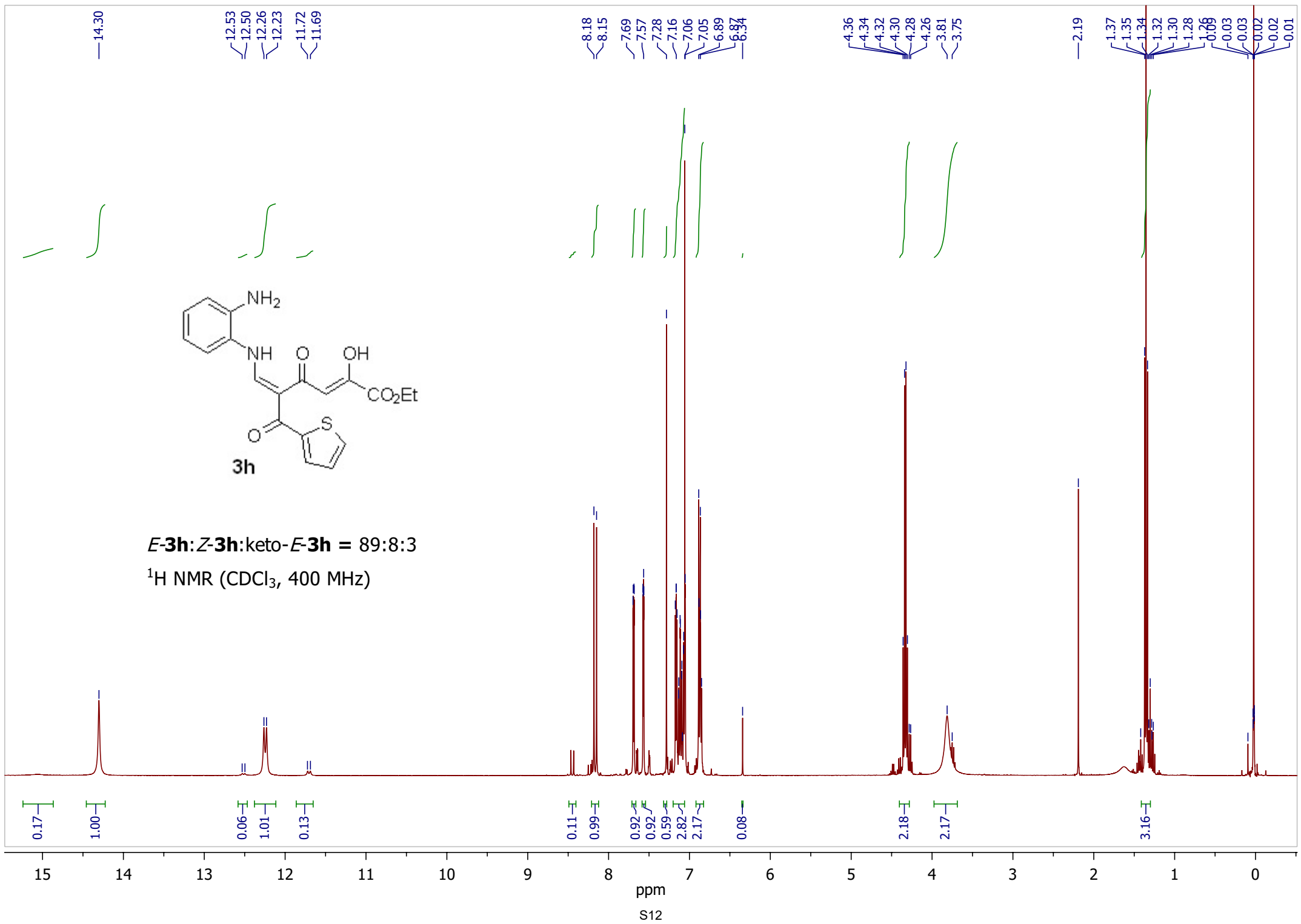


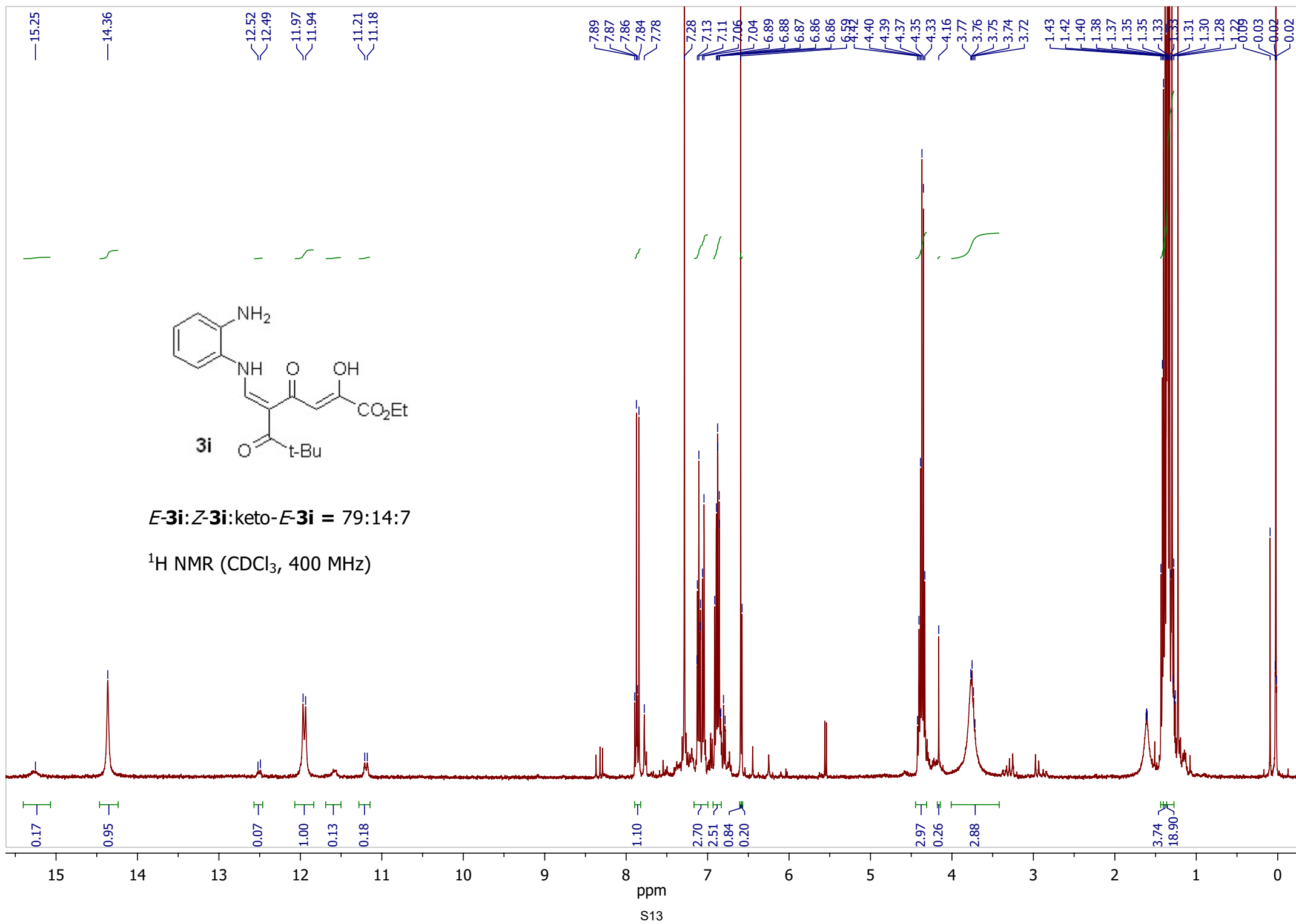


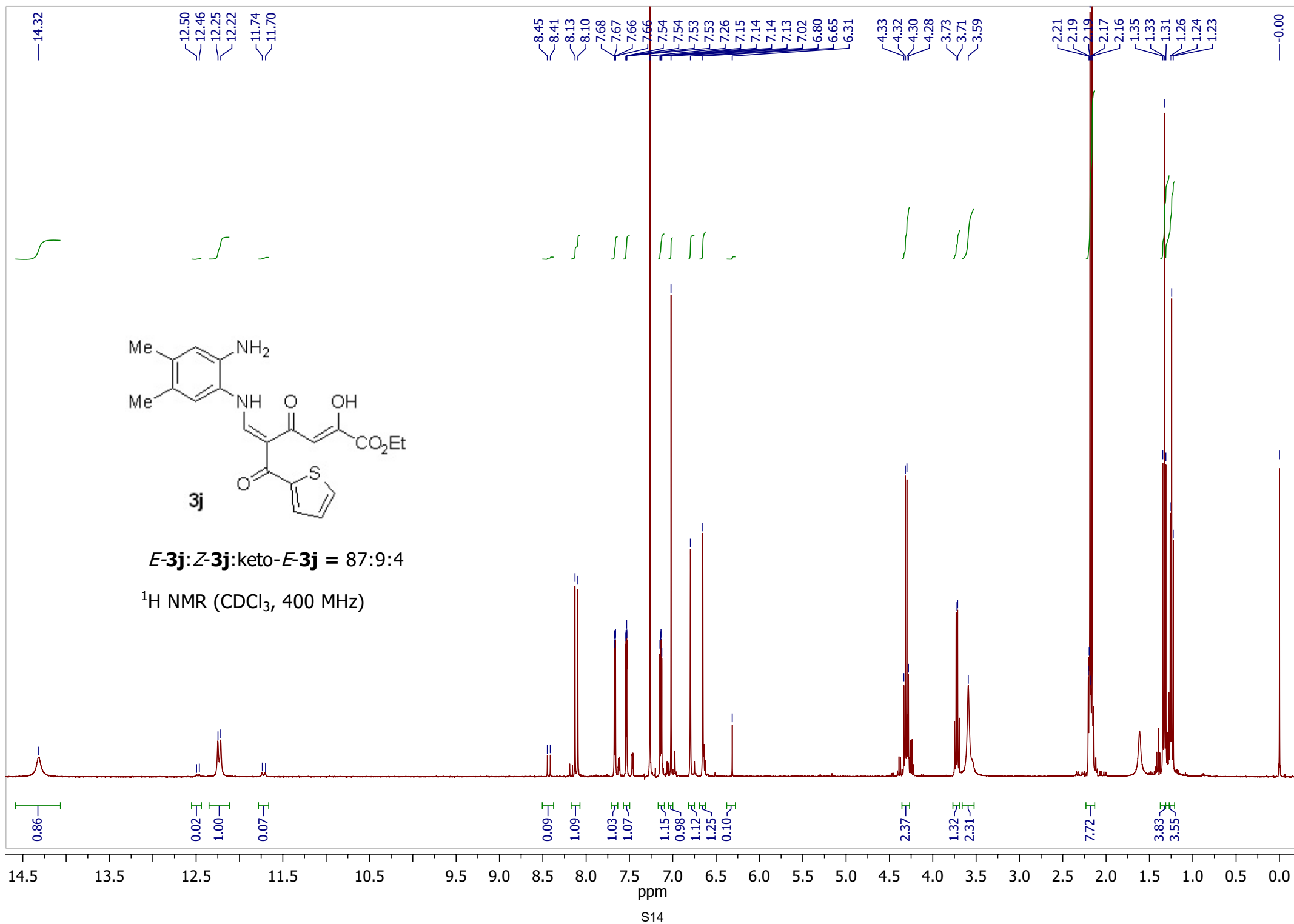


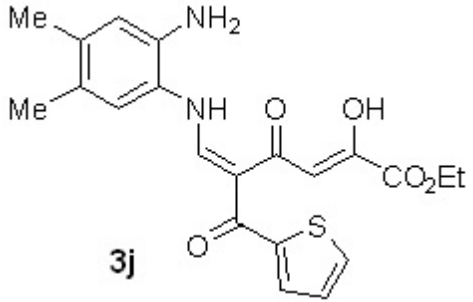




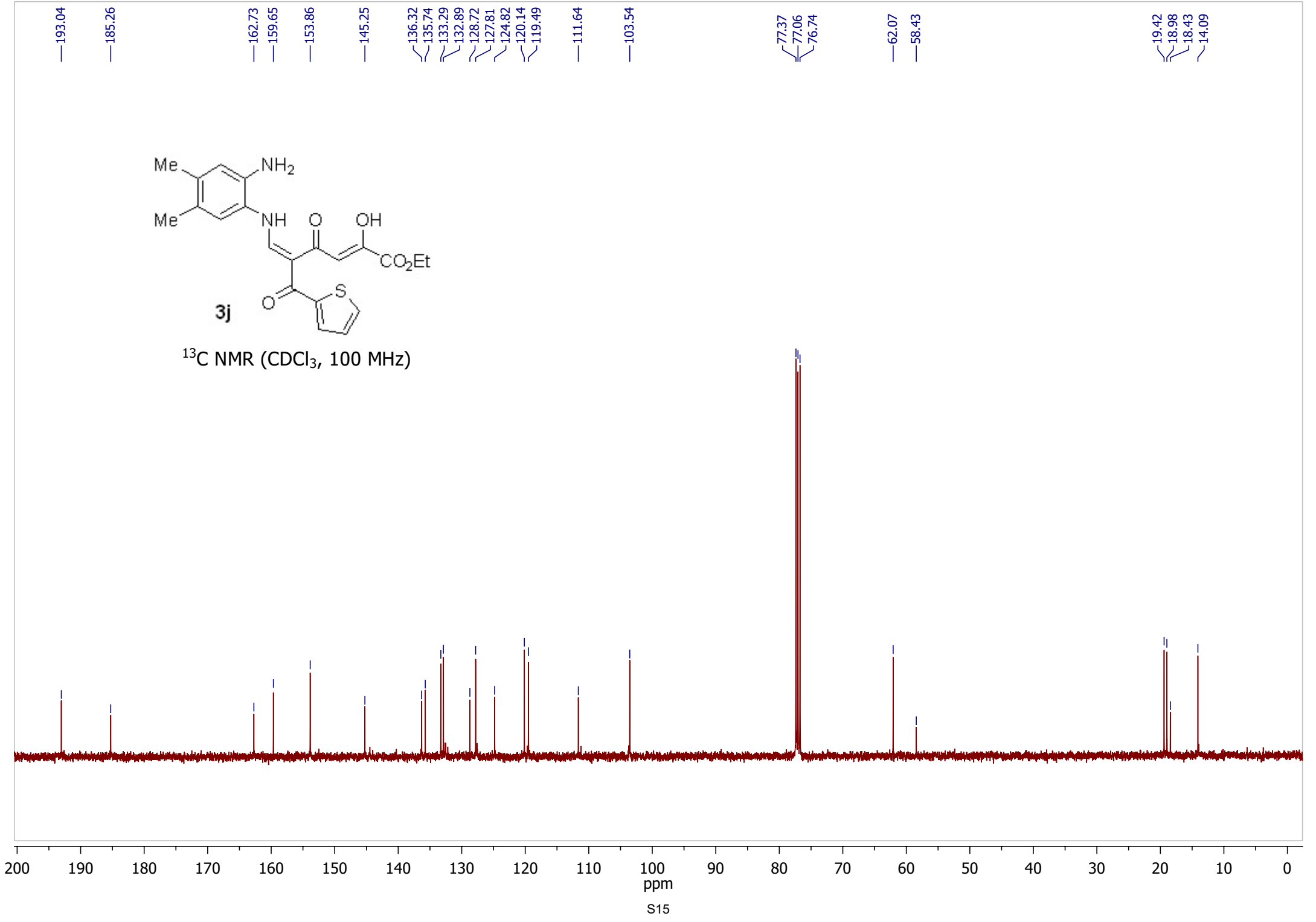


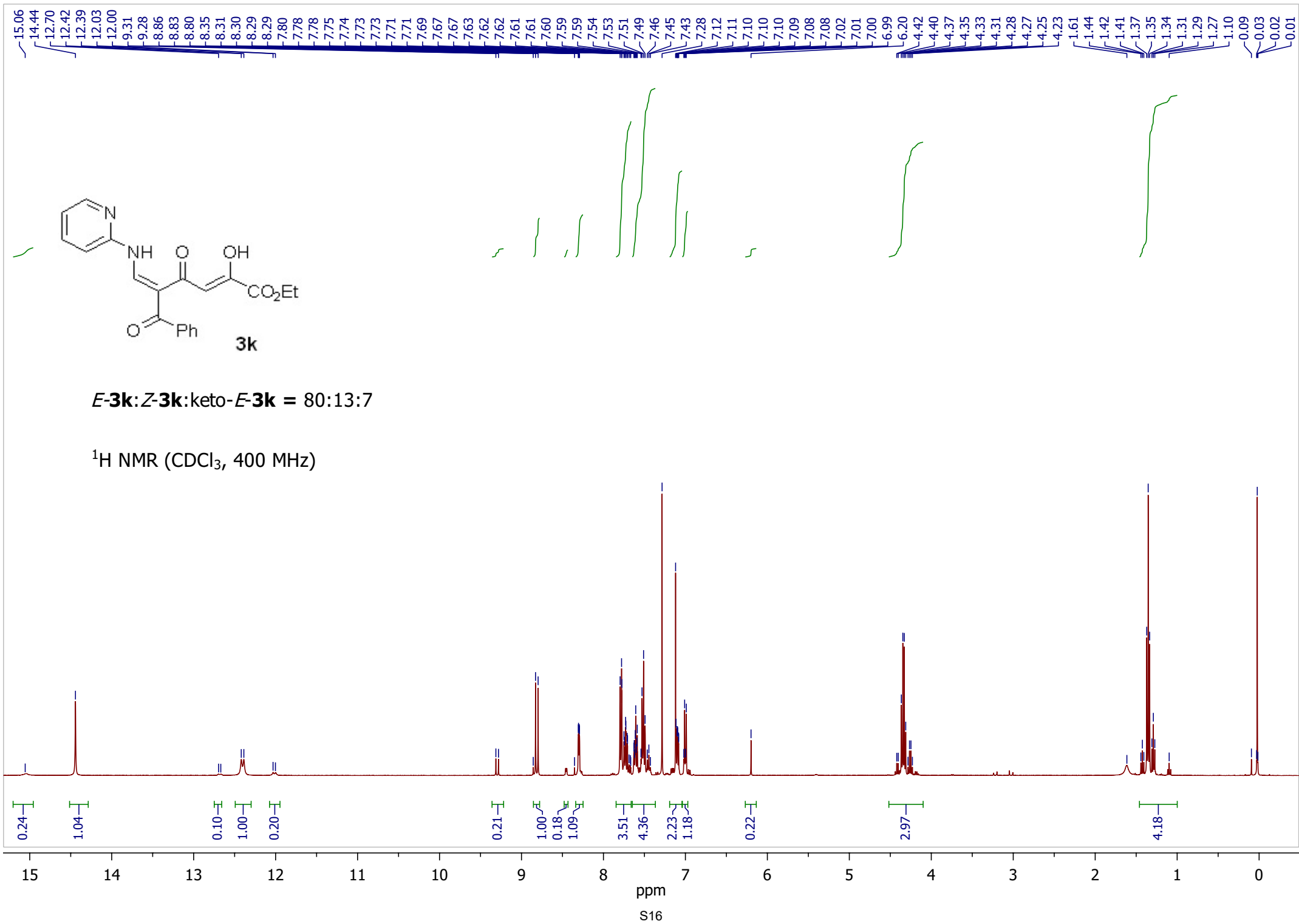






¹³C NMR (CDCl₃, 100 MHz)





SOS-4989
SOS-4989

194.82
194.43

162.54
160.75

151.21
149.88
149.08

148.96
139.37
138.86
138.82

132.28
129.61
128.56

126.89
120.70

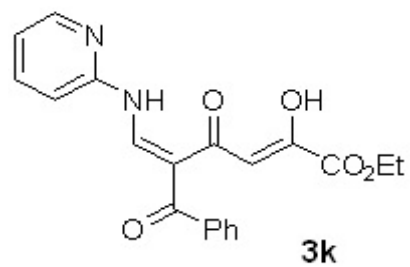
112.85
112.81
112.29

103.80
102.51

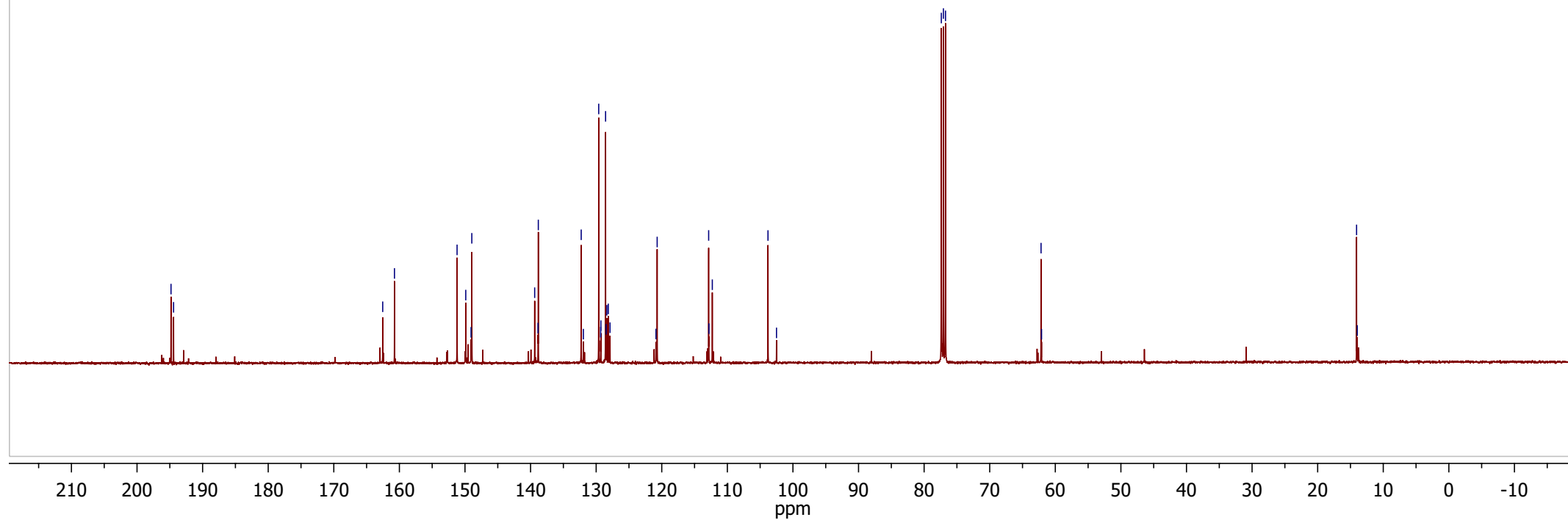
77.38
77.06
76.74

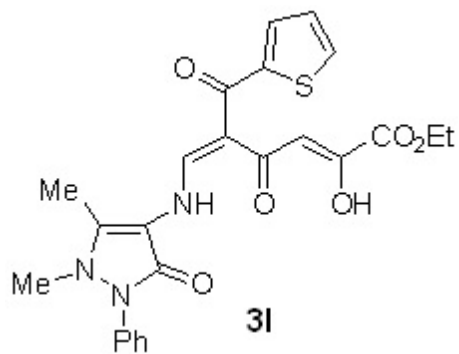
62.17
62.10

14.07
13.96



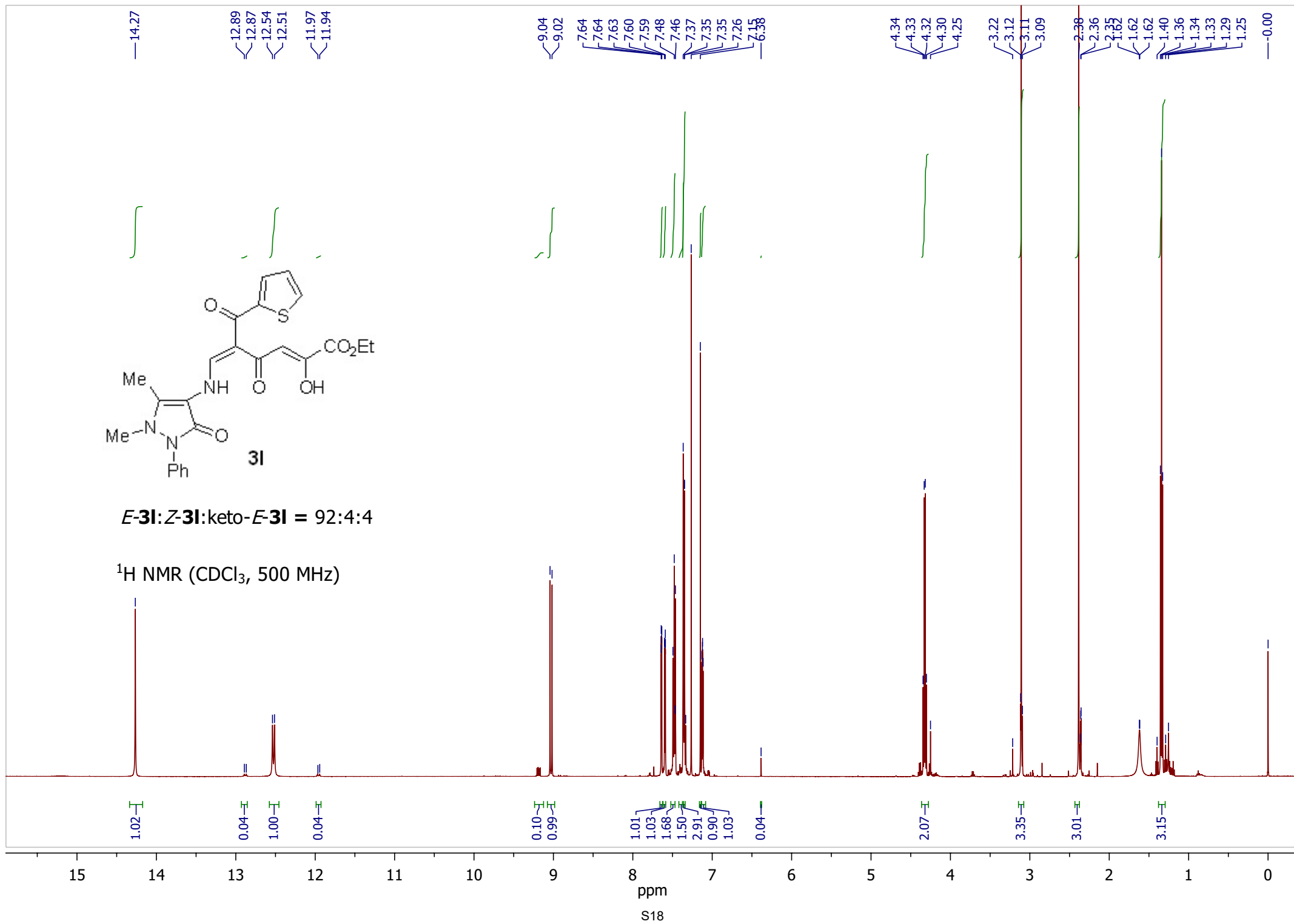
¹³C NMR (CDCl₃, 100 MHz)

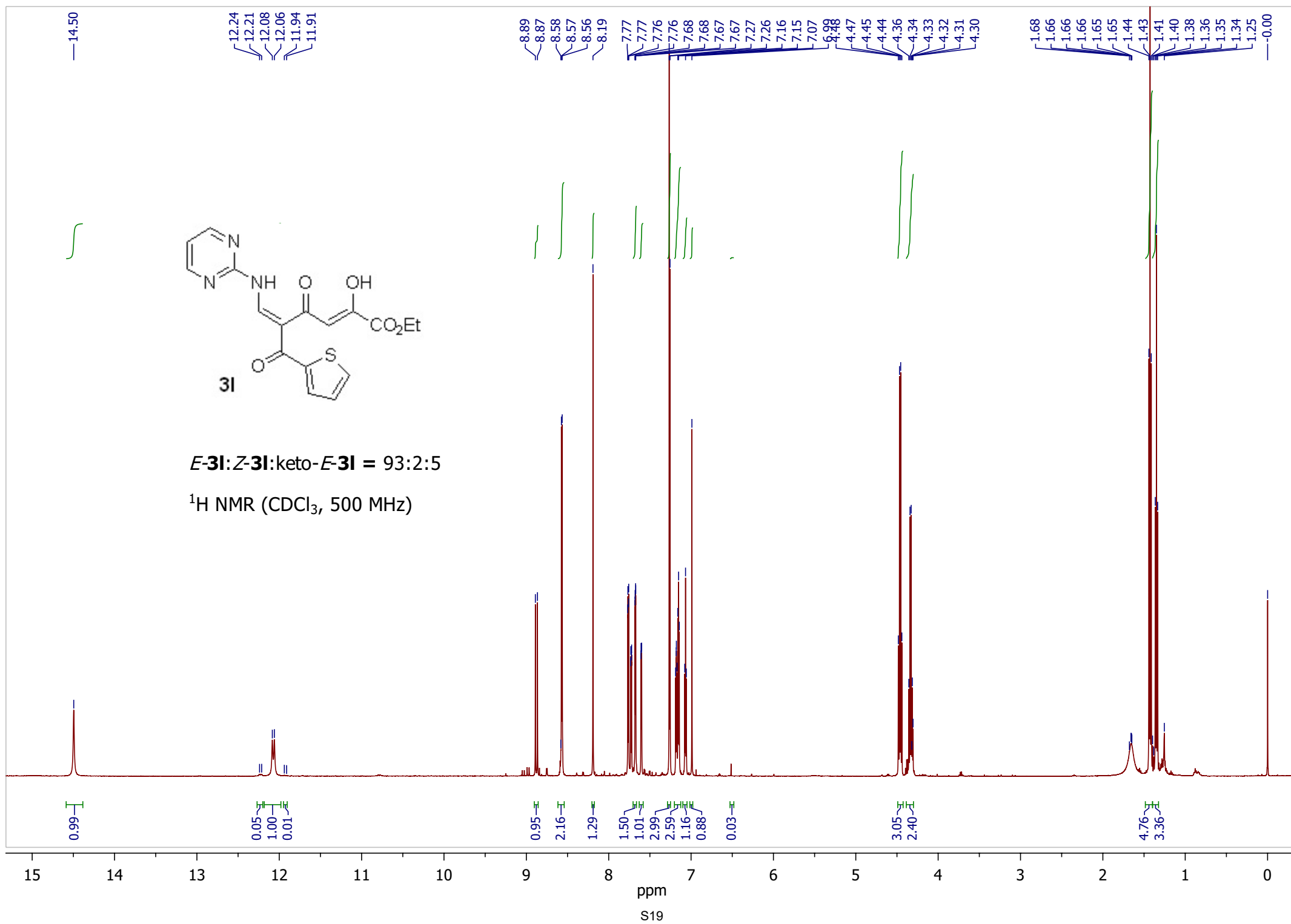


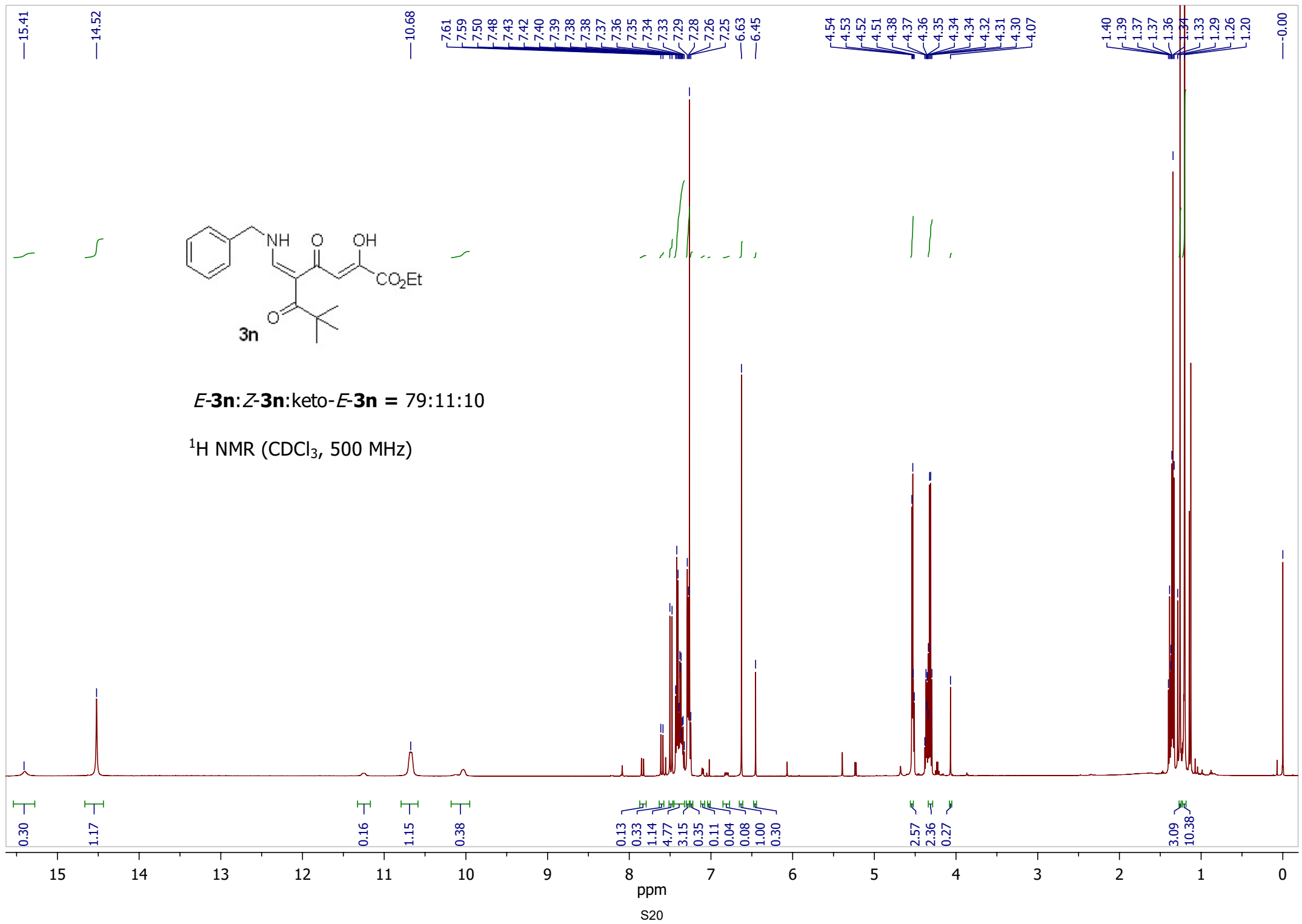


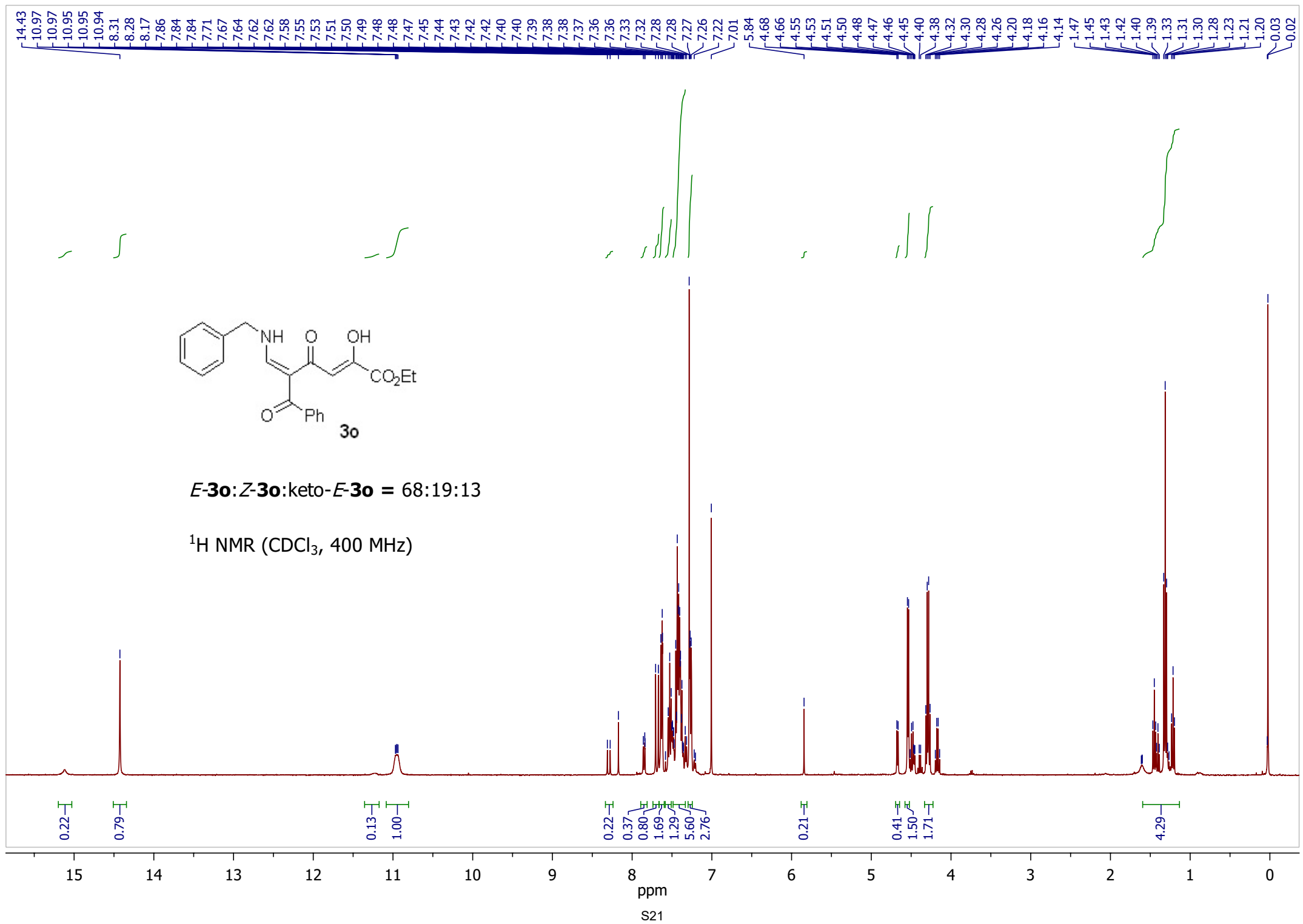
E-**31**:*Z*-**31**:keto-*E*-**31** = 92:4:4

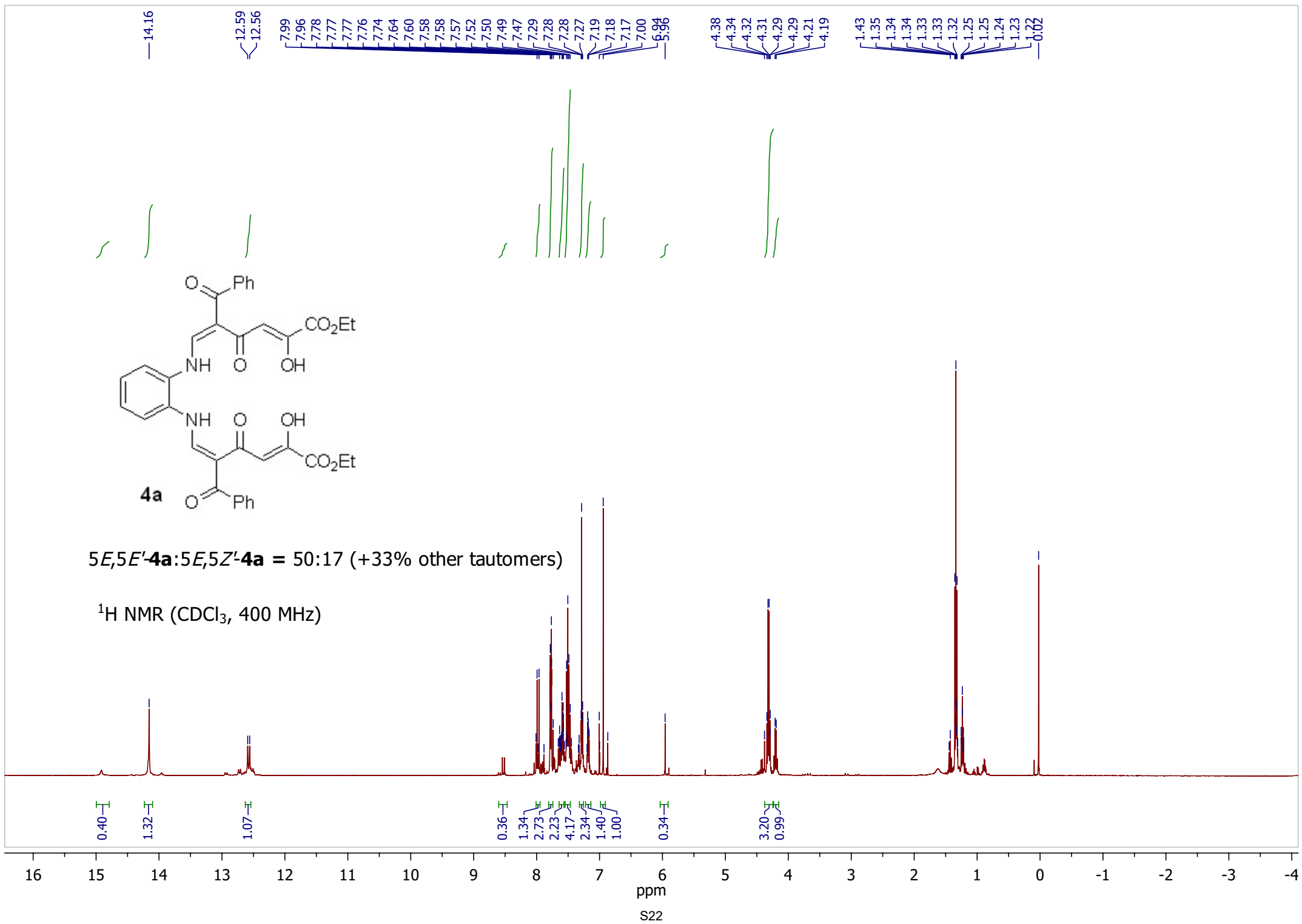
¹H NMR (CDCl₃, 500 MHz)

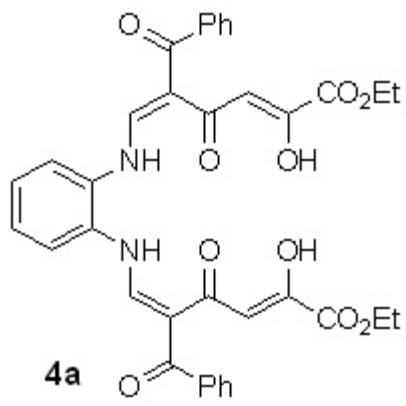




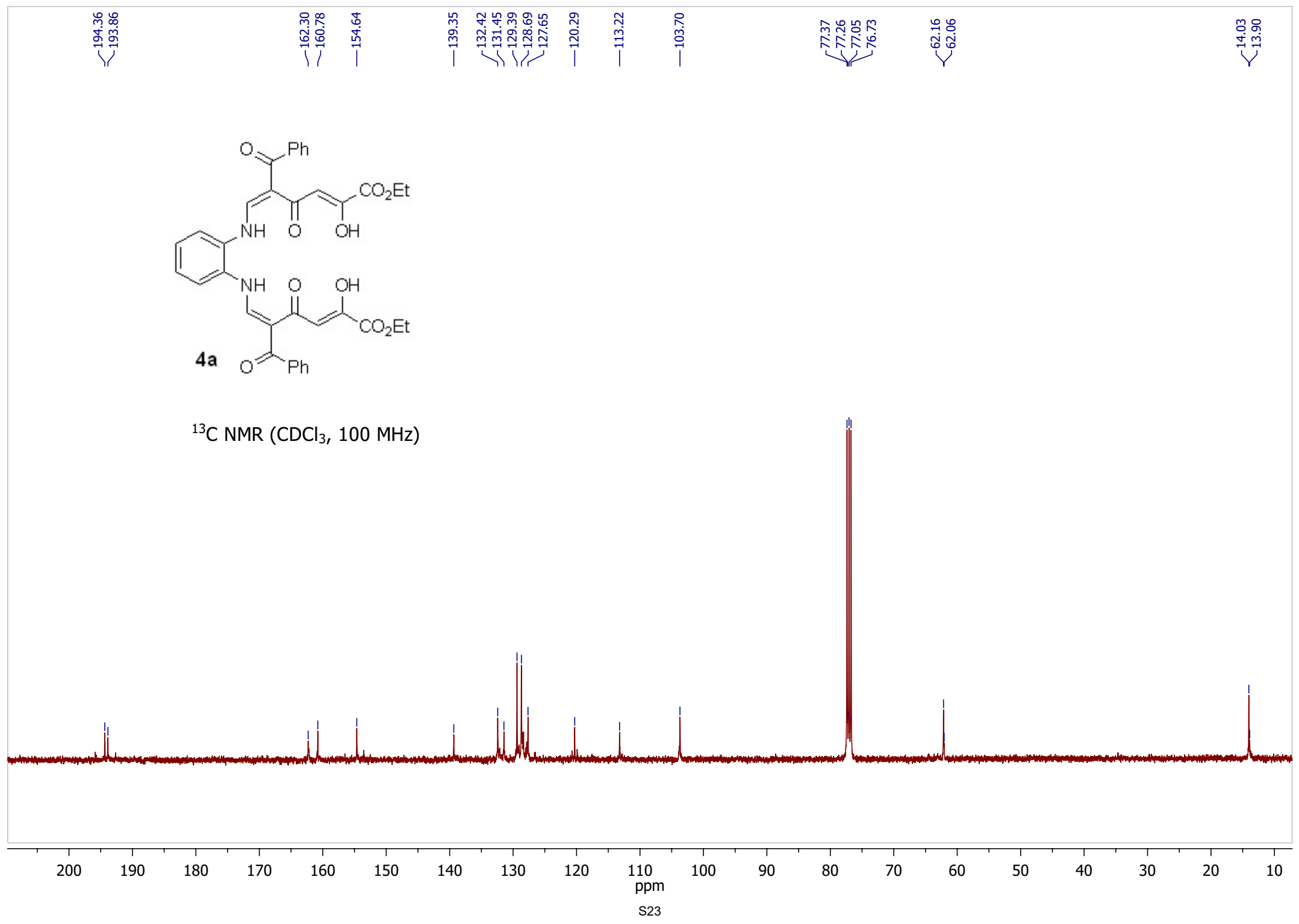


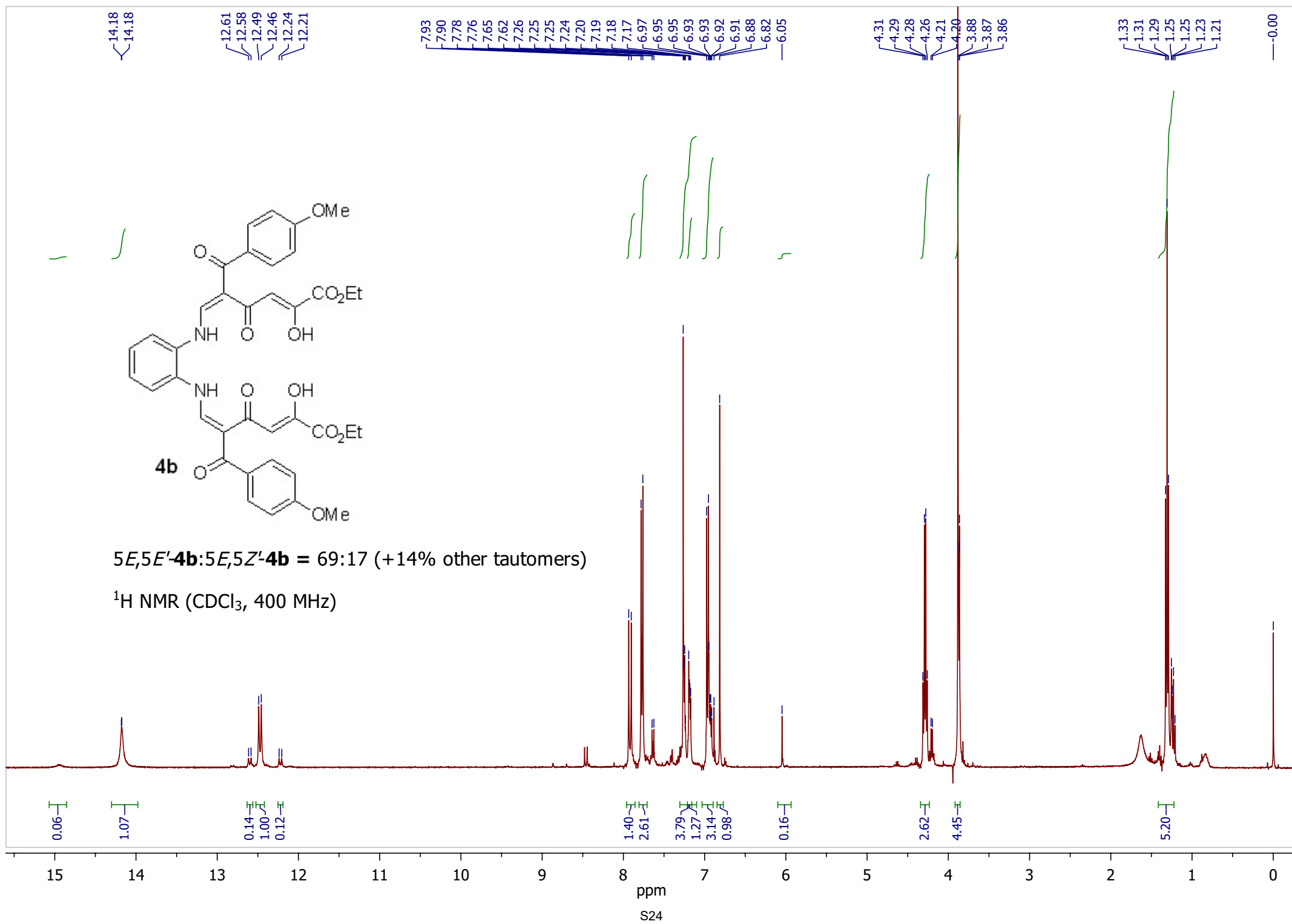






^{13}C NMR (CDCl_3 , 100 MHz)





194.17
192.65

163.28
162.36
160.55
156.82
153.62

132.18
131.87
131.68
131.49
127.46

120.21

113.92
113.85

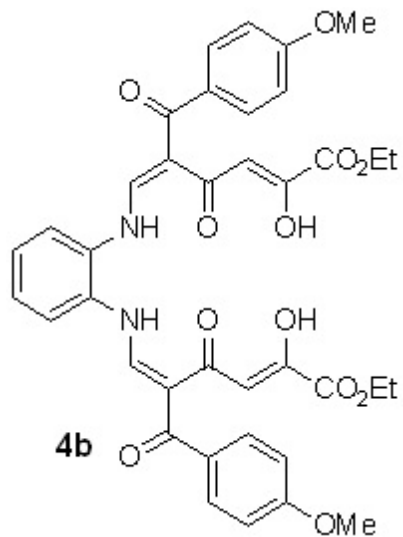
103.69

77.35
77.24
77.03
76.72

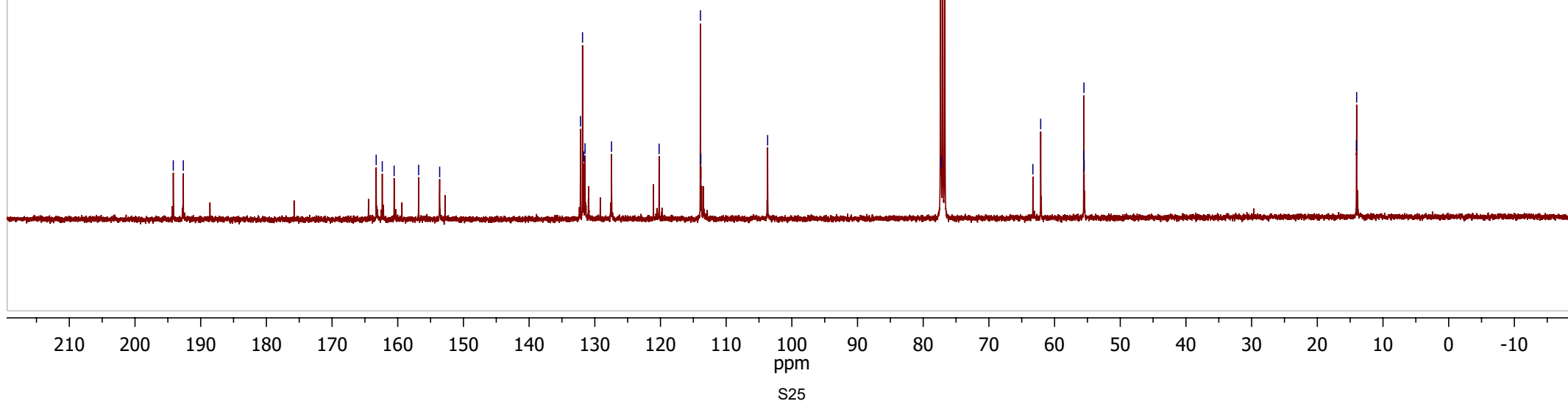
63.30
62.11

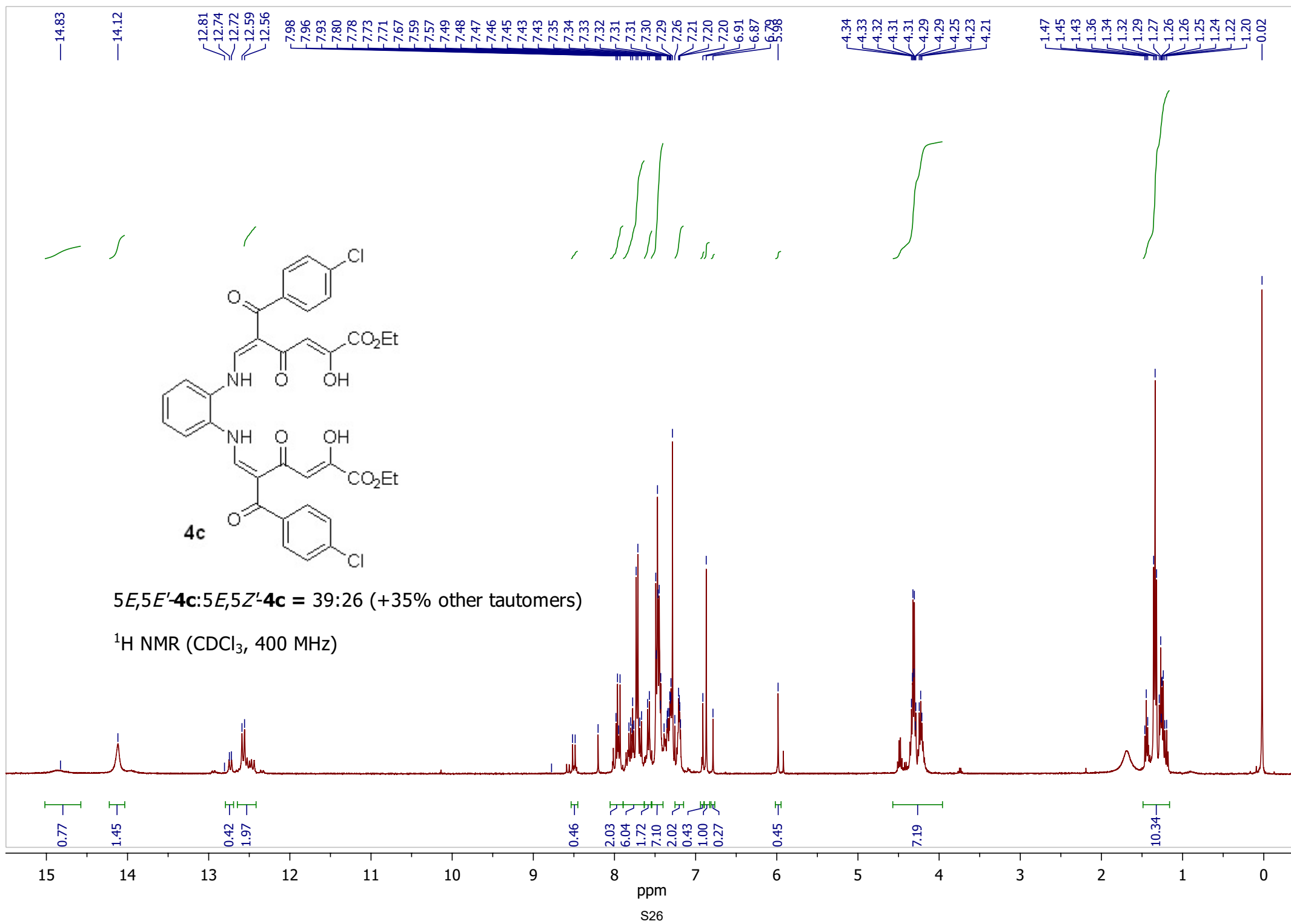
55.57
55.53
55.50

14.04
14.01



¹³C NMR (CDCl₃, 100 MHz)





194.14
192.49

162.18
160.93

154.50

138.82
137.64

130.77
129.00
128.97
126.30

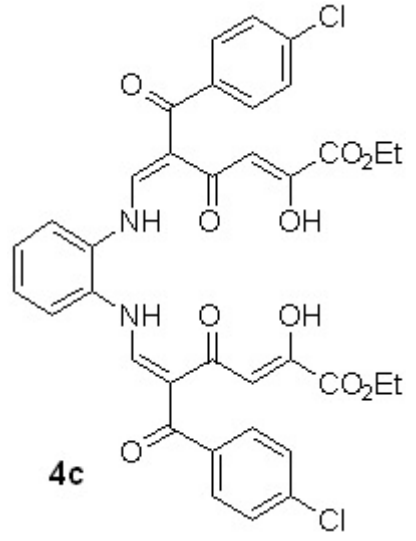
112.96

103.56

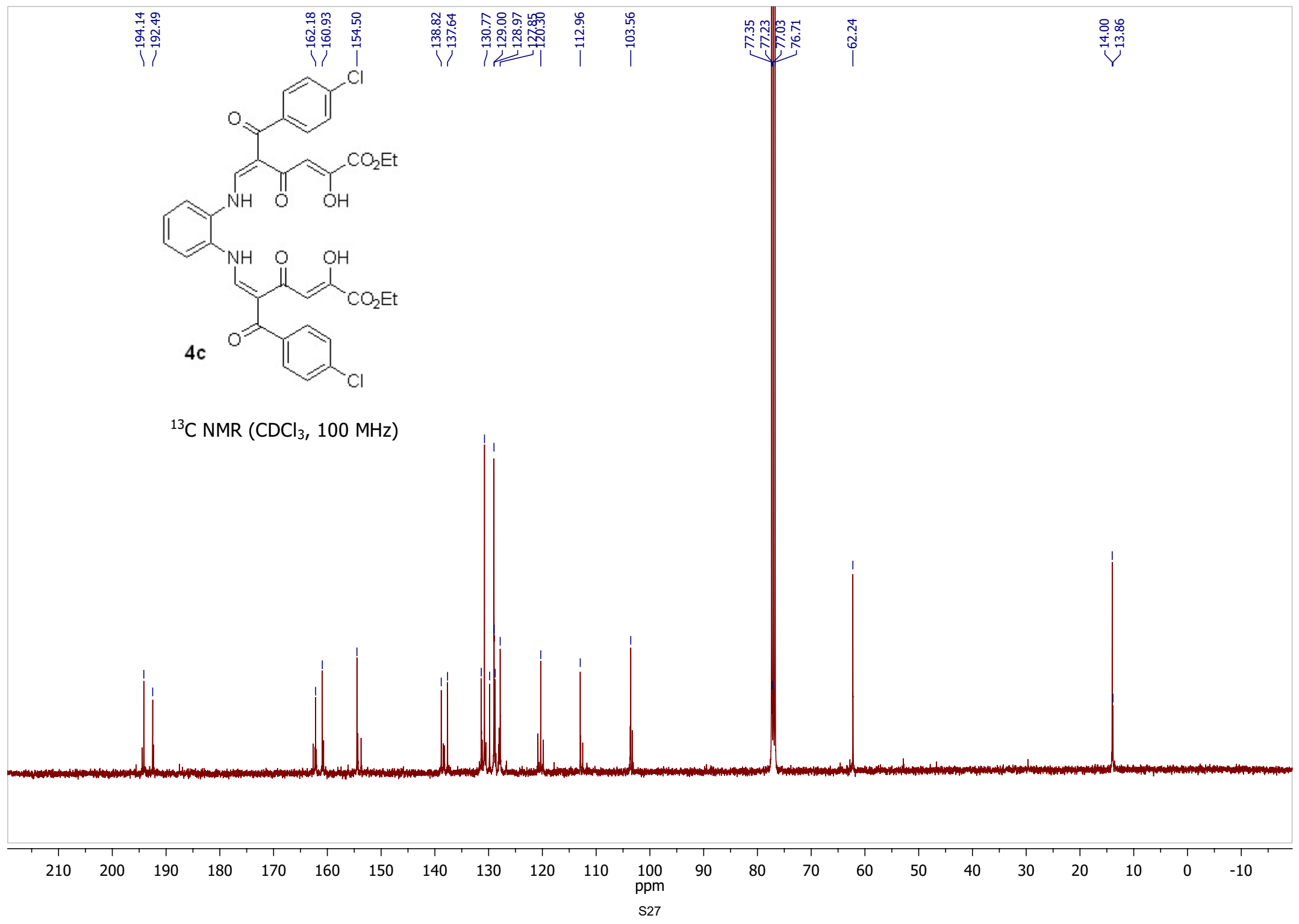
77.35
77.23
77.03
76.71

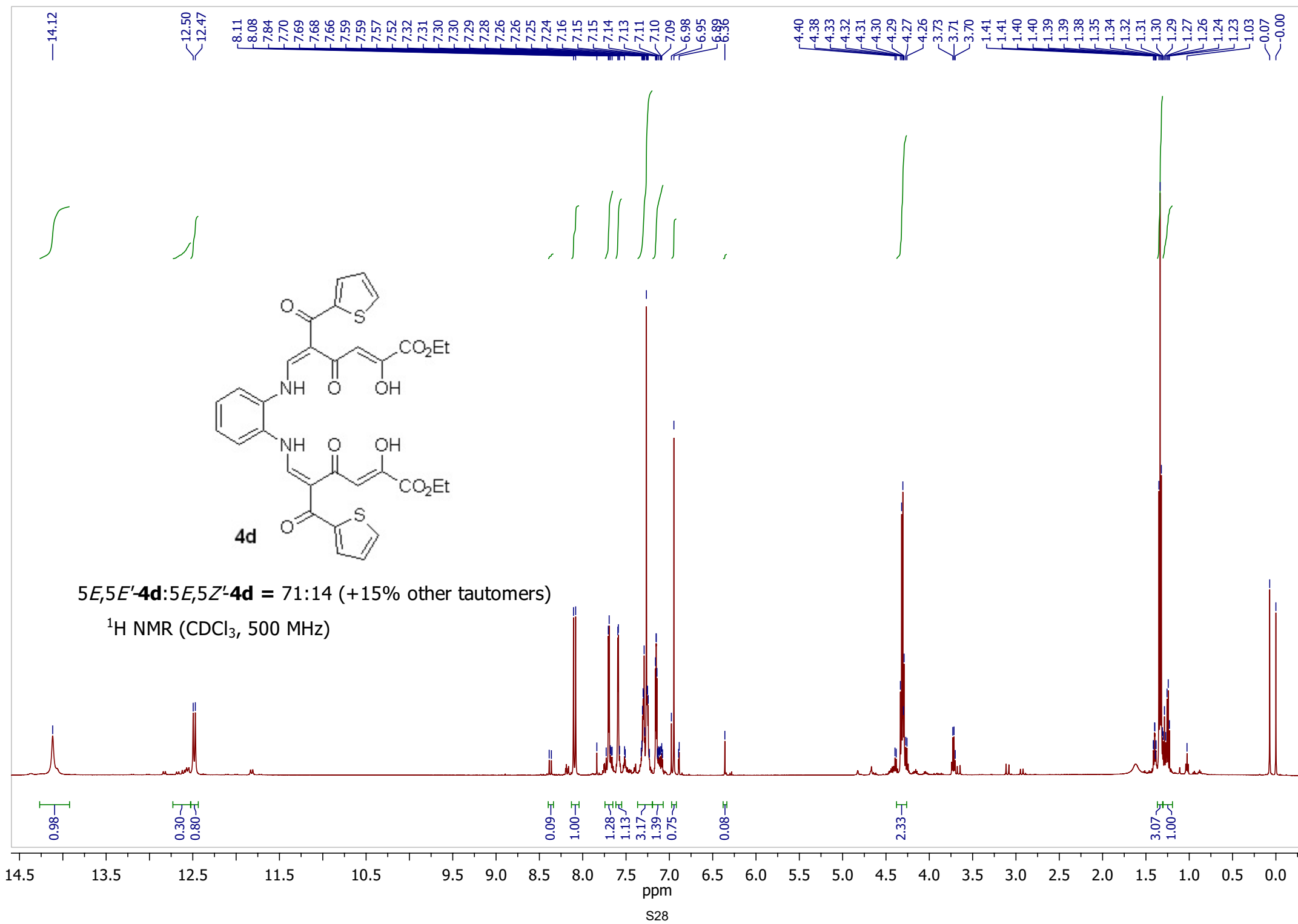
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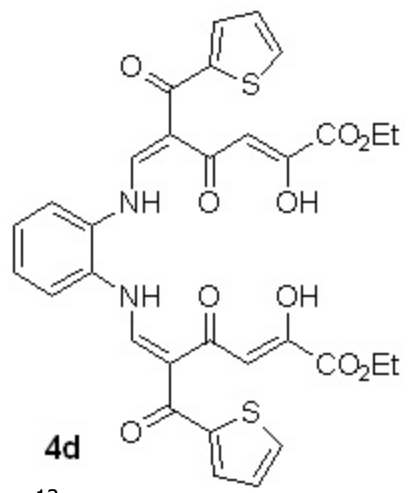
14.00
13.86



¹³C NMR (CDCl₃, 100 MHz)

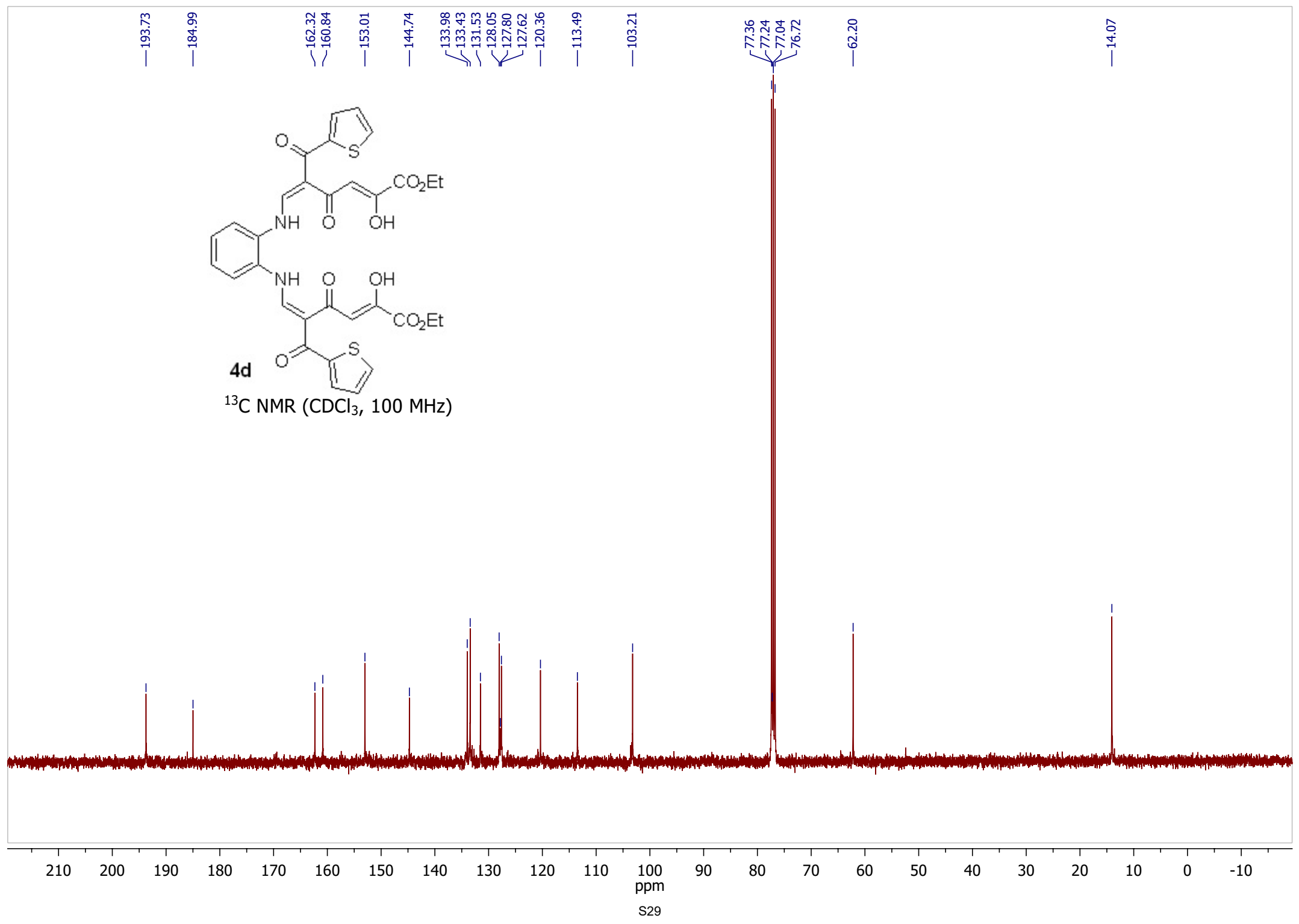


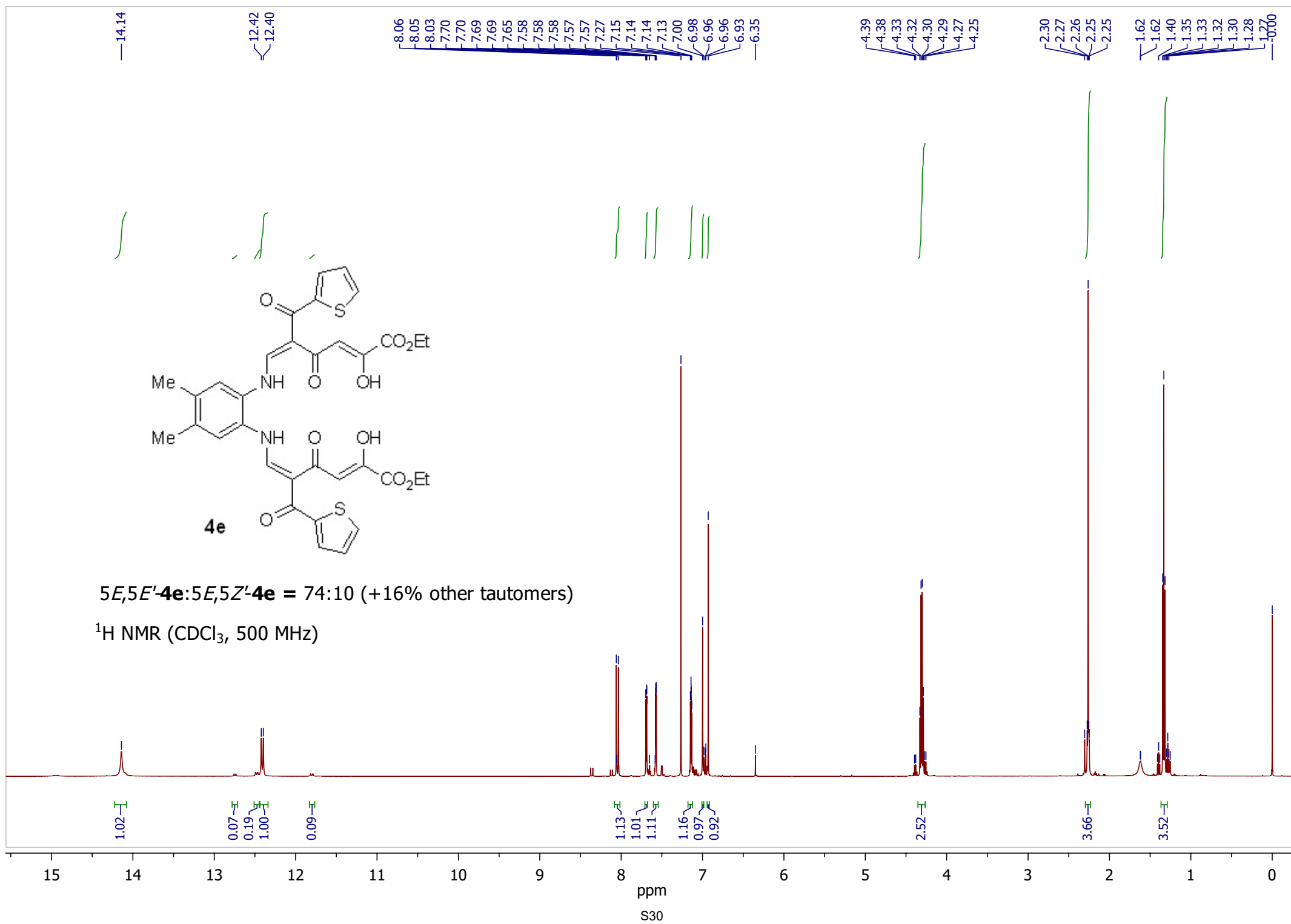




¹³C NMR (CDCl₃, 100 MHz)

- 193.73
- 184.99
- 162.32
- 160.84
- 153.01
- 144.74
- 133.98
- 133.43
- 131.53
- 128.05
- 127.80
- 127.62
- 120.36
- 113.49
- 103.21
- 77.36
- 77.24
- 77.04
- 76.72
- 62.20
- 14.07





193.53
193.48

185.04

162.38
160.52

153.44
153.22

144.89

136.90
133.85

133.79
133.39

129.05
128.00

121.54

113.03

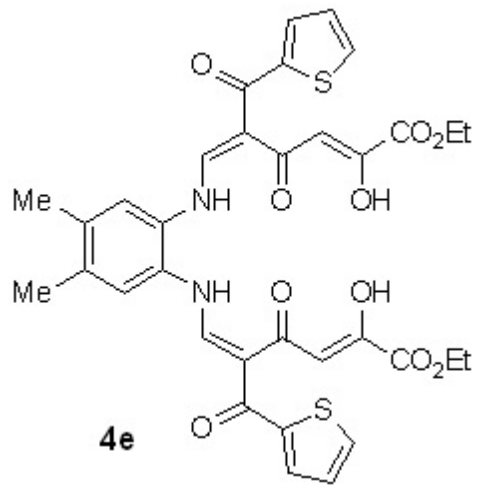
103.28

77.37
77.26
77.06

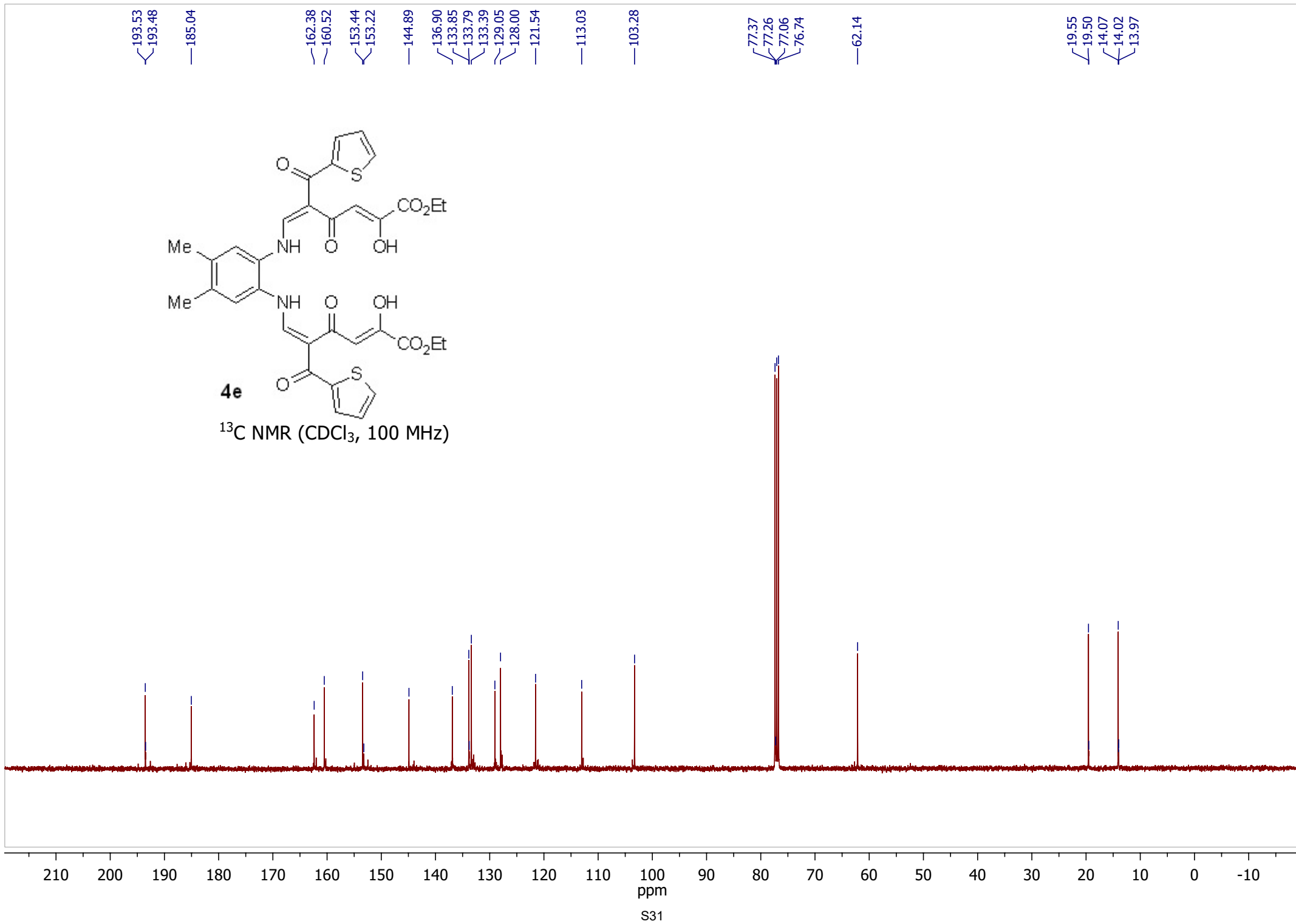
62.14

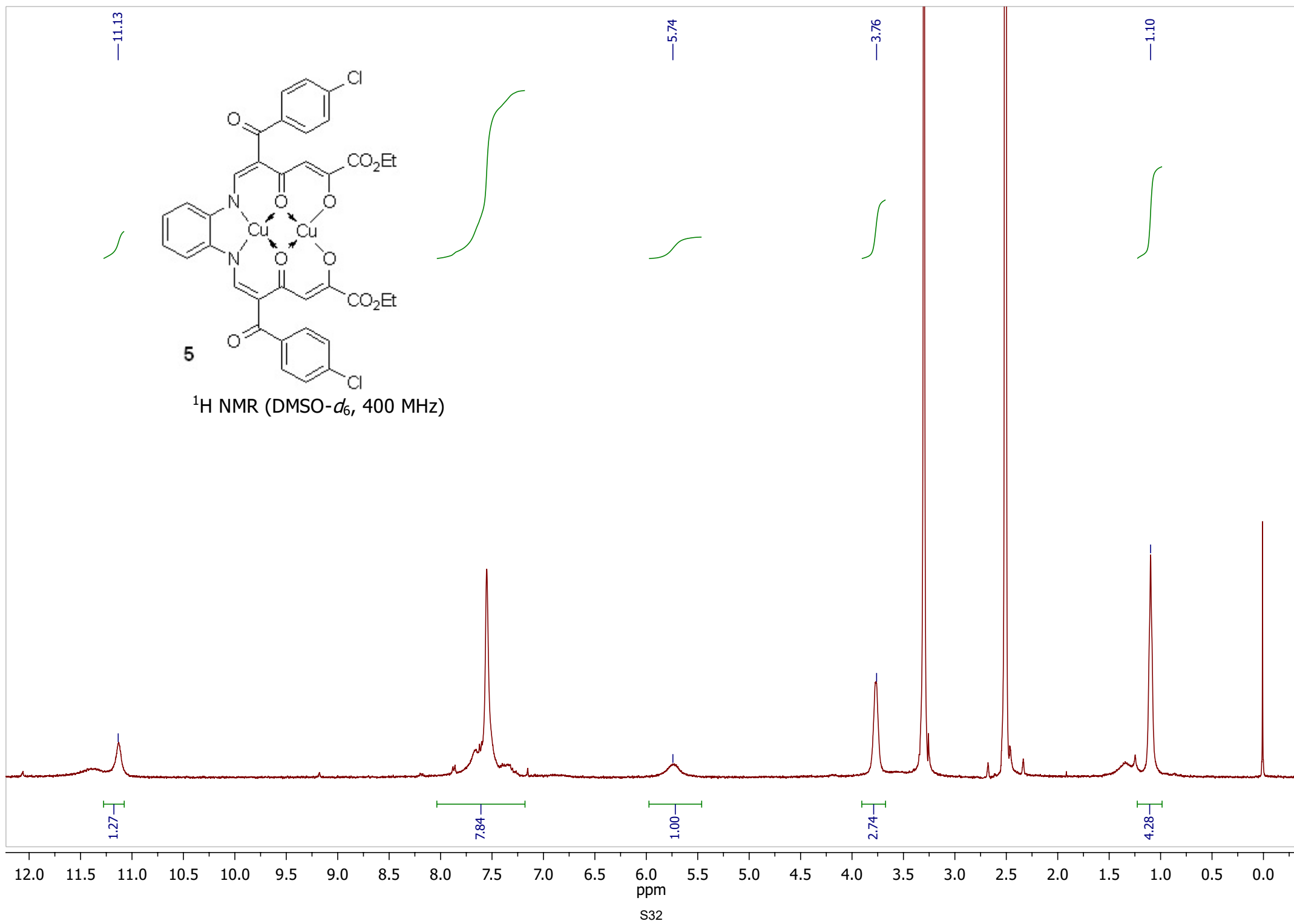
19.55
19.50

14.07
14.02
13.97



¹³C NMR (CDCl₃, 100 MHz)





Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -0.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

162 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: 2-2 O: 1-200 Cl: 2-2 Cu: 2-2

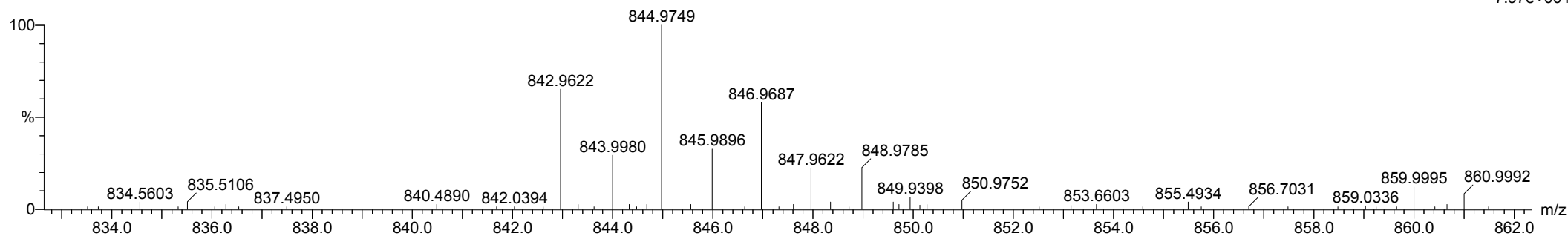
OD 18.11.2019

HRMS-CB-65 10 (0.088)

18-Nov-2019 13:09:37

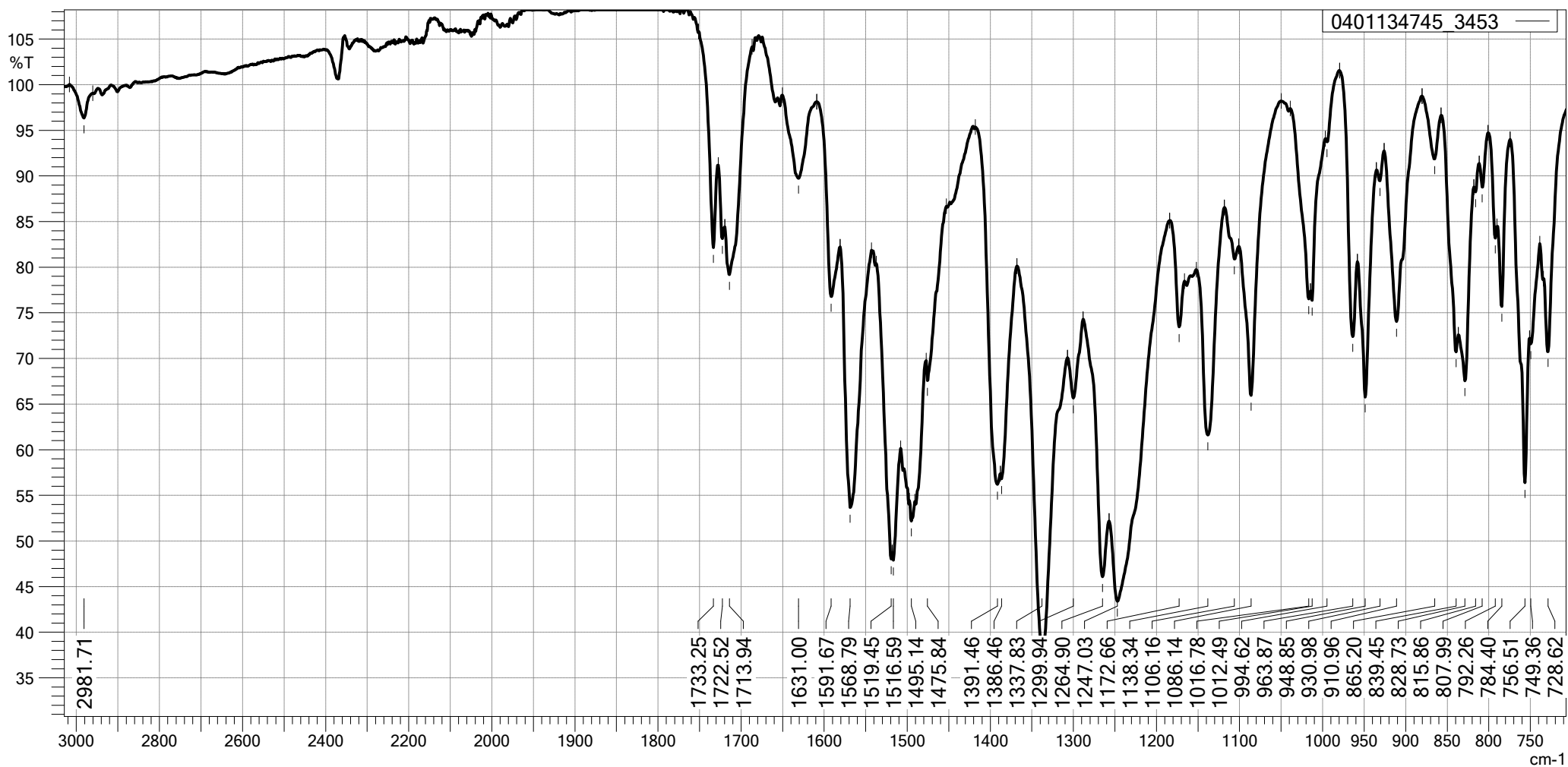
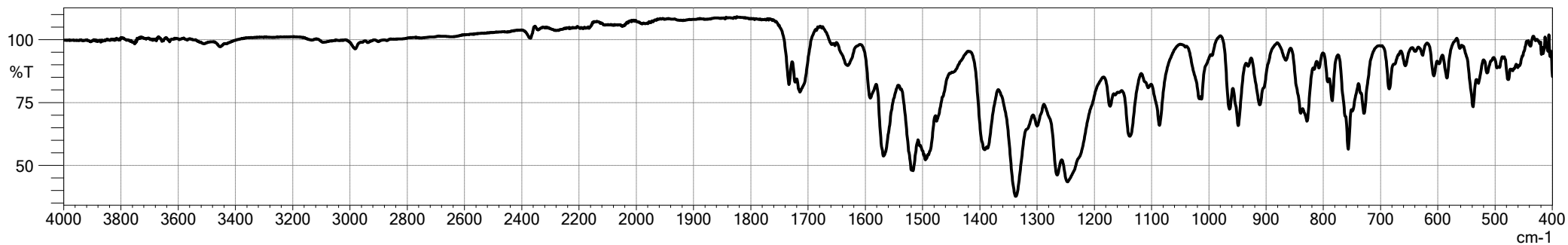
TOF MS ES+

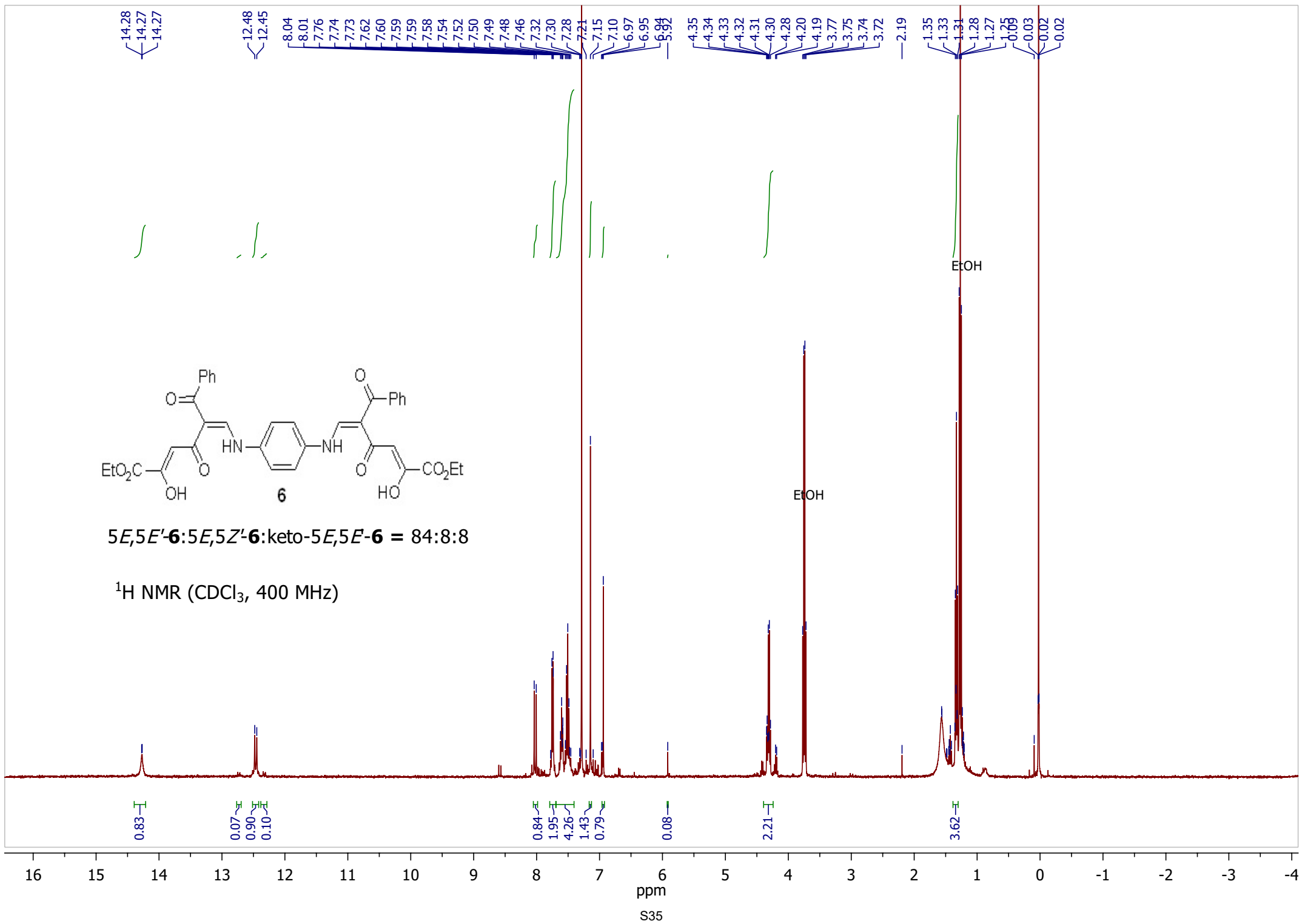
7.97e+001

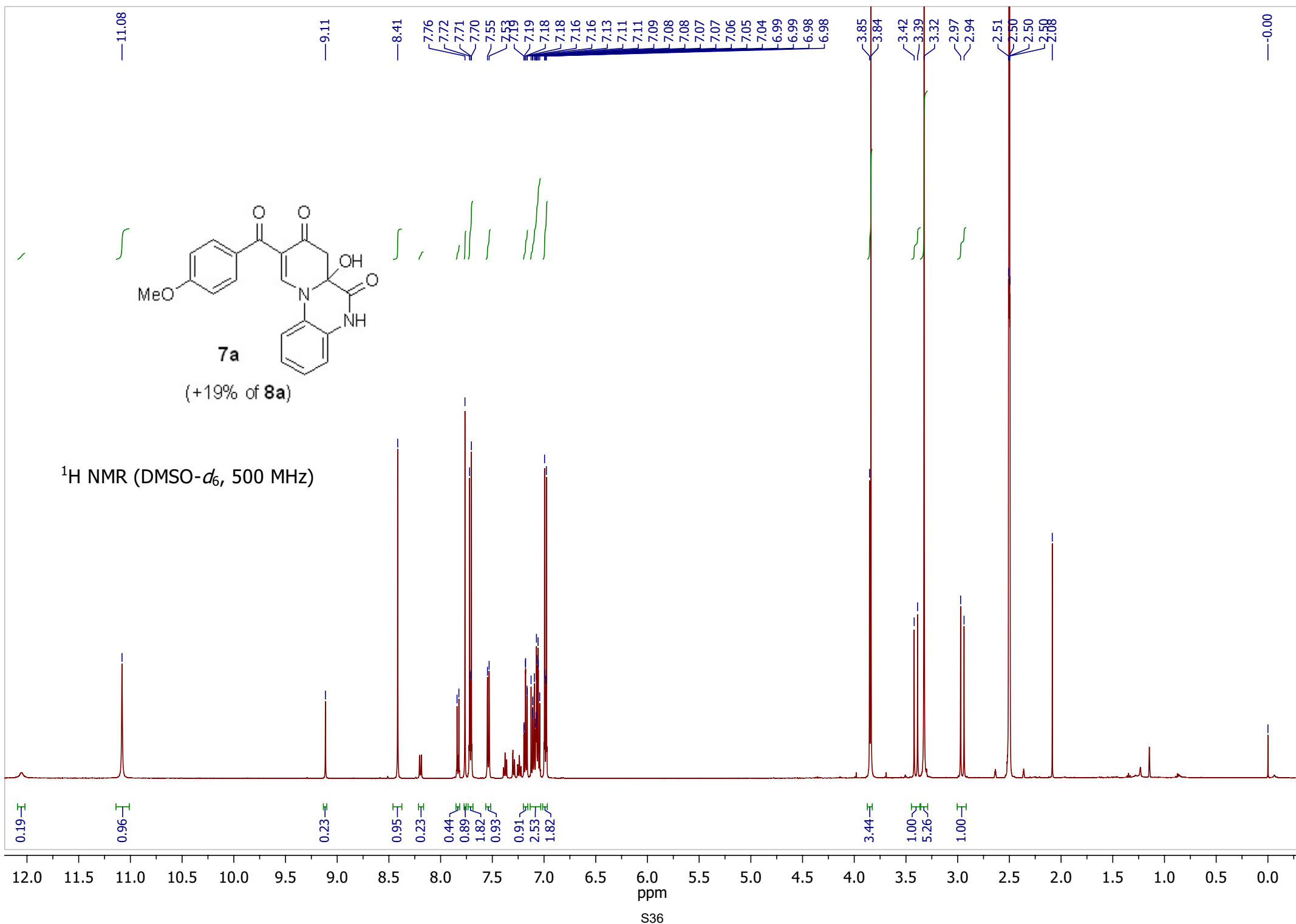


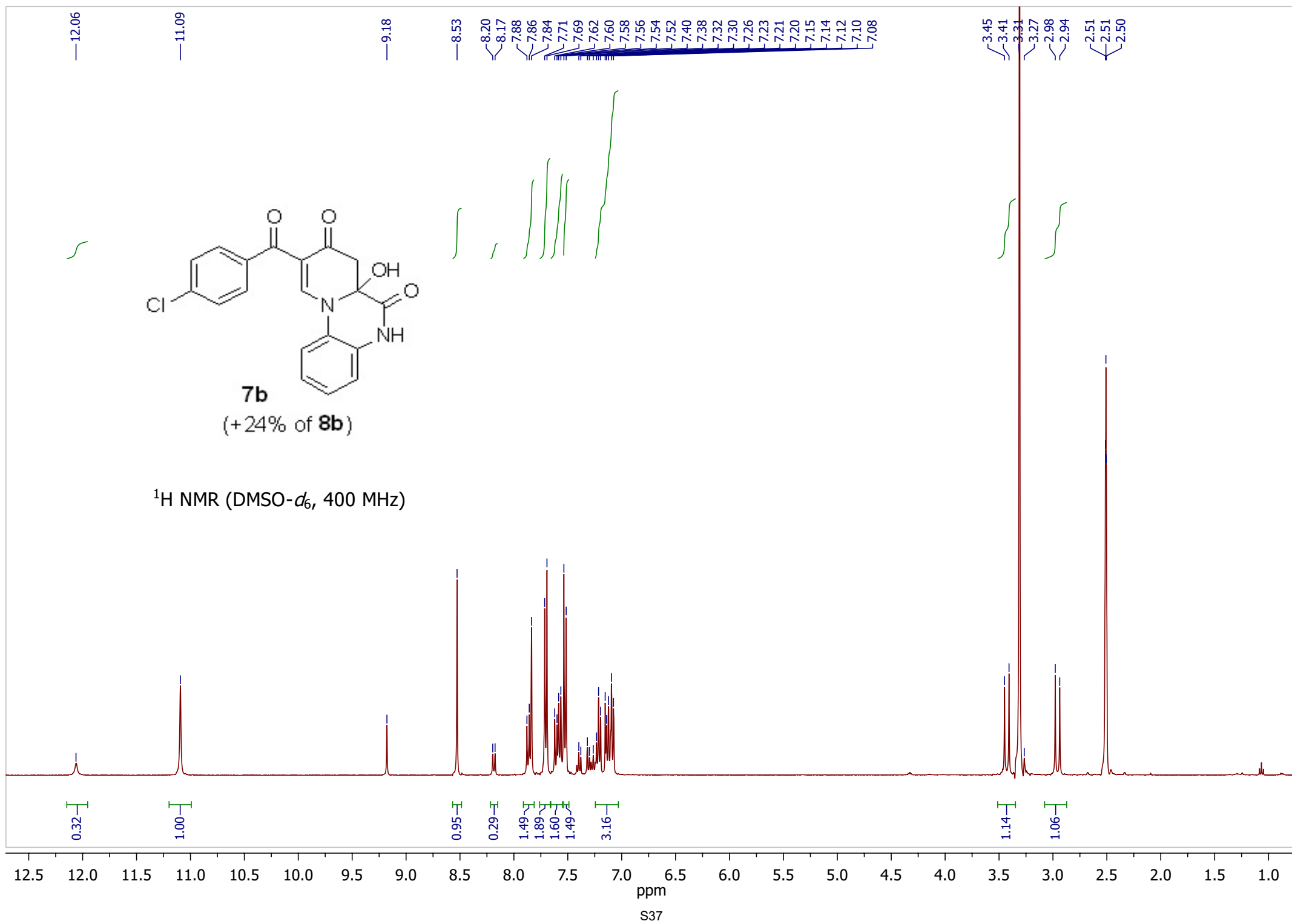
Minimum: -0.5
 Maximum: 5.0 5.0 50.0

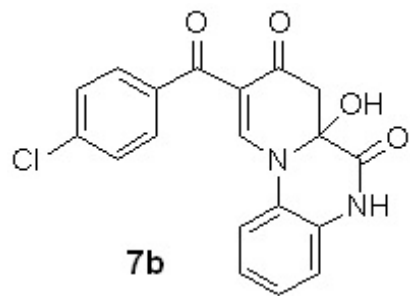
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
842.9622	842.9635	-1.3	-1.5	23.5	25.3	0.1	C36 H27 N2 O10 Cl2 Cu2
	842.9600	2.2	2.6	1.5	27.8	2.6	C18 H35 N2 O23 Cl2 Cu2



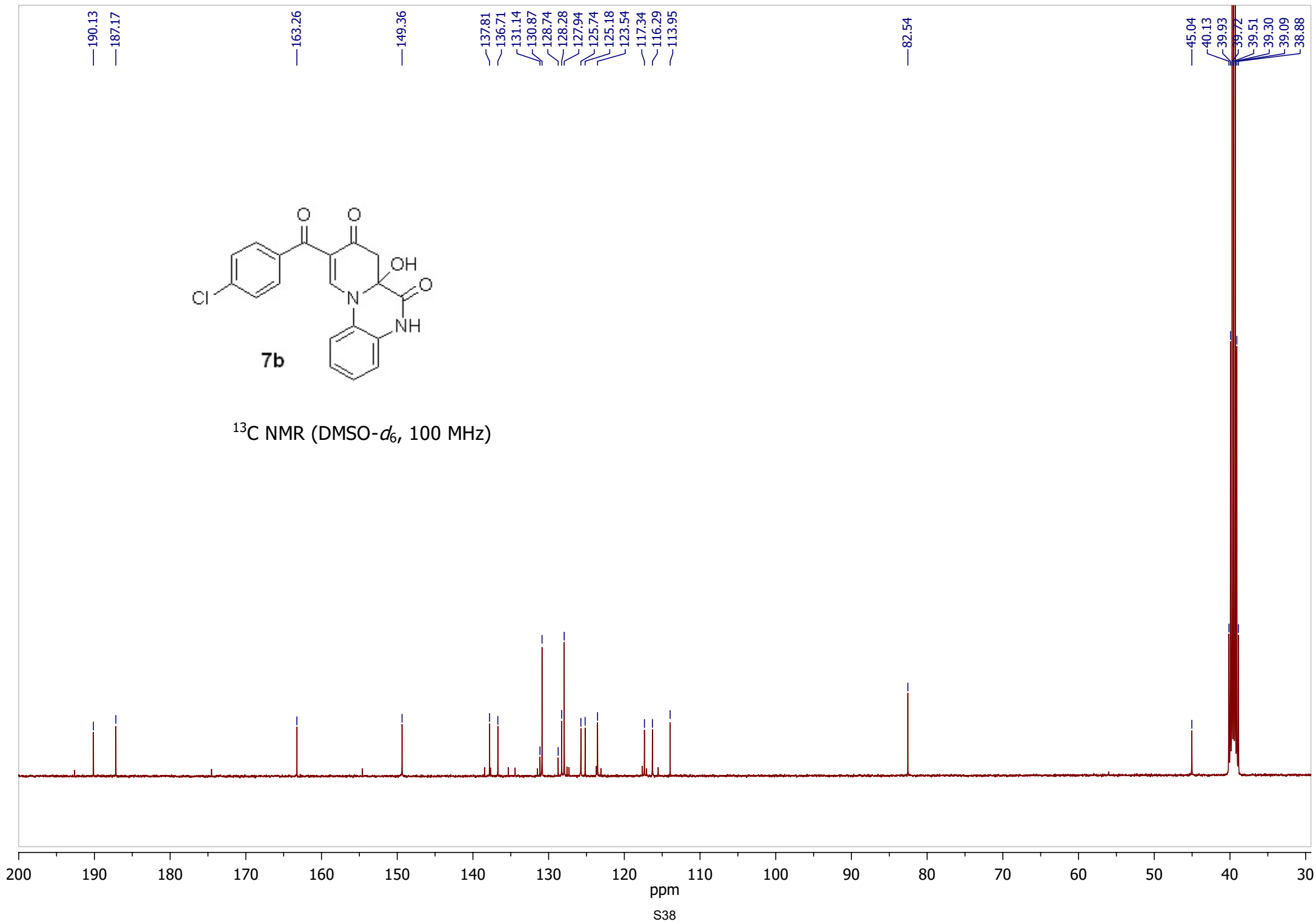


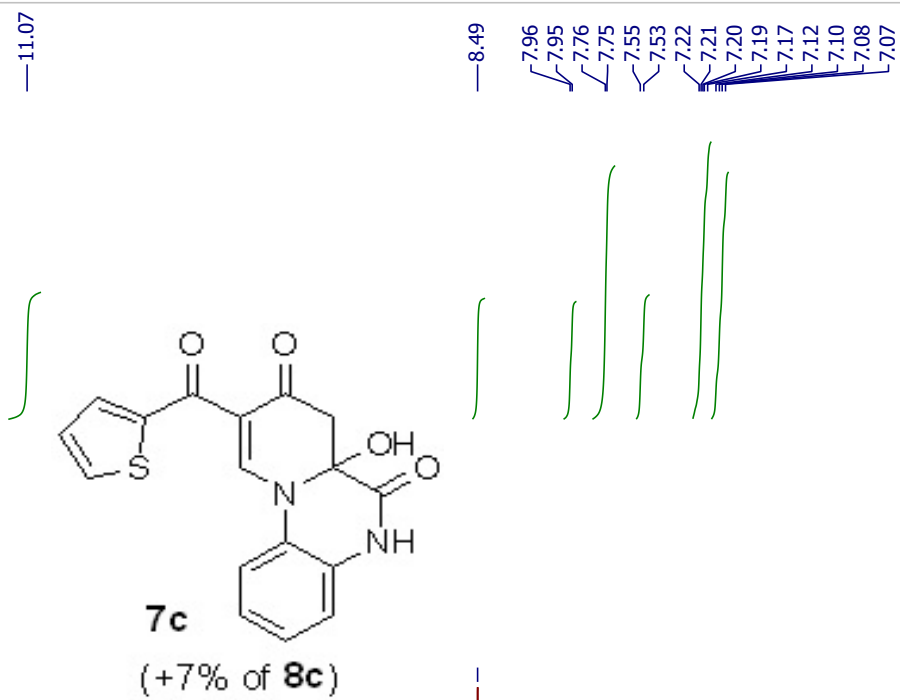




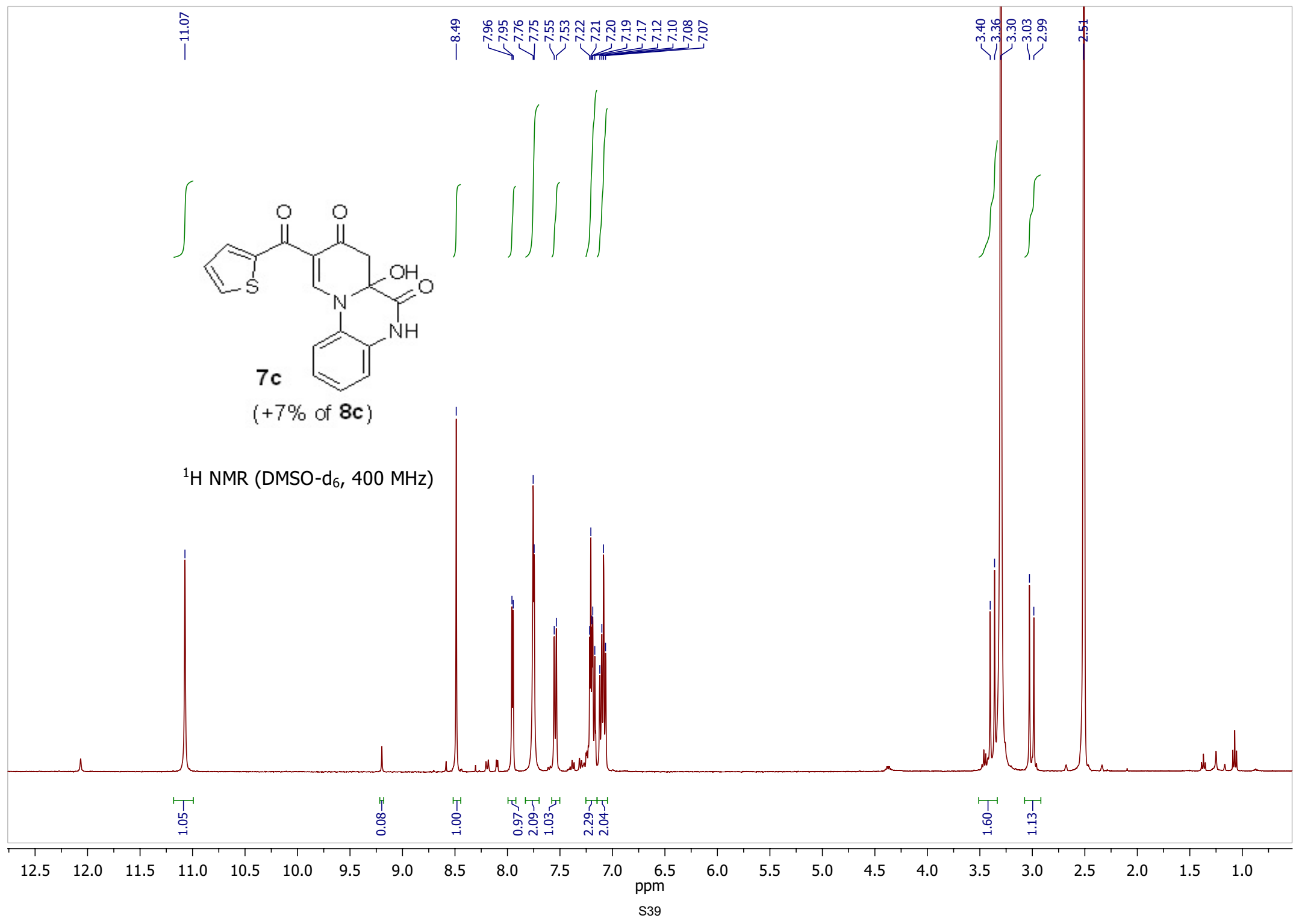


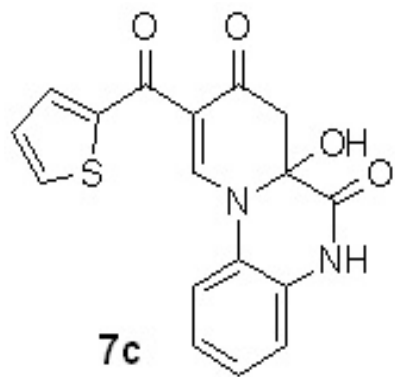
^{13}C NMR (DMSO- d_6 , 100 MHz)



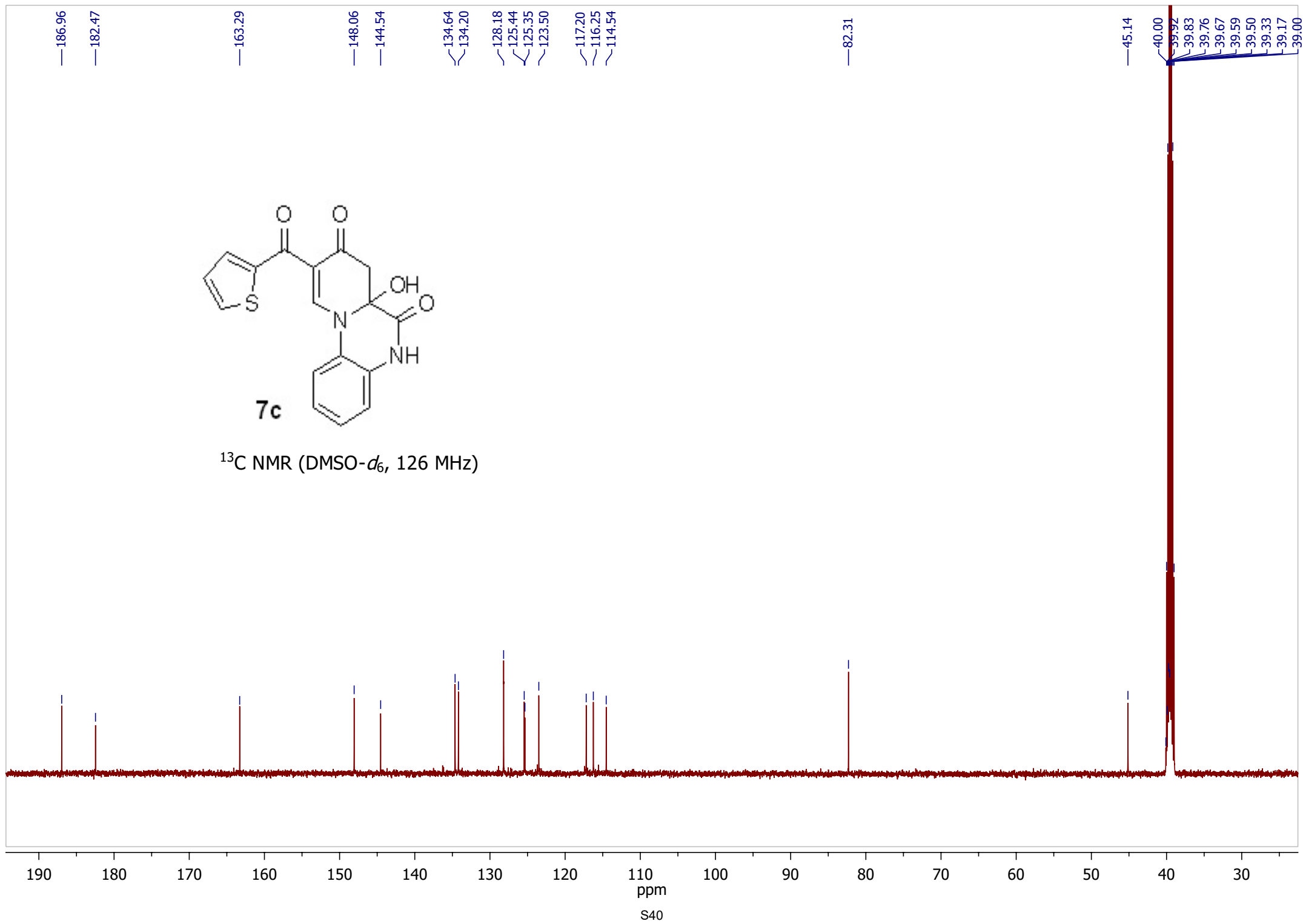


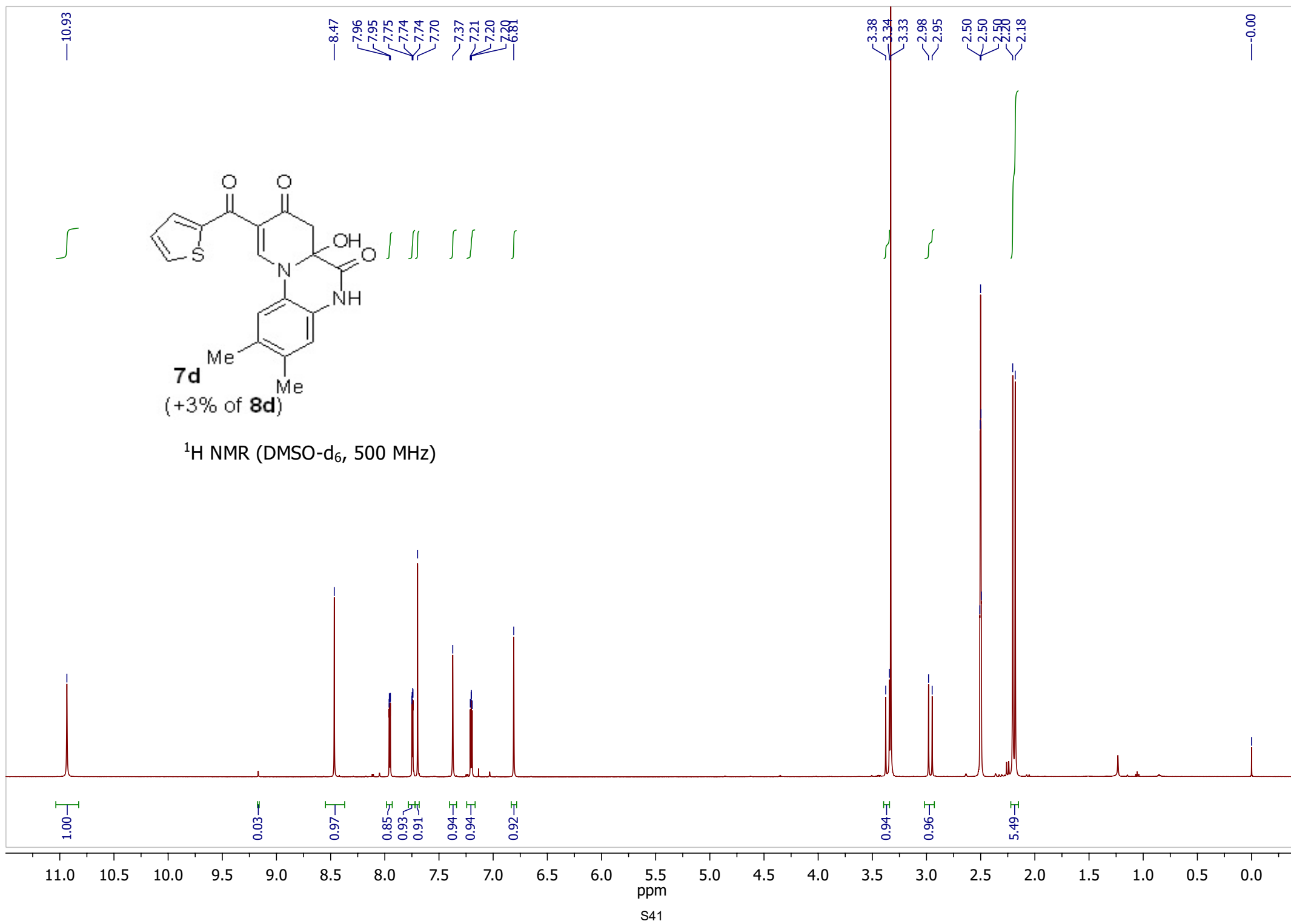
¹H NMR (DMSO-d₆, 400 MHz)

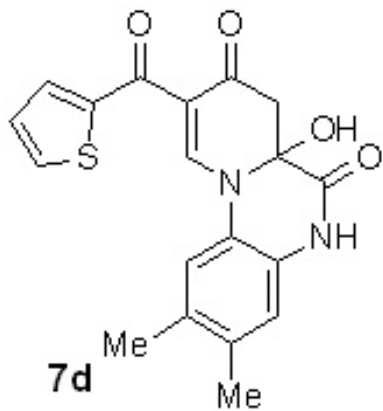




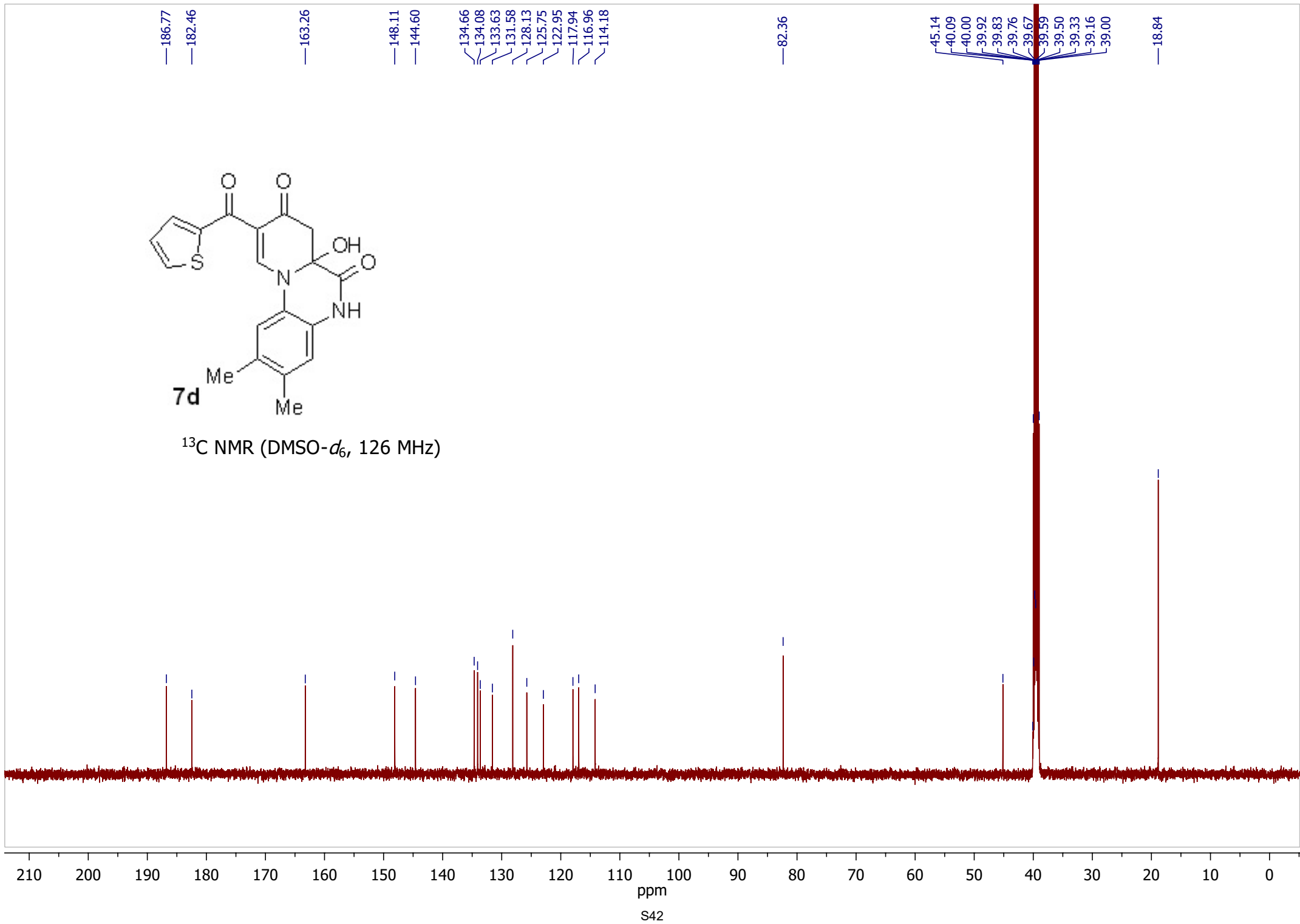
^{13}C NMR (DMSO- d_6 , 126 MHz)

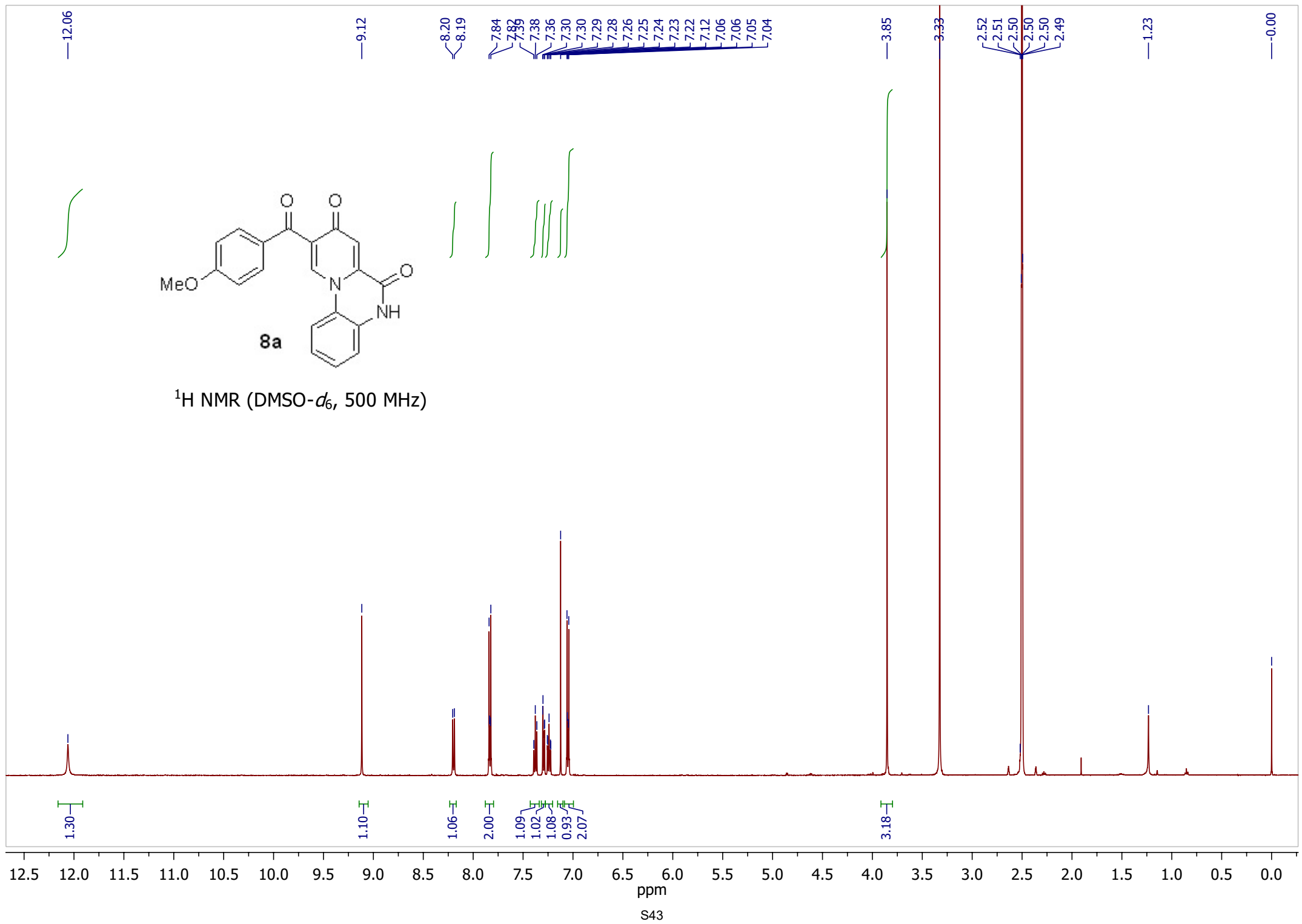


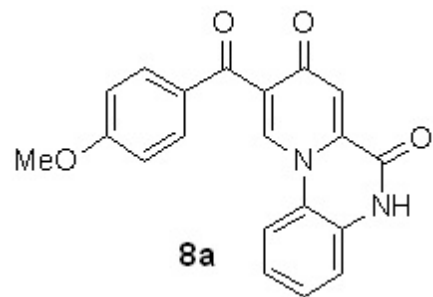




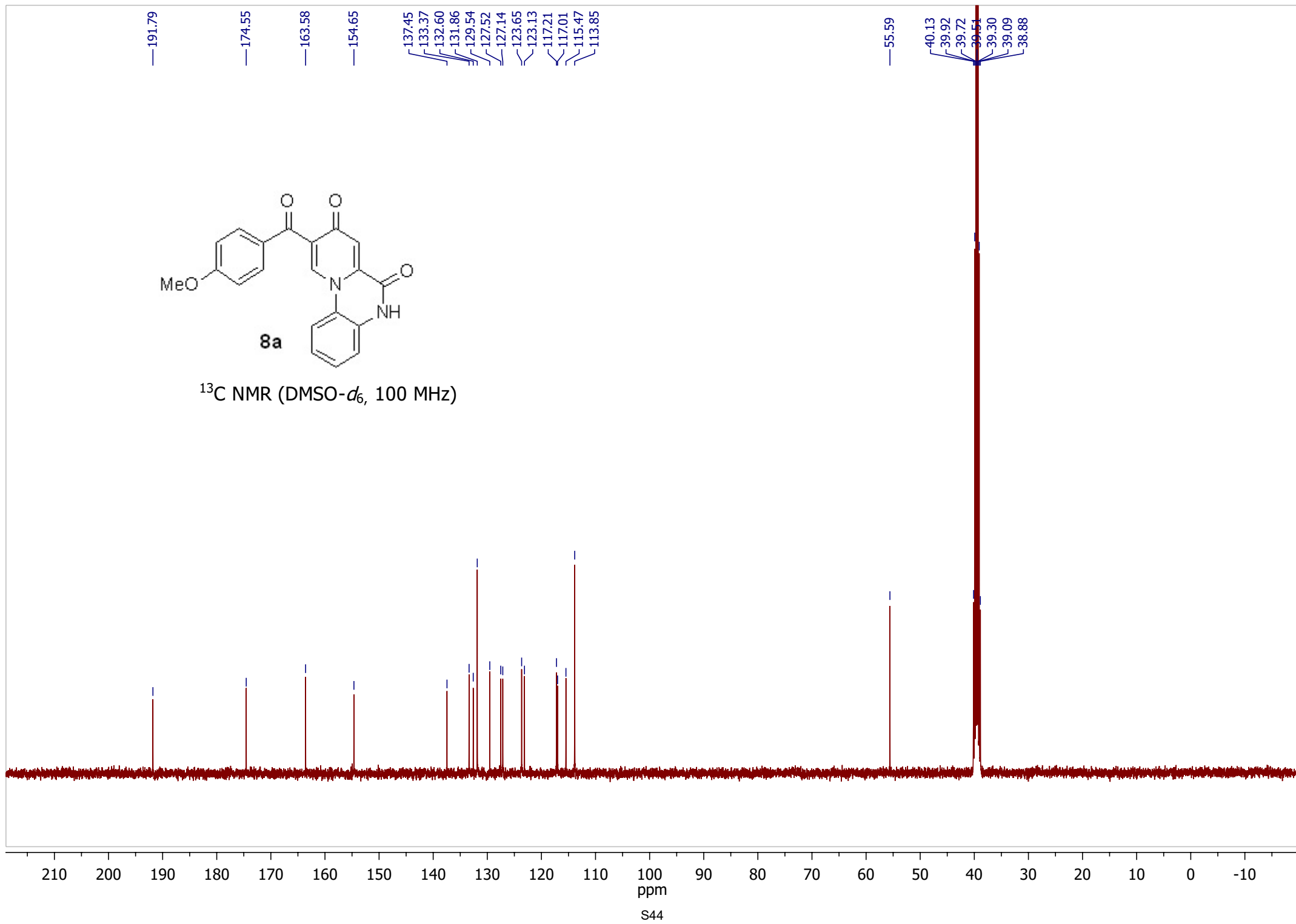
^{13}C NMR (DMSO- d_6 , 126 MHz)

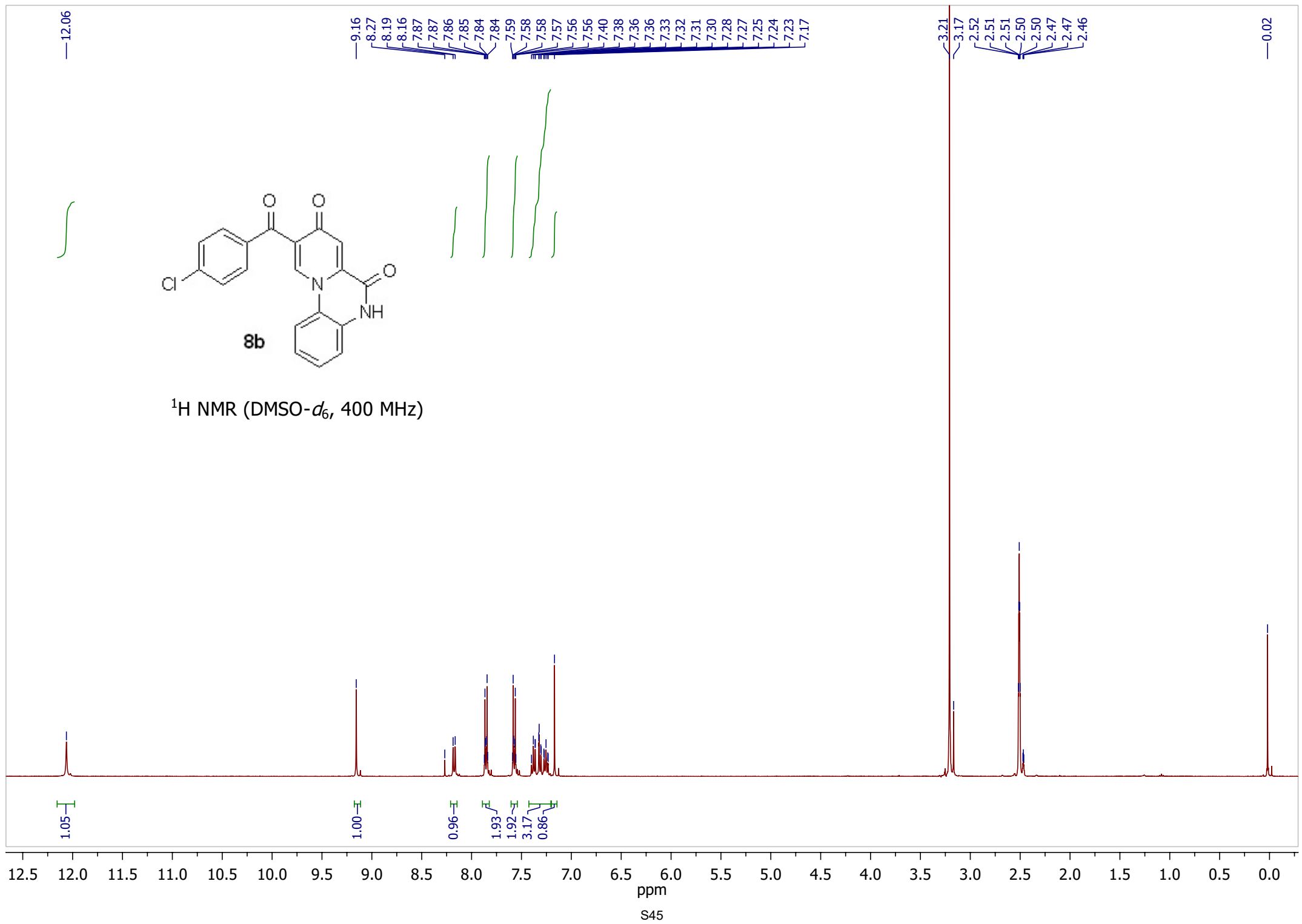


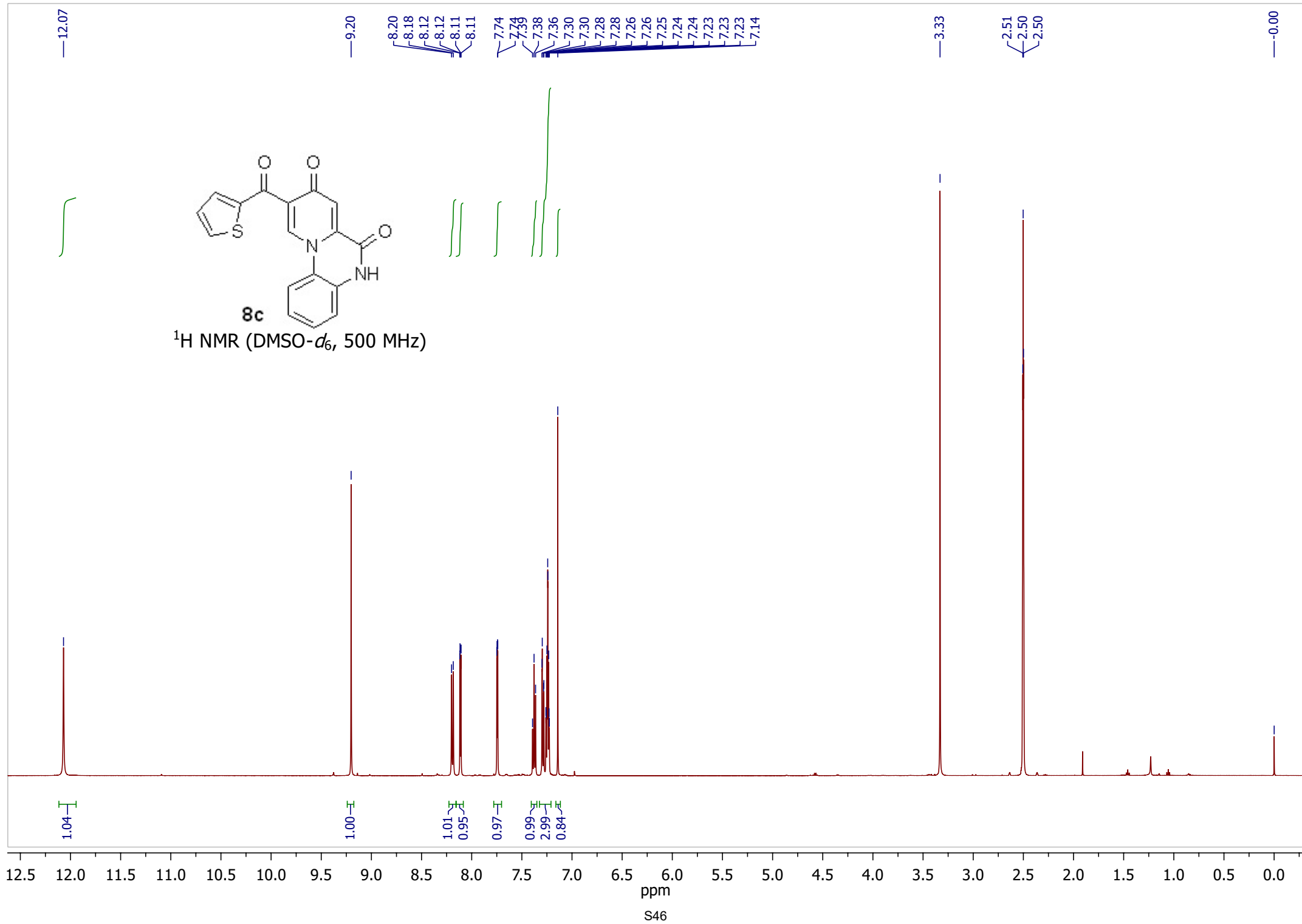
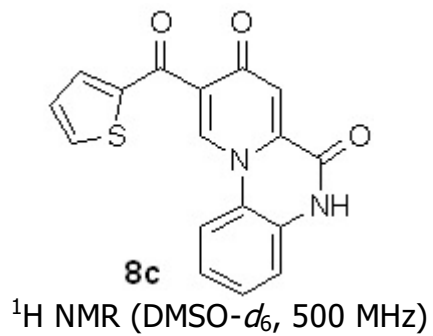


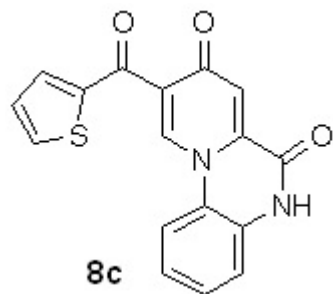


^{13}C NMR (DMSO- d_6 , 100 MHz)





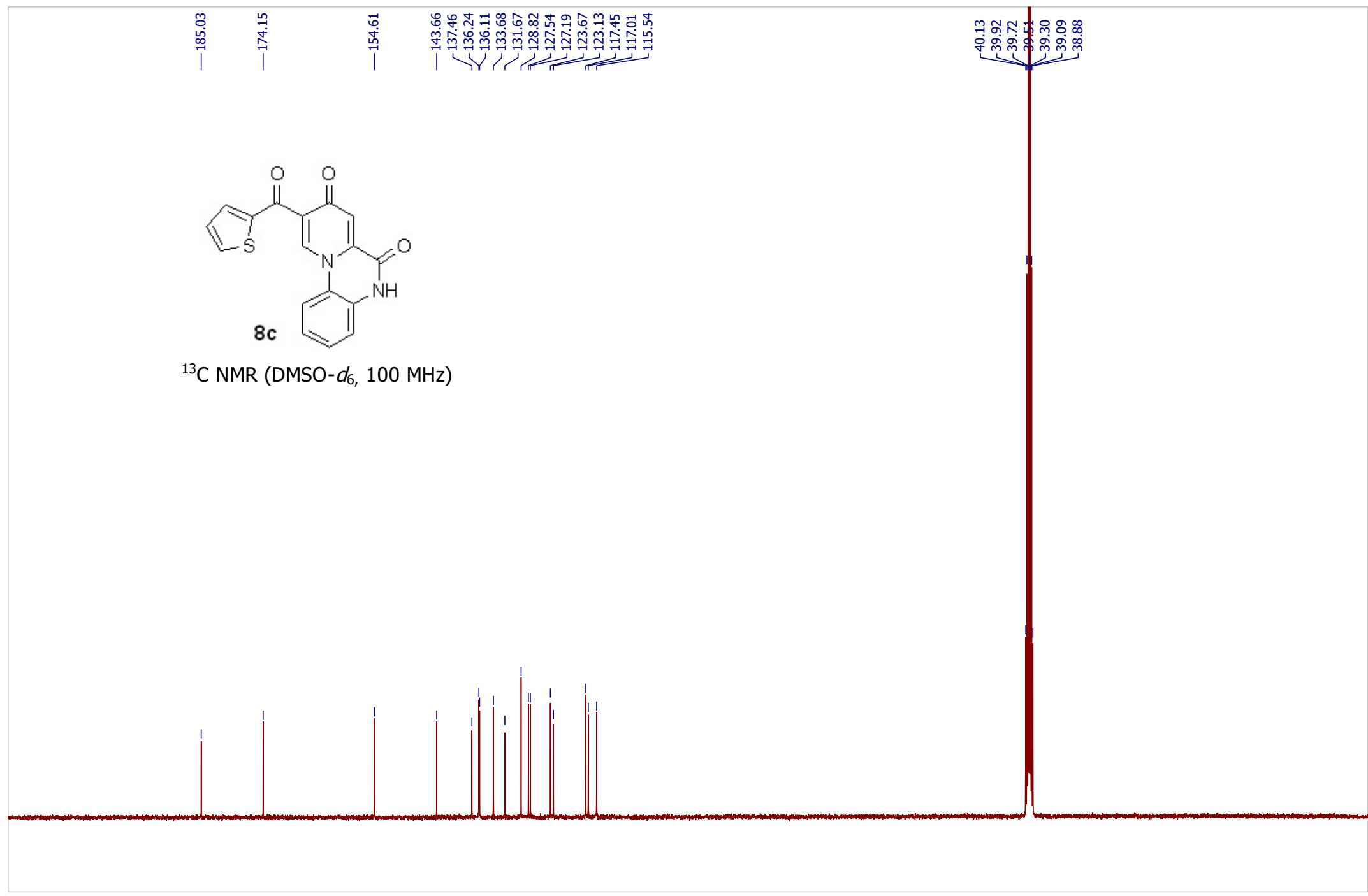




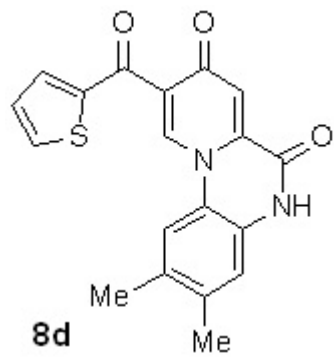
^{13}C NMR (DMSO- d_6 , 100 MHz)

185.03
174.15
154.61
143.66
137.46
136.24
136.11
133.68
131.67
128.82
127.54
127.19
123.67
123.13
117.45
117.01
115.54

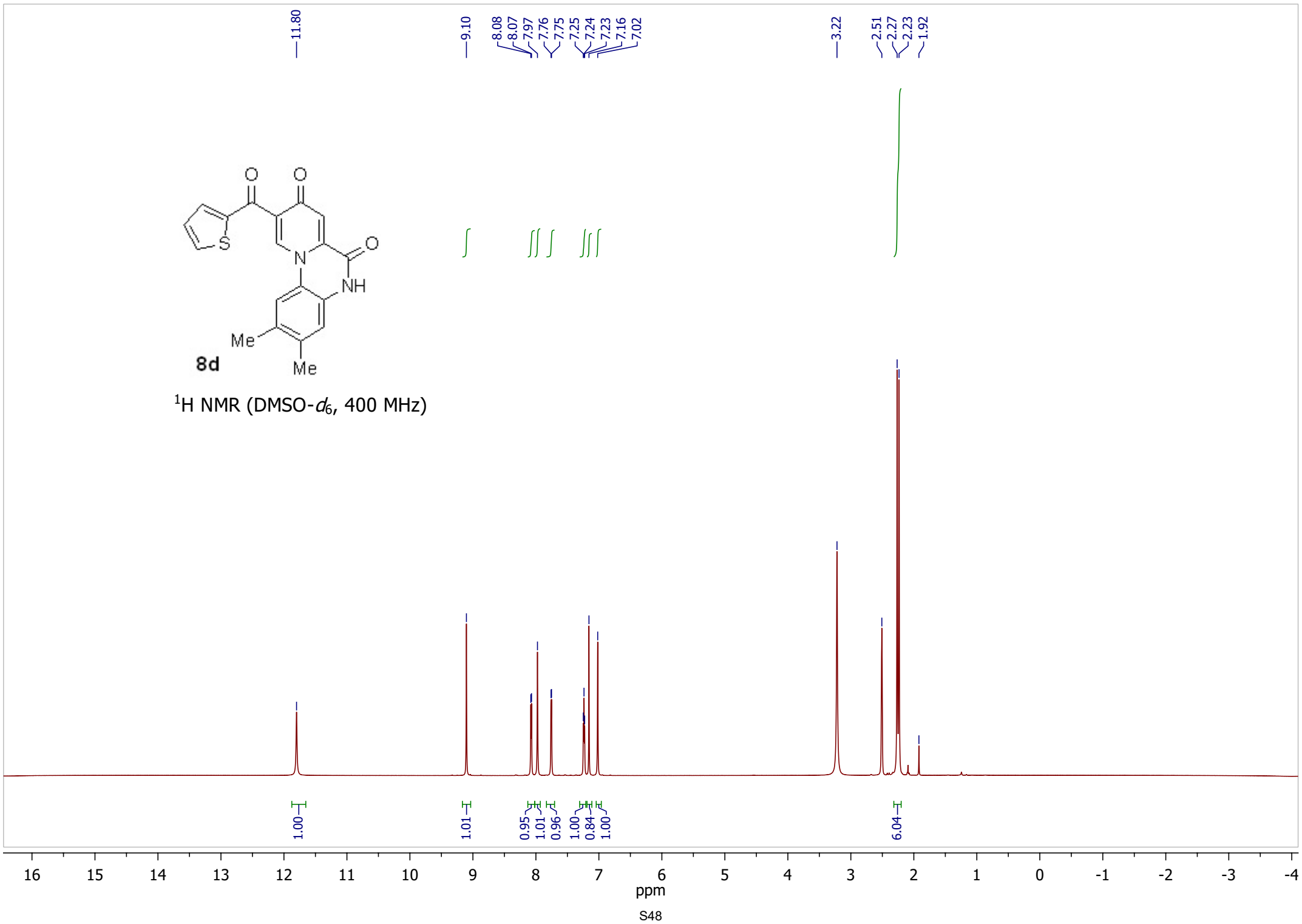
40.13
39.92
39.72
39.54
39.30
39.09
38.88



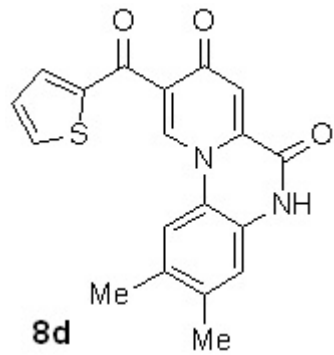
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10



^1H NMR (DMSO- d_6 , 400 MHz)



185.09
173.95
154.42
143.67
137.26
135.95
135.82
135.80
133.41
132.33
131.87
128.70
125.10
120.80
117.63
117.36
115.90



¹³C NMR (DMSO-*d*₆, 100 MHz)

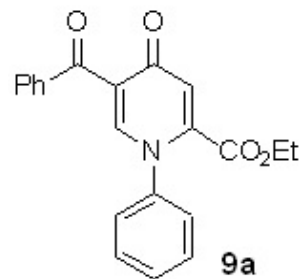
40.32
40.11
39.90
39.69
39.49
39.28
39.07

18.82
18.78

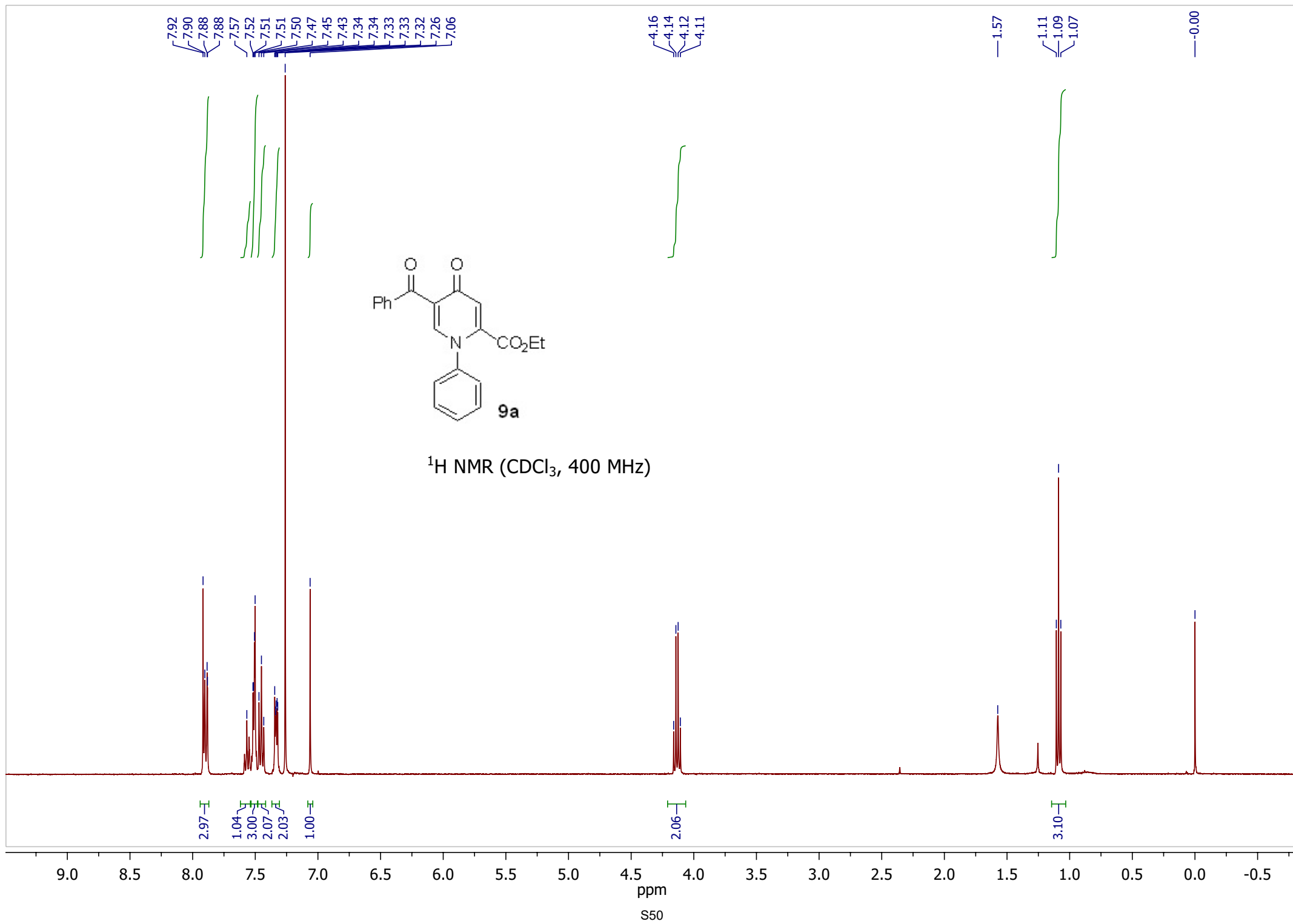
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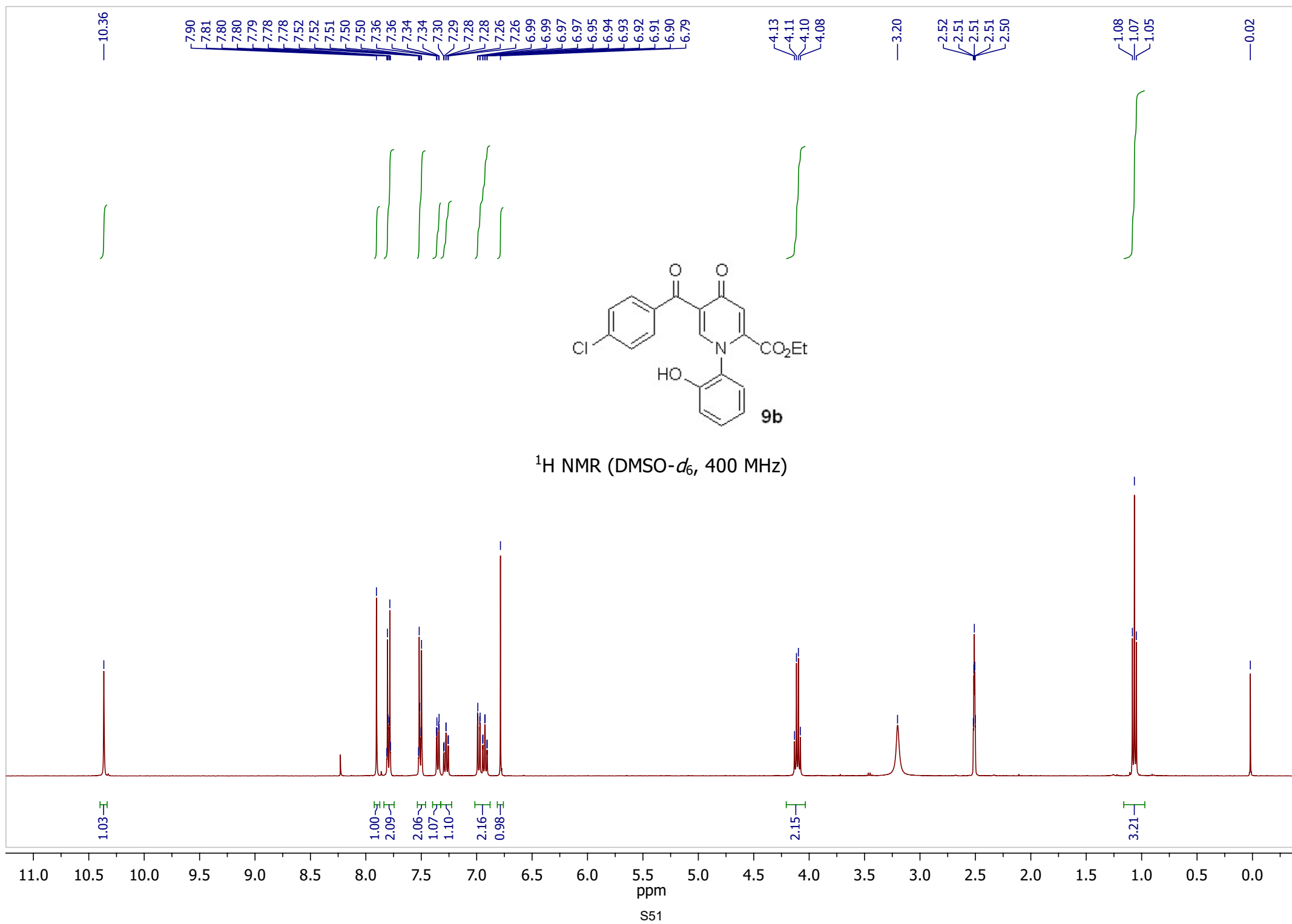
ppm

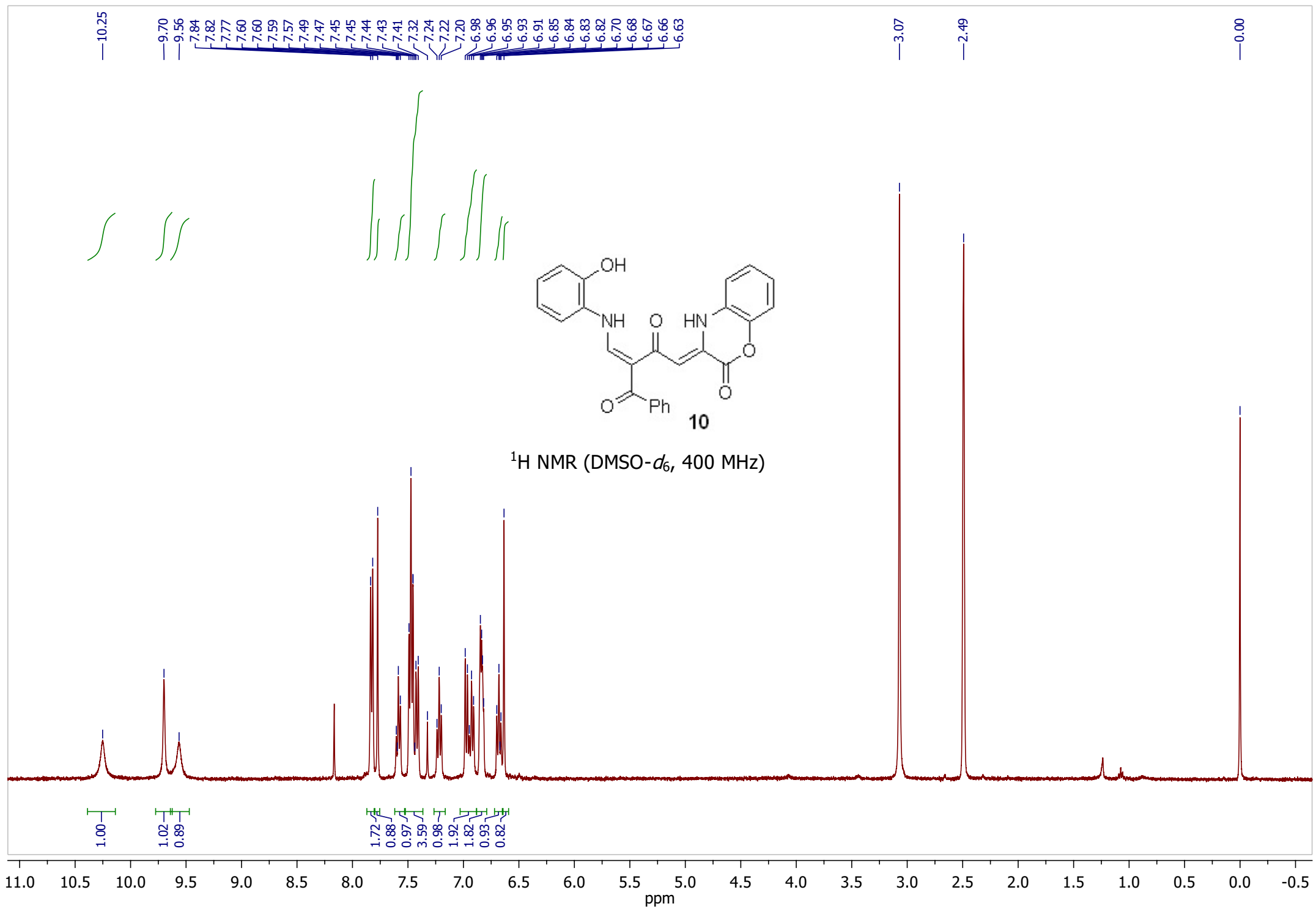
S49

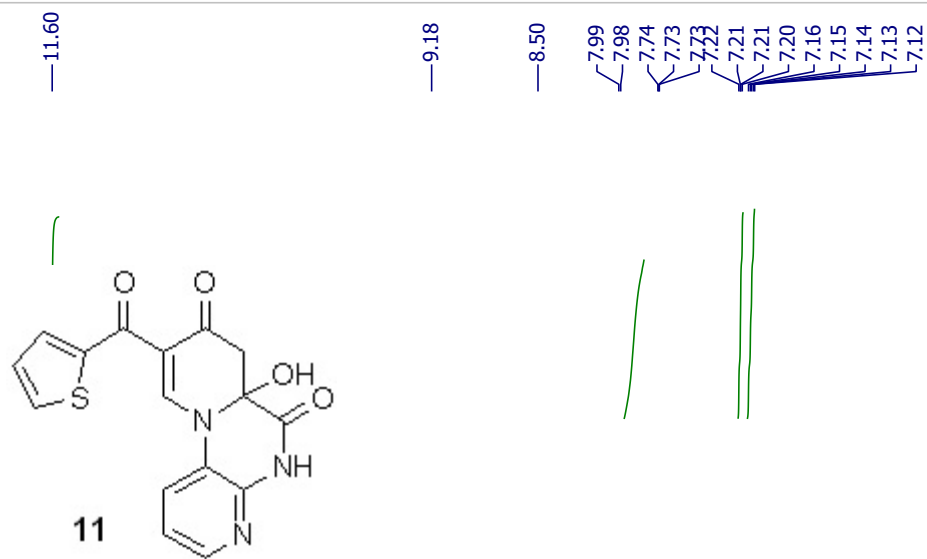


$^1\text{H NMR}$ (CDCl_3 , 400 MHz)

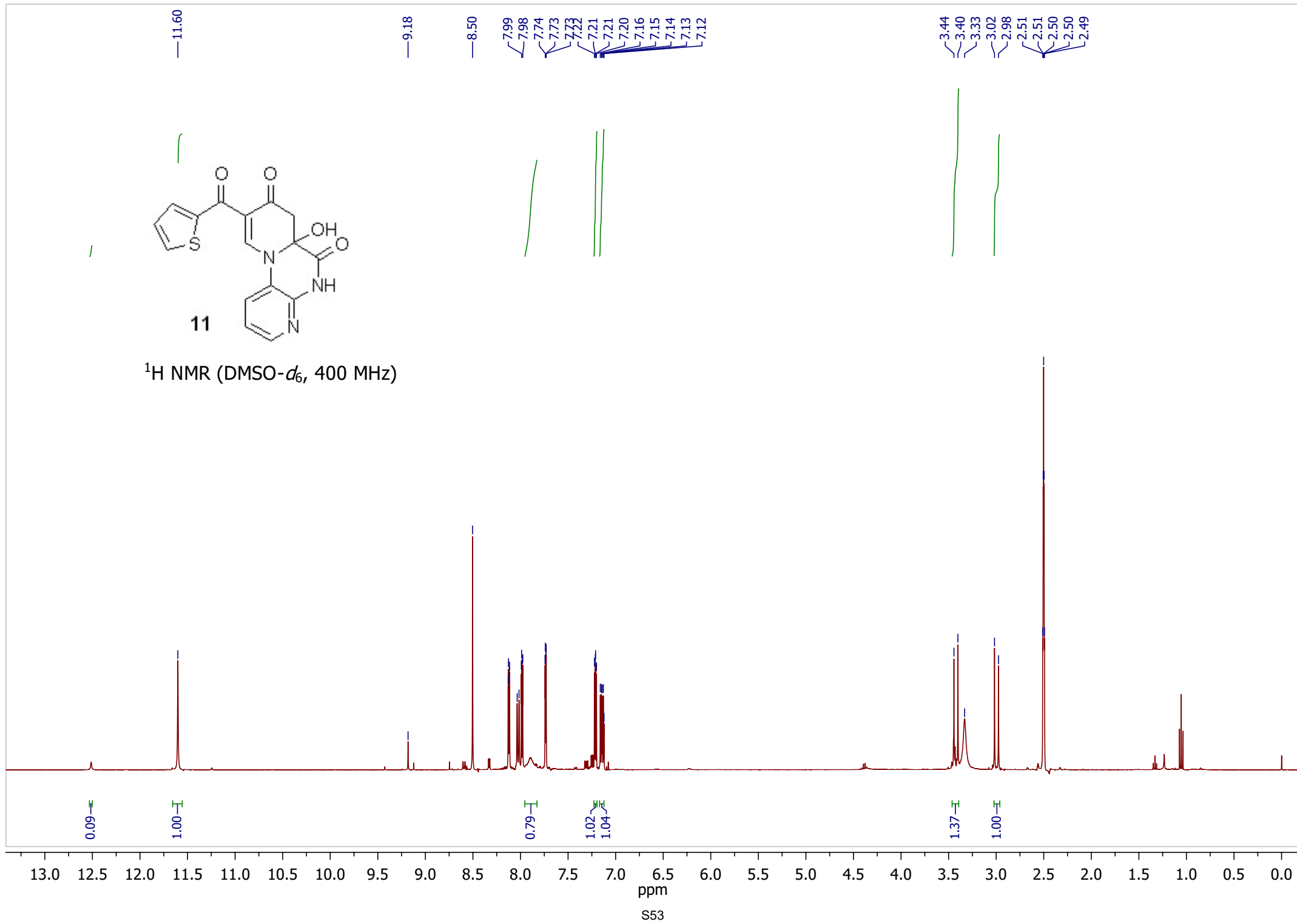


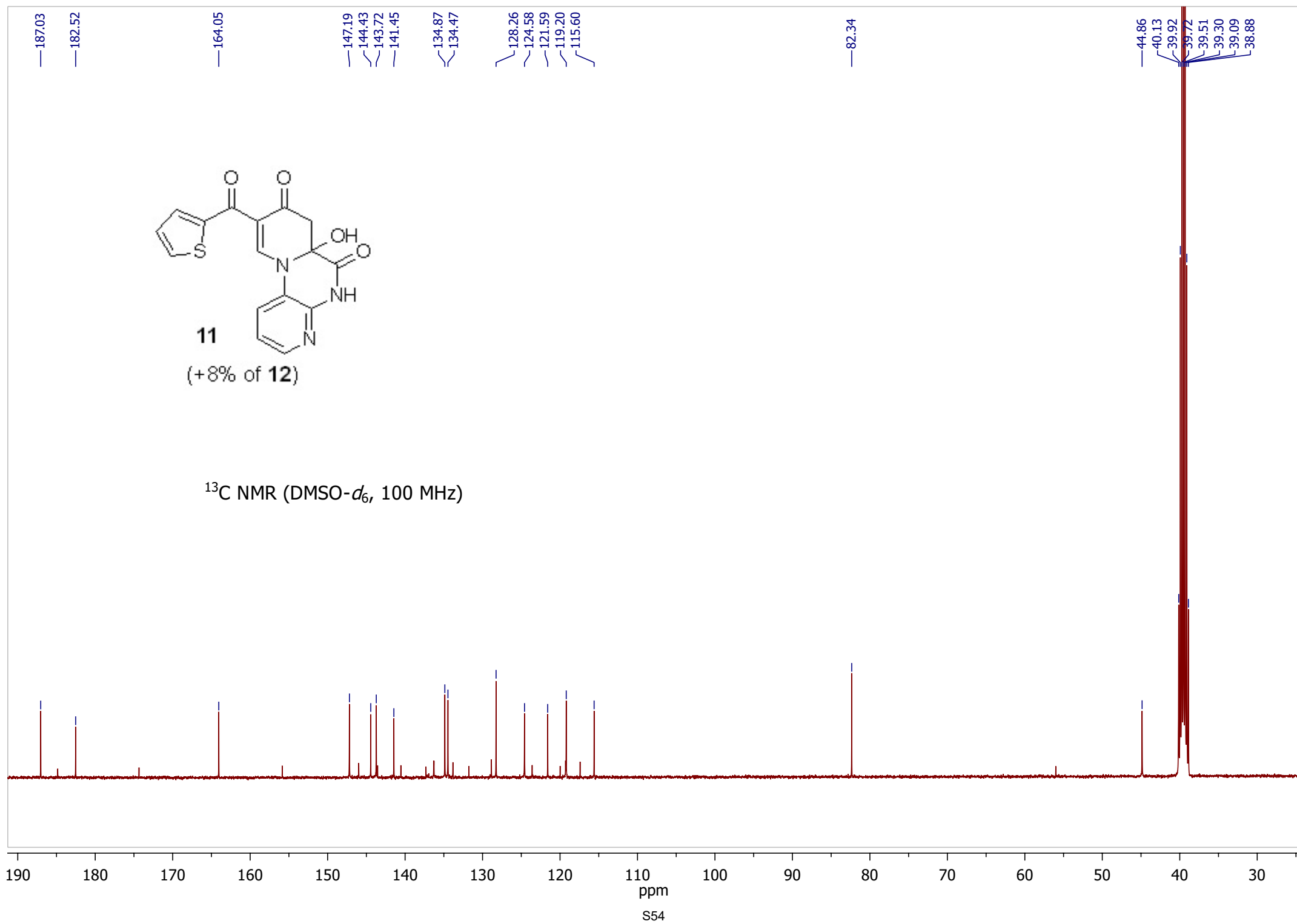


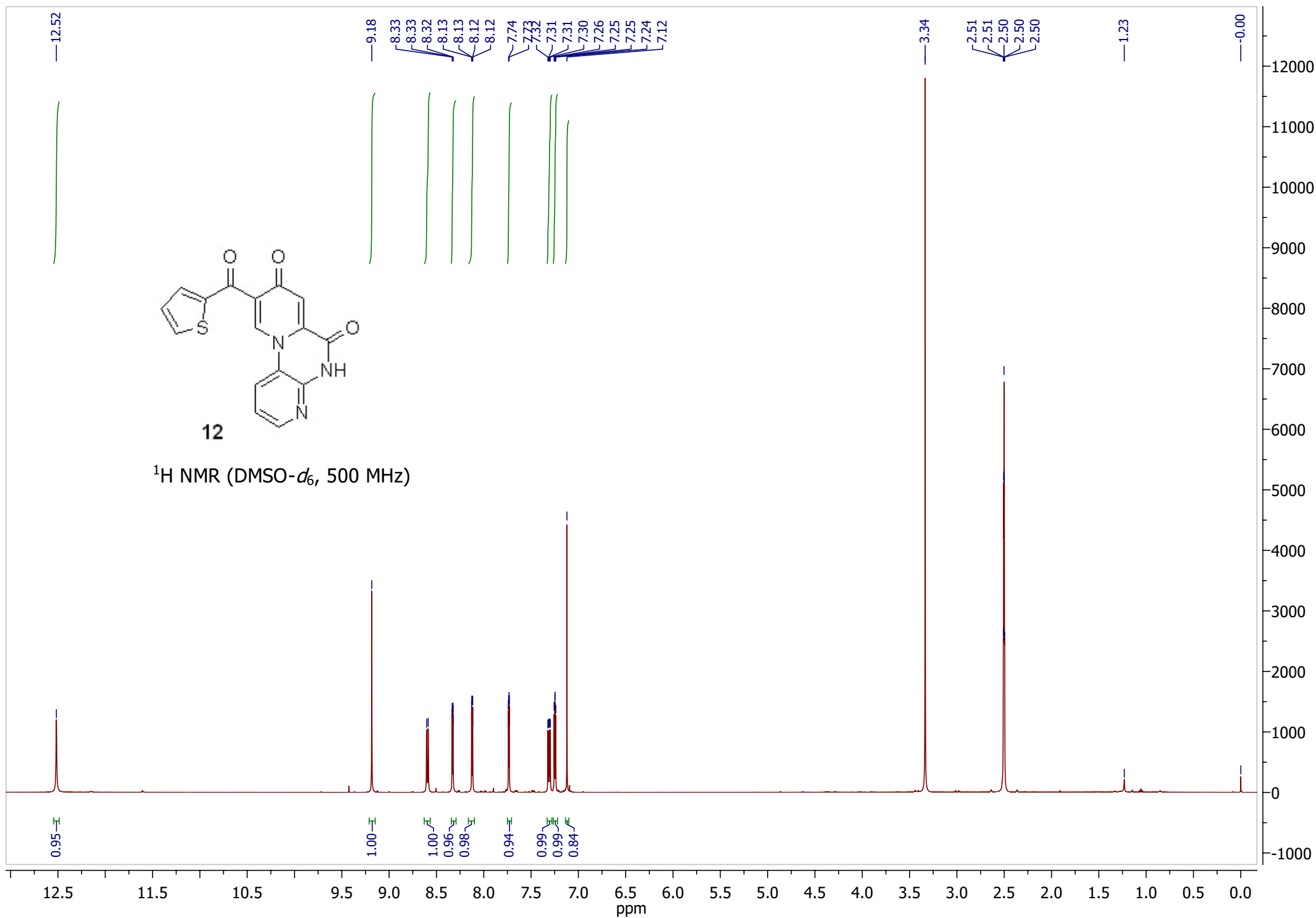


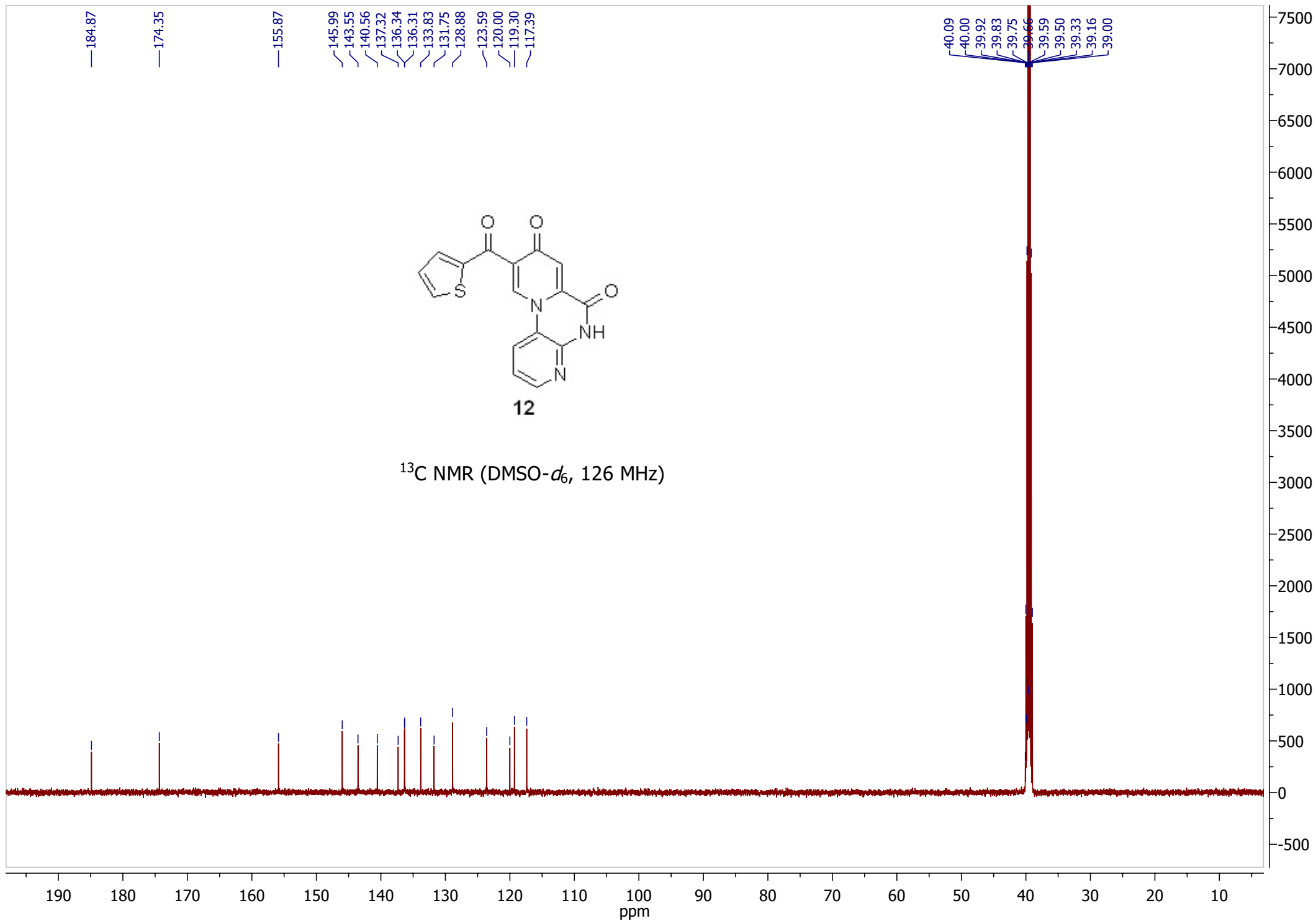


^1H NMR (DMSO- d_6 , 400 MHz)

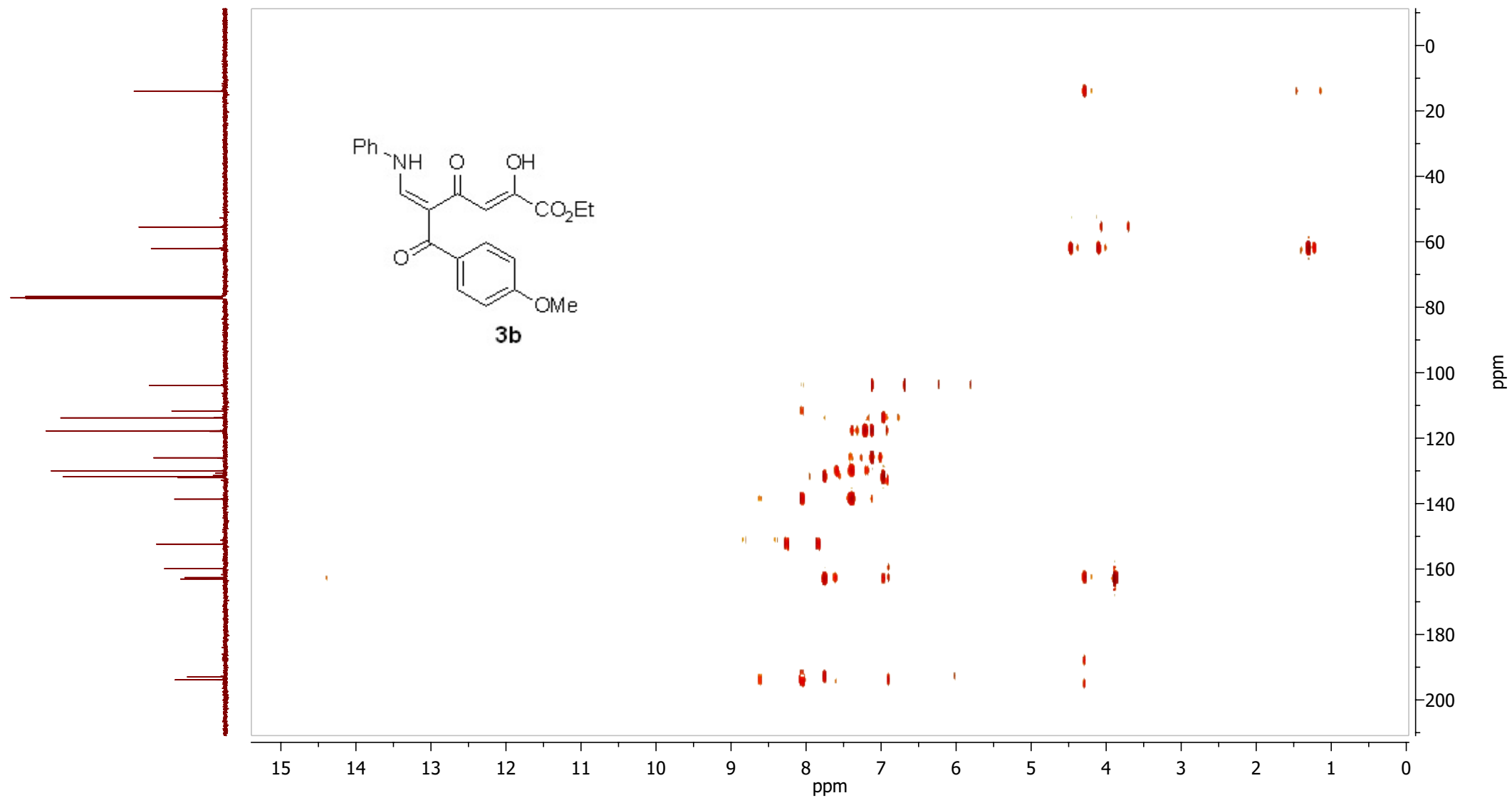








2D ^1H - ^{13}C HMBC (CDCl_3)



2D ^1H - ^{13}C HMBC (CDCl_3)

