#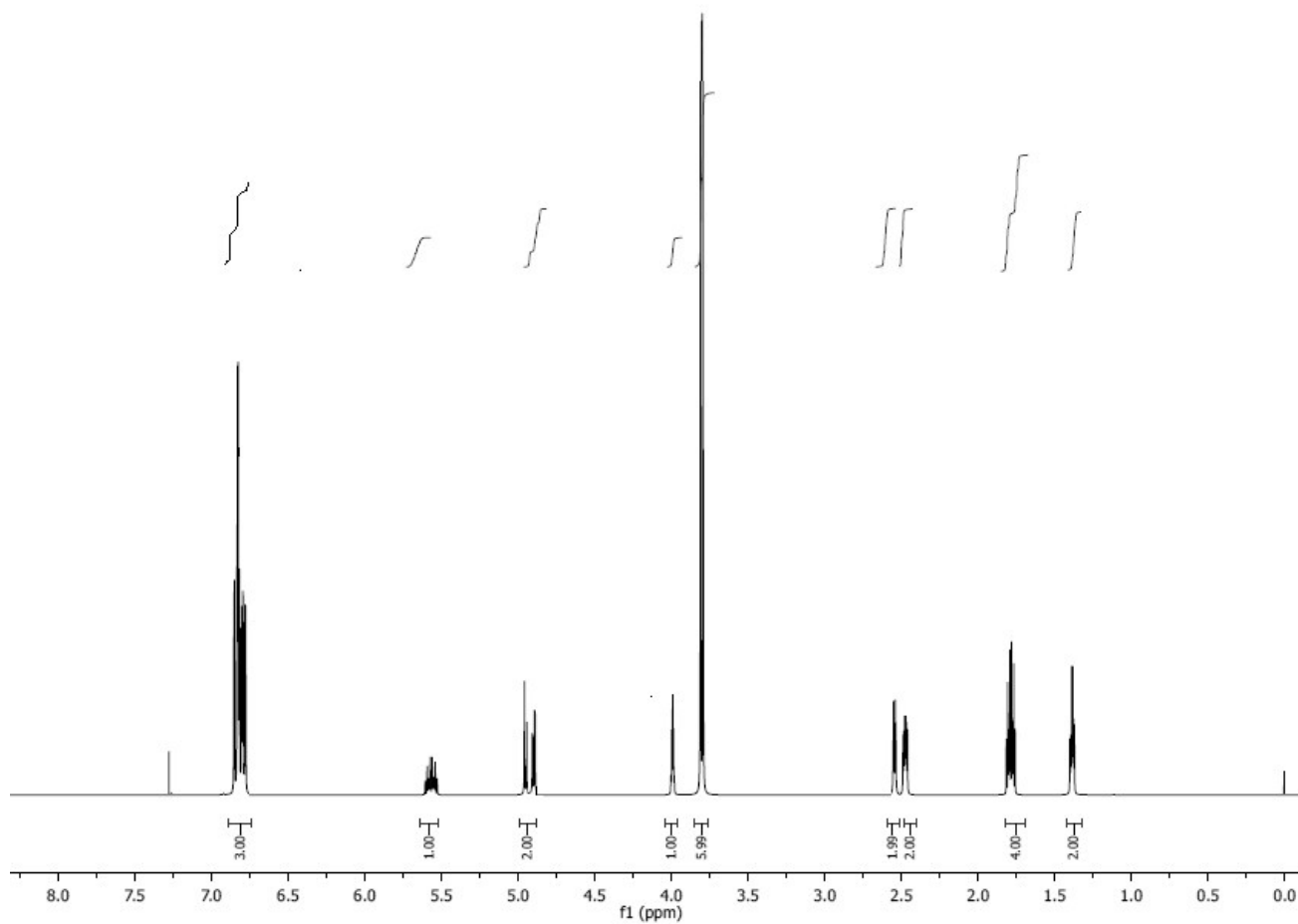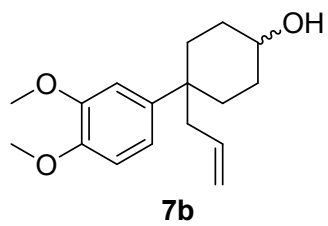 Total Synthesis of *Sceletium* Alkaloids (±)-Joubertinamine, (±)-Epijoubertinamine, (±)-Tortuosamine and Formal Synthesis of (±)-Mesembrine, (±)-*N*-Formyltortuosamine

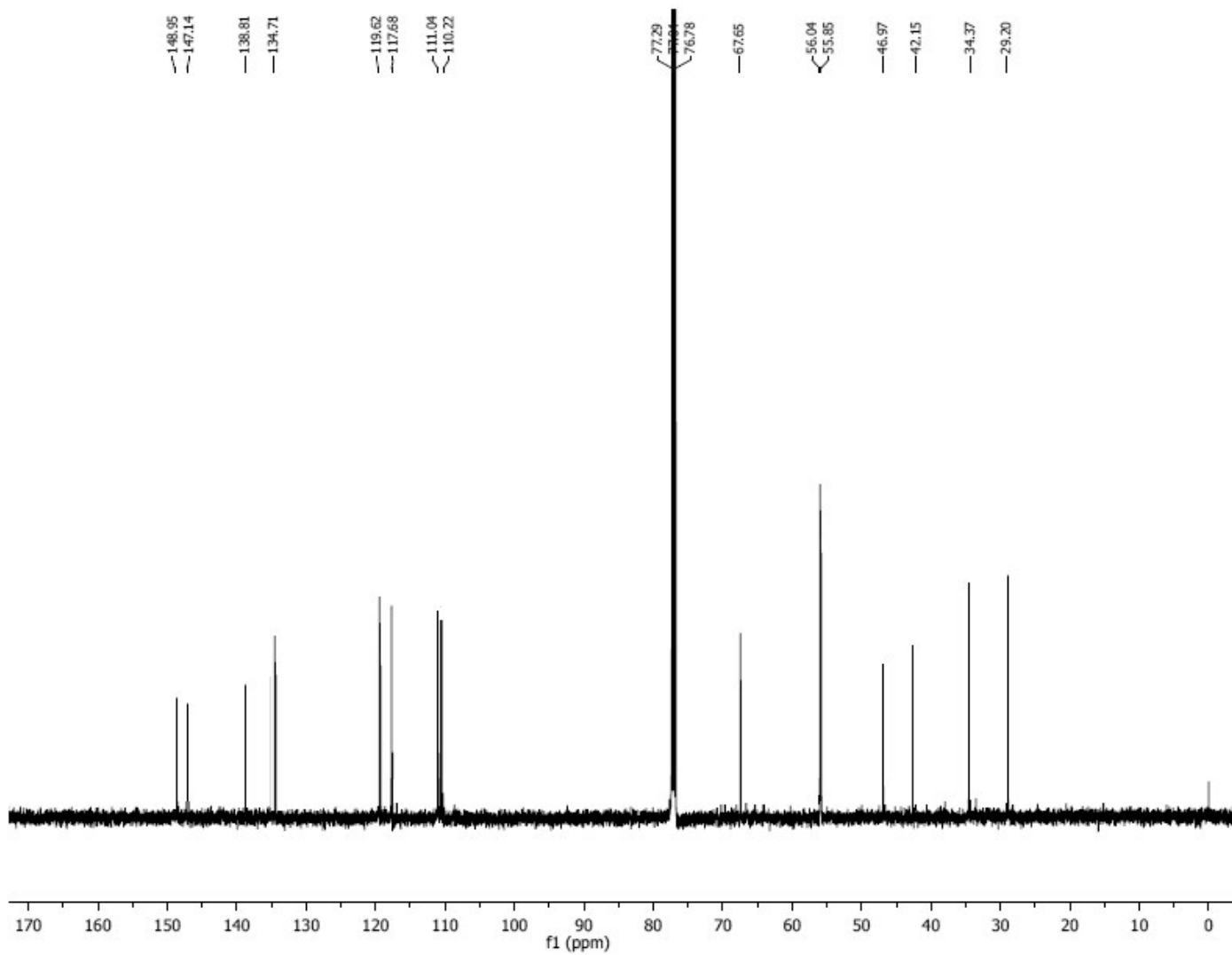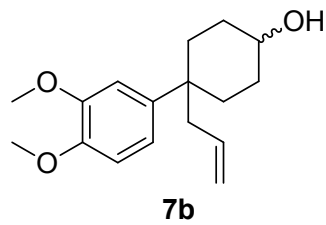Viraj A. Bhosale*, Dattatraya U. Ukale and Suresh B. Waghmode*

Garware Research Center, Department of Chemistry, Savitribai Phule Pune University (formerly Pune University of Pune), Ganeshkhind, Pune 411007, India
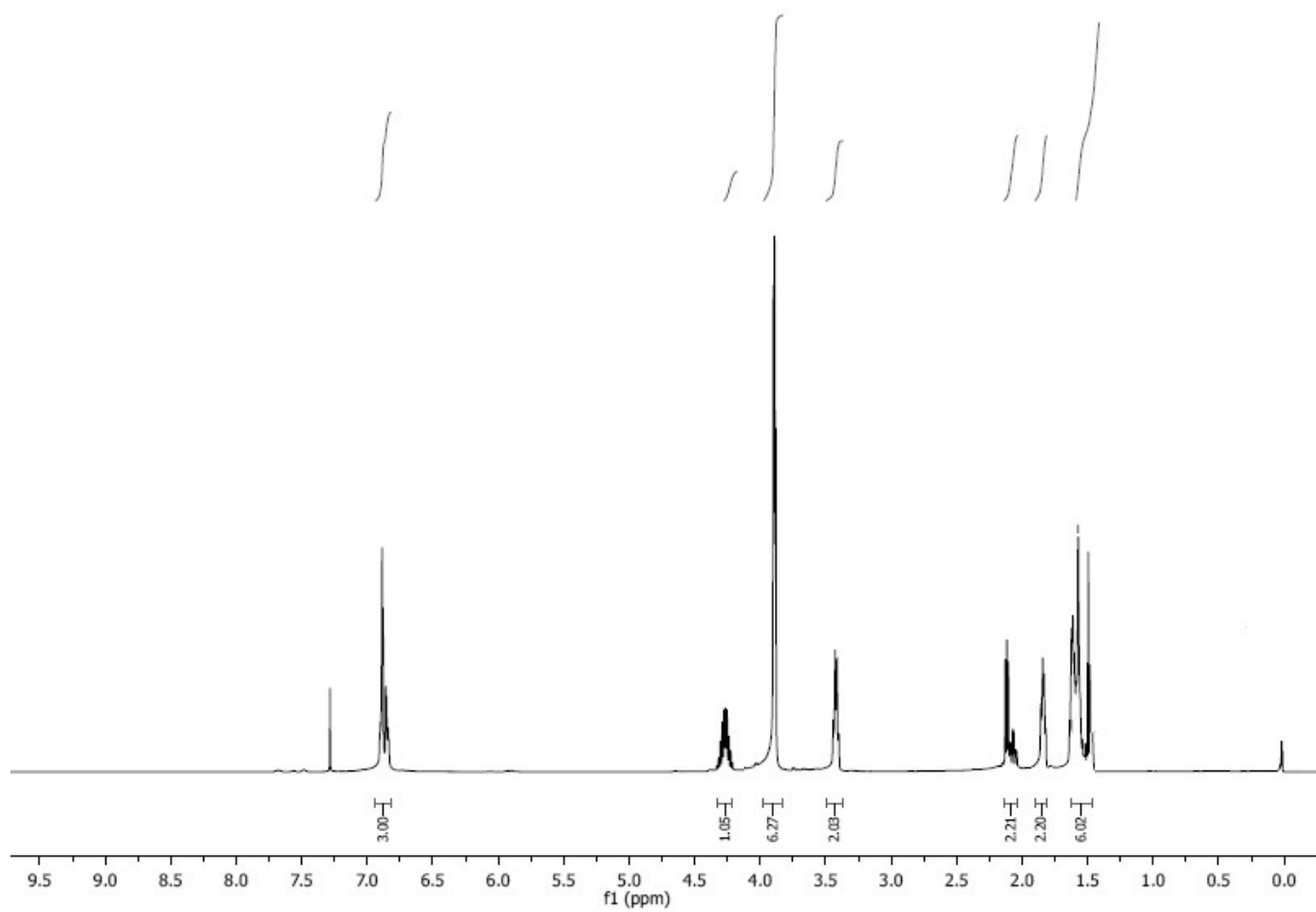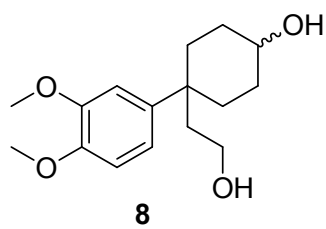
Table of contents

7b

^{1}H NMR of (±)-7b (500 MHz, CDCl$_3$)

7b

^{13}C NMR of (±)-7b (126 MHz, CDCl$_3$)

3

¹H NMR of (±)-8 (500 MHz, CDCl₃)

8

^{13}C NMR of (±)-8 (126MHz, CDCl$_3$)

9

¹H NMR of (±)-9 (500 MHz, CDCl₃)

C13CPD CDCl3 {D:\MGK}

198.34

153.77
149.23
148.17
145.03

133.99
132.71
129.89
129.84

127.81

119.08

111.11
109.63

77.31
77.06
76.80

66.90

55.97
55.89

42.65
40.11
36.33
34.34

21.66

¹³C NMR of (±)-9 (126MHz, CDCl₃)

(±)-10a

¹H NMR of (±)-10a (500 MHz, CDCl₃)

(±)-10a

148.17
147.26
145.03
137.91
133.99
133.70
132.71
129.79
127.81
119.08
111.11
109.63
77.31
77.06
76.80
67.65
66.90
55.97
55.89
42.65
40.11
34.41
28.09
21.66
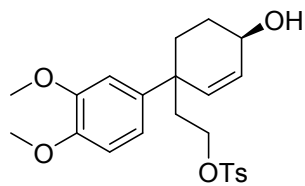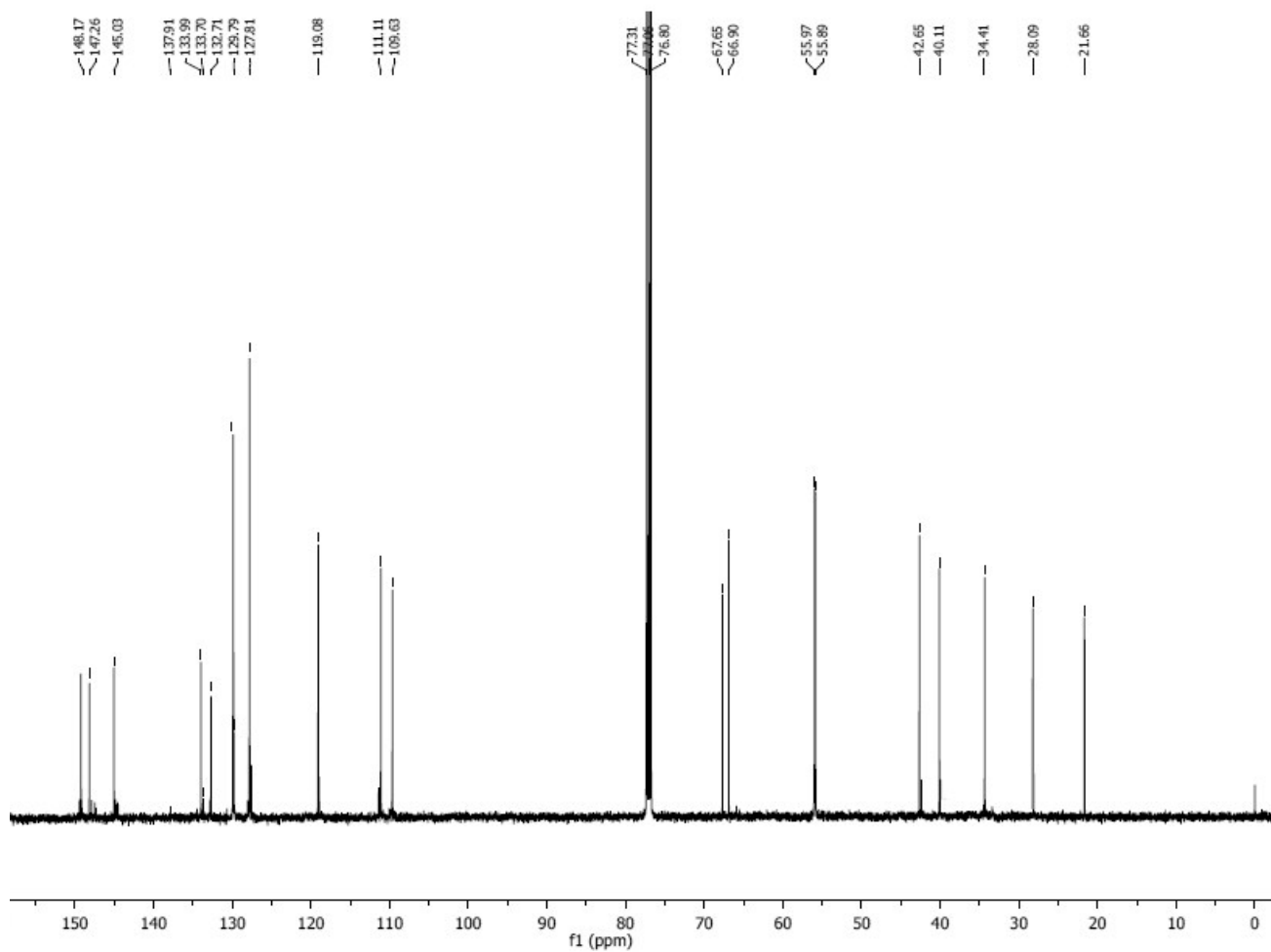
^{13}C NMR of (±)-10a (126MHz, CDCl$_3$)
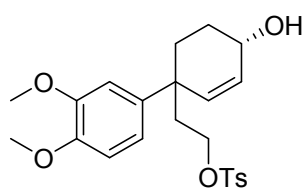
(±)-10b
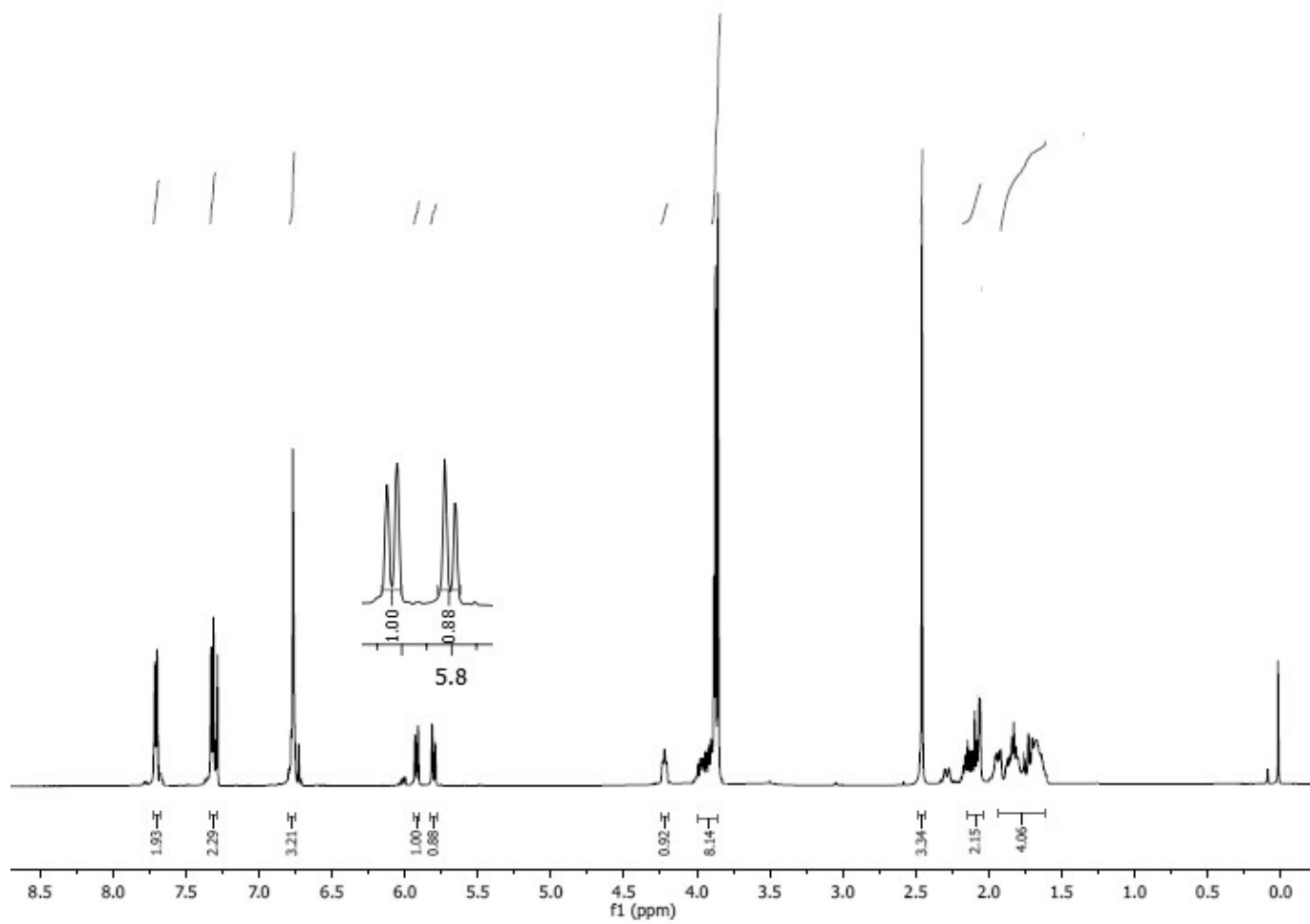
¹H NMR of (±)-10b (500 MHz, CDCl₃)

(±)-10b

149.44
147.44
144.89
137.86
133.99
133.86
132.84
129.89
127.54
119.00
111.38
109.73
77.31
77.06
76.80
67.65
66.90
56.02
55.97
42.39
40.30
34.16
28.28
21.00

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
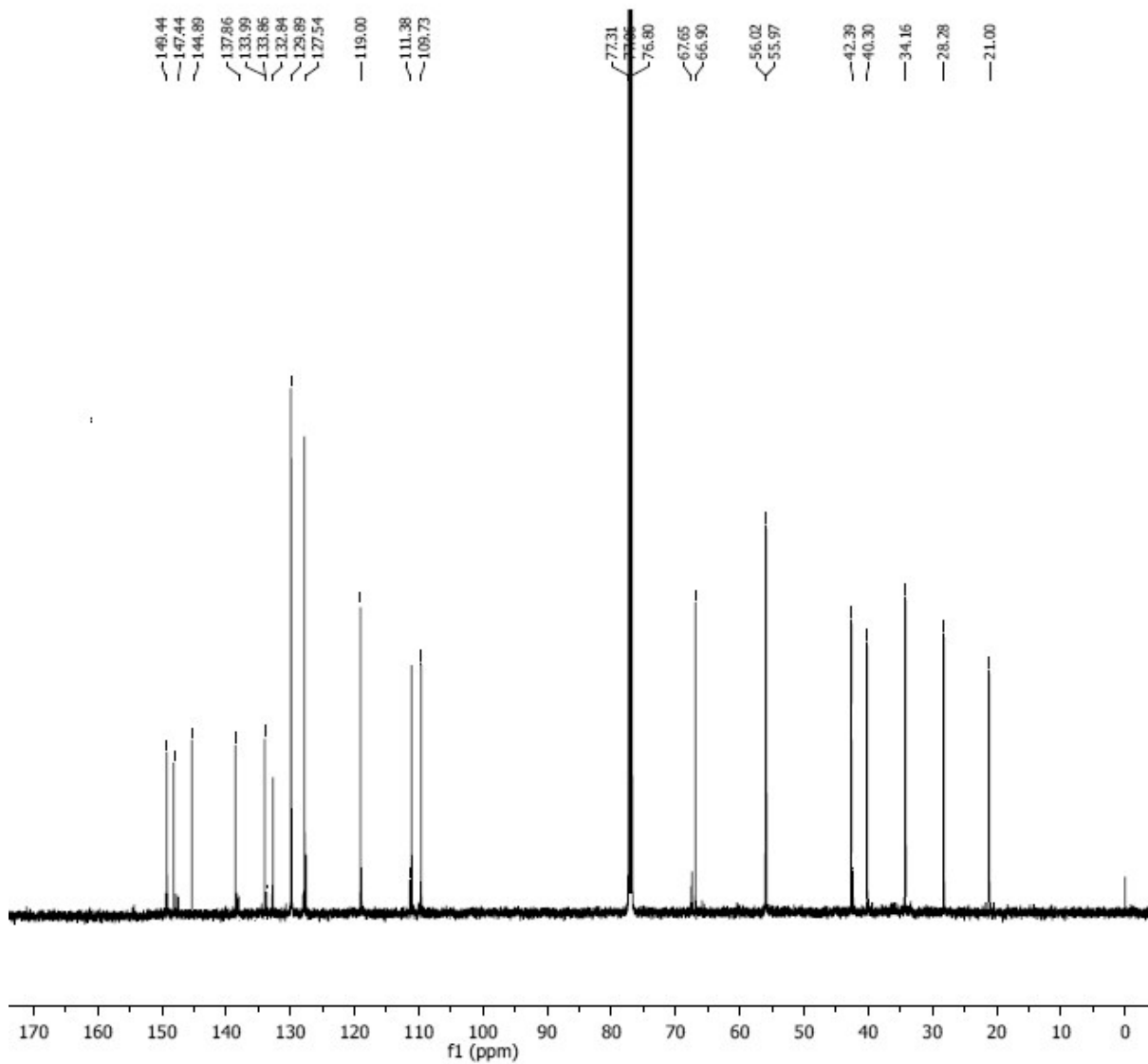
^{13}C NMR of (±)-10b (126MHz, CDCl$_3$)

1a
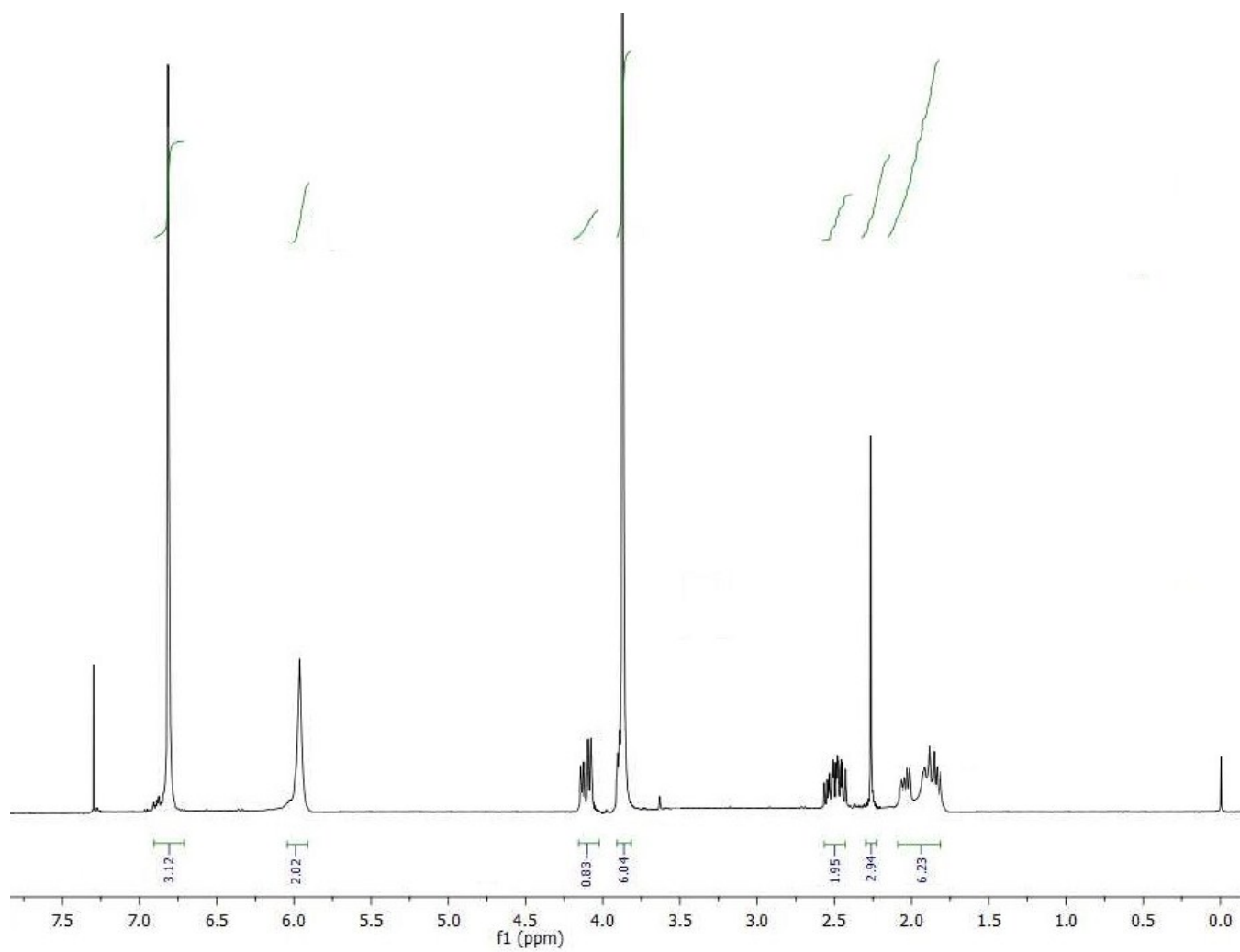
^{1}H NMR of (±)-1a (500 MHz, CDCl₃)

1a

148.51
147.14
139.08
136.46
131.54
119.62
110.58
110.45
77.83
77.19
76.55
64.09
55.91
55.80
48.61
42.88
42.57
37.34
33.54
28.76
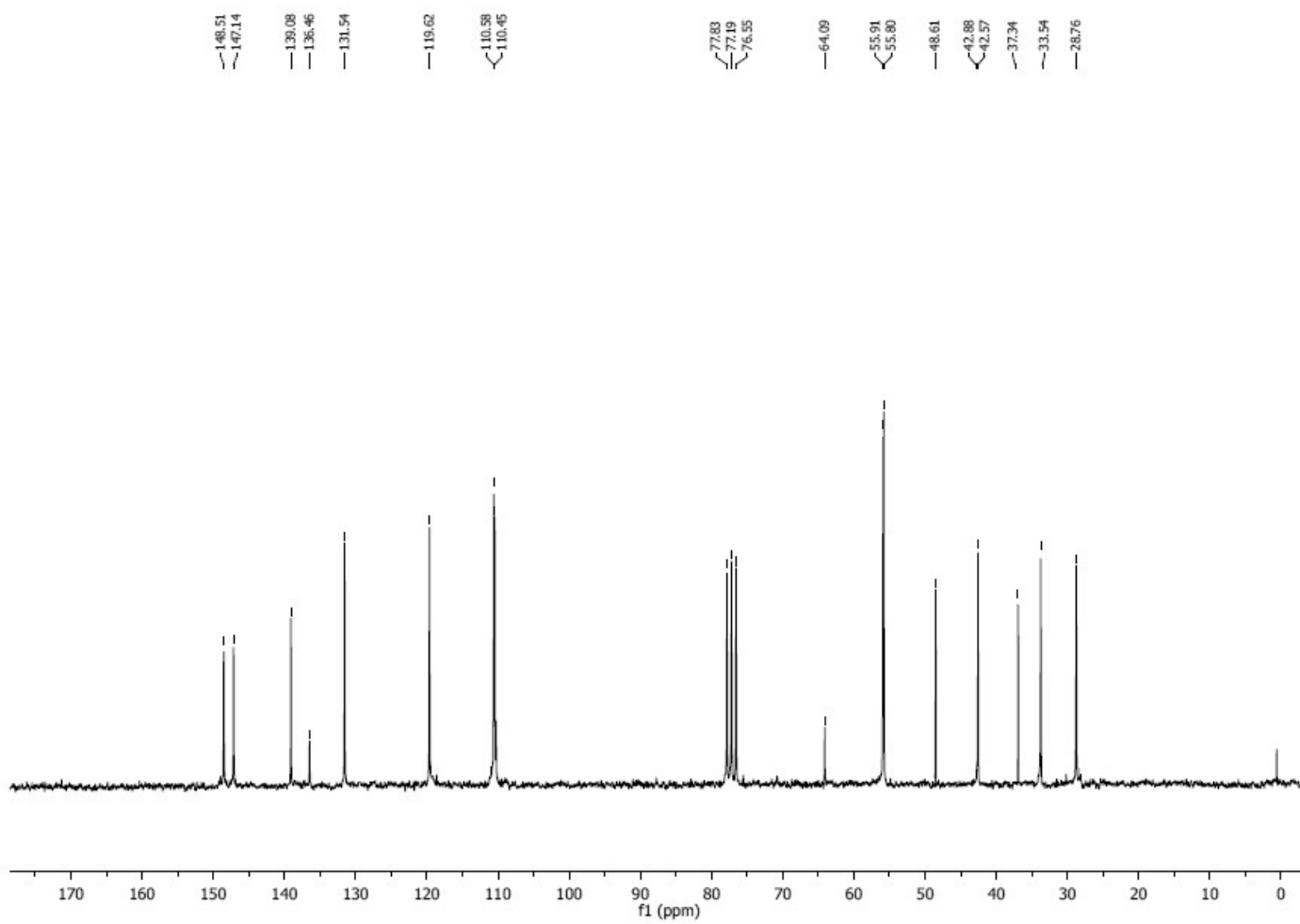
¹³C NMR of (±)-1a (126MHz, CDCl₃)

1b

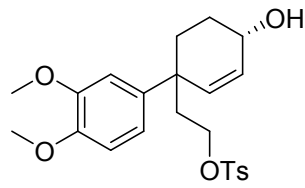^{1}H NMR of (±)-1b (500 MHz, CDCl$_3$)

1b

MR of (±)-1b (126MHz, CDCl₃)

11

¹H NMR 0f (±)-11 (500 MHz, CDCl₃)

11

148.62
147.48
144.45
135.09
132.83
129.83
127.79
118.93
111.21
109.82
77.29
76.78
67.67
55.97
55.86
39.90
37.89
35.91
32.12
21.64

f1 (ppm)
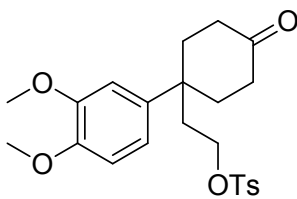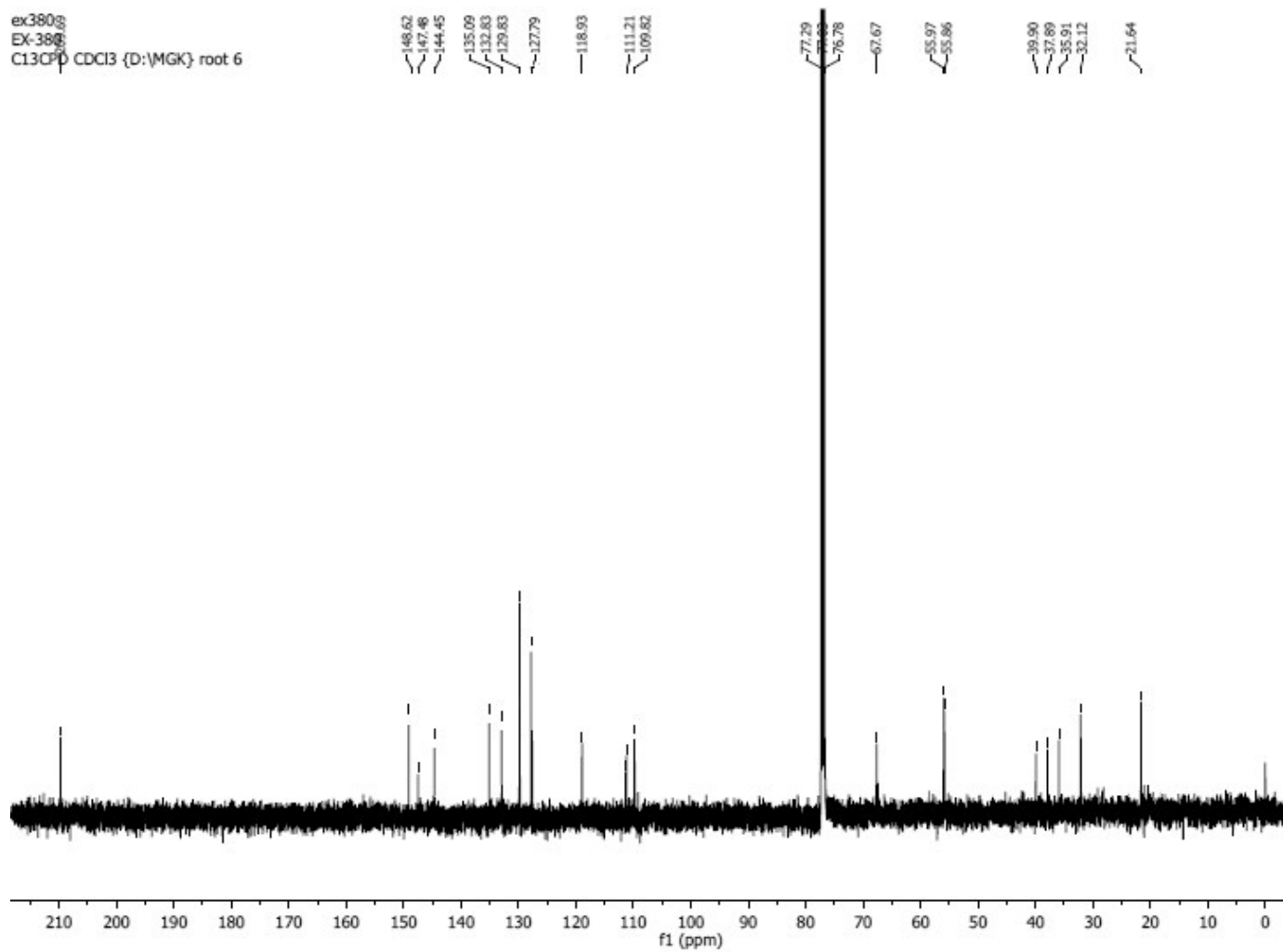
^{13}CNMR 0f (±)-11 (126MHz, CDCl$_3$)

13

¹H NMR 0f (±)-**13** (500 MHz, CDCl₃)

13

166.52
149.06
147.23
136.09
132.84
130.28
128.27
119.39
111.25
110.99
110.36
77.28
77.02
76.77
70.61
62.01
56.03
55.80
39.72
34.18
31.42
30.33

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
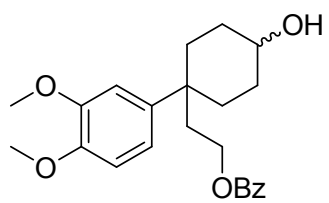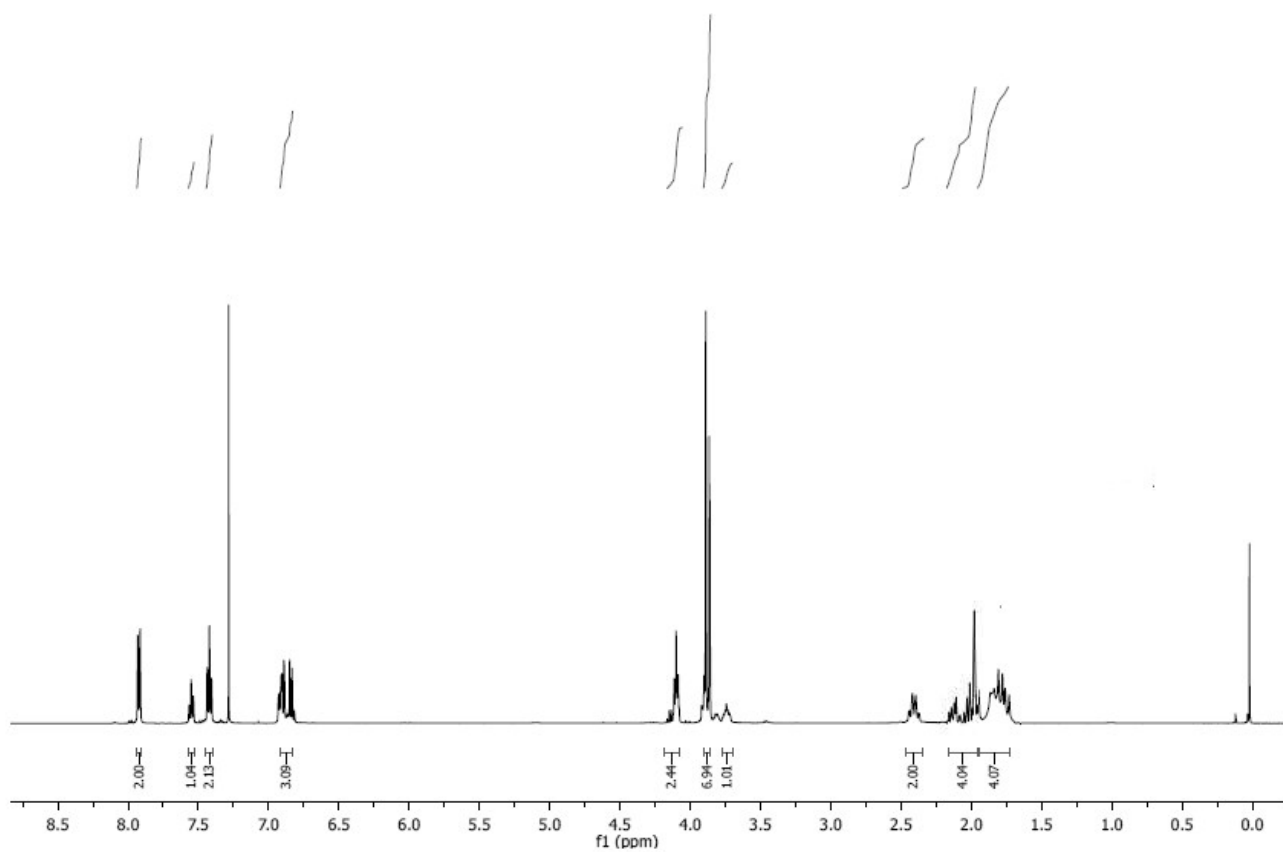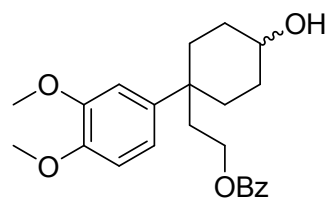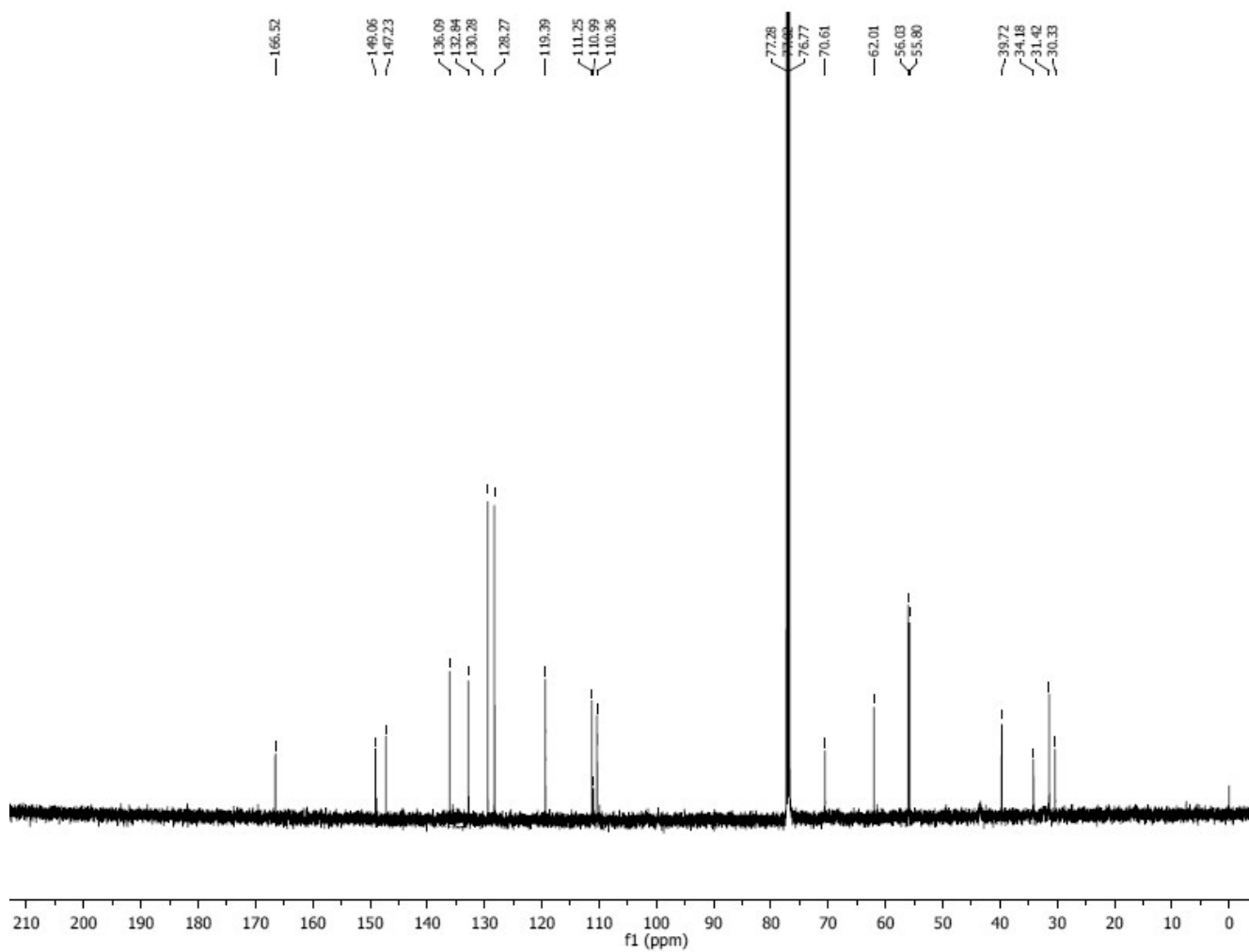
^{13}CNMR 0f (±)-**13** (126MHz, CDCl$_3$)

14
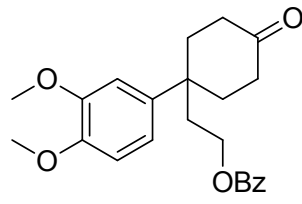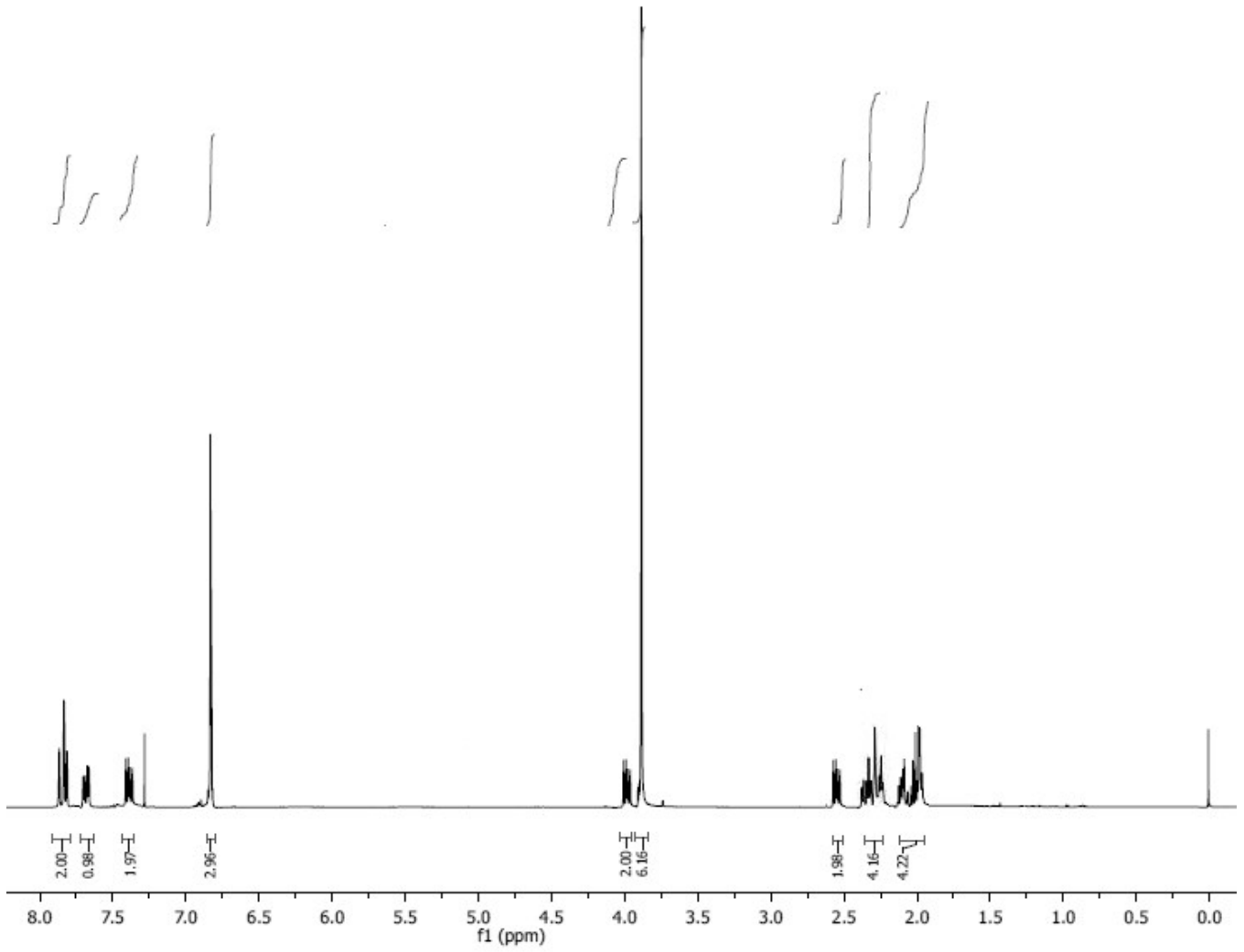
¹H NMR 0f (±)-14 (500 MHz, CDCl₃)
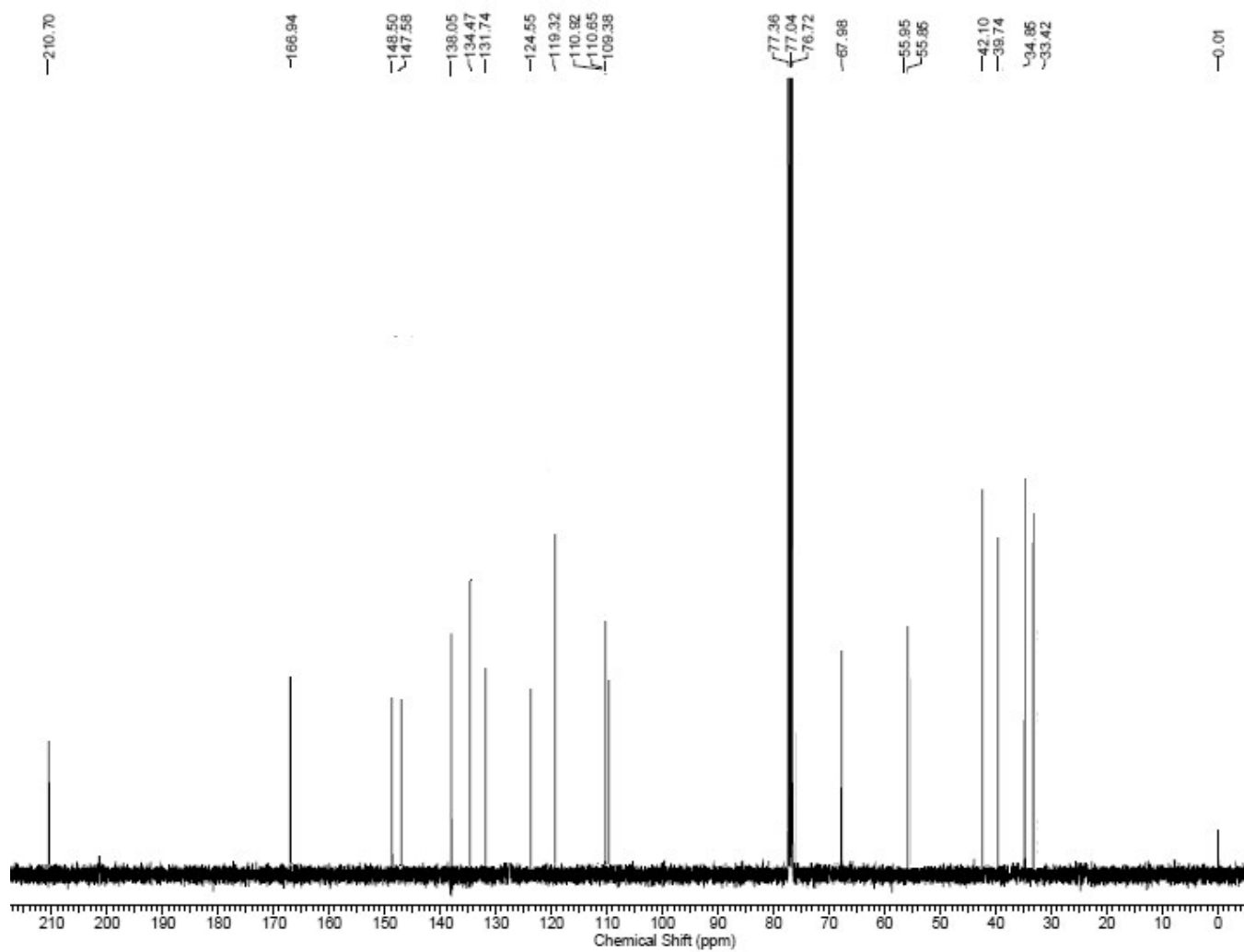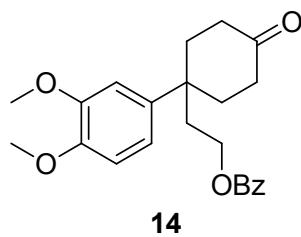
13CNMR 0f (±)-14 (126MHz, CDCl₃)

15
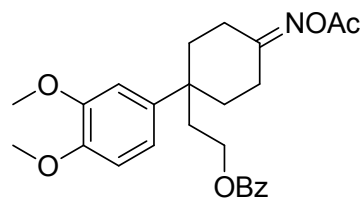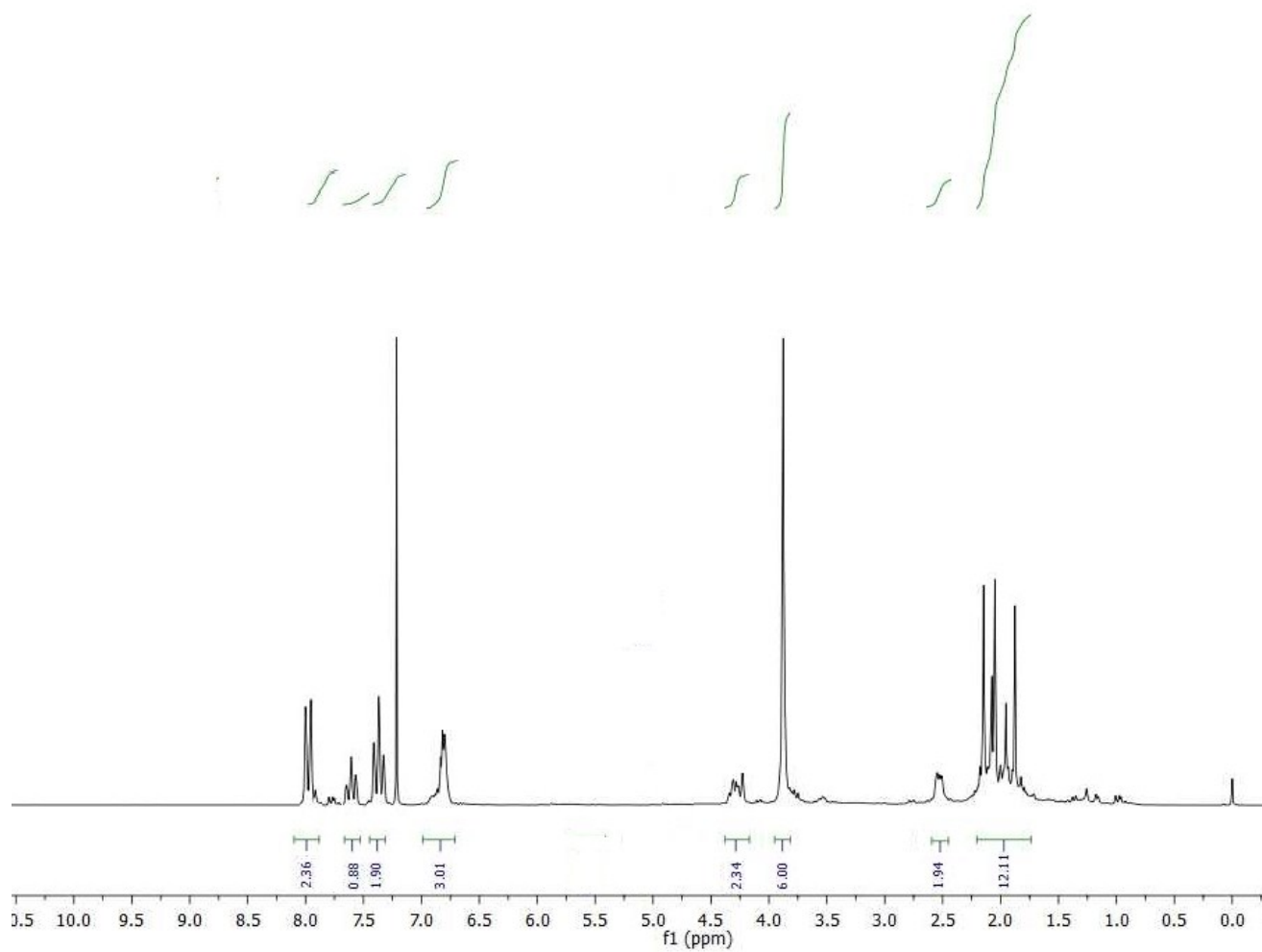
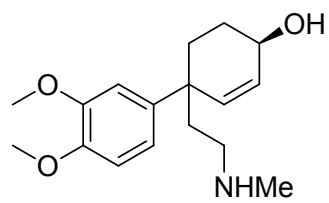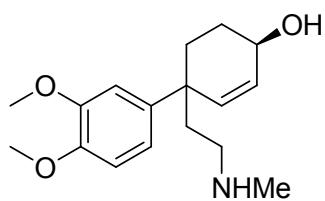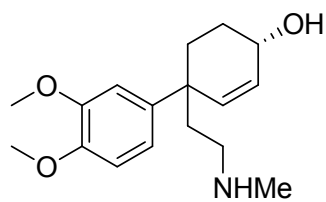^{1}H NMR 0f (±)-15 (500 MHz, CDCl₃)
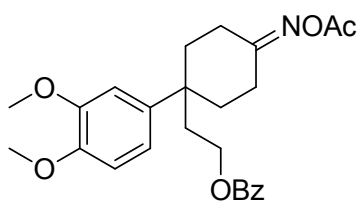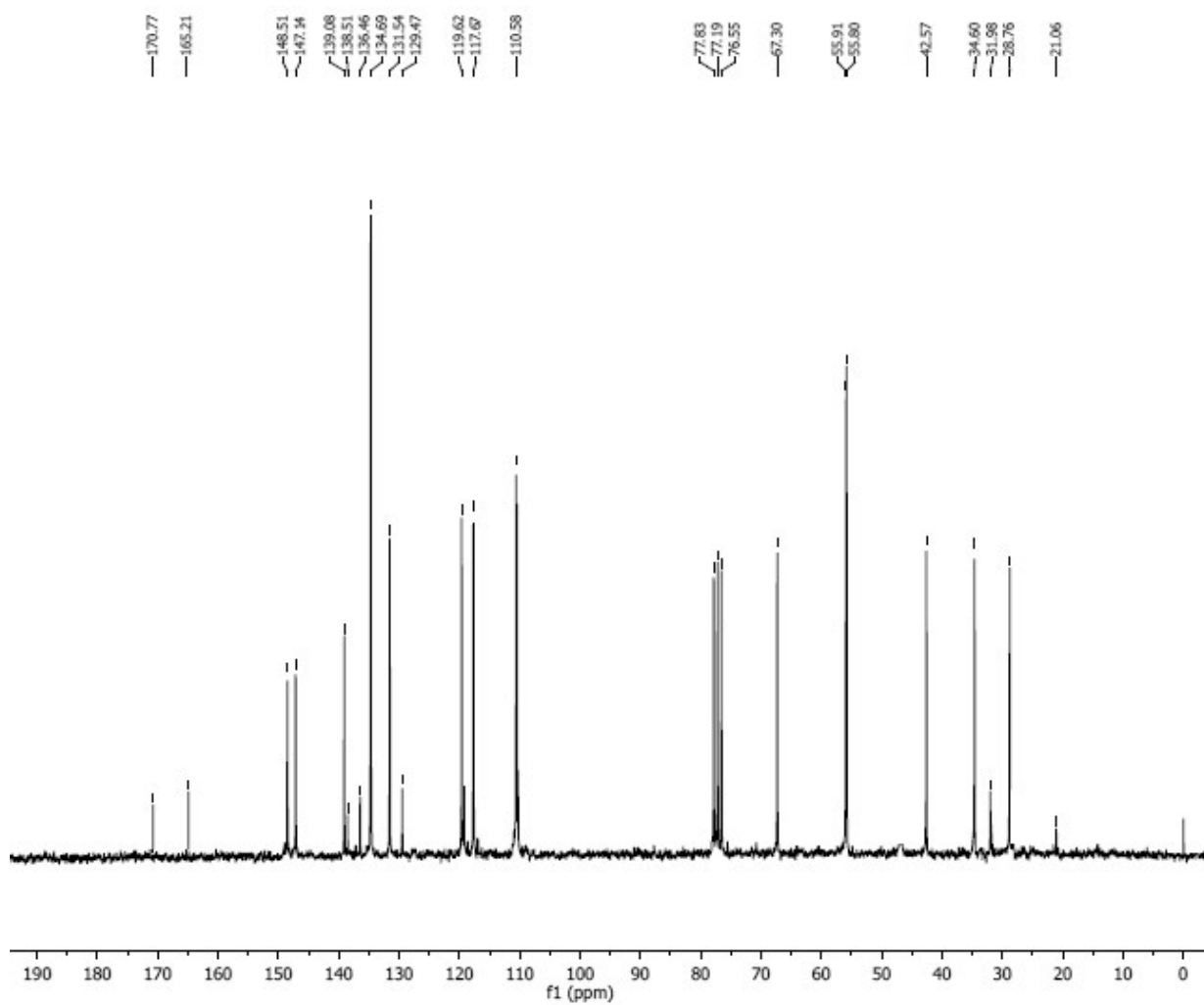
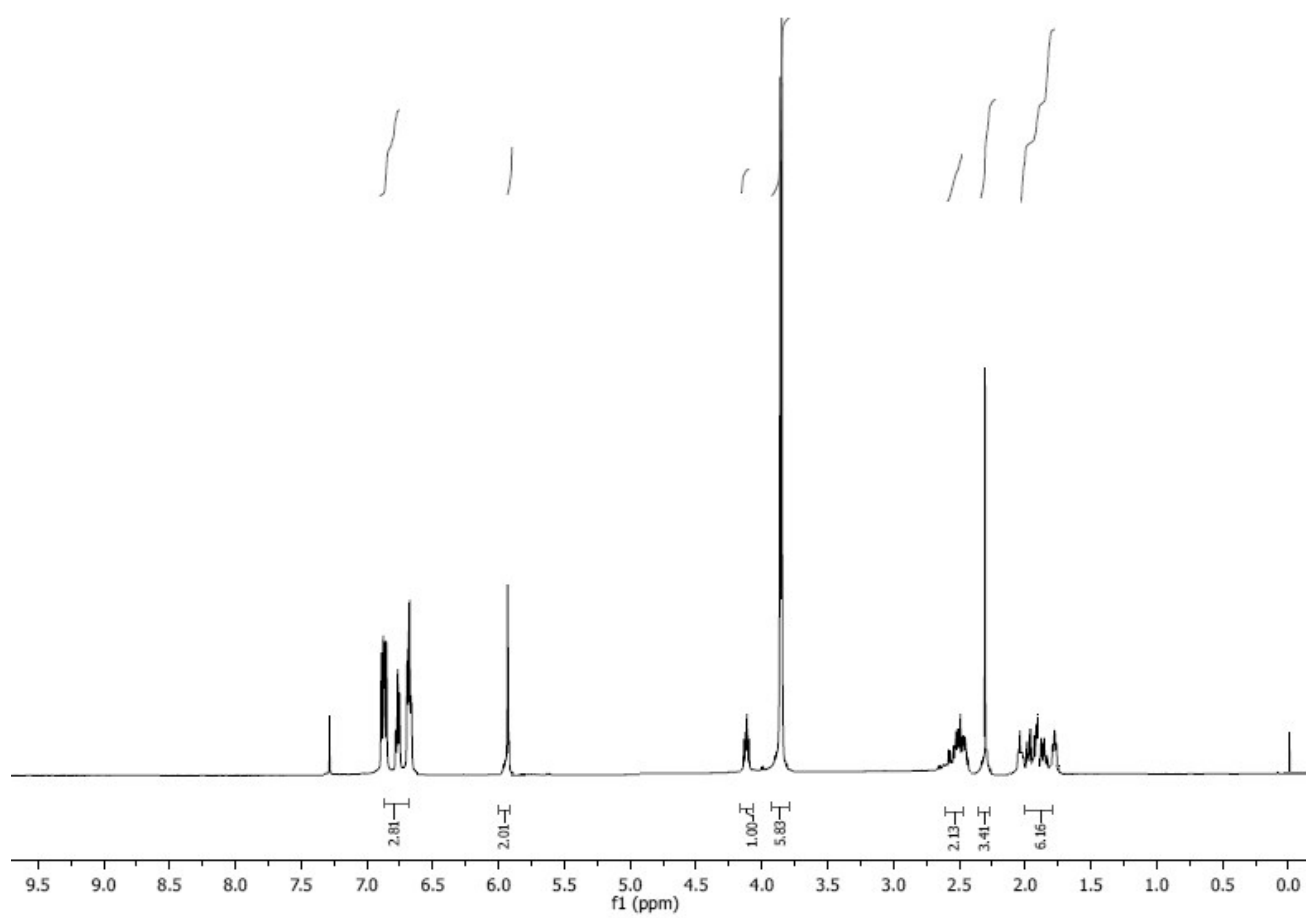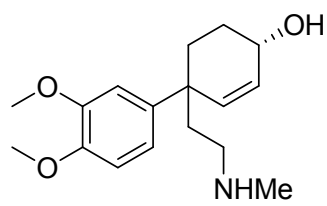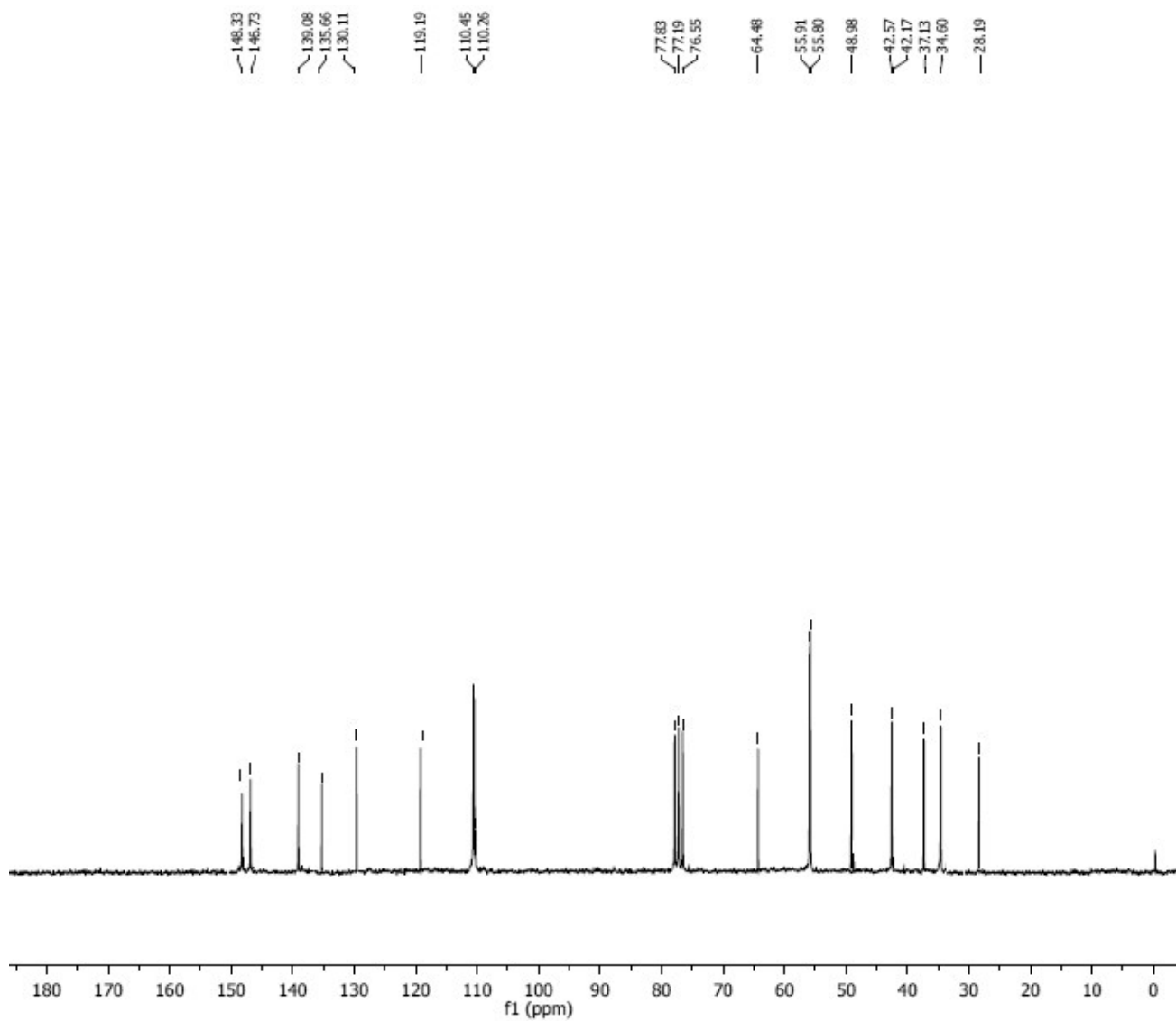13CNMR of (±)-15 (126MHz, CDCl₃)
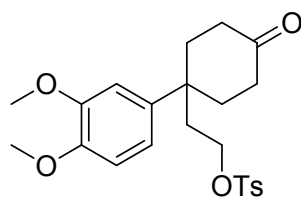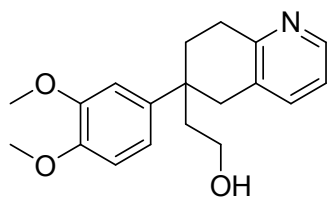
16
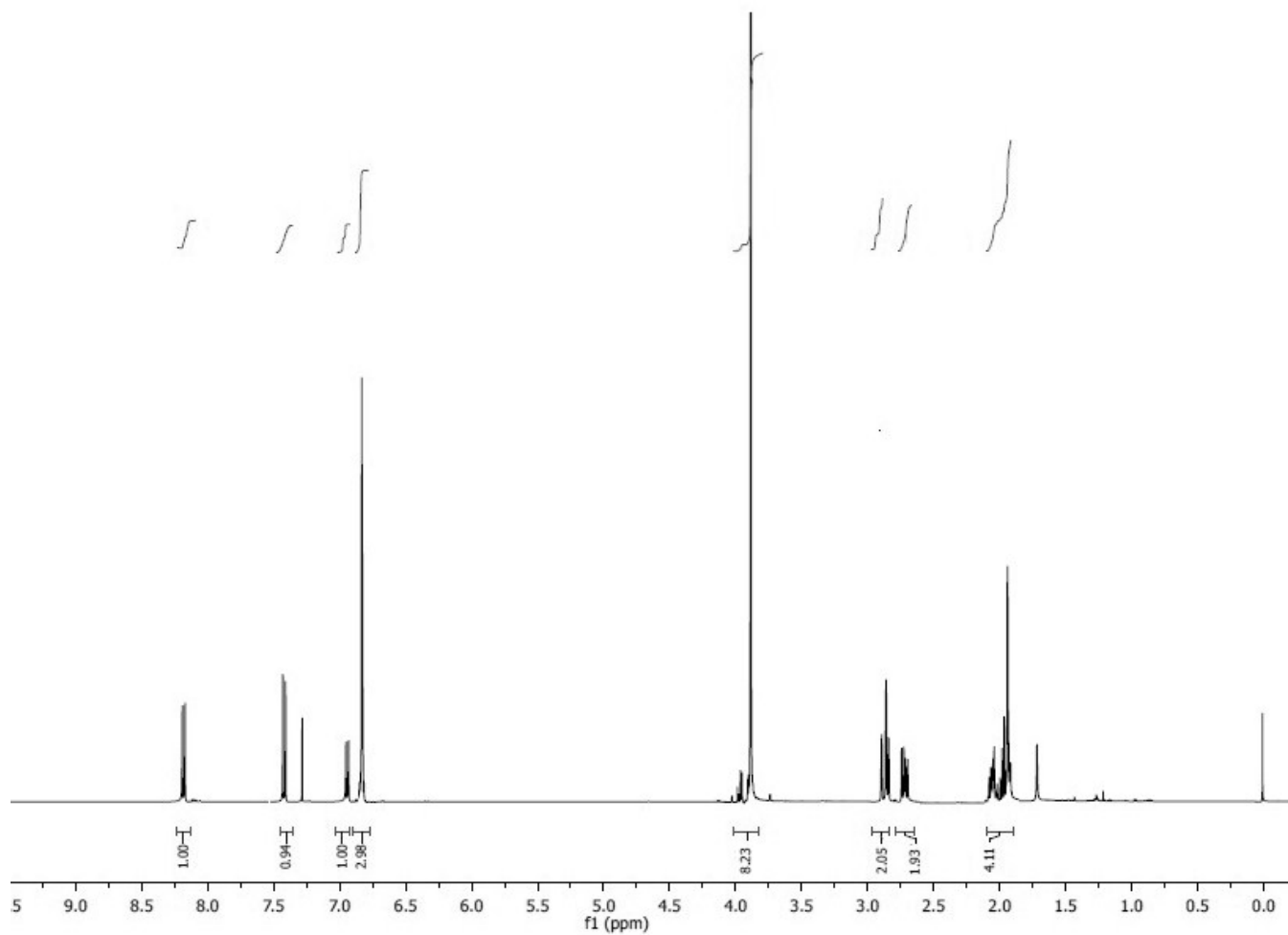
¹H NMR of (±)-16 (500 MHz, CDCl₃)
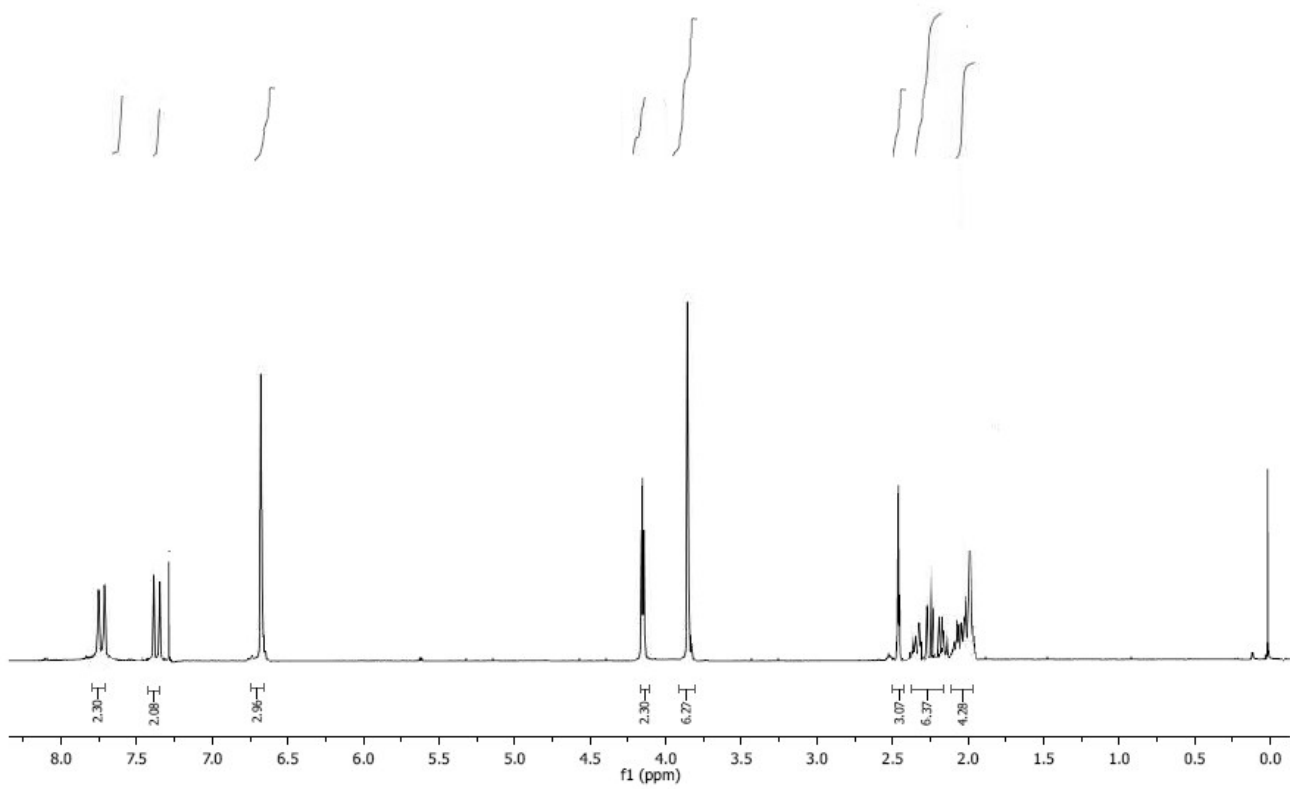
16

154.29
148.12
147.49
145.01
144.74
137.29
132.95
129.58
119.36
111.29
109.74
78.22
77.32
77.01
67.65
55.98
41.46
39.54
37.41
34.93
28.41
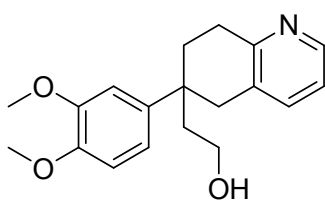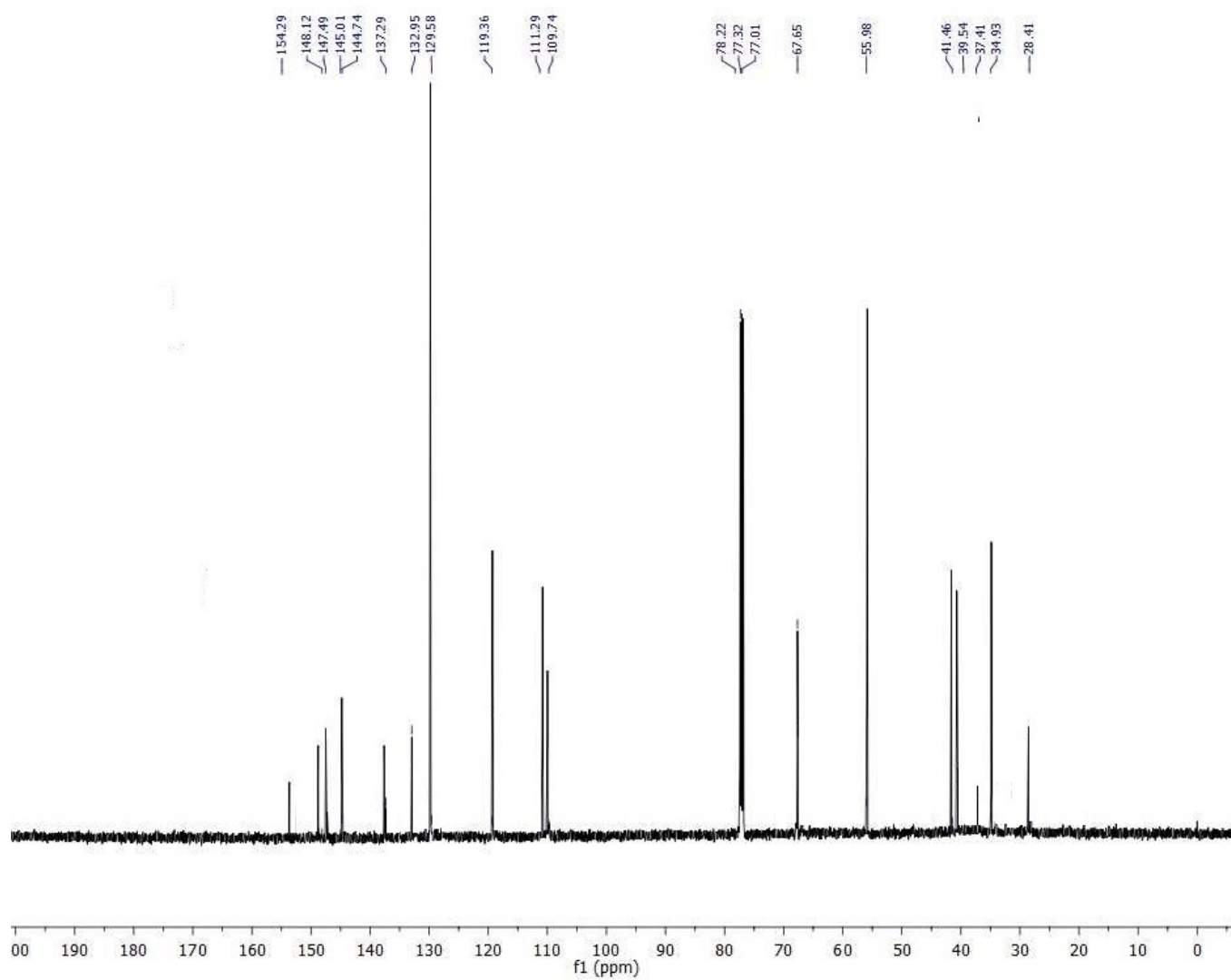
^{13}C NMR of (±)-**16** (126MHz, CDCl$_3$)

25

3a
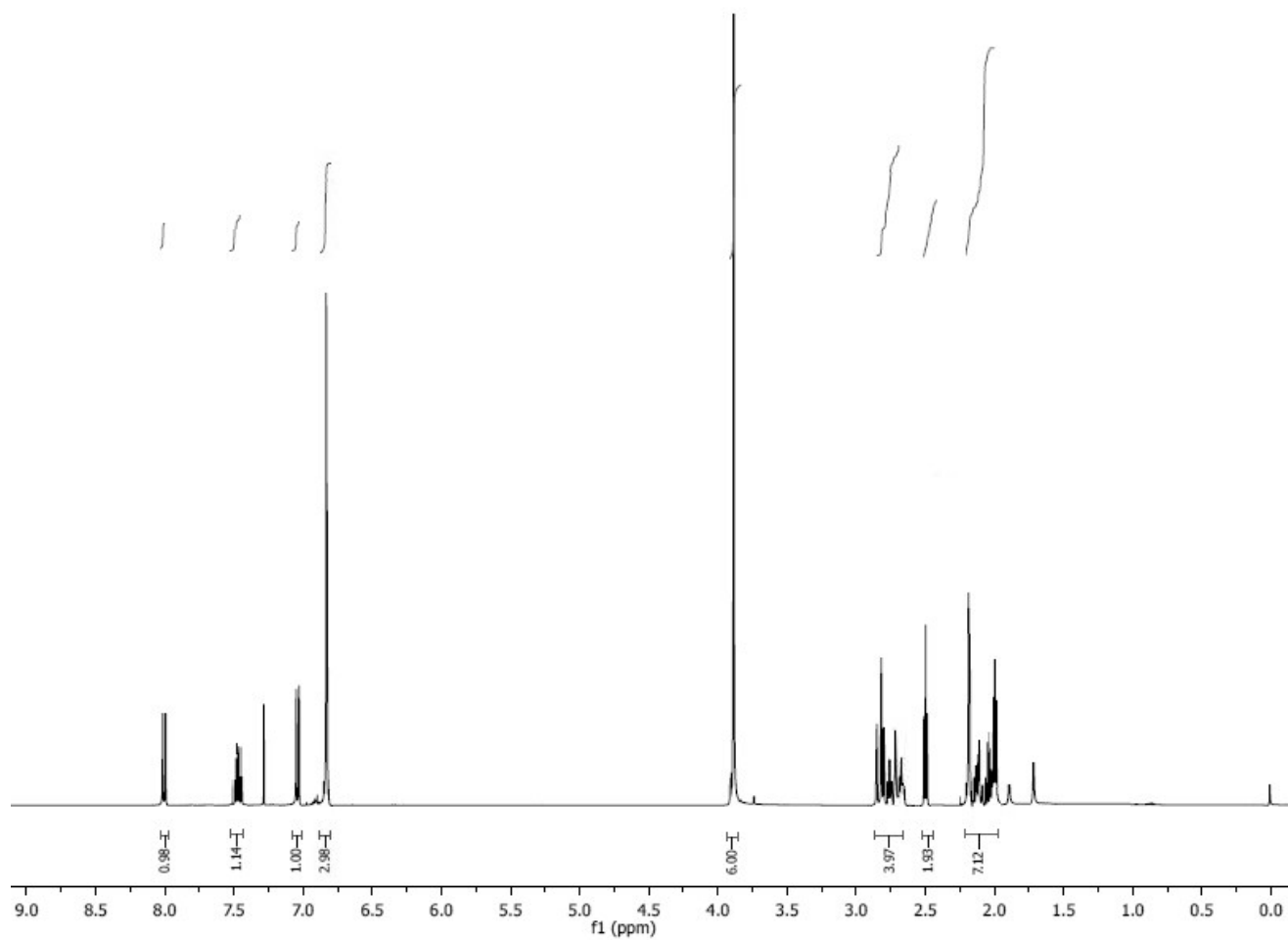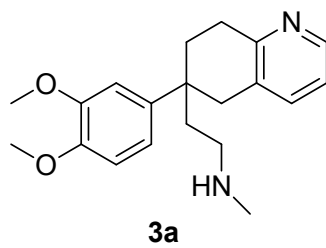
¹H NMR 0f (±)-tortuosamine3a (500 MHz, CDCl₃)

3a

C13CPD CDCl3 {D:\MGK} root 6

155.21
149.01
147.88
145.70
144.42
135.28
133.46
129.41
119.31
110.93
109.23
77.31
77.06
76.80
55.98
55.86
46.26
43.47
40.17
37.61
36.05
34.45
28.28
0.00
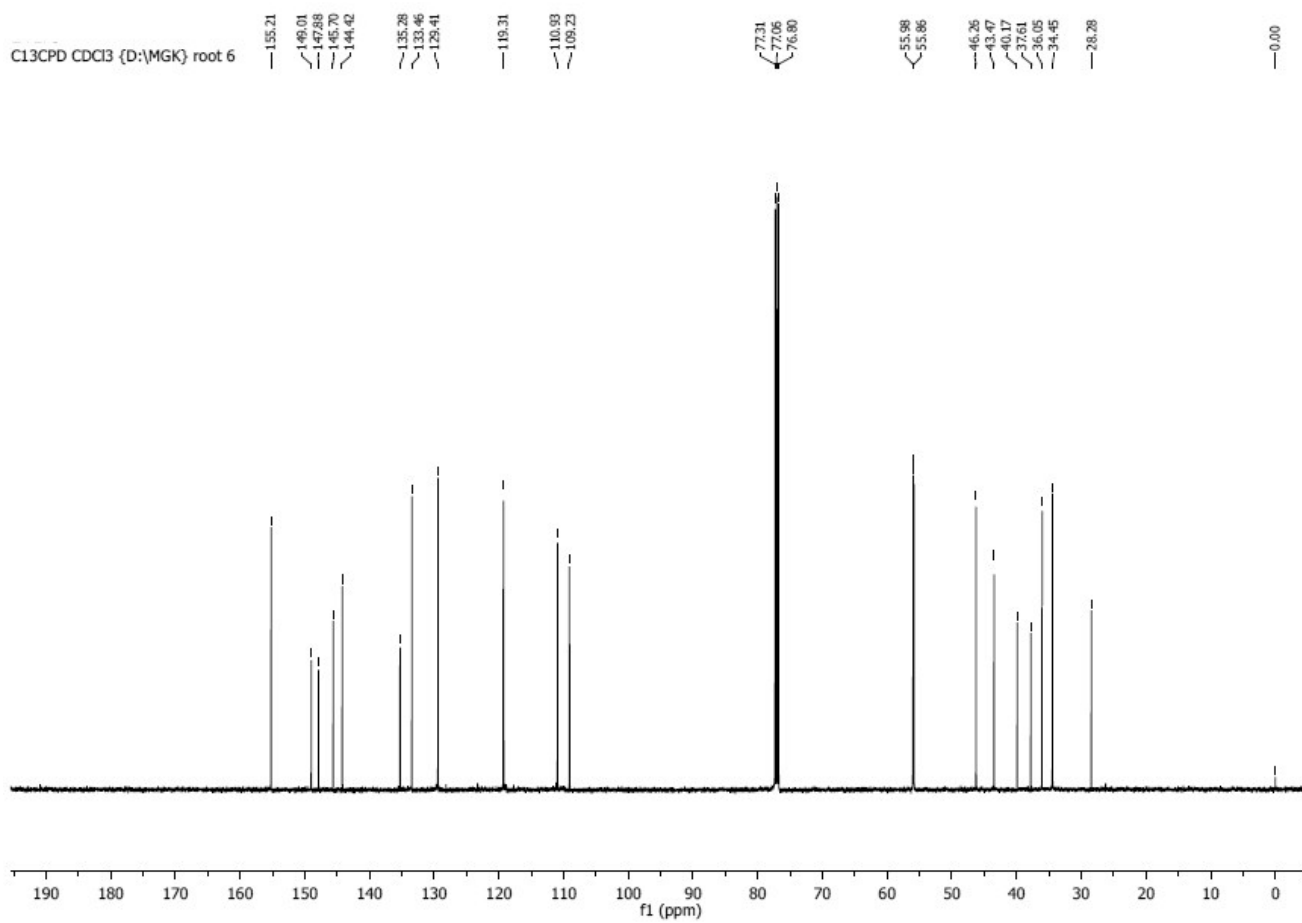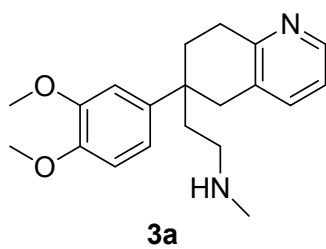
¹³CNMR of (±)-tortuosamine 3a (126MHz, CDCl₃)
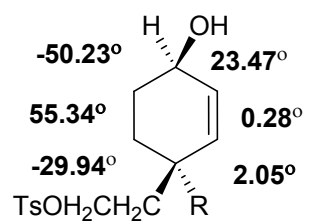
R = 3,4-dimethoxy benzene

10a^I

Fig. 1   Dihedral angles of conformer 10a^I obtained after the optimization by DFT

Fig. 2 DFT optimized structure of **10aᴵ**

Table 1. Coordinates of **10a^I** optimized structure by DFT

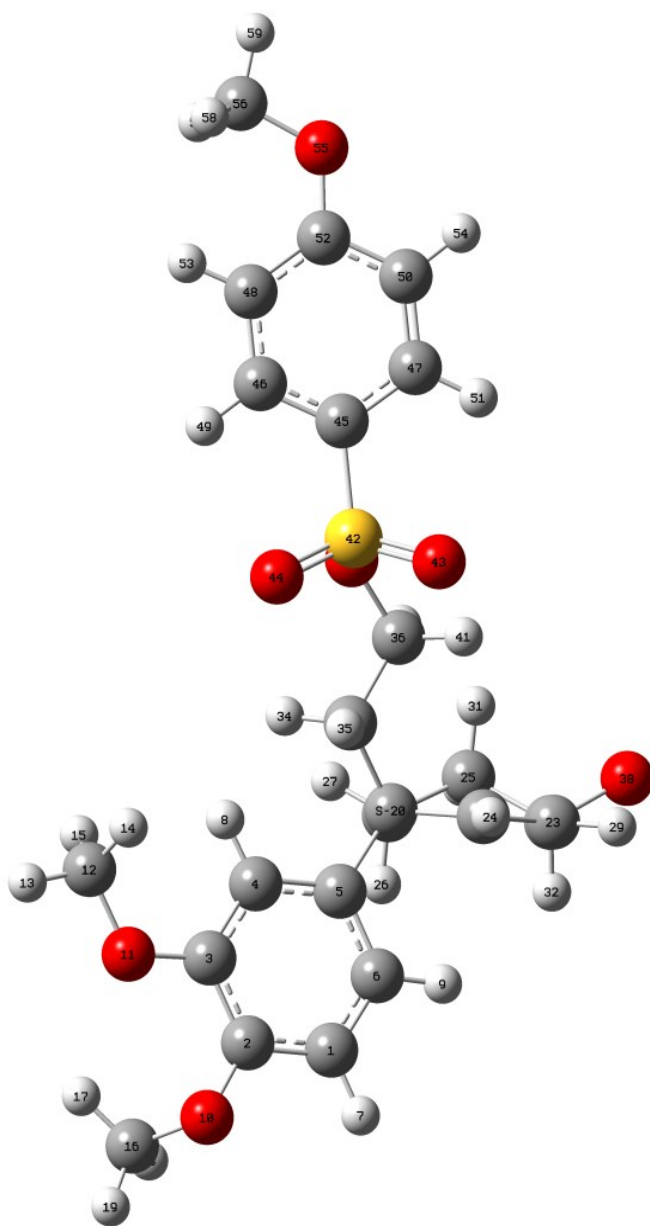| Atom	X	Y	Z
C	−5.48353600	−0.17264200	−0.64366400
C	−5.37300500	−1.52874400	−0.36374100
C	−4.13180400	−2.02993200	0.07194100
C	−3.05412500	−1.15694200	0.24279000
C	−3.16777200	0.21320600	−0.02975800
C	−4.40000900	0.68824300	−0.48616500
H	−6.43746800	0.19415400	−1.00509200
H	−2.11303700	−1.56535300	0.57682000
H	−4.52009000	1.73734900	−0.72805200
O	−6.44770200	−2.34810700	−0.60475000
O	−4.06517400	−3.37635800	0.29122700
C	−2.80836800	−3.95512200	0.62247400
H	−2.98737000	−5.02680600	0.69391600
H	−2.06251100	−3.76188800	−0.15493900
H	−2.43679500	−3.58612300	1.58479500
C	−7.03425300	−2.97840500	0.53927700
H	−6.32769100	−3.65258900	1.02723100
H	−7.38500000	−2.22498800	1.25389200
H	−7.88612800	−3.54616700	0.16580400
C	−2.00207000	1.20876500	0.20150900
C	−1.95000200	2.17028200	−0.97617300
C	−2.28800500	1.98210000	1.53132100
C	−2.08325600	3.49392800	−0.89970400
H	−1.79511700	1.70753500	−1.94782500
C	−1.76291800	3.42513500	1.56985300
H	−3.37051700	2.01401900	1.68089200
H	−1.88586800	1.40951900	2.37312400
C	−2.30204300	4.23407300	0.38931600
H	−2.04112600	4.10640200	−1.79528400
H	−2.06034300	3.89310900	2.51568400
H	−0.67200400	3.46743400	1.52358000
H	−3.38284900	4.40277100	0.52537100
C	−0.65544900	0.42870500	0.26182800
H	−0.65796500	−0.23607400	1.12970600
H	−0.58605200	−0.20524400	−0.62647700
C	0.61001700	1.27553400	0.34008300
H	0.65333200	1.88108700	1.24334600
O	−1.65181200	5.50707500	0.26113100
H	−1.86007200	6.03570600	1.03840500
O	1.79734900	0.43269300	0.47338500
H	0.73201700	1.92115900	−0.53004300
S	2.34256100	−0.36467300	−0.85712900
O	2.13399900	0.49776000	−2.01650800
O	1.79598400	−1.71619500	−0.84314800
C	4.07332400	−0.43521800	−0.45400300
C	4.57878200	−1.55599300	0.19300100
C	4.90332700	0.63778700	−0.79254400
C	5.93287400	−1.61534100	0.51518200
H	3.92175100	−2.38224900	0.43283100
C	6.24747300	0.58099500	−0.47308600
H	4.49605700	1.49626200	−1.31165400
C	6.77076800	−0.54433400	0.18386300
H	6.31820600	−2.49394200	1.01349800
H	6.91878100	1.39163000	−0.72756700
O	8.10001200	−0.50123900	0.44842900
C	8.71096700	−1.60997000	1.10284300
H	8.28150600	−1.76973900	2.09692200
H	8.61544100	−2.52353700	0.50754700
H	9.76317200	−1.35035400	1.20083800