Platinum-catalyzed *anti*-stereoselective ring opening of oxabicyclic alkenes with Grignard reagents

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Supporting Information

Table of Contents **Page**

1. General

Reagents were obtained from commercial vendors and used without further purification. CH_3CN, 1,2-dichloroethane (DCE), CH_2Cl_2, and diethyl ether were distilled from calcium hydride. Toluene, DME, dioxane, THF, and tetrahydropyran (THP) were distilled from sodium benzophenone ketyl immediately prior to use. Oxabenzonorbornadienes **1a-e** were prepared according to the literature procedures.[1-5] All flasks were flame-dried under a stream of nitrogen and cooled to room temperature before use. Solvents and solutions were transferred with syringes and cannulae using standard inert atmosphere techniques. All ^1H and ^{13}C NMR spectra were recorded at 400 and 100 M NMR, respectively, using $CDCl_3$ as solvent. The chemical shifts of all ^1H and ^{13}C NMR spectra are referenced to the residual signal of $CDCl_3$ (δ 7.26 ppm) for the ^1H NMR spectra and (δ 77.16 ppm) for the ^{13}C NMR spectra. Spectral features are tabulated in the following order: Chemical shift (δ, ppm); multiplicity (s-singlet, d-doublet, t-triplet, m-multiplet); coupling constants (*J*, Hz); number of protons. IR spectra were obtained using CH_2Cl_2 liquid film. MS were recorded using EI at 70 eV. High resolution mass spectra (HRMS) (ion trap) were obtained from (double focusing) mass spectrometer at 70 eV or mass spectrometer (APCI or ESI). The melting points are uncorrected. Crystal structure was determined by X-ray diffraction apparatus.

(1) H. Hart, A. Bashir-Hashemi, J. Luo, M. A. Meador, *Tetrahedron,* 1986, **42**, 1641−1654.
(2) H. Hart, C. Y. Lai, G. C. Nwokogu, S. Shamouilian, *Tetrahedron*, 1987, **43**, 5203−5224.
(3) G.. Stork, E. E. Van Tamelen, L. J. Friedman, A. W. Burgstahler, *J. Am. Chem. Soc*., 1953, **75**, 384−392.
(4) M. Davoust, J. A. Kitching, M. J. Fleming, M. Lautens, *Chem. Eur. J*., 2010, **16**, 50−54.
(5) W. M. Best, P. A. Collins, R. K. McCulloch, D. Wege, *Aust. J. Chem*., 1982, **35**, 843−848.

2. Crystal structure and data of (1*S**,2*R**)-6,7-dibromo-2-isopropyl -1,2-

dihydronaphthalen-1-ol (5i) (CCDC 946820)

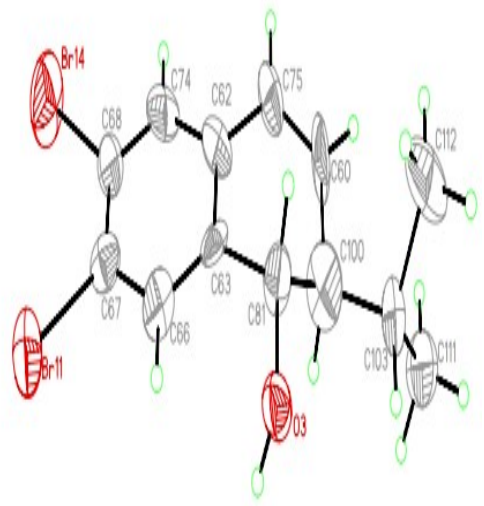


Table 1. Crystal data and structure refinement for 5i.

Identification code	**5i**
Empirical formula	$C_{13}H_{14}Br_2O$
Formula weight	346.04
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 12.698(9) A alpha = 108.667(14) deg.
	b = 15.704(11) A beta = 96.252(14) deg.
	c = 15.785(19) A gamma = 111.779(10) deg.
Volume	2675(4) A^3
Z, Calculated density	8, 1.719 Mg/m^3
Absorption coefficient	6.038 mm^-1
F(000)	1360
Crystal size	0.2 x 0.1 x 0.1 mm
Theta range for data collection	1.41 to 24.00 deg.
Limiting indices	-14<=h<=14, -17<=k<=17, -18<=l<=18
Reflections collected / unique	12433 / 8383 [R(int) = 0.1037]

Completeness to theta = 24.00	98.7 %
Max. and min. transmission	0.547 and 0.489
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8273 / 0 / 589
Goodness-of-fit on F^2	0.890
Final R indices [I>2 sigma (I)]	R1 = 0.0789, wR2 = 0.1502
R indices (all data)	R1 = 0.2821, wR2 = 0.2223
Largest diff. peak and hole	0.683 and -0.633 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 5i. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Br(11)	-4041(2)	427(2)	6348(1)	96(1)
Br(14)	-4073(2)	-75(2)	8287(2)	124(1)
C(60)	1516(17)	2707(16)	9266(12)	92(7)
C(62)	-528(18)	1605(14)	8616(12)	60(5)
C(63)	-550(17)	1731(11)	7760(13)	52(4)
O(3)	625(10)	2522(9)	6844(7)	64(3)
C(66)	-1582(19)	1377(13)	7097(12)	69(5)
C(67)	-2648(16)	855(12)	7232(11)	61(5)
C(68)	-2674(16)	694(12)	8047(14)	65(5)
C(74)	-1650(20)	1056(14)	8711(12)	74(6)
C(75)	553(18)	2011(14)	9278(10)	69(6)
C(81)	666(15)	2283(13)	7653(10)	67(5)
C(100)	1509(19)	3048(15)	8466(12)	97(7)
C(103)	2806(15)	3637(14)	8431(12)	73(5)
C(111)	3356(15)	4619(13)	9294(11)	91(6)

C(112)	3499(17)	3046(16)	8354(12)	111(7)

Table 3. Bond lengths [A] and angles [deg] for 5i.

Br(11)-C(67)	1.874(17)
Br(14)-C(68)	1.898(16)
C(60)-C(75)	1.31(2)
C(60)-C(100)	1.52(2)
C(60)-H(60)	0.9300
C(62)-C(75)	1.41(2)
C(62)-C(74)	1.42(2)
C(62)-C(63)	1.425(19)
C(63)-C(66)	1.38(2)
C(63)-C(81)	1.52(2)
O(3)-C(81)	1.443(15)
O(3)-H(3)	0.8200
C(66)-C(67)	1.38(2)
C(66)-H(66)	0.9300
C(67)-C(68)	1.389(19)
C(68)-C(74)	1.38(2)
C(74)-H(74)	0.9300
C(75)-H(75)	0.9300
C(81)-C(100)	1.41(2)
C(81)-H(81)	0.9800
C(100)-C(103)	1.58(2)
C(100)-H(100)	0.9800
C(103)-C(112)	1.49(2)
C(103)-C(111)	1.54(2)
C(103)-H(103)	0.9800
C(111)-H(11D)	0.9600

C(111)-H(11E)	0.9600
C(111)-H(11F)	0.9600
C(112)-H(11M)	0.9600
C(112)-H(11N)	0.9600
C(112)-H(11O)	0.9600
C(75)-C(60)-C(100)	119.2(17)
C(75)-C(60)-H(60)	120.4
C(100)-C(60)-H(60)	120.4
C(75)-C(62)-C(74)	125.8(18)
C(75)-C(62)-C(63)	119.9(18)
C(74)-C(62)-C(63)	114.2(17)
C(66)-C(63)-C(62)	122.6(17)
C(66)-C(63)-C(81)	124.0(17)
C(62)-C(63)-C(81)	113.4(17)
C(81)-O(3)-H(3)	109.5
C(67)-C(66)-C(63)	120.5(16)
C(67)-C(66)-H(66)	119.7
C(63)-C(66)-H(66)	119.7
C(66)-C(67)-C(68)	119.2(16)
C(66)-C(67)-Br(11)	119.9(14)
C(68)-C(67)-Br(11)	120.8(15)
C(74)-C(68)-C(67)	120.2(17)
C(74)-C(68)-Br(14)	116.4(16)
C(67)-C(68)-Br(14)	123.3(16)
C(68)-C(74)-C(62)	123.2(17)
C(68)-C(74)-H(74)	118.4
C(62)-C(74)-H(74)	118.4
C(60)-C(75)-C(62)	123.1(18)
C(60)-C(75)-H(75)	118.4
C(62)-C(75)-H(75)	118.4

O(3)-C(81)-C(63)	112.8(14)
C(100)-C(81)-H(81)	103.3
O(3)-C(81)-H(81)	103.3
C(63)-C(81)-H(81)	103.3
C(81)-C(100)-C(60)	111.3(17)
C(81)-C(100)-C(103)	120.1(16)
C(60)-C(100)-C(103)	110.4(16)
C(81)-C(100)-H(100)	104.5
C(60)-C(100)-H(100)	104.5
C(103)-C(100)-H(100)	104.5
C(112)-C(103)-C(111)	113.2(16)
C(112)-C(103)-C(100)	112.8(17)
C(111)-C(103)-C(100)	106.8(14)
C(112)-C(103)-H(103)	107.9
C(111)-C(103)-H(103)	107.9
C(100)-C(103)-H(103)	107.9
C(103)-C(111)-H(11D)	109.5
C(103)-C(111)-H(11E)	109.5
H(11D)-C(111)-H(11E)	109.5
C(103)-C(111)-H(11F)	109.5
H(11D)-C(111)-H(11F)	109.5
H(11E)-C(111)-H(11F)	109.5
C(103)-C(112)-H(11M)	109.5
C(103)-C(112)-H(11N)	109.5
H(11M)-C(112)-H(11N)	109.5
C(103)-C(112)-H(11O)	109.5
H(11M)-C(112)-H(11O)	109.5
H(11N)-C(112)-H(11O)	109.5

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 5i. The

anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

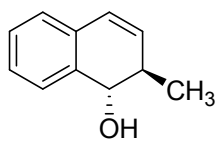
	U11	U22	U33	U23	U13	U12
Br(11)	67(2)	99(2)	107(2)	39(1)	9(1)	23(1)
Br(14)	90(2)	141(2)	142(2)	73(2)	50(2)	30(2)
C(60)	30(14)	127(19)	85(15)	47(14)	-20(10)	2(13)
C(62)	73(16)	75(15)	56(12)	21(11)	31(12)	59(13)
C(63)	66(15)	20(10)	76(14)	22(9)	29(11)	21(10)
O(3)	60(9)	82(10)	64(7)	43(7)	19(6)	33(7)
C(66)	74(16)	68(14)	69(13)	27(11)	30(12)	32(12)
C(67)	72(16)	55(13)	58(12)	29(10)	20(10)	23(11)
C(68)	50(14)	68(14)	91(14)	37(12)	32(11)	32(11)
C(74)	93(18)	81(15)	87(15)	38(13)	43(14)	69(14)
C(75)	57(15)	86(16)	50(11)	9(11)	-5(11)	36(12)
C(81)	64(15)	76(14)	51(12)	34(11)	9(10)	15(11)
C(100)	110(20)	105(18)	47(12)	18(13)	-2(12)	34(15)
C(103)	45(13)	78(15)	83(14)	27(12)	9(10)	18(12)
C(111)	88(16)	87(16)	88(14)	33(13)	10(11)	32(13)
C(112)	130(20)	150(20)	111(16)	59(15)	52(14)	111(18)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 5i.

	x	y	z	U(eq)
H(60)	2195	2989	9741	111
H(3)	194	2802	6839	96

H(66)	-1557	1492	6556	82
H(74)	-1691	935	9249	88
H(75)	583	1773	9745	83
H(81)	966	1775	7500	80
H(100)	1207	3553	8644	116
H(103)	2765	3802	7883	88
H(11D)	3397	4476	9841	137
H(11E)	2881	4974	9299	137
H(11F)	4132	5019	9280	137
H(11M)	4270	3429	8318	166
H(11N)	3114	2444	7805	166
H(11O)	3559	2882	8887	166

3. Copies of ^{1}H and ^{13}C NMR spectra of 2a-g, 2ff, 2gg, 3a-f, 4a, 4aa, 4e, 4ee, 5a, 5d, 5e, 5i, 5f, and 6a, 6e



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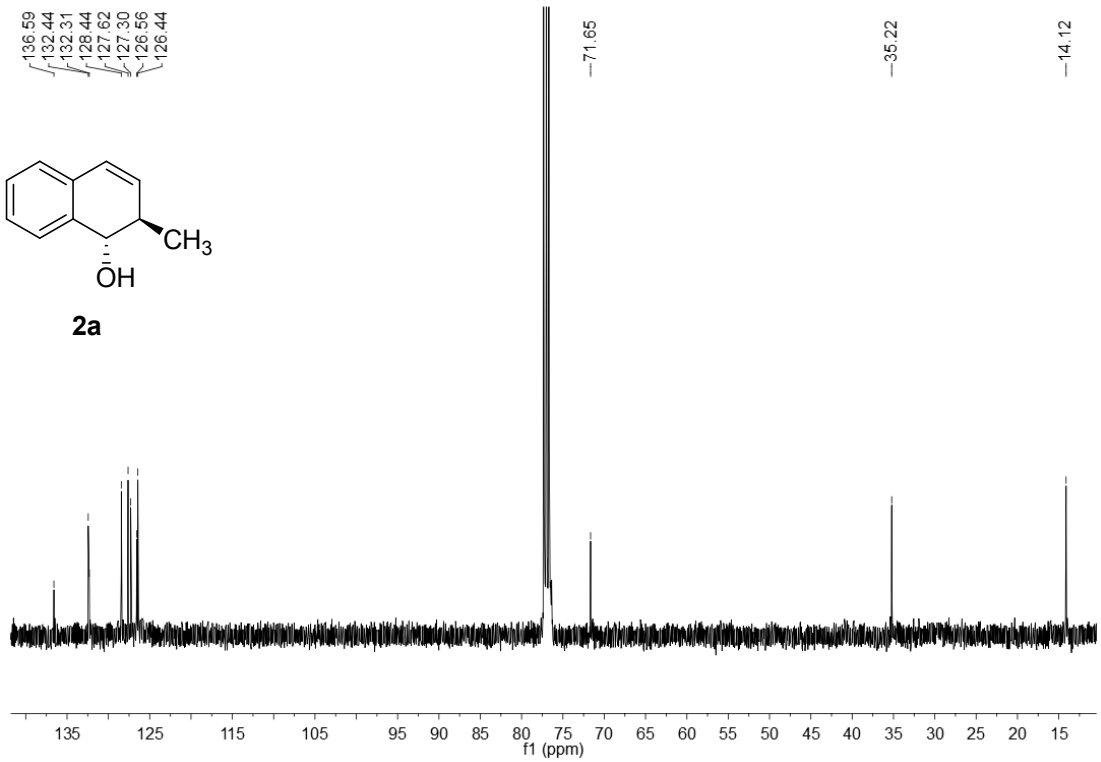
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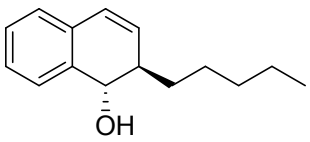
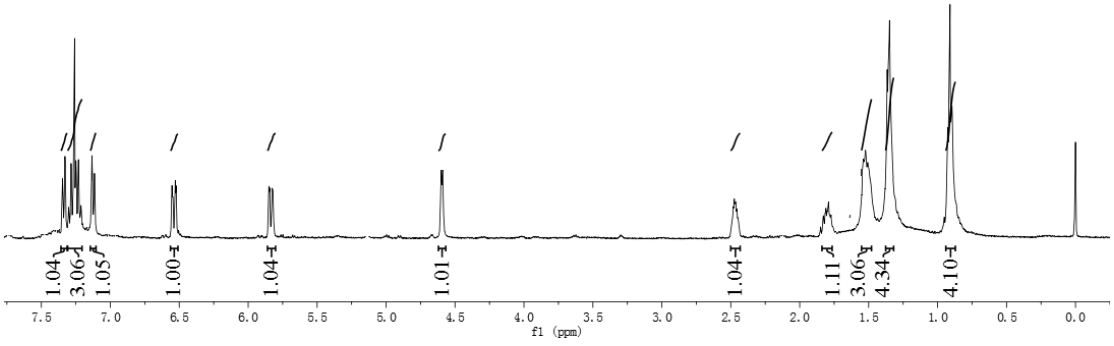
CH3
OH
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
f1 (ppm)

2a


OH

2b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1.04
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6.5
6.0
5.5
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4.0
3.5
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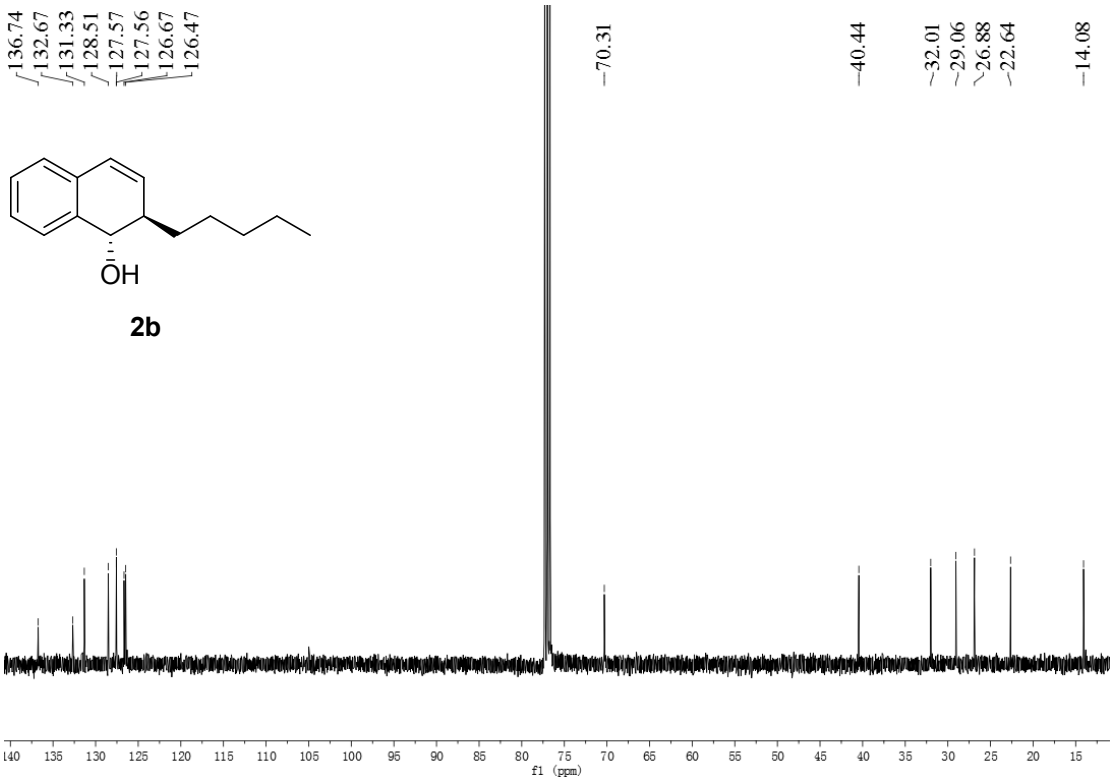
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OH
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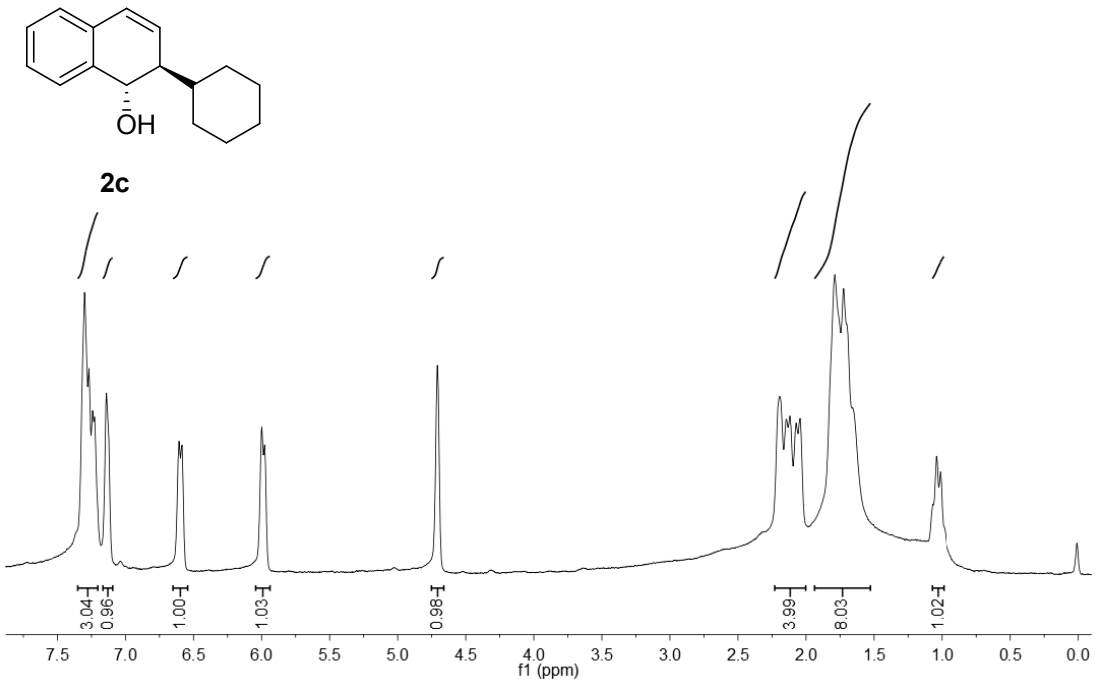
2b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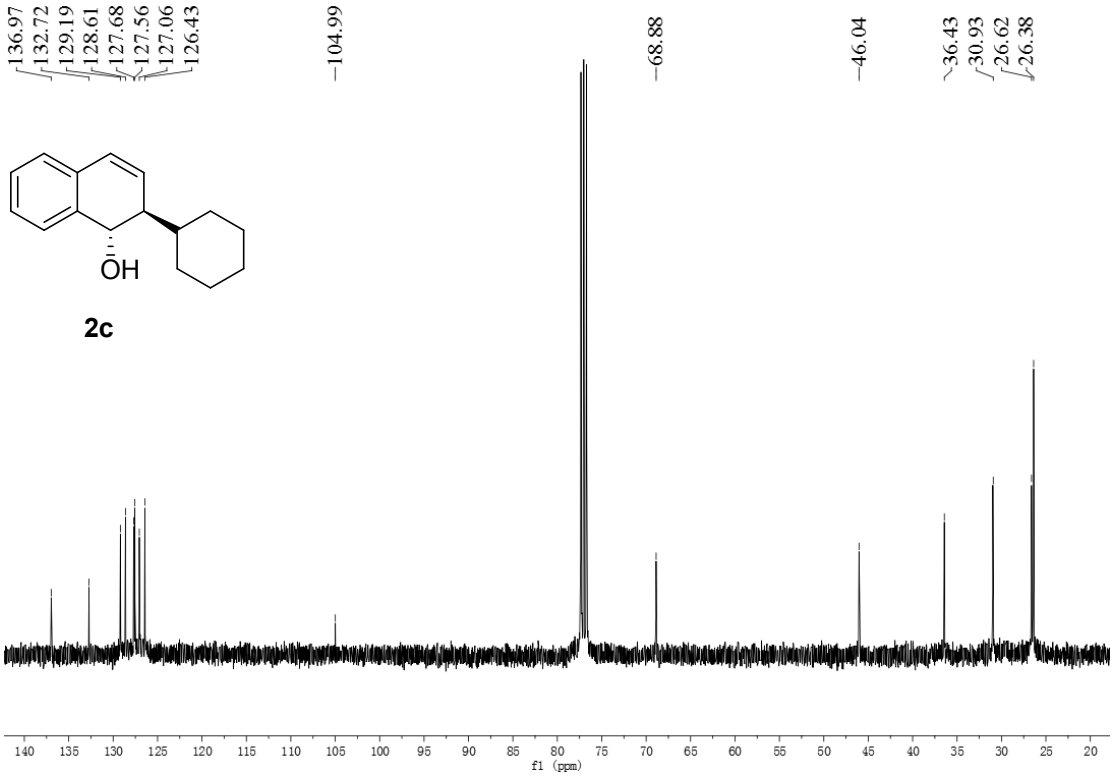
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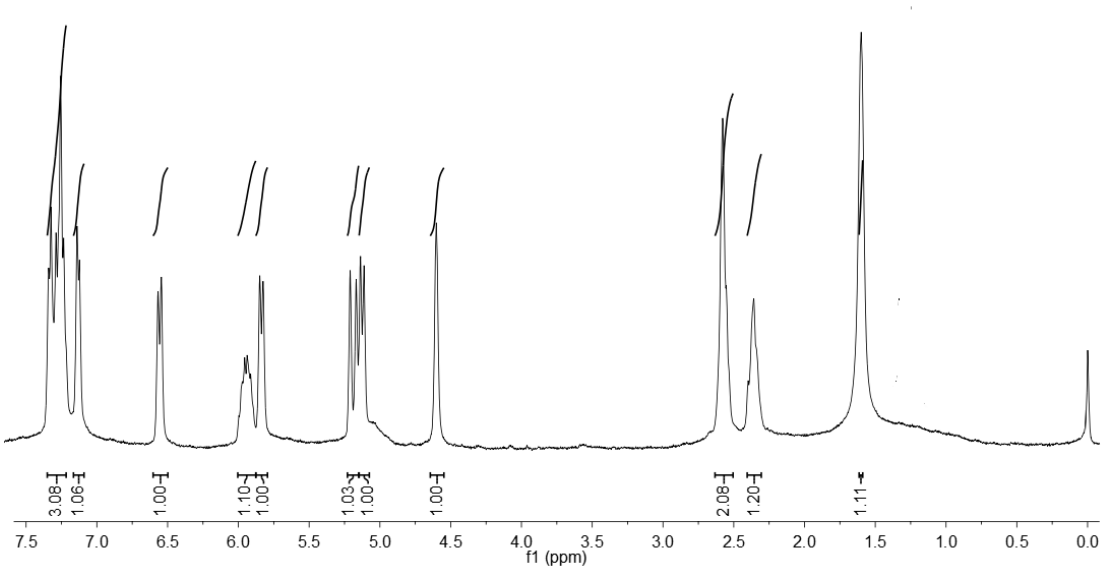
2c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1.00
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1.20
1.11
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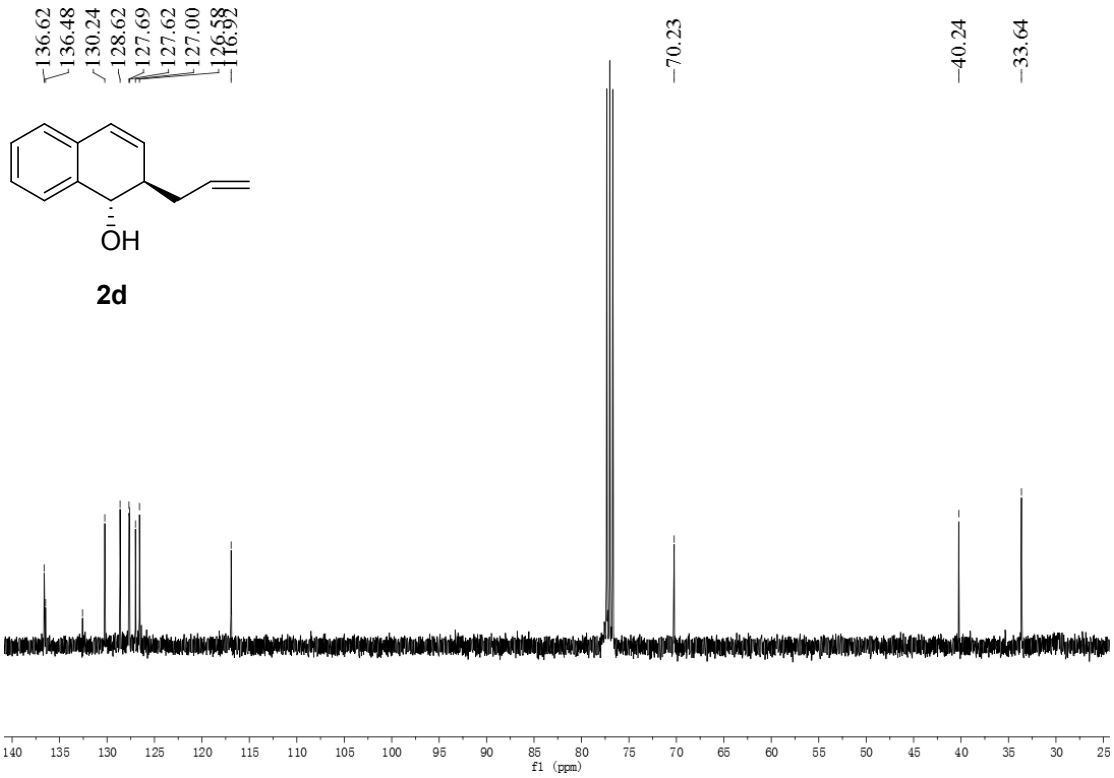
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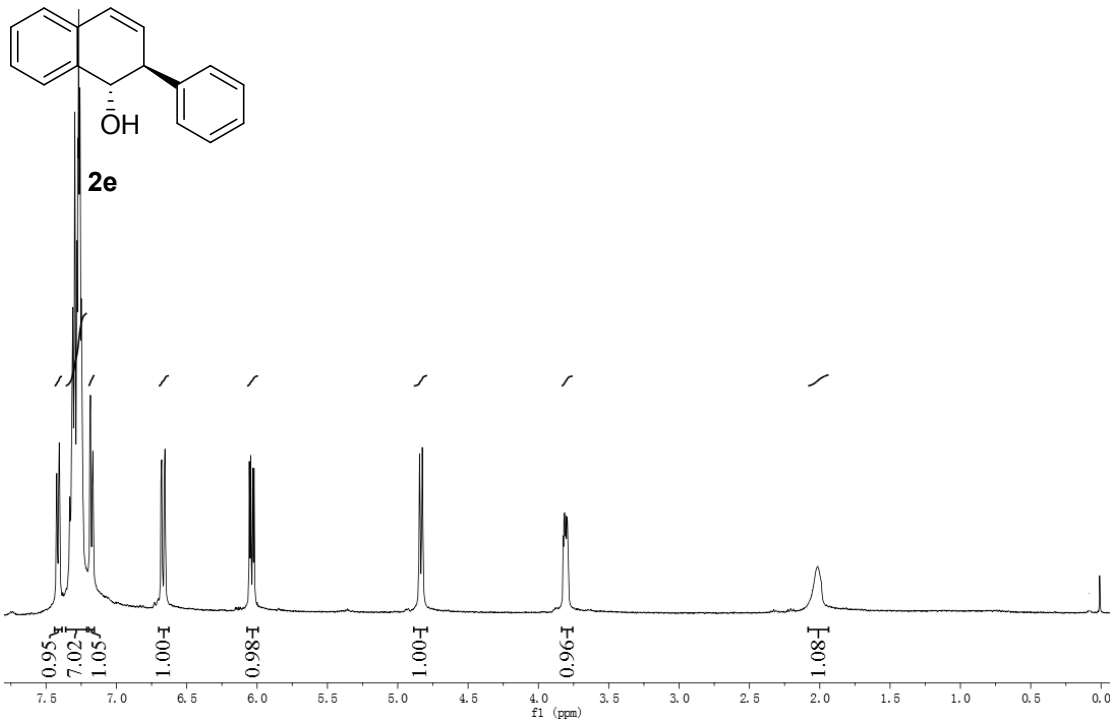
OH
2d
f1 (ppm)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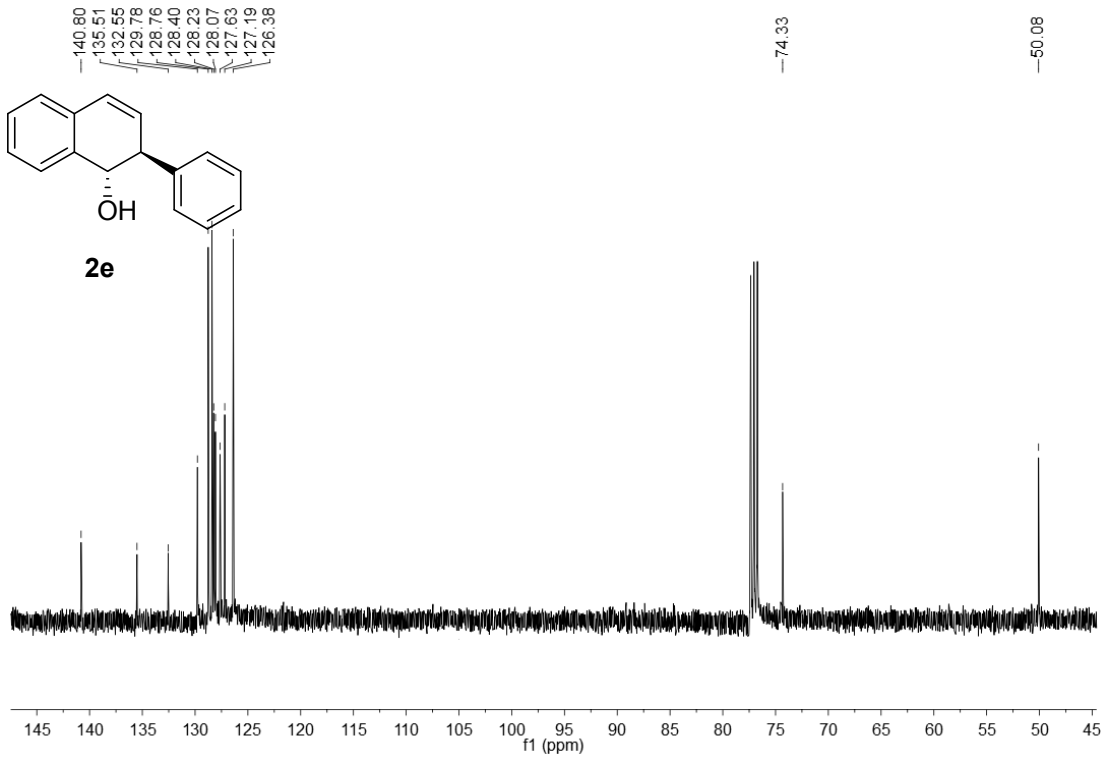
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2e
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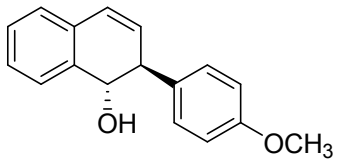
f1 (ppm)


OH
OCH3

2f

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2.07
2.96
2.01
1.04
1.00
1.00
1.03
3.00
0.83
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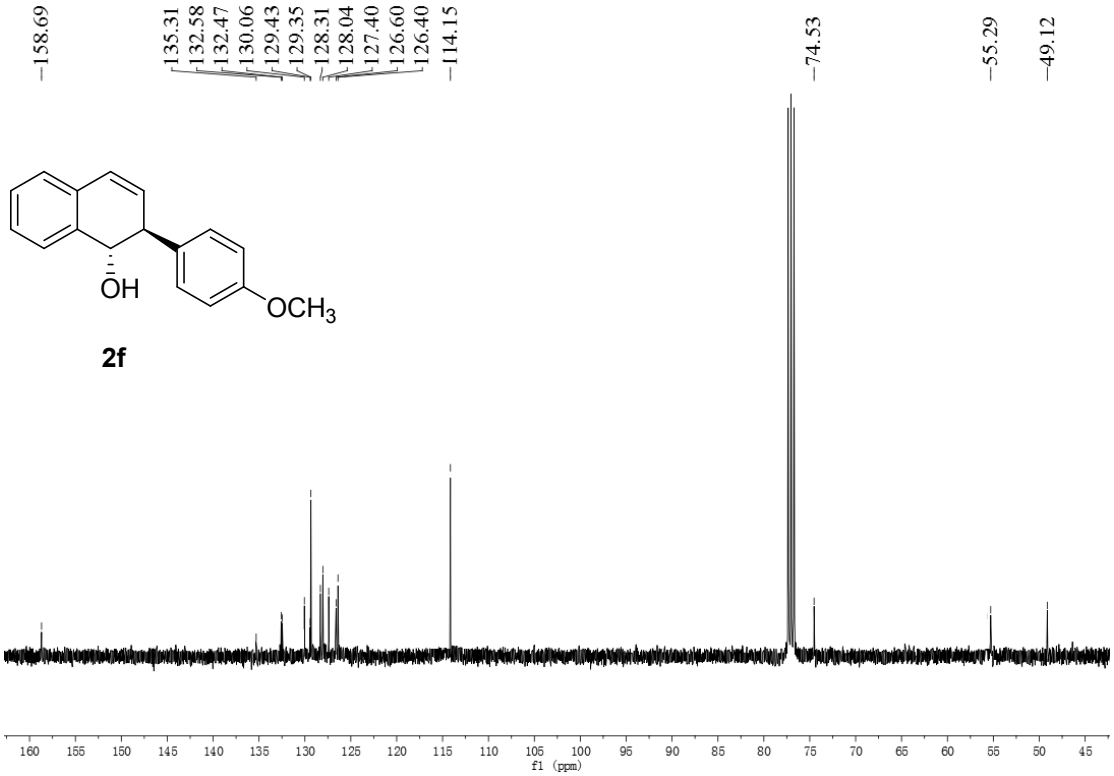
f1 (ppm)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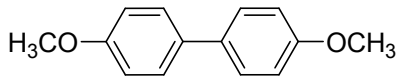
f1 (ppm)

OH
OCH3

2f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OCH3

2ff

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6.0
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4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
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f1 (ppm)


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OCH3

2ff

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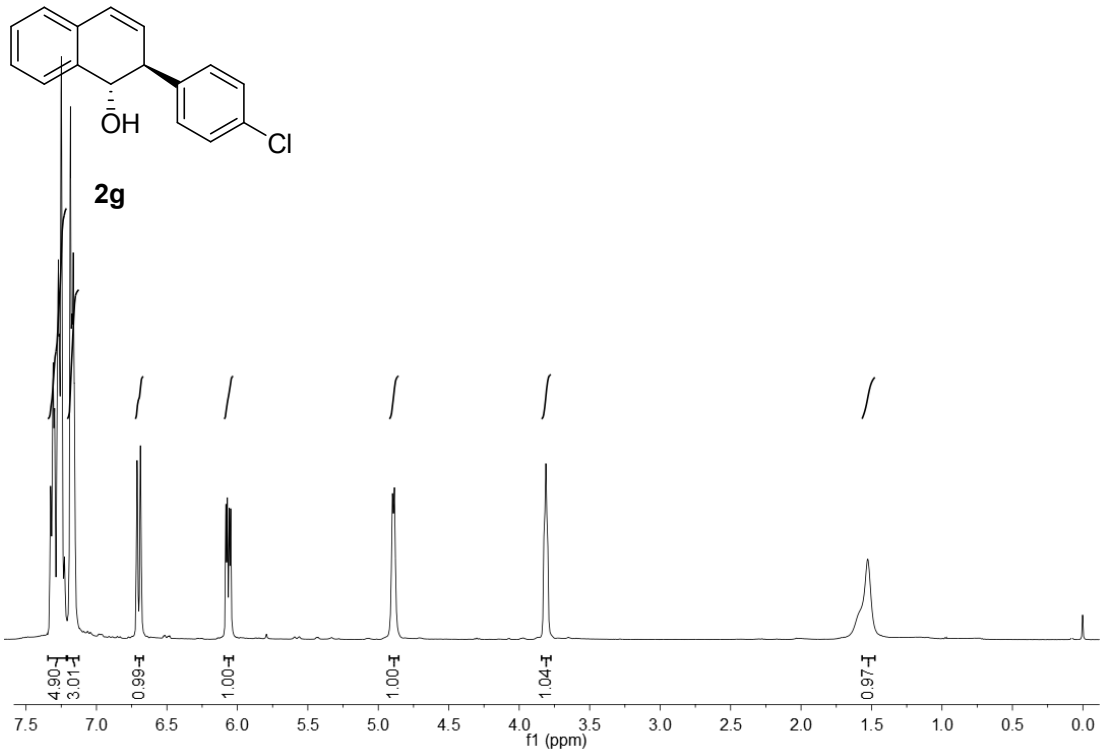
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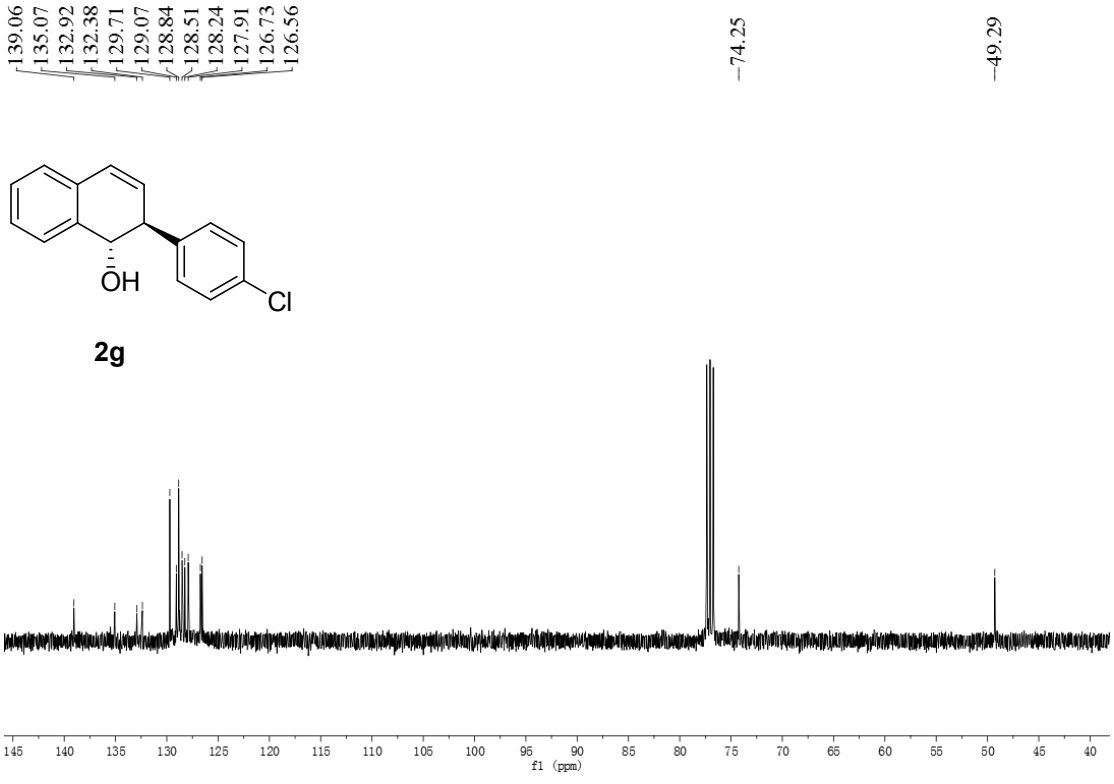
f1 (ppm)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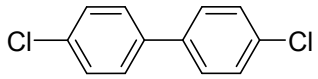
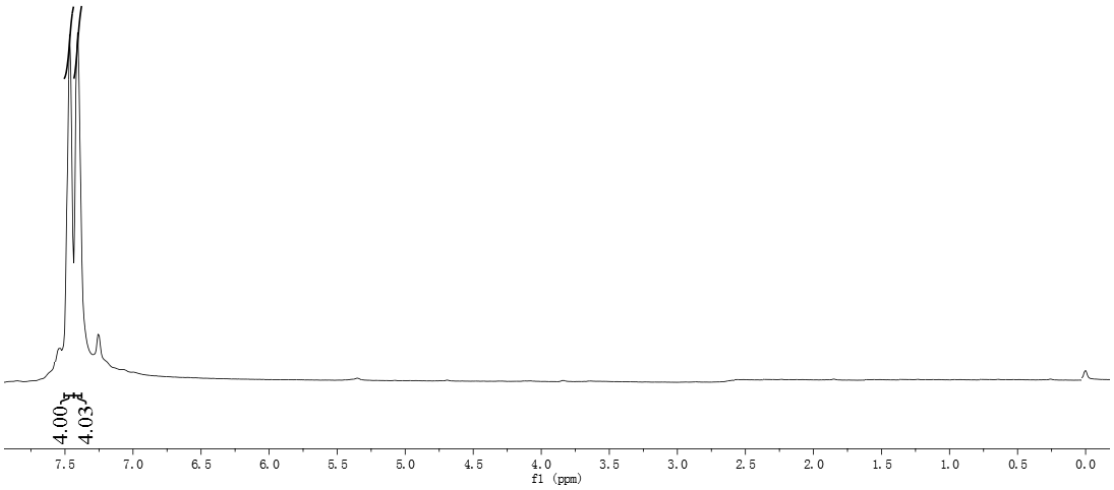
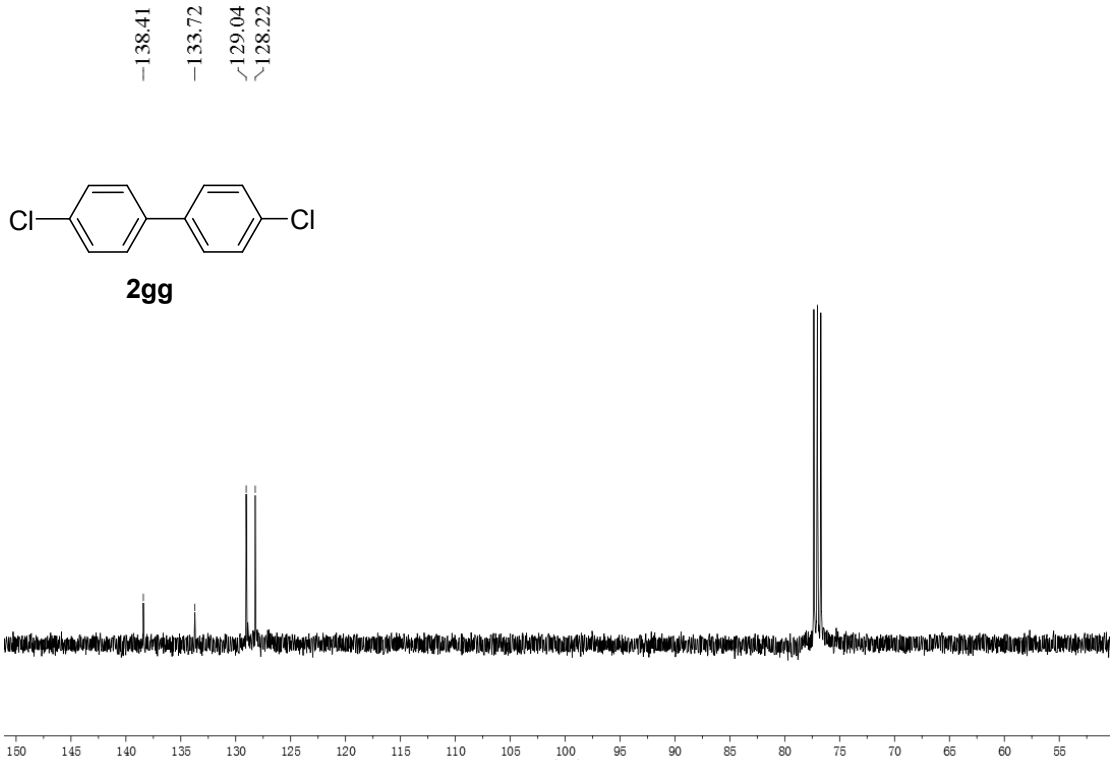
74.25
49.29
OH
Cl
2g
145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40
f1 (ppm)


Cl
Cl

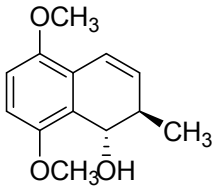
2gg


4.00
4.03
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


138.41
133.72
129.04
128.22
150
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
f1 (ppm)

Cl
Cl

2gg


OCH3
CH3
OCH3OH

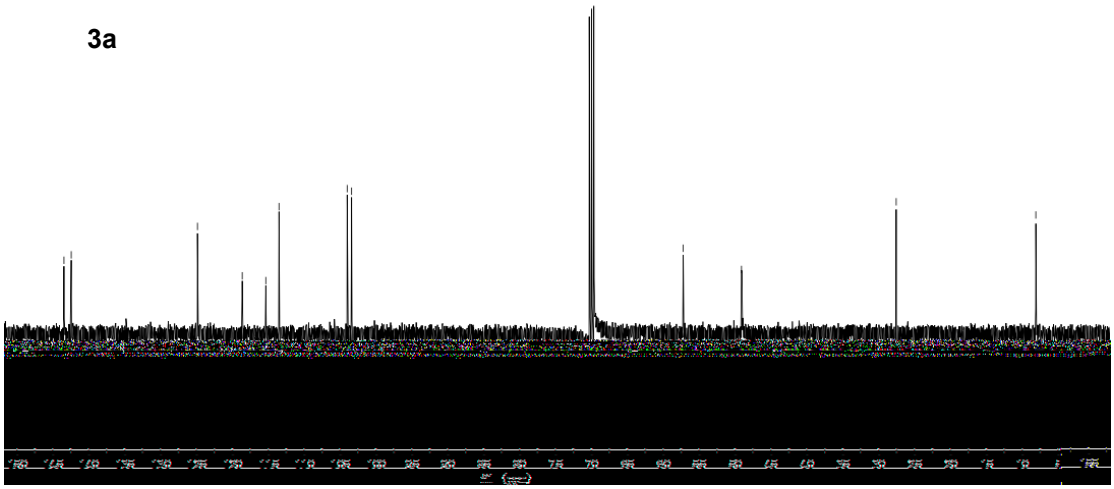
3a

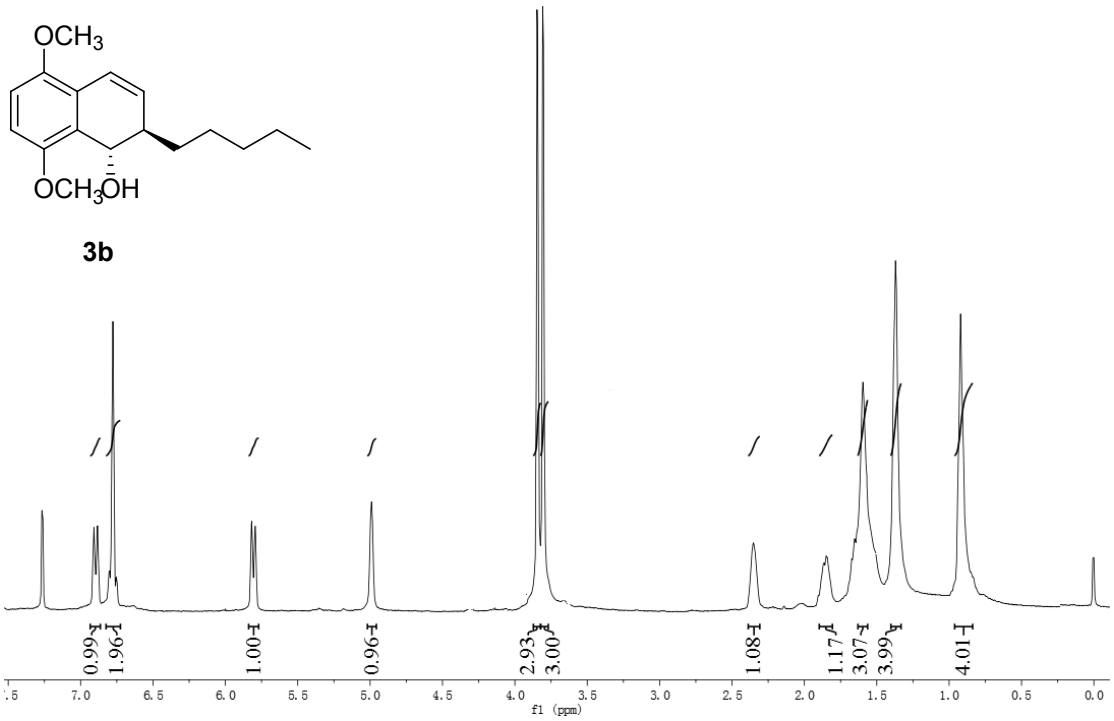
0.95
2.02
1.00
1.01
3.07
3.08
1.06
1.18
3.04
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

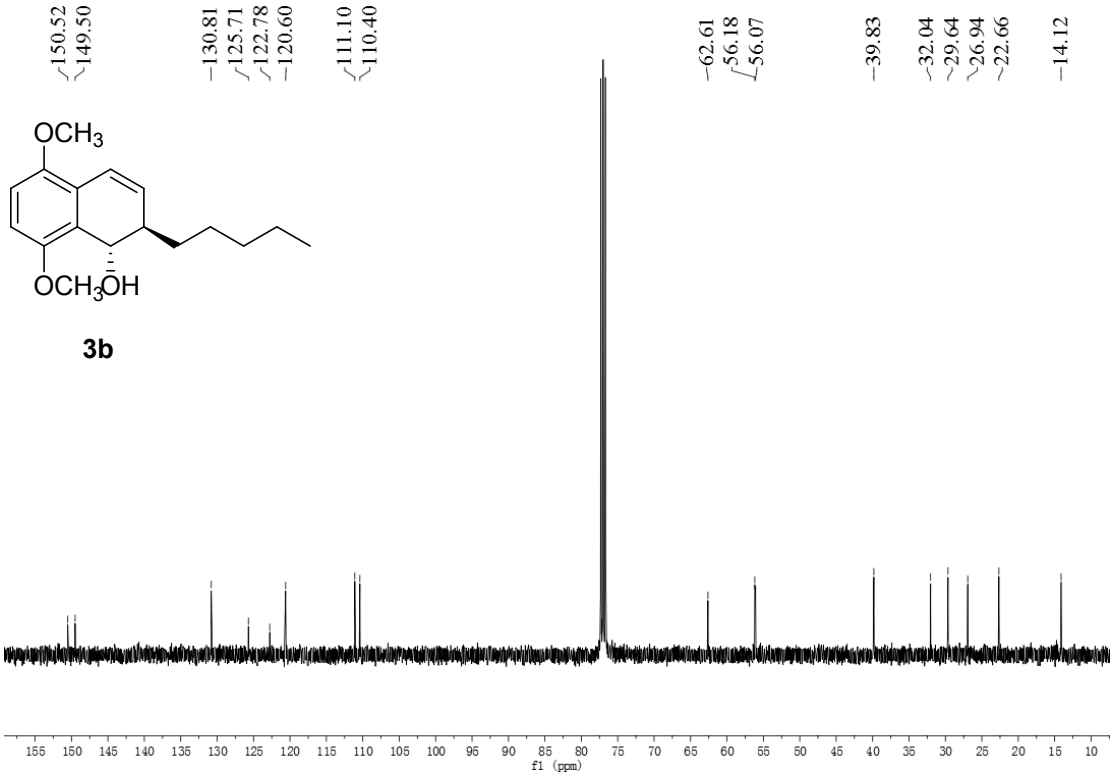

150.49
149.48
131.90
125.67
122.38
120.54
111.05
110.43
64.25
56.14
34.59
15.15

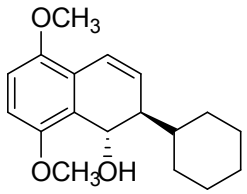
OCH3
CH3
OCH3OH

3a



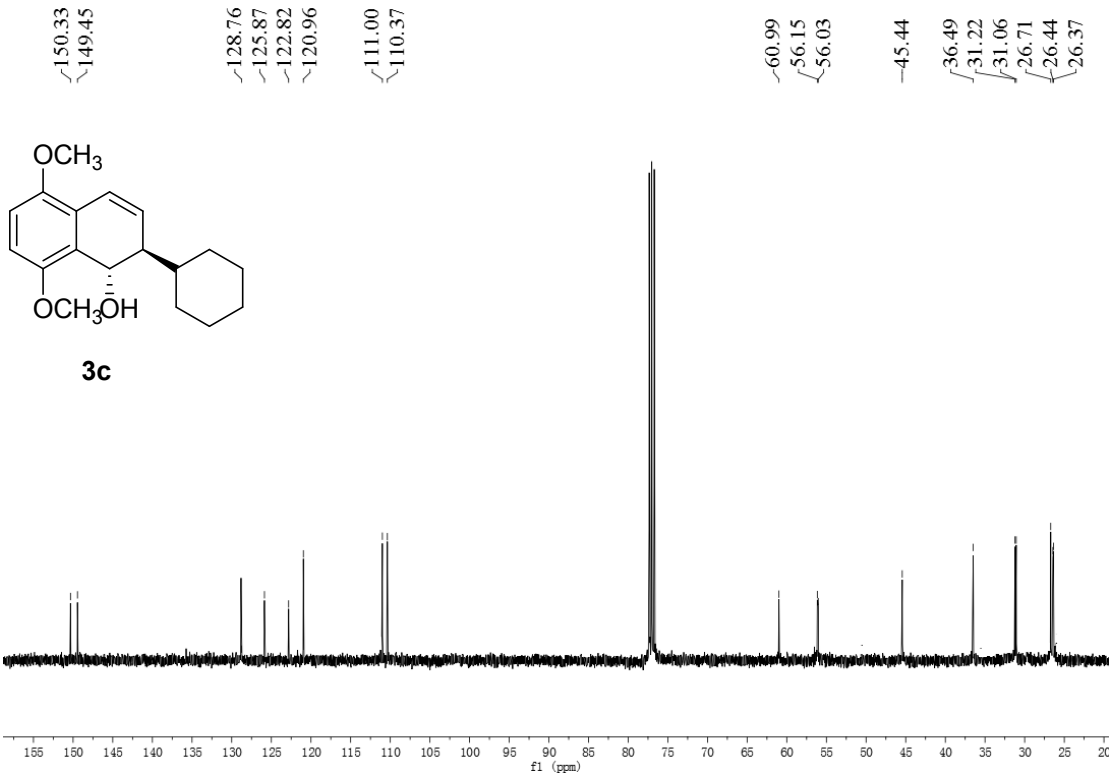

OCH3
OCH3
OH
3b
0.99
1.96
1.00
0.96
2.93
3.00
1.08
1.17
3.07
3.99
4.01
f1 (ppm)


150.52
149.50
130.81
125.71
122.78
120.60
111.10
110.40
62.61
56.18
56.07
39.83
32.04
29.64
26.94
22.66
14.12
OCH3
OCH3
OH
3b
f1 (ppm)

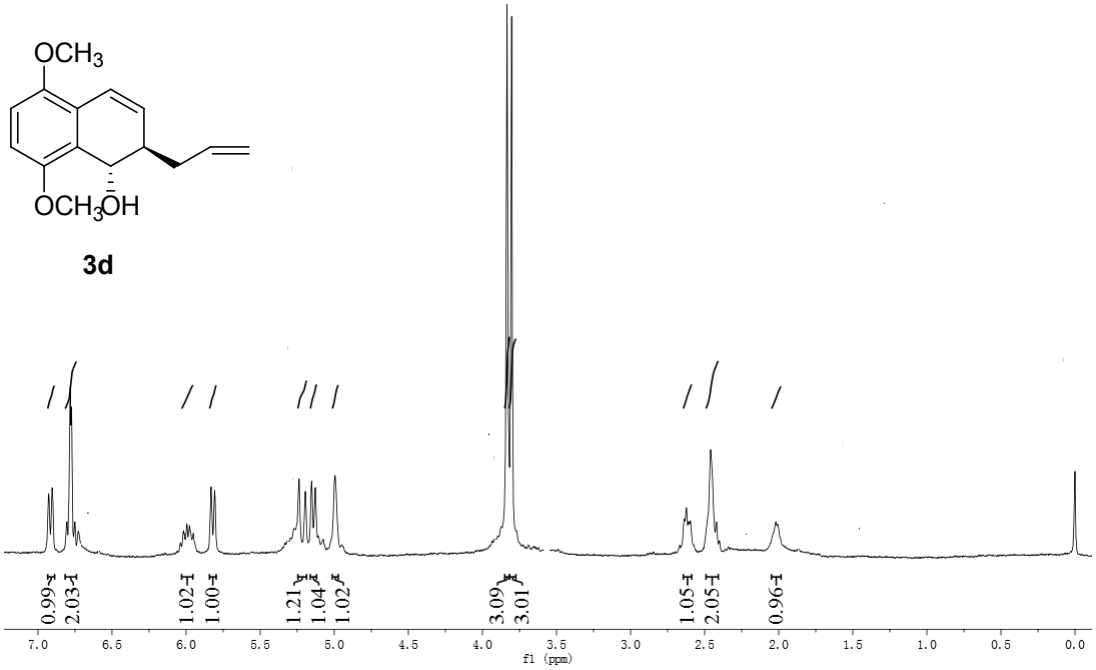

OCH3
OCH3
OH

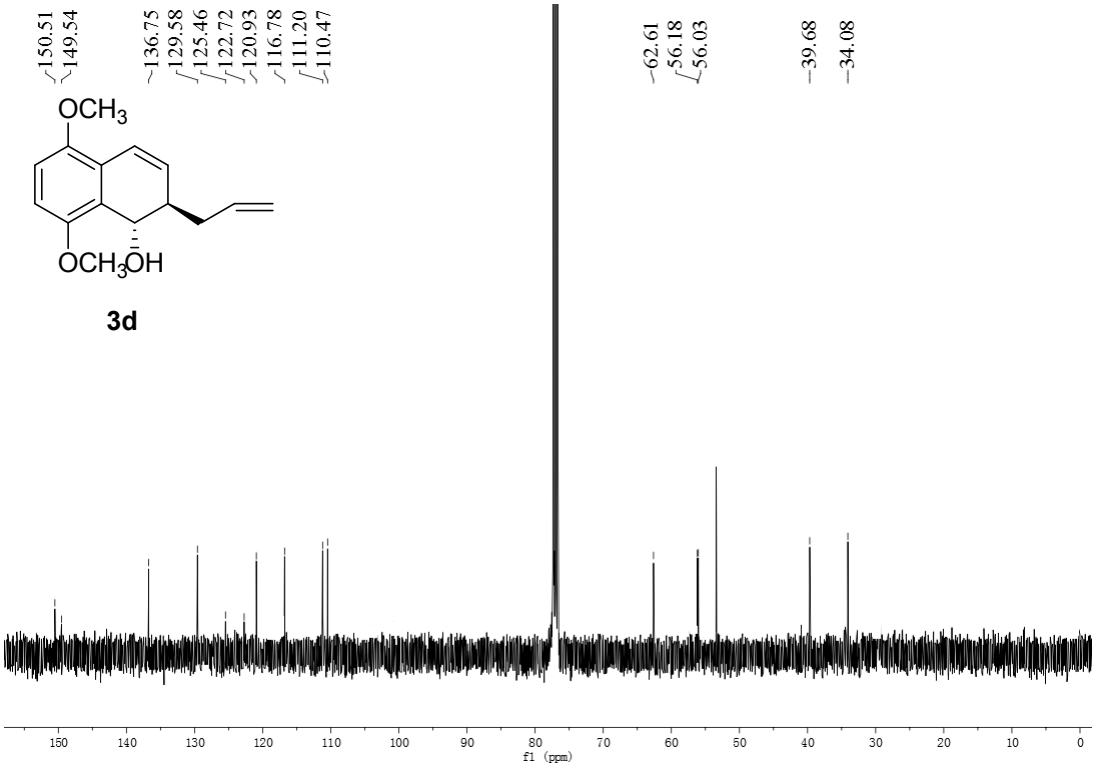
3c

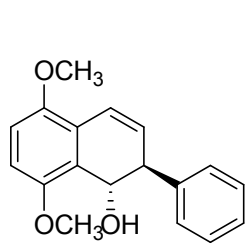
1.02
1.96
1.00
1.04
0.65
2.95
3.03
1.15
1.12
1.25
6.07
2.00
0.98
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


150.33
149.45
128.76
125.87
122.82
120.96
111.00
110.37
60.99
56.15
56.03
45.44
36.49
31.22
31.06
26.71
26.44
26.37
OCH3
OCH3
OH
155
150
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
f1 (ppm)

3c

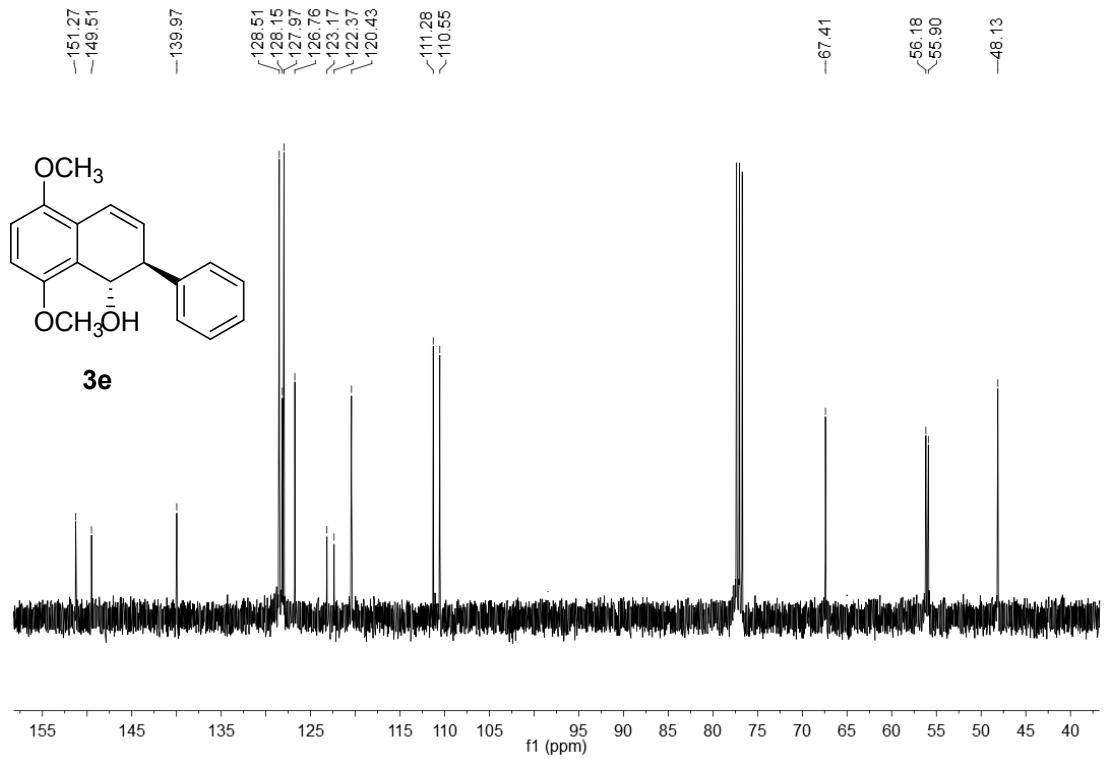

OCH3
OCH3
OH
3d
0.99
2.03
1.02
1.00
1.21
1.04
1.02
3.09
3.01
1.05
2.05
0.96
f1 (ppm)


150.51
149.54
136.75
129.58
125.46
122.72
120.93
116.78
111.20
110.47
62.61
56.18
56.03
39.68
34.08
OCH3
OCH3
OH
3d
f1 (ppm)


OCH3
OCH3
OH

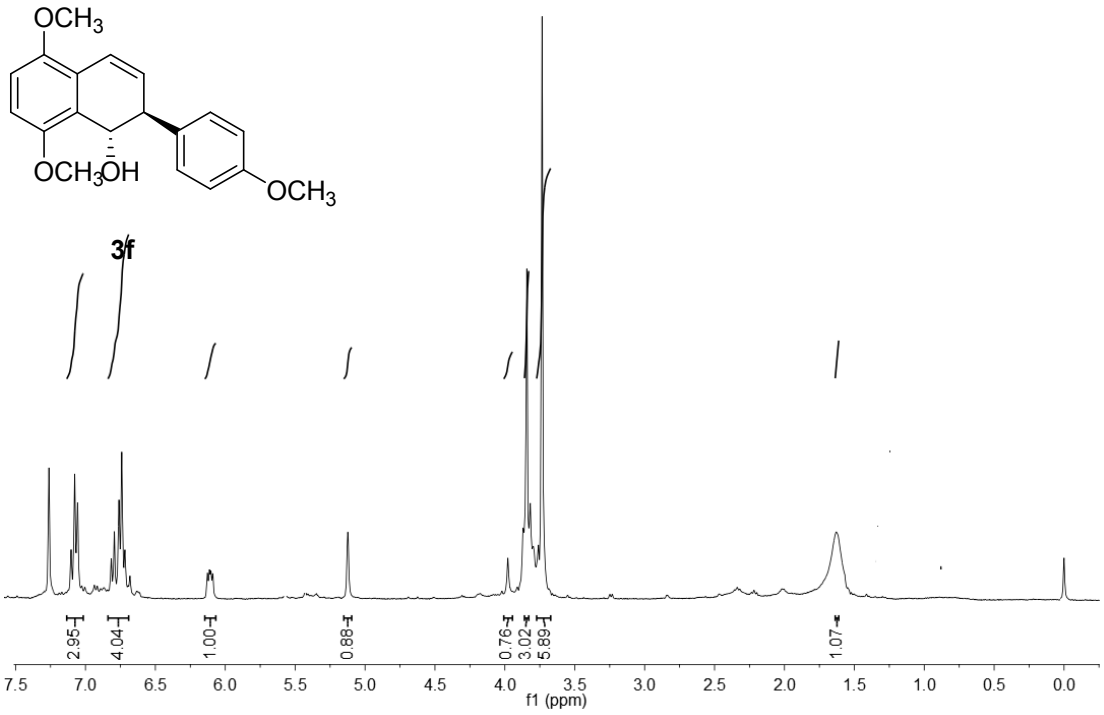
3e

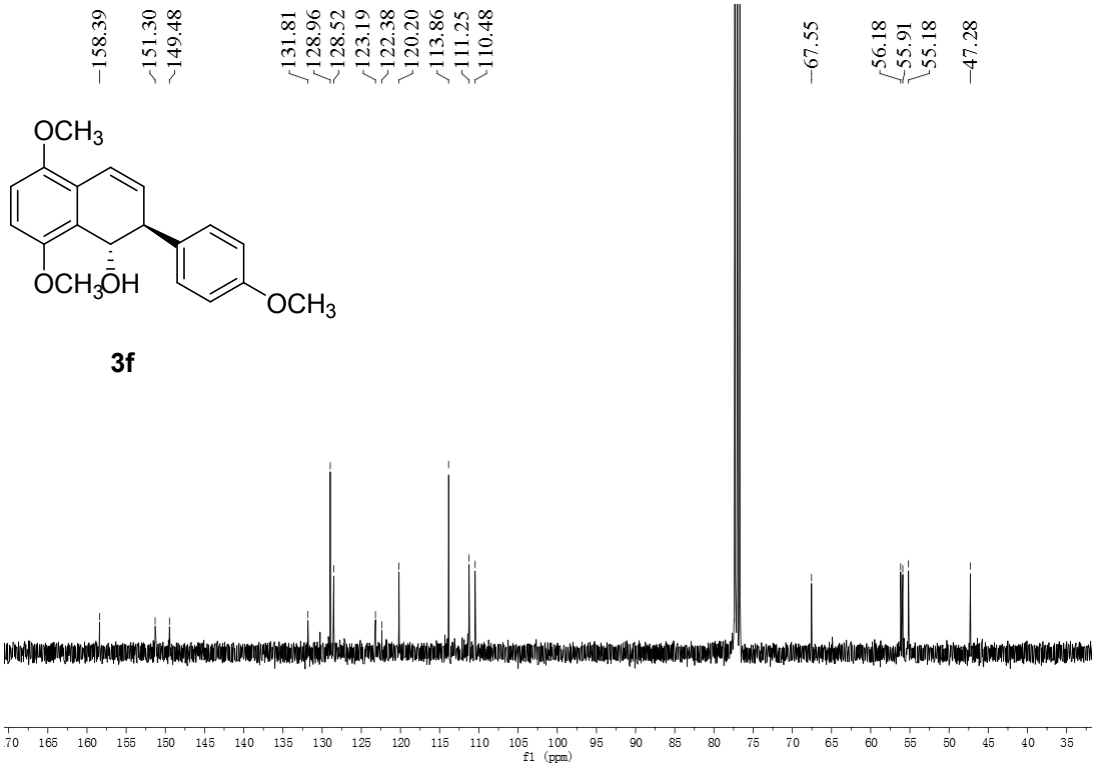
4.80
1.04
1.04
1.01
1.00
1.01
1.03
2.86
2.75
0.88
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

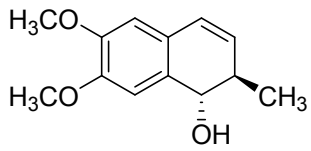

151.27
149.51
139.97
128.51
128.15
127.97
126.76
123.17
122.37
120.43
111.28
110.55
67.41
56.18
55.90
48.13
155
145
135
125
115
110
105
95
90
85
80
75
70
65
60
55
50
45
40
f1 (ppm)

OCH3
OCH3
OH

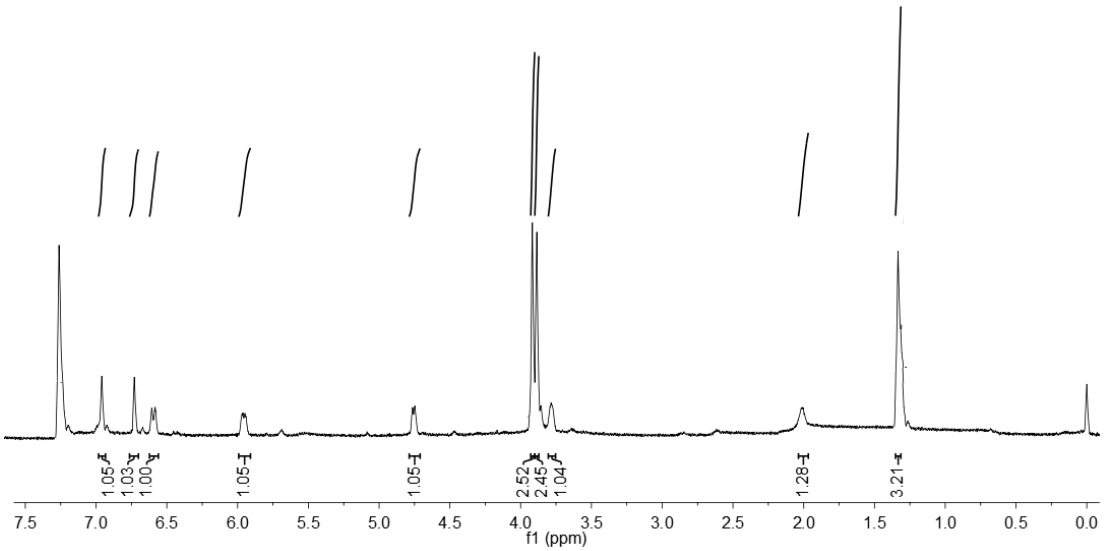
3e

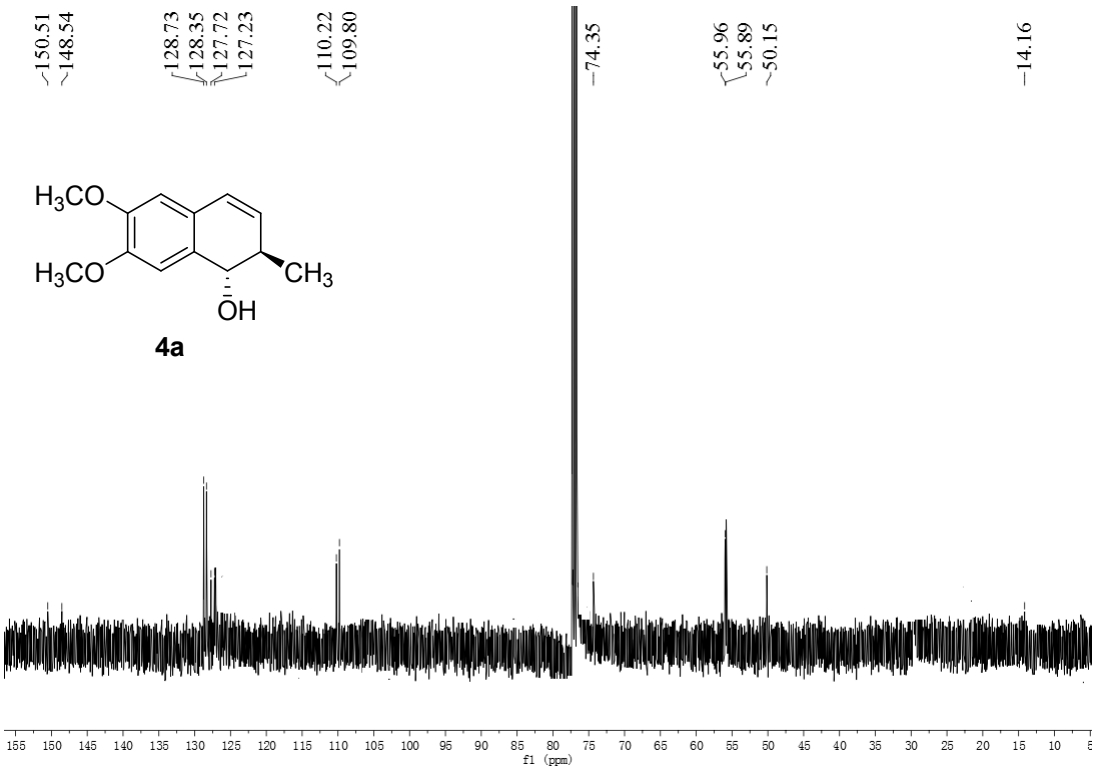

OCH3
OCH3
OH
OCH3
3f
2.95
4.04
1.00
0.88
0.76
3.02
5.89
1.07
f1 (ppm)


158.39
151.30
149.48
131.81
128.96
128.52
123.19
122.38
120.20
113.86
111.25
110.48
67.55
56.18
55.91
55.18
47.28
OCH3
OCH3
OH
OCH3
3f
f1 (ppm)

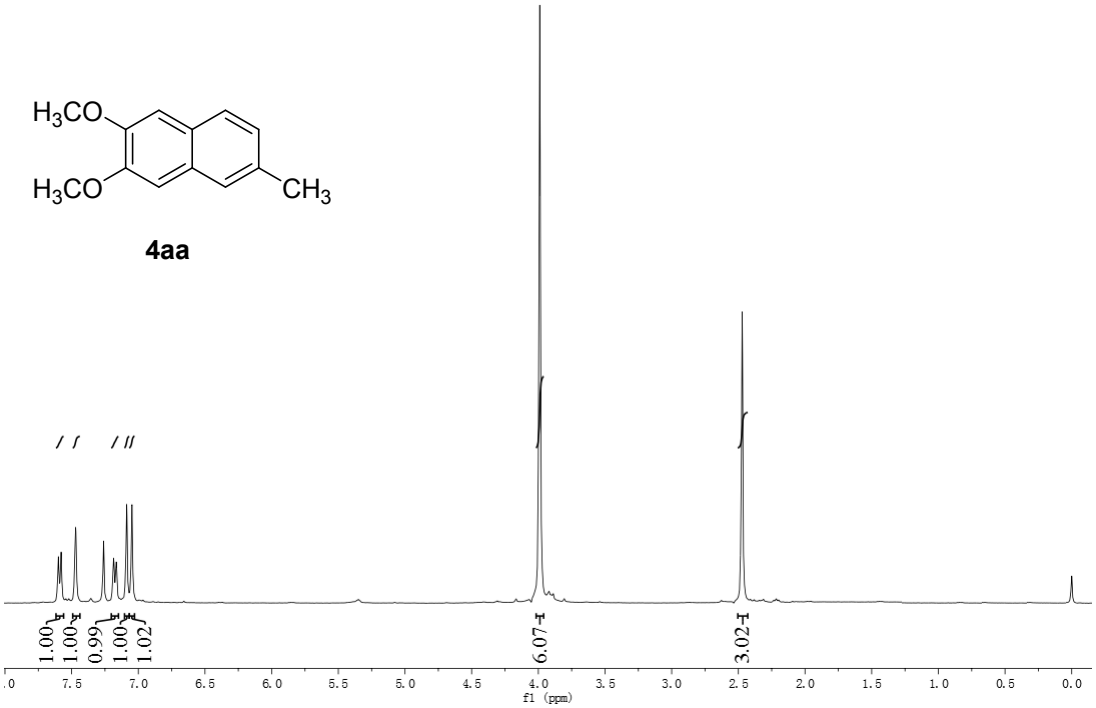

H3CO
H3CO
CH3
OH

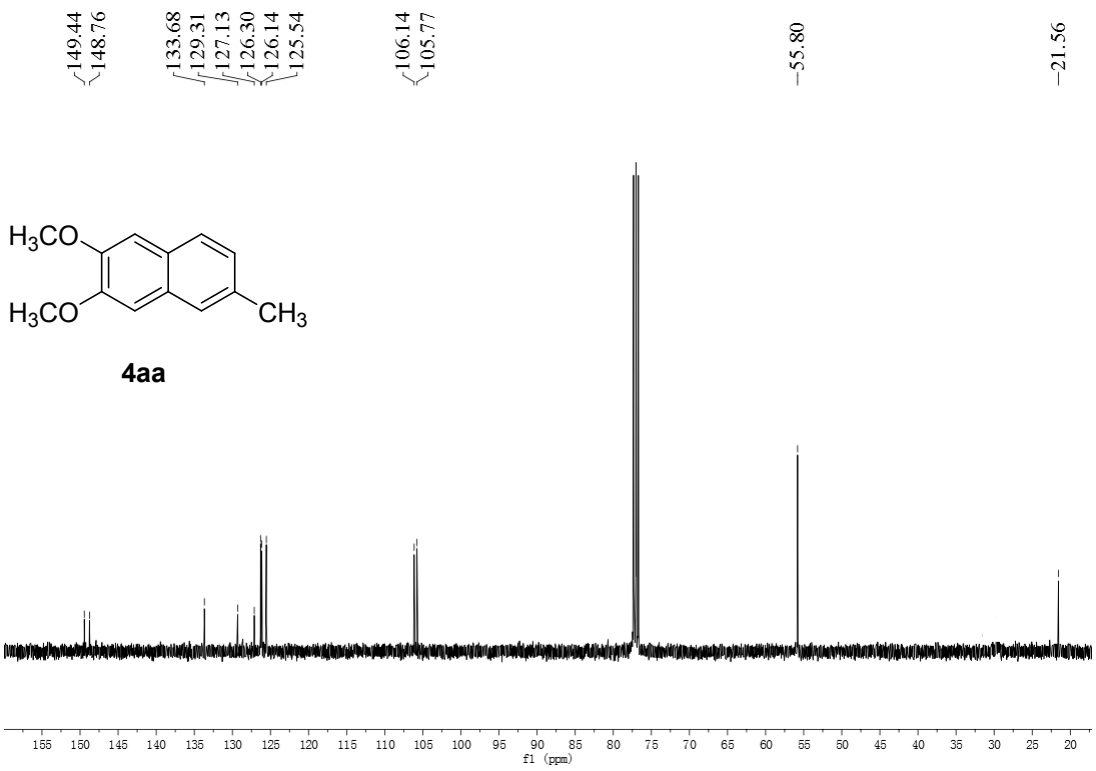
4a

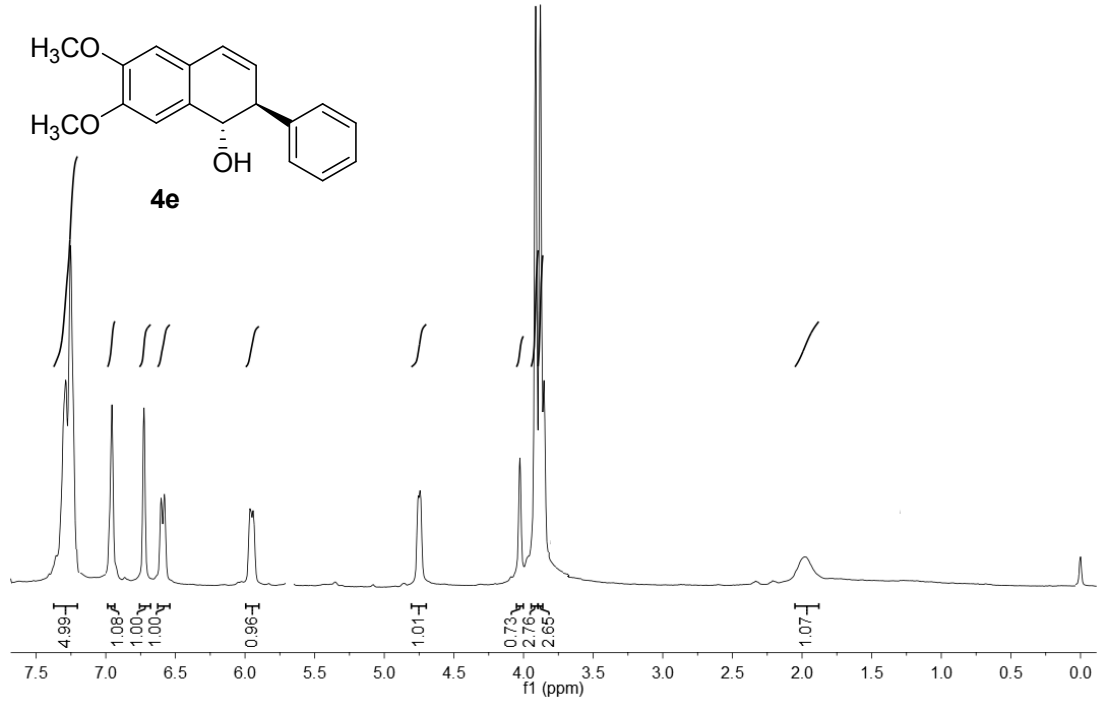

1.05
1.03
1.00
1.05
1.05
2.52
2.45
1.04
1.28
3.21
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

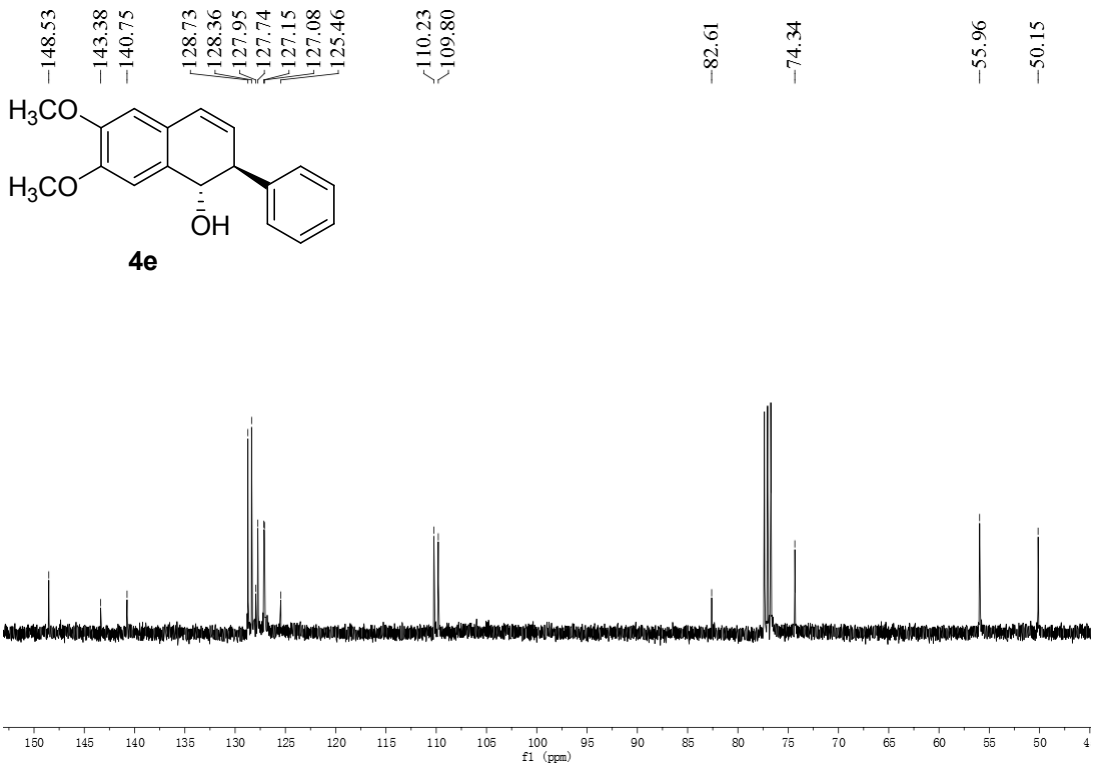

150.51
148.54
128.73
128.35
127.72
127.23
110.22
109.80
74.35
55.96
55.89
50.15
14.16
H3CO
H3CO
CH3
OH
155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10
f1 (ppm)

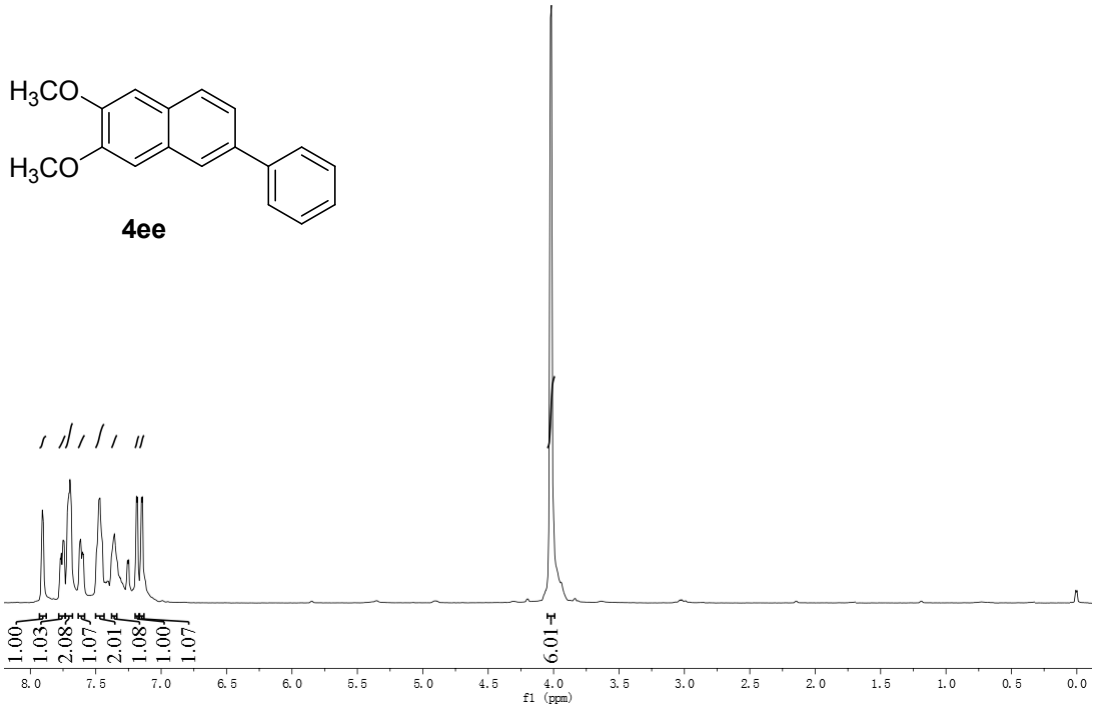
4a

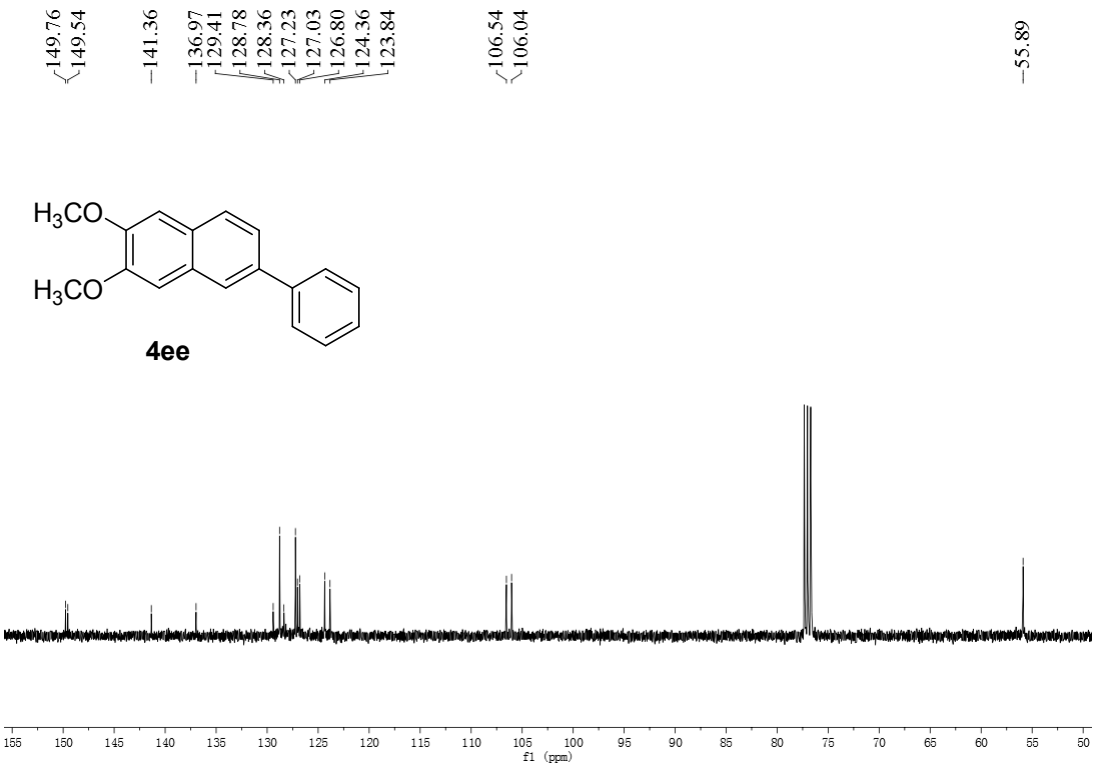

H3CO
H3CO
CH3
4aa
1.00
1.00
0.99
1.00
1.02
6.07
3.02
f1 (ppm)

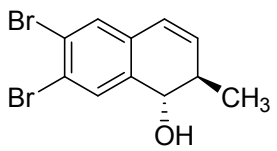

149.44
148.76
133.68
129.31
127.13
126.30
126.14
125.54
106.14
105.77
55.80
21.56
H3CO
H3CO
CH3
4aa
f1 (ppm)


H3CO
H3CO
OH
4e
4.99
1.08
1.00
1.00
0.96
1.01
0.73
2.76
2.65
1.07
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

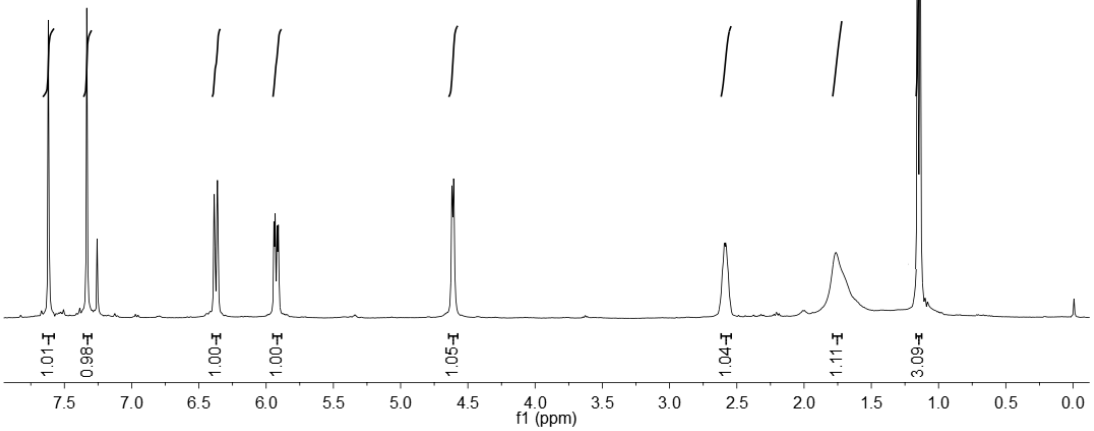

148.53
143.38
140.75
128.73
128.36
127.95
127.74
127.15
127.08
125.46
110.23
109.80
82.61
74.34
55.96
50.15
H3CO
H3CO
OH
4e
150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 4
f1 (ppm)

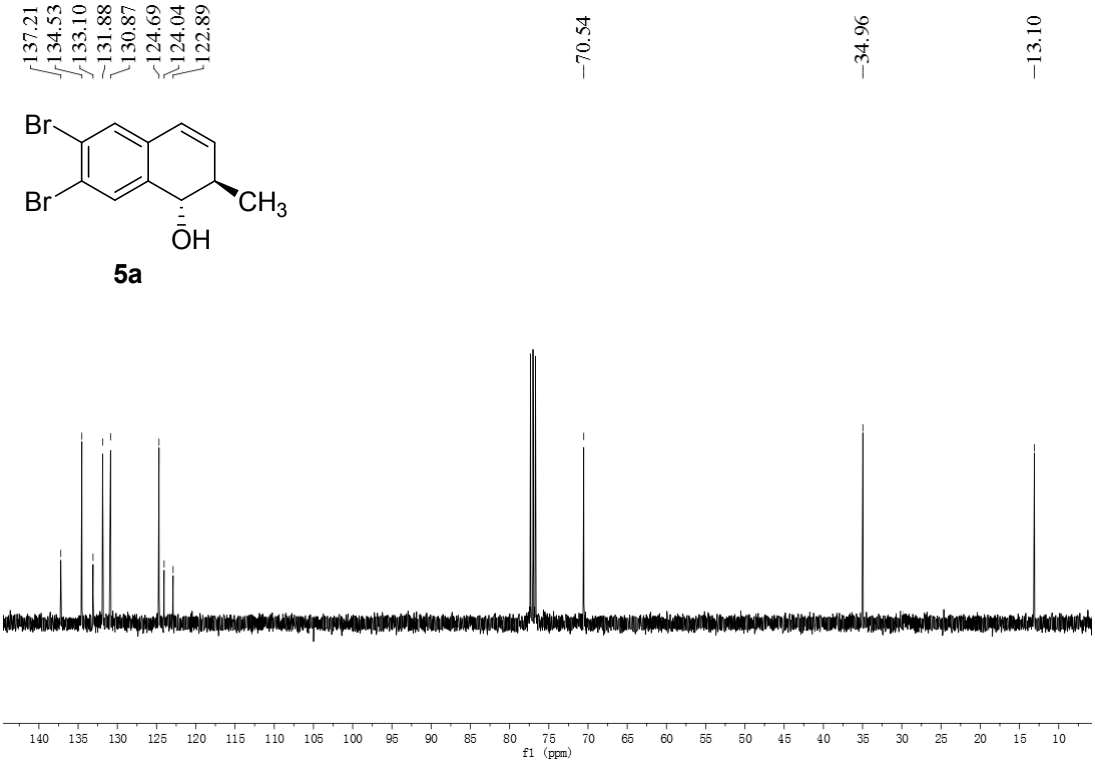

H3CO
H3CO
4ee
1.00
1.03
2.08
1.07
2.01
1.08
1.00
1.07
6.01
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


149.76
149.54
141.36
136.97
129.41
128.78
128.36
127.23
127.03
126.80
124.36
123.84
106.54
106.04
55.89
H3CO
H3CO
4ee
155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50
f1 (ppm)

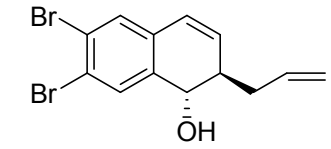

Br
Br
CH3
OH

5a

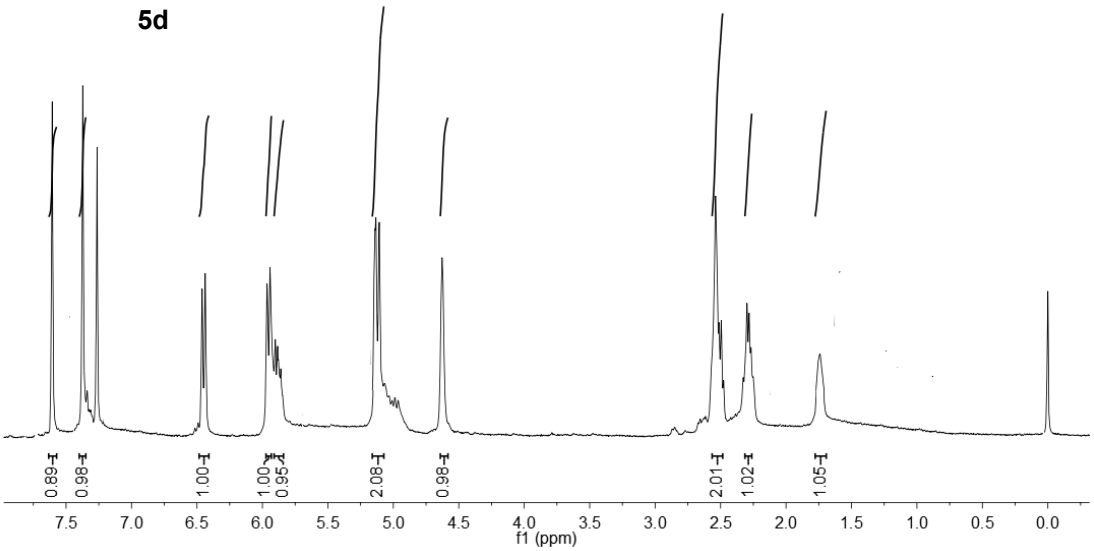

1.01
0.98
1.00
1.00
1.05
1.04
1.11
3.09
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

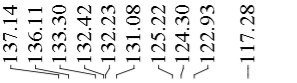

137.21
134.53
133.10
131.88
130.87
124.69
124.04
122.89
70.54
34.96
13.10
Br
Br
CH3
OH
140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10
f1 (ppm)

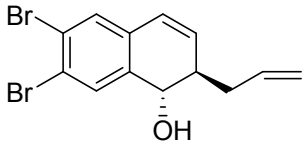
5a


Br
Br
OH

5d

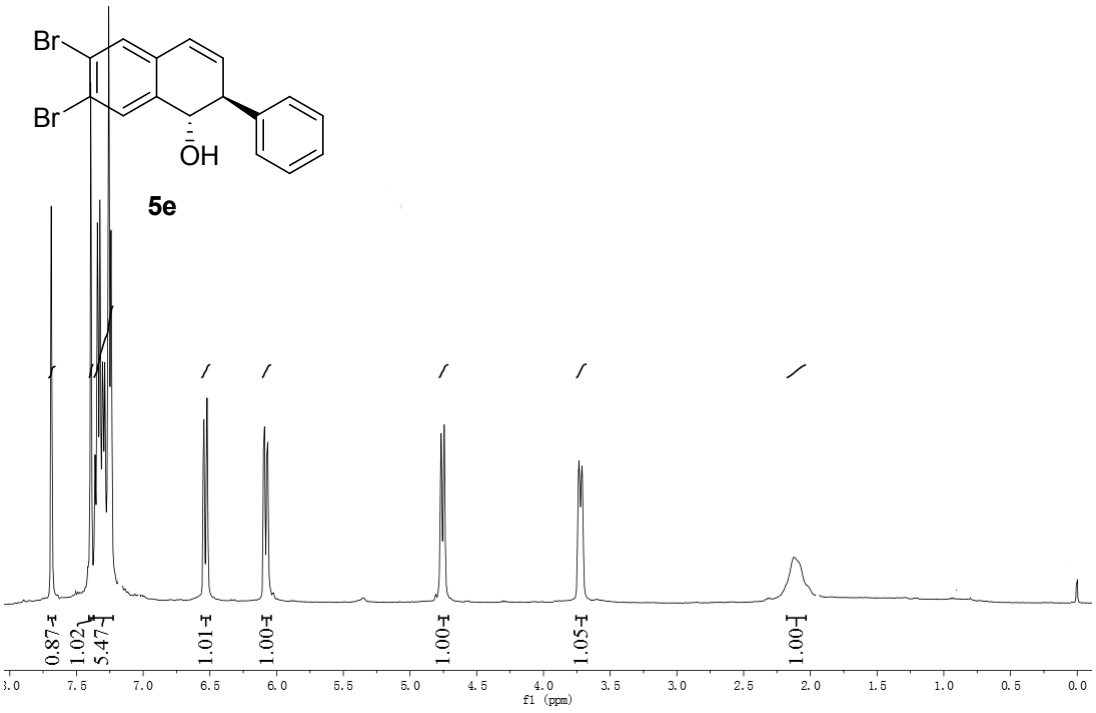

0.89
0.98
1.00
1.00
0.95
2.08
0.98
2.01
1.02
1.05
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

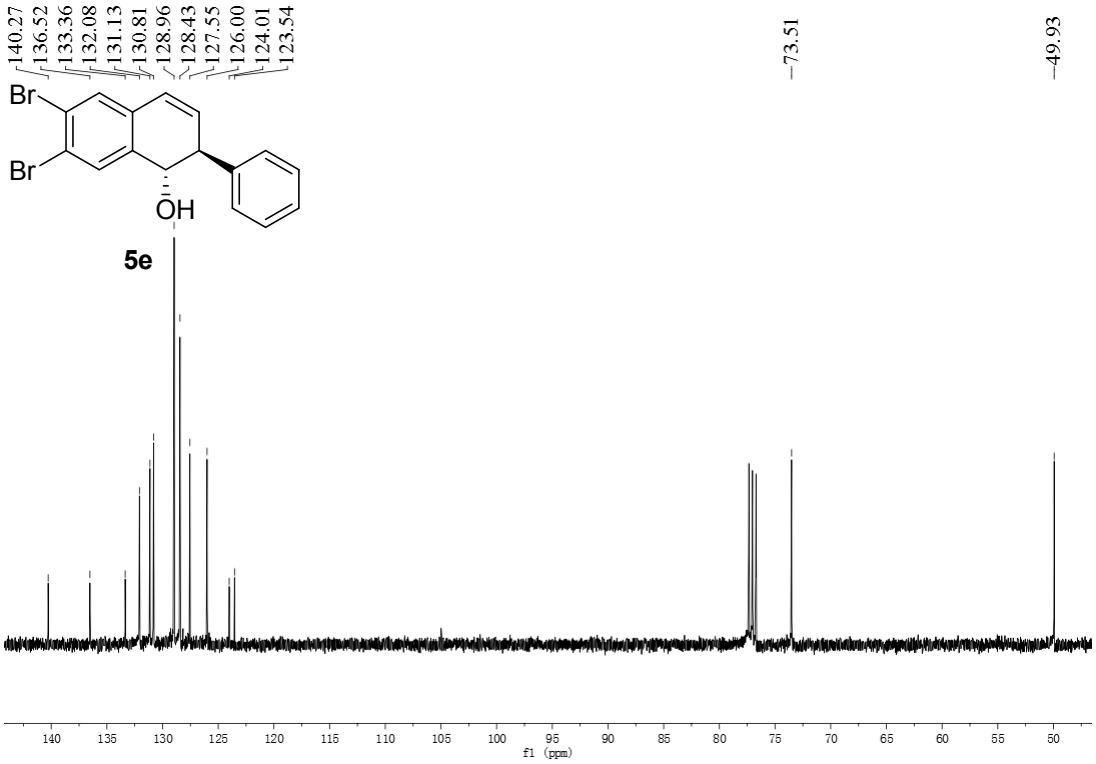

137.14
136.11
133.30
132.42
132.23
131.08
125.22
124.30
122.93
117.28

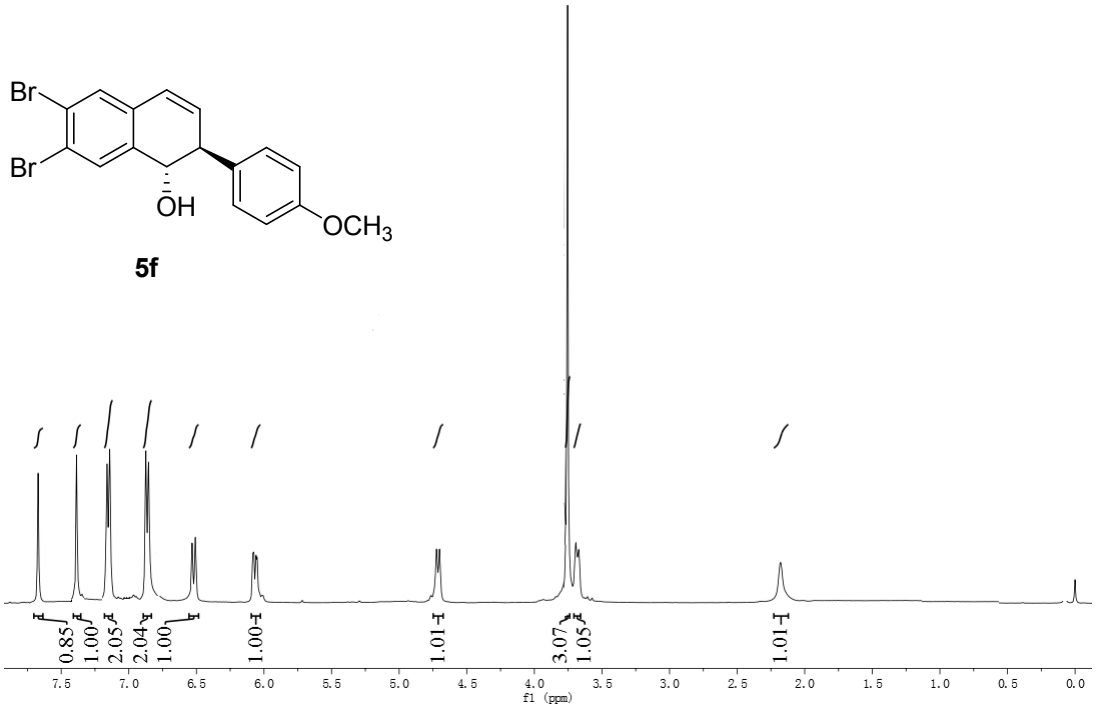

Br
Br
OH

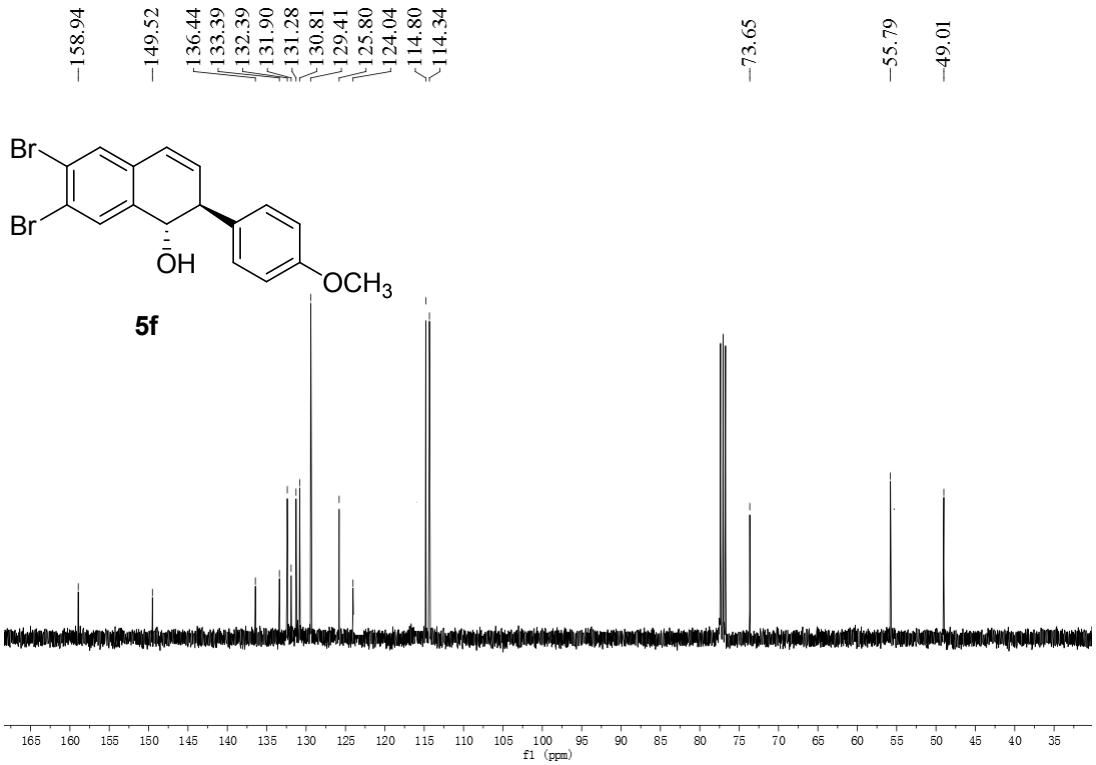
5d

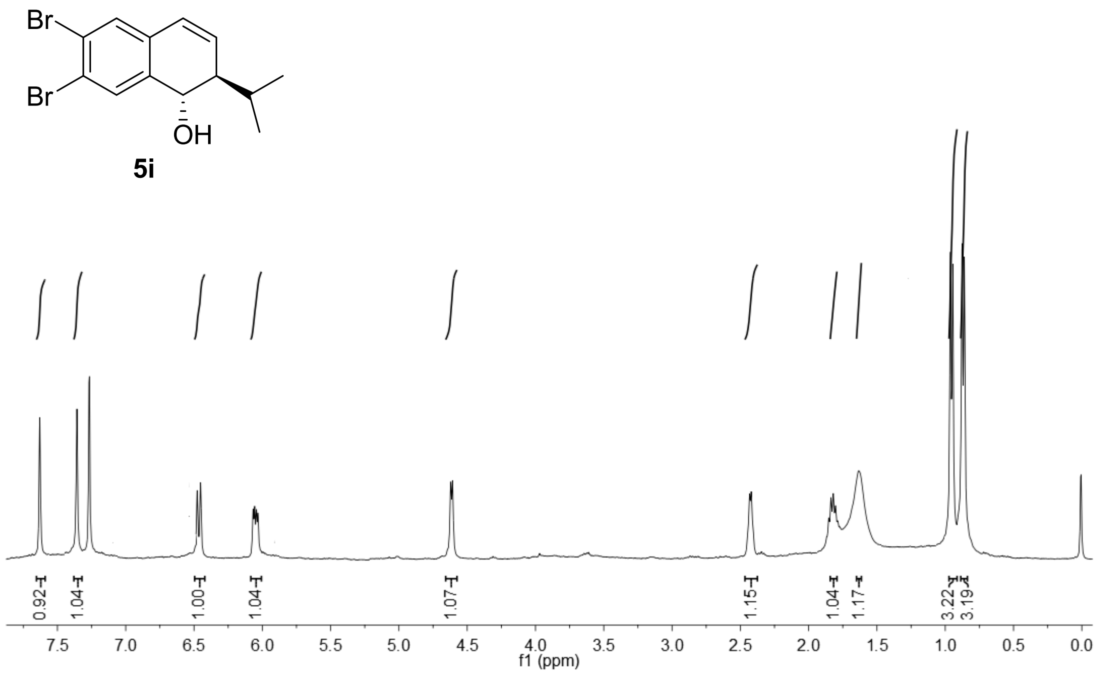
69.36
39.93
33.04
140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35
f1 (ppm)

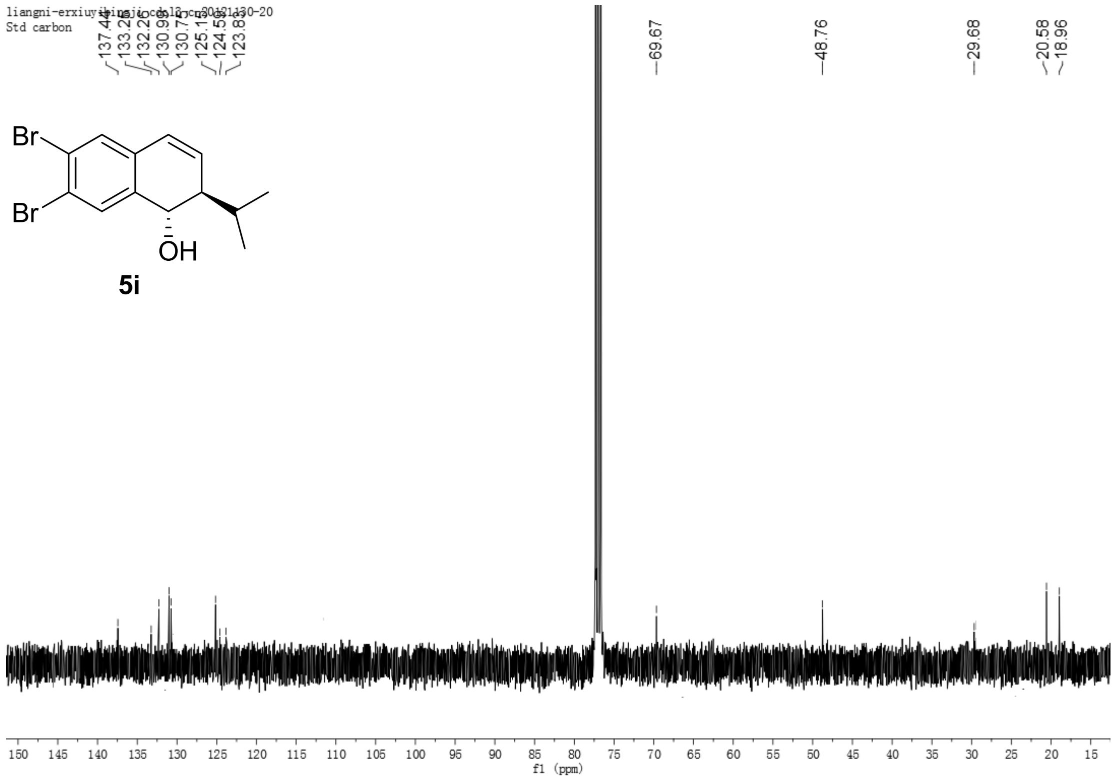

Br
Br
OH
5e
0.87
1.02
5.47
1.01
1.00
1.00
1.05
1.00
f1 (ppm)

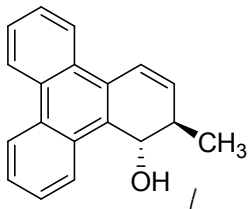

140.27
136.52
133.36
132.08
131.13
130.81
128.96
128.43
127.55
126.00
124.01
123.54
73.51
49.93
Br
Br
OH
5e
f1 (ppm)


Br
Br
OH
OCH3
5f
0.85
1.00
2.05
2.04
1.00
1.00
1.01
3.07
1.05
1.01
f1 (ppm)

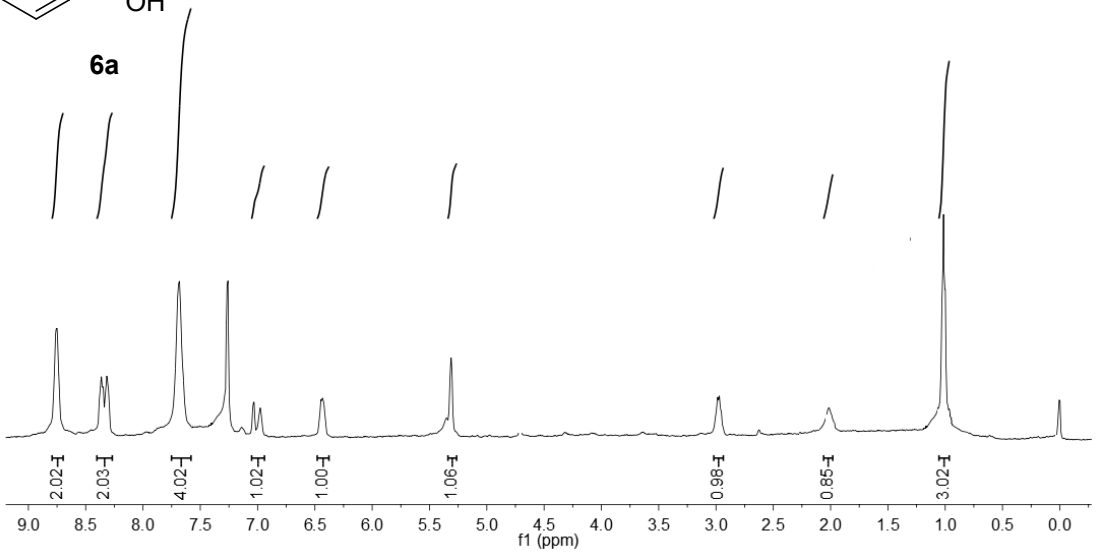

158.94
149.52
136.44
133.39
132.39
131.90
131.28
130.81
129.41
125.80
124.04
114.80
114.34
73.65
55.79
49.01
Br
Br
OH
OCH3
5f
f1 (ppm)


Br
Br
OH
5i
0.92
1.04
1.00
1.04
1.07
1.15
1.04
1.17
3.22
3.19
f1 (ppm)

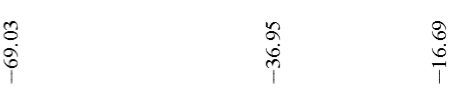

Std carbon
69.67
48.76
29.68
20.58
18.96
Br
Br
OH
5i
f1 (ppm)

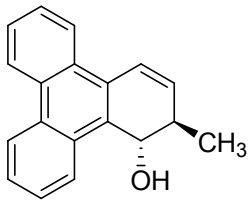

CH3
OH

6a

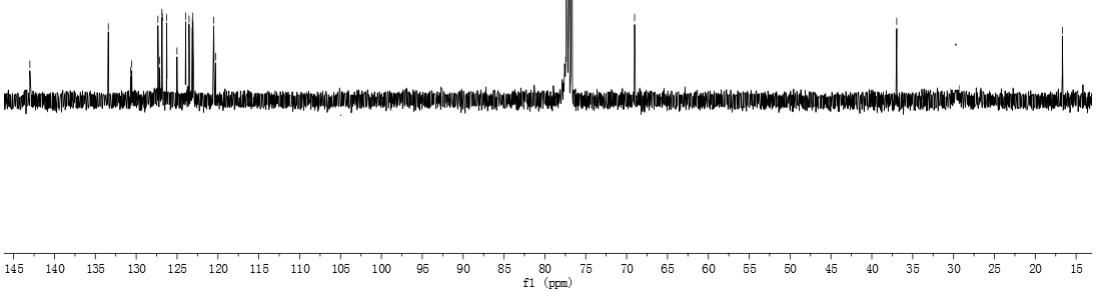

2.02
2.03
4.02
1.02
1.00
1.06
0.98
0.85
3.02
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

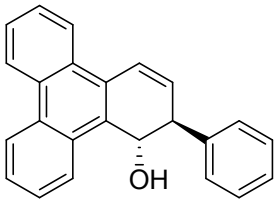

143.02
133.41
130.68
130.55
127.34
127.13
126.85
126.81
126.27
125.01
123.95
123.53
123.13
123.07
120.52
120.29


69.03
36.95
16.69

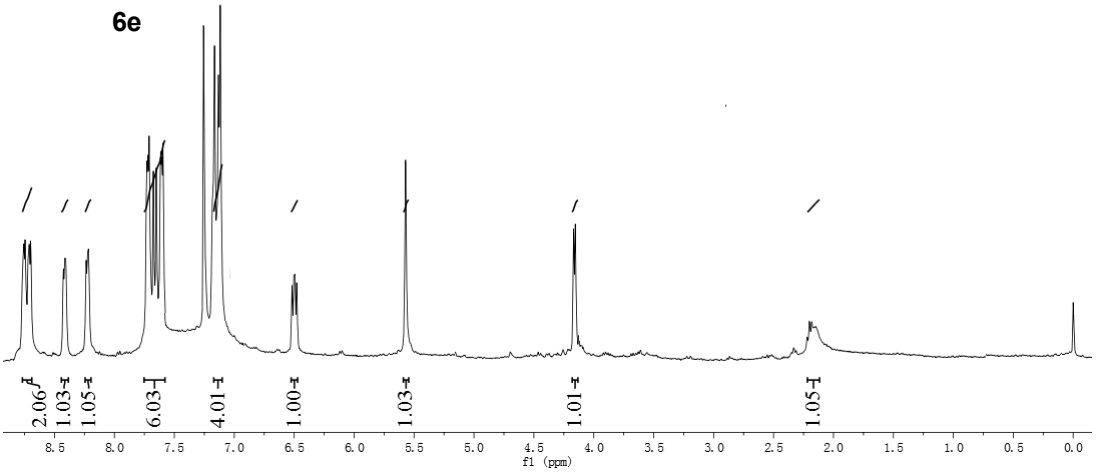

CH3
OH

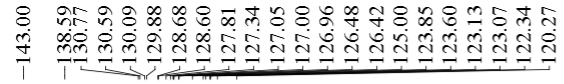
6a

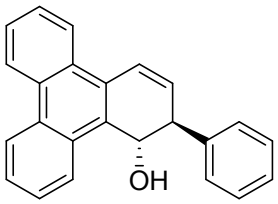

145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15
f1 (ppm)


OH

6e


2.06
1.03
1.05
6.03
4.01
1.00
1.03
1.01
1.05
f1 (ppm)


143.00
138.59
130.77
130.59
130.09
129.88
128.68
128.60
127.81
127.34
127.05
127.00
126.96
126.48
126.42
125.00
123.85
123.60
123.13
123.07
122.34
120.27
69.46
48.79


OH

6e

f1 (ppm)