Supporting Information

Rh(I) catalyzed insertion of allenes into C-C bonds of benzocyclobutenols

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1 General Information

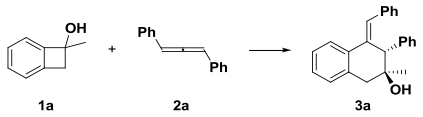
Components were visualized by UV and/or phosphomolybdic acid staining. ^{1}H-, ^{13}C- NMRs were recorded on a Bruker Ascend^{TM} 400 spectrometers. Chemical shifts (in ppm) were referenced to internal solvent peaks (^{1}H, ^{13}C). All operation was in flame-dried glassware using Schlenk techniques under a static pressure of argon. Toluene and dichloromethane (DCM) were purified by a solvent processing system. Silica gel (200-300 meshes) was used for column chromatography. High-resolution mass spectral analysis (HRMS) data were measured by means of the ESI.

2 Reaction optimization

The effect of catalyst and reaction temperature in two kinds of capable solvents (toluene and dioxane) was reported in Table 1 of the manuscript.

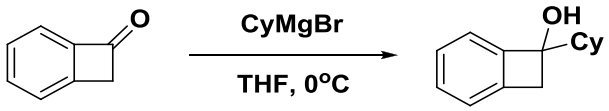
Other solvents were also tested under the otherwise optimized conditions (e.g., 2.0 mol % $[Rh(cod)(OH)]_2$, 100 ^{o}C with 0.1 mmol of **1a** and 0.11 mmol of **2a**). The result is compiled below:

Table S1. Screening of solvent



entry	solvent catalyst	Time (h)	yield[b] (%)
1	THF	4	15
2	CH_2Cl_2	4	35
3	DMF	24	nd
4	DMSO	24	nd
5	MeOH	24	nd

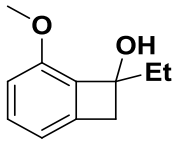
3 Typical procedure for the synthesis of benzocyclobutenols



1f

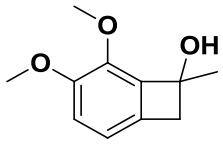
Under argon, benzocyclobutenone (116 mg, 1.0 mmol) was dissolved in THF (2 mL), a solution of cyclohexylmagnesium bromide was added dropwise at 0 °C. After 15 min, the mixture was warmed to room temperature for 1 h. The mixture was quenched by saturated NH_4Cl and the aqueous solution was extracted with diethyl ether for three times. The resulting oil was purified by silica gel chromatography (eluted by ethyl acetate/petroleum ether v/v=1/20) to afford pure product **1f** as a white oil (161.6 mg, 0.80 mmol, 80%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29-7.15 (m, 4H), 3.41 (d, *J* = 14.0 Hz, 1H), 3.04 (d, *J* = 14.0 Hz, 1H), 2.03 (s, 1H), 1.95-1.67 (m, 6H), 1.30-1.21 (m, 5H) . **^{13}C NMR** (101 MHz, $CDCl_3$) δ 150.10, 142.23, 129.24, 127.09, 124.01, 121.81, 83.67, 45.52, 45.04, 27.55, 27.50, 26.54, 26.50, 26.44. **HRMS** (ESI) calcd for $[M+Na]^+$ $C_{14}H_{18}O$: 225.1250, found 225.1250.

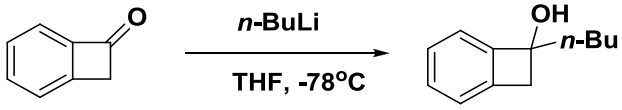


According to the procedure analogous to that described for **1f**, **1j** (160 mg, 0.9 mmol, 90%) was prepared from 6-methoxycyclobutabenzen-1(2H)-one (148 mg, 1.0 mmol), Purified by silica gel chromatography (eluted by ethyl acetate/petroleum ether v/v=1/20) as a white solid. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.22 (t, *J* = 8.0 Hz, 1H), 6.75 (d, *J* = 7.2 Hz, 1H), 6.70 (d, *J*= 8.4 Hz, 1H), 3.87 (s, 3H), 3.32 (d, *J* = 14.0 Hz, 1H), 3.05 (d, *J* = 13.6 Hz, 1H), 2.28 (s, 3H), 2.09-2.00 (m, 1H), 1.96-1.87 (m, 1H), 1.02 (t, *J* = 7.6 Hz , 3H) . **^{13}C NMR** (101 MHz, $CDCl_3$) δ 153.93, 143.37, 134.35, 130.93, 116.24,

112.17, 81.29, 56.49, 45.33, 32.43, 9.38. **HRMS** (ESI) calcd for $[M+Na]^+$ $C_{11}H_{14}O_2$: 201.0886, found 201.0883.



According to the procedure analogous to that described for **1f**, **1k** (178 mg, 0.92 mmol, 92%) was prepared from 5,6-dimethoxycyclobutabenzen-1(2H)-one (178 mg, 1.0 mmol), Purified by silica gel chromatography (eluted by ethyl acetate/petroleum ether v/v=1/15) as a white solid. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.81 (d, J = 7.6 Hz, 1H), 6.66 (d, J = 7.6 Hz, 1H), 4.07 (s, 3H), 3.82 (s, 3H), 3.27 (d, J = 14.0 Hz, 1H), 3.11 (d, J = 14.0 Hz, 1H), 2.57 (s, 1H), 1.73 (s, 3H) . **^{13}C NMR** (101 MHz, $CDCl_3$) δ 148.14, 144.35, 134.23, 133.42, 116.12, 113.96, 77.39, 58.81, 56.66, 47.55, 28.01. **HRMS** (ESI) calcd for $[M+Na]^+$ $C_{11}H_{14}O_3$: 217.0835, found 217.0832.

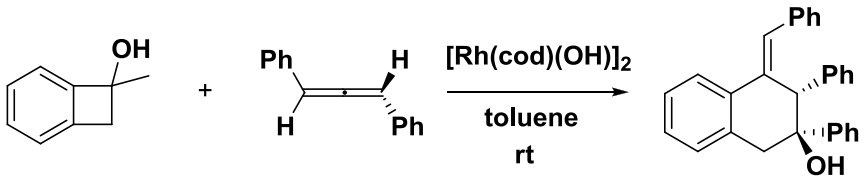


1i

Under argon, benzocyclobutenone (116 mg, 1.0 mmol) was dissolved in THF (2 mL), a solution of *n*-butyllithium was added dropwise at -78^{o}C. After 30 min, the mixture was warmed to room temperature for 1 h. The mixture was quenched by saturated NH_4Cl and the aqueous solution was extracted with diethyl ether for three times. The resulting oil was purified by silica gel chromatography (eluted by ethyl acetate/petroleum ether v/v=1/15) to afford pure product **1i** (167.2 mg , 0.95 mmol , 95 %) as a yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.29-7.15 (m, 4H), 3.35 (d, J = 14.0 Hz, 1H), 3.15 (d, J = 14.4 Hz, 1H), 2.27 (s, 1H), 1.92-1.86 (m, 2H), 1.56-1.49 (m, 2H),

1.39-1.34 (m, 2H), 0.92 (t, *J* = 7.2 Hz, 3H) . **^{13}C NMR** (101 MHz, $CDCl_3$) δ 150.56, 141.68, 129.34, 127.22, 124.09, 121.21, 81.12, 47.01, 38.95, 27.19, 23.14, 14.20. **HRMS** (ESI) calcd for $[M-H]^-$ $C_{12}H_{16}O$: 175.1128, found 175.1128.

4. Mechanistic proposal



(+)-**2a** (±)-**3a**

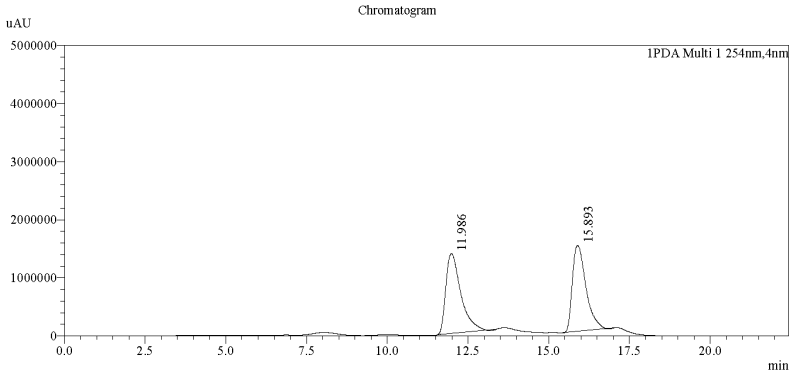
Under argon atmosphere, in an 10 mL Schlenk tube equipped with a stir bar, $[Rh(cod)OH]_2$ (1.8 mg, 0.004 mmol, 2 mol%), benzocyclobutenol **1a** (0.20 mmol, 1.0 equiv) were placed and 1.0 mL of toluene was added. The reaction tube is degassed three times with argon. Then chiral allene **(*S*)-2a** (0.22 mmol, 1.1 equiv) was added by syringe. The reaction was stirring at room temperature and monitored by HPLC. The enantiomeric ratio was determined by HPLC using Daicel Chiralcel OD-H column, column temperature 35 °C.

Table S2.

Conversion of **1a**	Time	**2a** *ee* [%]	**3a** *ee* [%]
0	-	99	-
17	1h	55	0
40	4h	25	0
100	24h	0	0

2a (Chiralcel-OD , 1% IPA in hexane, 0.4 mL / min)

Racemic **2a**

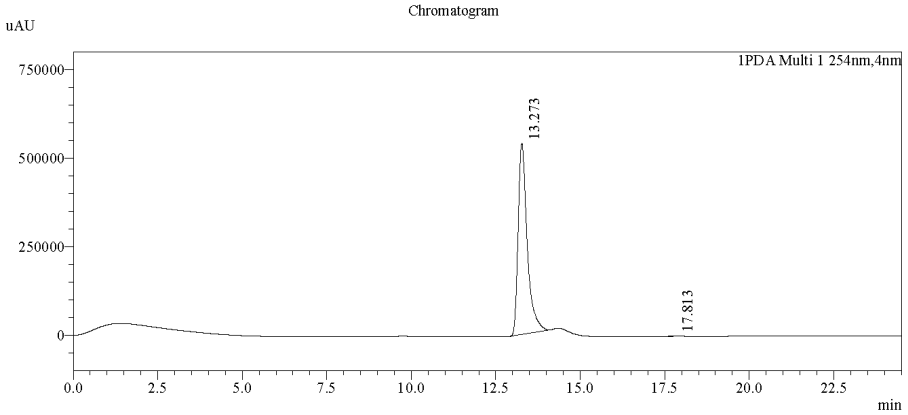


Peak Table

PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	11.986	44285743	50.738
2	15.893	42997871	49.262
Total		87283614	100.000

(*R*)-**2a**

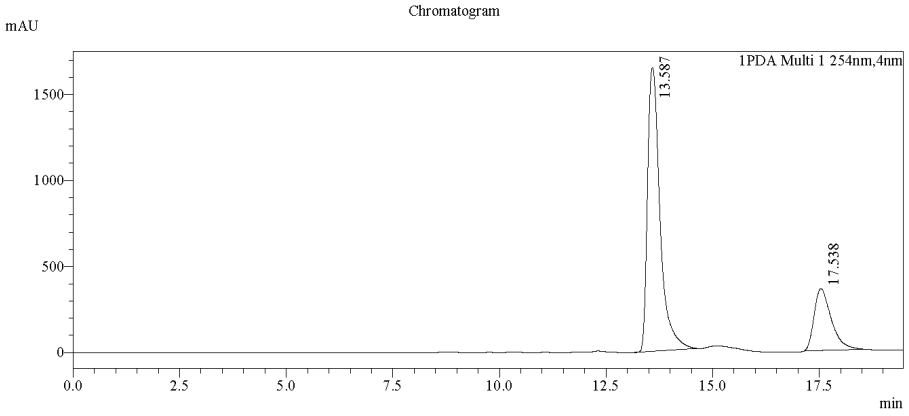


Peak Table

PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	13.273	10052263	99.773
2	17.813	22824	0.227
Total		10075087	100.000

Stirring at room temperature for 1h

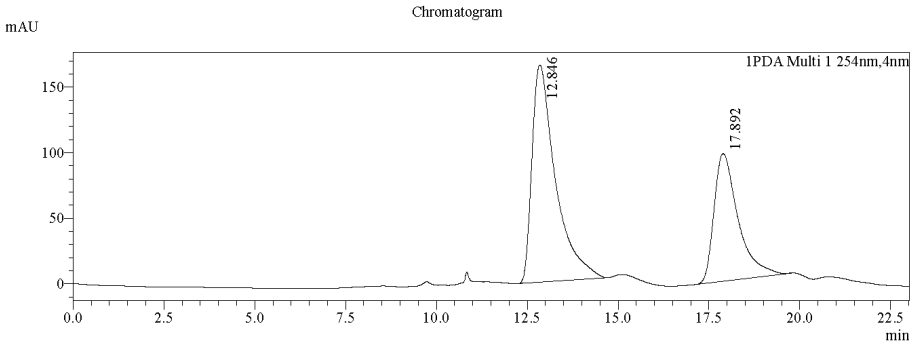


Peak Table

PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	13.587	33705966	77.207
2	17.538	9950592	22.793
Total		43656558	100.000

Stirring at room temperature for 4h

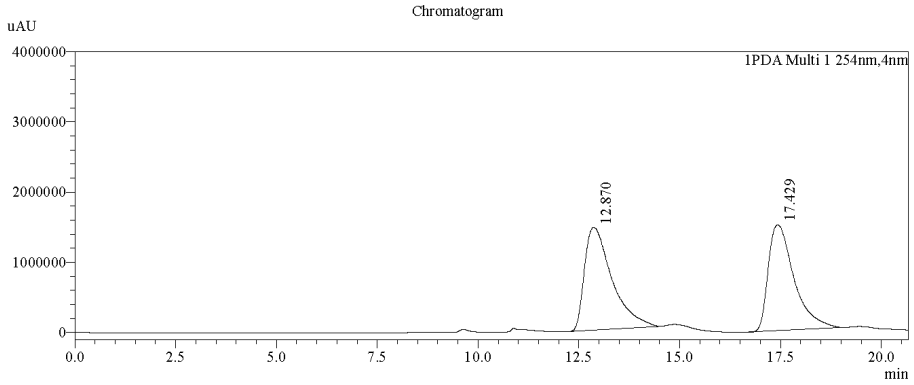


Peak Table

PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	12.846	7448843	62.394
2	17.892	4489619	37.606
Total		11938462	100.000

Stirring at room temperature for 24h



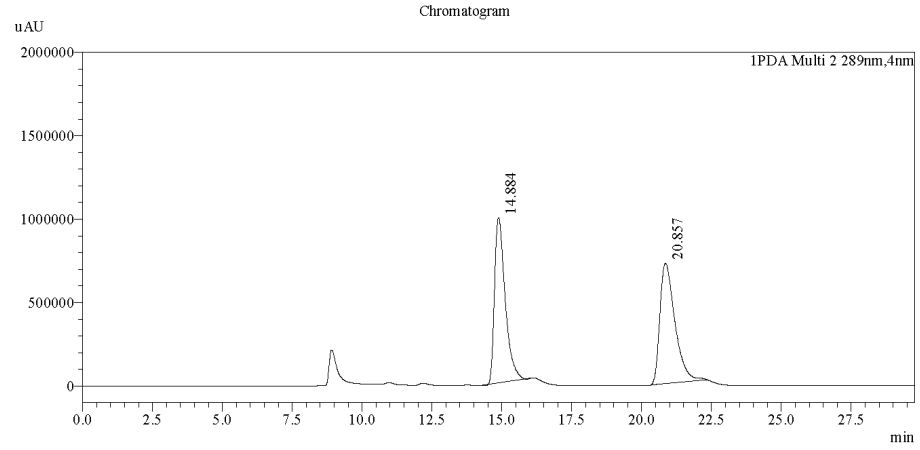
Peak Table

PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	12.870	69597291	50.919
2	17.429	67083795	49.081
Total		136681086	100.000

3a (Chiralcel-OD , 5% IPA in hexane, 0.5 mL / min)

Racemic **3a**

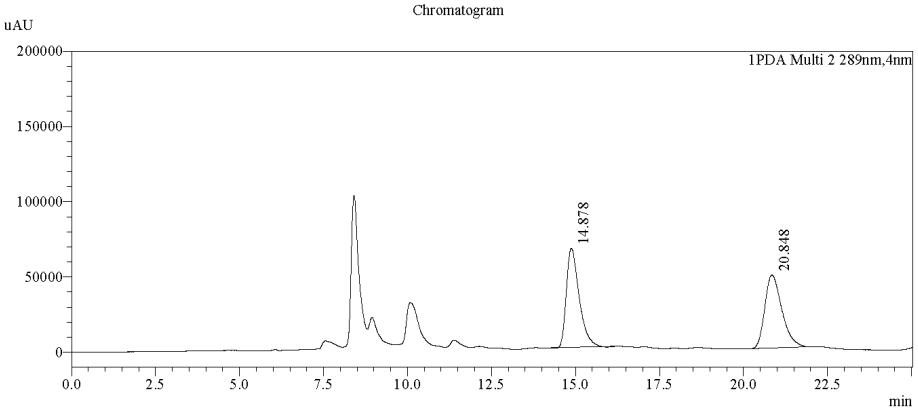


Peak Table

PDA Ch2 289nm

Peak#	Ret. Time	Area	Area%
1	14.884	26064506	49.042
2	20.857	27082869	50.958
Total		53147375	100.000

Stirring at room temperature for 1h

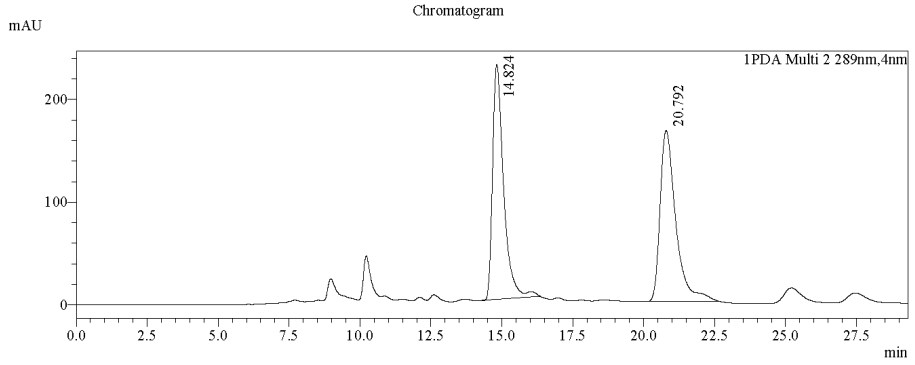


Peak Table

PDA Ch2 289nm

Peak#	Ret. Time	Area	Area%
1	14.878	1729547	50.358
2	20.848	1704975	49.642
Total		3434521	100.000

Stirring at room temperature for 4h

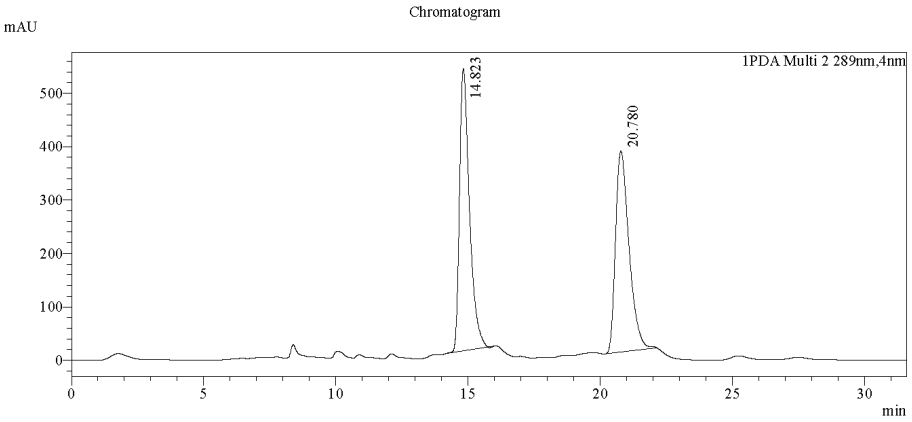


Peak Table

PDA Ch2 289nm

Peak#	Ret. Time	Area	Area%
1	14.824	6182584	49.168
2	20.792	6391748	50.832
Total		12574332	100.000

Stirring at room temperature for 24h



Peak Table

PDA Ch2 289nm

Peak#	Ret. Time	Area	Area%
1	14.823	13827969	50.866
2	20.780	13357271	49.134
Total		27185239	100.000

5. Typical procedure for rhodium-catalyzed reactions of 1 and 2

Under argon atmosphere, in an 10 mL Schlenk tube equipped with a stir bar, $[Rh(cod)OH]_2$ (1.8 mg, 0.004 mmol, 2 mol%), benzocyclobutenol **1**[1] (0.20 mmol, 1.0 equiv) were placed and 1.0 mL of toluene was added. The reaction tube is degassed three times with argon. Then allene **2**[2] (0.22 mmol, 1.1 equiv) was added by syringe. The reaction was heated in 100 ^{o}C oil bath with stirring for 2 h. The reaction solution was then cooled down to room temperature, and solvent was removed *in vacuo* to leave a crude mixture and the resulting oil was purified by silica gel chromatography (eluted by ethyl acetate/ petroleum ether v/v= 1:10 to 1:20) to afford pure product **3**.

6 Hydrogenation of tetralin 3l

A mixture of **3l** (0.02 mmol) and 5% palladium/C (7.6 mg) in methanol (0.2 mL) was treated 2h with hydrogen at ambient temperature. The catalyst was removed by filtration through silica gel

and solvent was removed *in vacuo* and purified by silica gel chromatography (eluted by ethyl acetate/ petroleum ether = 1:20 to 1:10) to give the tetralin **4** (8.2 mg, 0.019 mmol).

The relative stereochemistry was assigned according to the following figure S1.

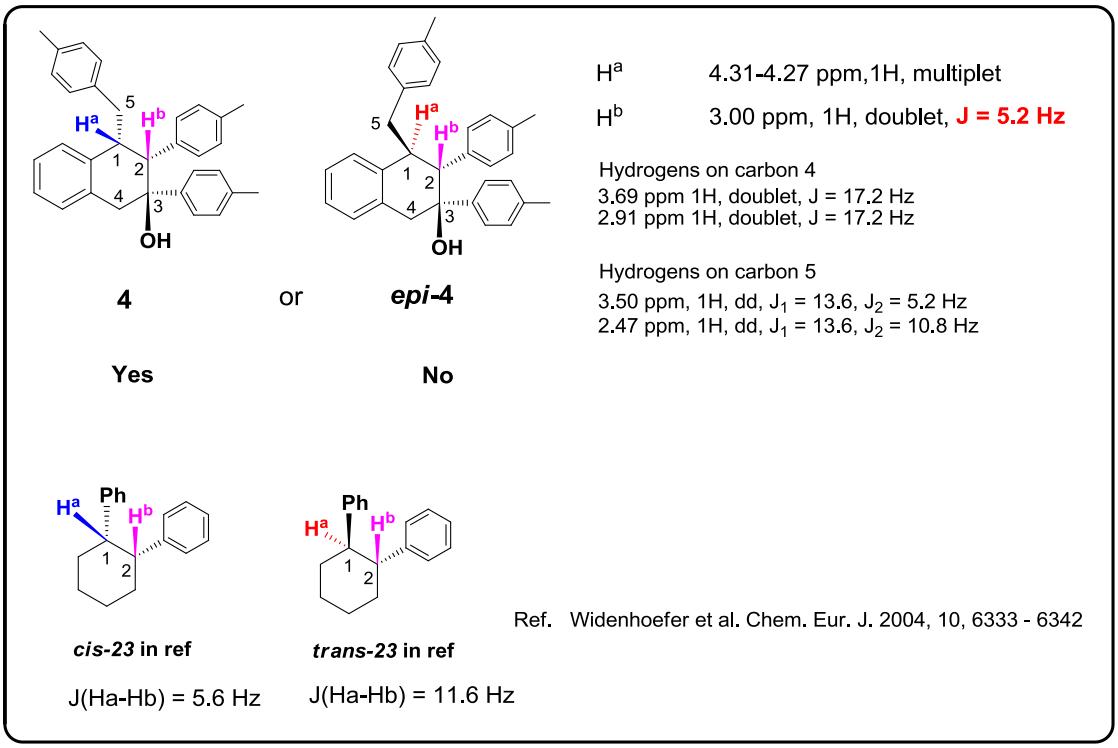
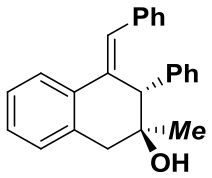


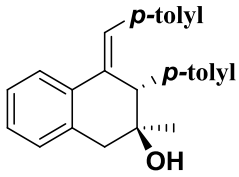
Figure S1. Assignment of relative stereochemistry of 4.

7 Compound Characterization Data.



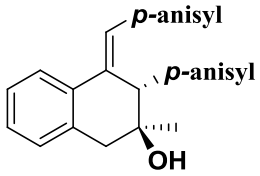
4-benzylidene-2-methyl-3-phenyl-1,2,3,4-tetrahydronaphthalen-2-ol **(3a)**

3a was obtained by silica gel chromatography eluted by (ethyl acetate/petroleum ether v/v= 1:20) 52.2 mg (80% yield), yellow oil. **^{1}H NMR** (400 MHz, acetone-d6) δ 7.90-7.88 (m, 1H), 7.34-7.16 (m, 14H), 4.17 (s, 1H), 3.55 (s, 1H), 2.86 (d, *J* = 17.1 Hz, 1H), 2.76 (d, *J* = 17.1 Hz, 1H), 1.17 (s, 3H). **^{13}C NMR** (100 MHz, acetone-d6) δ 143.75, 139.33, 138.88, 137.20, 136.38, 130.48, 130.03, 129.62, 129.22, 128.80, 128.44, 127.56, 127.48, 127.31, 124.97, 72.03, 55.58, 40.53, 28.97. **HRMS** (ESI) calcd for $[M+H]^+$ $C_{24}H_{22}O$: 327.1743, found 327.1742. dr > 19:1.



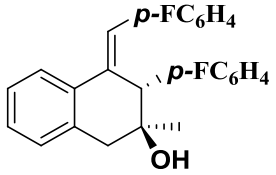
2-methyl-4-(4-methylbenzylidene)-3-p-tolyl-1,2,3,4-tetrahydronaphthalen-2-ol **(3b)**

3b was obtained by silica gel chromatography eluted by (ethyl acetate/petroleum ether v/v= 1:20), 58.1 mg (82% yield), white solid. **^{1}H NMR** (400 MHz, acetone-d6) δ 7.87-7.85 (m, 1H), 7.28-7.25 (m, 3H), 7.15-7.10 (m, 5H), 7.06 (m, 4H), 4.13 (d, *J* = 1.2 Hz, 1H), 3.46 (d, *J* = 0.4 Hz, 1H), 2.85 (d, *J* = 17.2 Hz, 1H), 2.73 (d, *J* = 17.2 Hz, 1H), 2.32 (s, 3H), 2.27 (s, 3H), 1.17 (s, 3H). **^{13}C NMR** (100 MHz, acetone-d6) δ 140.77, 138.80, 137.40, 137.12, 136.81, 136.30, 136.06, 130.43, 130.02, 129.83, 129.55, 129.44, 128.27, 128.24, 127.24, 124.89, 72.04, 55.15, 40.52, 28.99, 21.17, 21.01. **HRMS** (ESI) calcd for $[M+Na]^+$ $C_{26}H_{26}O$: 377.1876, found 377.1875. dr > 19:1.



4-(4-methoxybenzylidene)-3-(4-methoxyphenyl)-2-methyl-1,2,3,4-tetrahydronaphthalen-2-ol **(3c)**

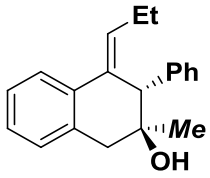
3c was obtained by silica gel chromatography eluted by (ethyl acetate/petroleum ether v/v= 1:20), 65.7 mg (85% yield), white solid. **^{1}H NMR** (400 MHz, acetone-d6) *δ* 7.86-7.83 (m, 1H), 7.29-7.21 (m, 5H), 7.19-7.08 (m, 3H), 6.88-6.81 (m, 4H), 4.12 (s, 1H), 3.80 (s, 3H), 3.75 (s, 3H), 3.44 (s, 1H), 2.83 (d, *J* = 17.2 Hz, 1H), 2.72 (d, *J* = 16.8 Hz, 1H), 1.17 (s, 3H). **^{13}C NMR** (101 MHz, acetone-d6) *δ* 159.61, 159.35, 137.92, 137.48, 136.14, 135.63, 131.40, 131.34, 130.62, 130.43, 128.08, 127.90, 127.23, 124.82, 114.51, 114.23, 72.07, 55.52, 55.36, 54.60, 40.51, 28.96. dr > 19:1. **HRMS** (ESI) calcd for $[M+Na]^+$ $C_{26}H_{26}O_3$: 409.1774, found 409.1772.



4-(4-fluorobenzylidene)-3-(4-fluorophenyl)-2-methyl-1,2,3,4-tetrahydronaphthalen-2-ol **(3d)**

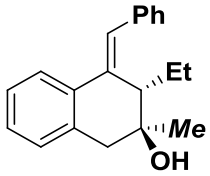
3d was obtained by silica gel chromatography eluted by (ethyl acetate/petroleum ether v/v= 1:10), 64.5 mg (89% yield), off white solid. **^{1}H NMR** (400 MHz, acetone-d6) *δ* 7.89-7.87 (m, 1H), 7.31-7.28 (m, 3H), 7.24-7.16 (m, 5H), 7.10-7.00 (m, 4H), 4.13 (s, 1H), 3.64 (s, 1H), 2.84 (d, *J* = 17.2 Hz, 1H), 2.77 (d, *J* = 17.6 Hz, 1H), 1.17 (s, 3H) . **^{13}C NMR** (101 MHz, acetone-d6) *δ* 162.53 (d, *J* = 245 Hz), 162.47 (d, *J* = 244 Hz), 139.66 (d, *J* = 3.0 Hz), 139.35, 136.73, 136.25, 135.21 (d, *J* = 3.0 Hz), 131.79 (d, *J* = 8.0 Hz), 131.34 (d, *J* = 8.0 Hz), 130.54, 128.58, 127.38, 127.26, 125.00, 115.93 (d, *J* = 21.2 Hz), 115.62 (d, *J* = 21.2 Hz), 71.89, 54.62, 40.37, 28.87. dr > 19:1. **HRMS** (ESI) calcd for $[M+Na]^+$

$C_{24}H_{20}F_2O$: 385.1374, found 385.1377.



2-methyl-3-phenyl-4-propylidene-1,2,3,4-tetrahydronaphthalen-2-ol **(3ea)**

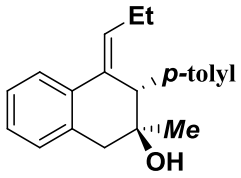
3ea was obtained by silica gel chromatography eluted by (ethyl acetate/petroleum ether v/v= 1:12) 23.9 mg, (43% yield), yellow oil. **^{1}H NMR** (400 MHz, acetone-d6) δ 7.76 (d, *J* = 6.8 Hz, 1H), 7.22-7.14 (m, 5H), 7.13-7.11 (m, 3H), 6.27 (t, *J* = 7.1 Hz, 1H), 4.04 (s, 1H), 3.45 (s, 1H), 2.91 (d, *J* = 16.7 Hz, 1H), 2.73 (dd, *J* = 16.7, 1.1 Hz, 1H), 2.32 – 2.12 (m, 1H), 2.06-1.95 (m, 1H), 1.11 (s, 3H), 0.88 (t, *J* = 7.5 Hz, 3H). **^{13}C NMR** (100 MHz, acetone-d6) δ 143.83, 136.69, 136.39, 135.35, 130.55, 129.93, 129.51, 128.87, 127.51, 127.12, 127.01, 123.67, 71.20, 54.99, 40.83, 28.75, 22.04, 14.14. **HRMS** (ESI) calcd for $[M+Na]^+$ $C_{20}H_{22}O$: 301.1563, found 301.1564. dr > 10:1.



4-benzylidene-3-ethyl-2-methyl-1,2,3,4-tetrahydronaphthalen-2-ol **(3eb)**

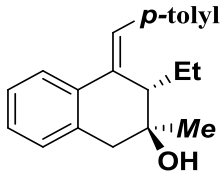
3eb was obtained by silica gel chromatography eluted by (ethyl acetate/petroleum ether v/v= 1:20) 24.0 mg (43% yield), yellow oil. **^{1}H NMR** (400 MHz, acetone-d6) δ 7.77 (dd, *J* = 5.6, 3.6 Hz, 1H), 7.45-7.37 (m, 4H), 7.29-7.18 (m, 4H), 7.15-7.12 (m, 1H), 3.70 (s, 1H), 3.06 (d, *J* = 16.8 Hz, 1H), 2.98 (dd, *J* = 10.4, 3.2 Hz, 1H), 2.76 (d, *J* = 16.9 Hz, 1H), 2.02-1.93 (m, 1H), 1.23 (d, *J* = 0.8 Hz, 3H), 1.17-1.02 (m, 1H), 0.77 (t, *J* = 7.5 Hz, 3H). **^{13}C NMR** (100 MHz, acetone-d6) δ 142.36, 139.34, 136.37, 135.15, 130.16, 129.92, 128.98, 128.30, 127.32, 127.29, 127.11, 125.82, 71.53, 49.41,

41.47, 29.13, 21.59, 12.88. **HRMS** (ESI) calcd for $[M+Na]^+$ $C_{20}H_{22}O$: 301.1563, found 301.1564. dr > 19:1.



2-methyl-4-propylidene-3-p-tolyl-1,2,3,4-tetrahydronaphthalen-2-ol **(3fa)**

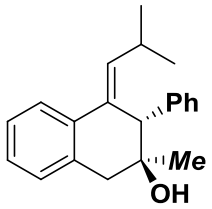
3fa was obtained by silica gel chromatography eluted by (ethyl acetate/petroleum ether v/v= 1:20), 22.0 mg (38% yield), white solid. **^{1}H NMR** (400 MHz, acetone-d6) δ 7.77-7.75 (m, 1H), 7.19-7.15 (m, 2H), 7.12-7.10 (m, 1H), 7.02-6.97 (m, 4H), 6.26 (t, *J* = 7.2 Hz, 1H), 3.99 (s, 1H), 3.40 (s, 1H), 2.90 (d, *J* = 16.8 Hz, 1H), 2.71 (d, *J* = 16.8 Hz, 1H), 2.30-2.23 (m, 4H), 2.02-1.95 (m, 1H), 1.11 (s, 3H), 0.89 (t, *J* = 7.5 Hz, 3H). **^{13}C NMR** (100 MHz, acetone-d6) δ 140.78, 136.82, 136.44, 136.42, 135.38, 130.55, 129.73, 129.50, 129.40, 127.48 , 126.98, 123.66, 71.23 54.58, 40.81, 28.78, 22.02, 20.97, 14.19. **HRMS** (ESI) calcd for $[M+Na]^+$ $C_{21}H_{24}O$: 315.1719, found 315.1719. dr > 10:1.



3-ethyl-2-methyl-4-(4-methylbenzylidene)-1,2,3,4-tetrahydronaphthalen-2-ol **(3fb)**

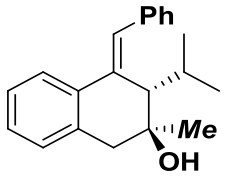
3fb was obtained by silica gel chromatography eluted by (ethyl acetate/petroleum ether v/v= 1:20), 22.4 mg (38% yield), white solid. **^{1}H NMR** (400 MHz, acetone-d6) δ 7.75-7.73 (m, 1H), 7.32 (m, 2H), 7.22-7.19 (m, 4H), 7.13-7.11 (m, 2H), 3.68 (s, 1H), 3.05 (d, *J* = 16.9 Hz, 1H), 3.00 (dd, *J* = 10.4, 3.5 Hz, 1H), 2.75 (d, *J* = 16.9 Hz, 1H), 2.34 (s, 3H), 2.00-1.92 (m, 1H), 1.22 (s, 3H), 1.11-1.02 (m, 1H), 0.78 (t, *J* = 7.5 Hz, 3H). **^{13}C NMR** (100 MHz, acetone-d6) δ 141.90, 136.82, 136.40, 136.28, 135.34,

130.14, 129.85, 129.64, 128.18, 127.36, 127.09, 125.79, 71.55, 49.40, 41.48, 29.13, 21.61, 21.14, 12.91. **HRMS** (ESI) calcd for $[M+Na]^+$ $C_{21}H_{24}O$: 315.1719, found 315.1719. dr > 19:1.



2-methyl-4-(2-methylpropylidene)-3-phenyl-1,2,3,4-tetrahydronaphthalen-2-ol **(3ga)**

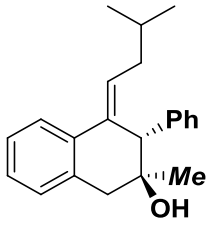
3ga was obtained by silica gel chromatography eluted by (ethyl acetate/petroleum ether v/v= 1:20), 22.3 mg (38% yield), yellow oil. **^{1}H NMR** (400 MHz, acetone-d6) δ 7.78-7.76 (m, 1H), 7.20-7.16 (m, 5H), 7.13-7.11 (m, 3H), 6.09 (d, *J* = 9.6 Hz, 1H), 4.09 (s, 1H), 3.43 (s, 1H), 2.90 (d, *J* = 16.7 Hz, 1H), 2.73 (m, 2H), 1.12 (s, 3H), 1.05 (d, *J* = 6.6 Hz, 3H), 0.63 (d, *J* = 6.6 Hz, 3H). **^{13}C NMR** (100 MHz, acetone-d6) δ 144.32, 136.47, 135.74, 135.46, 134.75, 130.53, 129.44, 128.87, 127.51, 127.11, 126.99, 123.76, 71.20, 55.09, 40.81, 28.76, 28.00, 23.33, 22.70. **HRMS** (ESI) calcd for $[M+Na]^+$ $C_{21}H_{24}O$: 315.1719, found 315.1708. dr > 10:1.



4-benzylidene-3-isopropyl-2-methyl-1,2,3,4-tetrahydronaphthalen-2-ol **(3gb)**

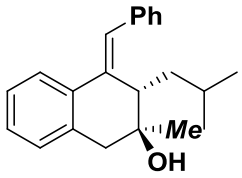
3gb was obtained by silica gel chromatography eluted by (ethyl acetate/petroleum ether v/v= 1:20), 13.4 mg (23% yield), yellow oil. **^{1}H NMR** (400 MHz, acetone-d6) δ 7.71-7.69 (m, 1H), 7.46-7.38 (m, 4H), 7.28-7.13 (m, 4H), 7.08 (s, 1H), 3.64 (s, 1H), 3.21 (d, *J* = 17.1 Hz, 1H), 2.93 (d, *J* = 7.3 Hz, 1H), 2.77 (d, *J* = 8.8 Hz, 1H), 1.91 (dt, *J* = 13.7, 6.8 Hz, 1H), 1.21 (s, 3H), 1.09 (d, *J* = 6.6 Hz, 3H), 0.73 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (100 MHz, MeOH-d3) δ 142.97, 139.79, 137.03, 136.34,

130.28, 130.18, 129.17, 128.58, 127.93, 127.58, 125.77, 73.63, 53.58, 41.16, 30.01, 28.42, 25.12, 22.49. **HRMS** (ESI) calcd for $[M+Na]^+$ $C_{21}H_{24}O$: 315.1719, found 315.1717. dr > 19:1.



2-methyl-4-(3-methylbutylidene)-3-phenyl-1,2,3,4-tetrahydronaphthalen-2-ol **(3ha)**

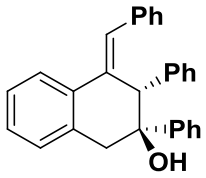
3ha was obtained by silica gel chromatography eluted by (ethyl acetate/petroleum ether v/v= 1:10), 34.7 mg (56% yield), white solid. **^{1}H NMR** (400 MHz, acetone-d6) δ 7.80-7.78 (m, 1H), 7.22-7.10 (m, 8H), 6.35 (t, *J* = 7.3 Hz, 1H), 4.05 (s, 1H), 3.42 (s, 1H), 2.91 (d, *J* = 16.8 Hz, 1H), 2.73 (d, *J* = 16.8 Hz, 1H), 2.15 (dt, *J* = 14.3, 7.0 Hz, 1H), 1.91 (dt, *J* = 14.6, 7.1 Hz, 1H), 1.59 (td, *J* = 13.4, 6.7 Hz, 1H), 1.12 (s, 3H), 0.87 (d, *J* = 6.8 Hz, 3H), 0.72 (d, *J* = 6.4 Hz, 3H). **^{13}C NMR** (100 MHz, acetone-d6) δ 143.82, 137.47, 136.52, 135.32, 130.58, 129.58, 128.85, 127.53, 127.47, 127.10, 127.04, 123.72, 71.29, 55.13, 40.88, 37.93, 29.51, 28.78, 22.91, 22.71. **HRMS** (ESI) calcd for $[M+Na]^+$ $C_{22}H_{26}O$: 329.1876, found 329.1876. dr > 10:1.



4-benzylidene-3-isobutyl-2-methyl-1,2,3,4-tetrahydronaphthalen-2-ol **(3hb)**

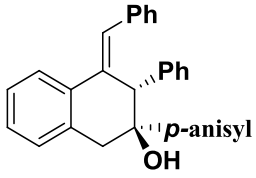
3hb was obtained by silica gel chromatography eluted by (ethyl acetate/petroleum ether v/v= 1:15), 19.8 mg (33% yield), white solid. **^{1}H NMR** (400 MHz, acetone-d6) δ 7.82-7.79 (m, 1H), 7.44-7.37 (dt, *J* = 13.2, 7.5 Hz, 4H), 7.28-7.20 (m, 4H), 7.15-7.14 (m, 1H), 3.73 (s, 1H), 3.18 (dd, *J* = 10.6, 2.2 Hz, 1H), 3.05 (d, *J* = 16.8 Hz, 1H), 2.76 (d, *J* = 16.8 Hz, 1H), 1.62 (ddd, *J* = 12.9, 7.4, 2.8 Hz,

1H), 1.54-1.47 (m, 1H), 1.34 (s, 3H), 1.05-0.98 (m, 1H), 0.68 (d, *J* = 6.6 Hz, 3H), 0.40 (d, *J* = 6.4 Hz, 3H). **^{13}C NMR** (100 MHz, acetone-d6) *δ* 142.96, 139.44, 136.49, 134.87, 130.26, 129.91, 129.00, 128.28, 127.24, 127.07, 126.47, 125.70, 71.27, 45.34, 41.55, 38.34, 29.12, 25.94, 24.59, 22.18. **HRMS** (ESI) calcd for $[M+Na]^+$ $C_{22}H_{26}O$: 329.1876, found 329.1874. dr > 19:1.



4-benzylidene-2,3-diphenyl-1,2,3,4-tetrahydronaphthalen-2-ol **(3i)**

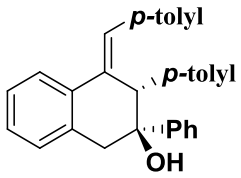
3i was obtained by silica gel chromatography eluted by (ethyl acetate/petroleum ether v/v= 1:15) , 65.3 mg (84% yield), white solid. **^{1}H NMR** (400 MHz, acetone-d6) *δ* 8.02-7.99 (m, 1H), 7.46 (s, 1H), 7.36-7.31 (m, 2H), 7.29-7.18 (m, 11H), 7.11-7.07 (m, 1H), 7.02-6.99 (m, 2H), 6.60-6.58 (m, 2H), 4.40 (d, *J* = 1.6 Hz, 1H), 4.18 (s, 1H), 3.68 (d, *J* = 16.8 Hz, 1H), 2.98 (dd, *J* = 16.8, 0.8 Hz, 1H). **^{13}C NMR** (100 MHz, acetone-d6) *δ* 147.36, 142.25, 138.93, 138.77, 137.02, 136.16, 131.07, 130.04, 129.87, 128.85, 128.61, 128.50, 128.33, 128.27, 127.74, 127.64, 127.44, 127.33, 127.24, 124.78, 75.92, 56.51, 37.92. **HRMS** (ESI) calcd for $C_{29}H_{24}O$ $[M+Na]^+$: 411.1719, found 411.1720. dr > 19:1.



4-benzylidene-2-(4-methoxyphenyl)-3-phenyl-1,2,3,4-tetrahydronaphthalen-2-ol **(3j)**

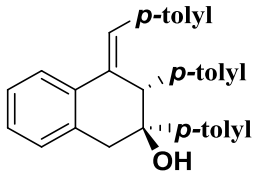
3j was obtained by silica gel chromatography eluted by (ethyl acetate/petroleum ether v/v= 1:10), 61.1 mg (73% yield), white solid. **^{1}H NMR** (400 MHz, acetone-d6) *δ* 8.00-7.98 (m, 1H), 7.45 (s, 1H), 7.35-7.20 (m, 8H), 7.12-7.08 (m, 3H), 7.04-7.00 (m, 2H), 6.77-6.73 (m, 2H), 6.62-6.60 (m, 2H), 4.38

(d, *J* = 1.2 Hz, 1H), 4.06 (s, 1H), 3.76 (s, 3H), 3.62 (d, *J* = 16.8 Hz, 1H), 2.95 (dd, *J* = 16.8, 1.2 Hz, 1H). **^{13}C NMR** (100 MHz, acetone-d6) *δ* 159.67, 142.44, 139.44, 139.09, 138.82, 137.07, 136.27, 131.07, 130.05, 129.91, 128.85, 128.60, 128.48, 128.37, 128.19, 127.62, 127.41, 127.29, 124.77, 113.55, 75.64, 56.64, 55.45, 38.17. **HRMS** (ESI) calcd for $[M+Na]^+$ $C_{30}H_{26}O_2$: 441.1825, found 441.1826. dr > 19:1.



4-(4-methylbenzylidene)-2-phenyl-3-p-tolyl-1,2,3,4-tetrahydronaphthalen-2-ol **(3k)**

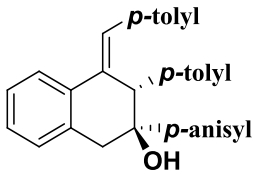
3k was obtained by silica gel chromatography eluted by (ethyl acetate/petroleum ether v/v= 1:12), 55.8 mg (67% yield), pale yellow solid. **^{1}H NMR** (400 MHz, DMSO-d6) *δ* 7.97-7.95 (m, 1H), 7.34-7.26 (m, 3H), 7.24-7.13 (m, 6H), 7.07 (m, 4H), 6.79 (d, *J* = 8.0 Hz, 2H), 6.33 (d, *J* = 8.0 Hz, 2H), 5.13 (s, 1H), 4.22 (s, 1H), 3.49 (d, *J* = 17.6 Hz, 1H), 2.98 (d, *J* = 16.0 Hz, 1H), 2.27 (s, 3H), 2.14 (s, 3H). **^{13}C NMR** (100 MHz, DMSO-d6) *δ* 146.88, 137.91, 137.41, 136.00, 135.88, 135.25, 135.15, 134.57, 130.08, 128.88, 128.67, 128.41, 128.36, 127.41, 127.27, 126.79, 126.32, 126.28, 126.05, 123.56, 74.19, 54.34, 36.30, 20.76, 20.53. **HRMS** (ESI) calcd for $[M+Na]^+$ $C_{31}H_{28}O$: 439.2032, found 439.2033. dr > 19:1.



4-(4-methylbenzylidene)-2,3-dip-tolyl-1,2,3,4-tetrahydronaphthalen-2-ol **(3l)**

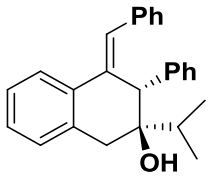
3l was obtained by silica gel chromatography eluted by (ethyl acetate/petroleum ether v/v= 1:10),

58.6 mg (68% yield), white solid. **^{1}H NMR** (400 MHz, acetone-d6) δ 7.97-7.95 (m, 1H), 7.39 (s, 1H), 7.34-7.23 (m, 3H), 7.13-7.07 (m, 6H), 7.02 (d, 2H), 6.82 (d, *J* = 7.9 Hz, 2H), 6.49 (d, *J* = 7.9 Hz, 2H), 4.37 (s,1H), 3.97 (s, 1H), 3.62 (d, *J* = 16.6Hz, 1H) , 2.93 (d, *J* = 16.6Hz, 1H), 2.30 (s, 3H), 2.29 (s, 3H), 2.19 (s, 3H). **^{13}C NMR** (100 MHz, acetone-d6) δ 144.57, 139.34, 137.29, 137.23, 137.04, 136.57, 136.19, 131.039, 130.07, 129.85, 129.51, 129.22, 128.90, 128.31, 128.12, 127.37, 127.26, 124.70, 75.80, 56.09, 38.11, 21.18, 21.02, 20.98. **HRMS** (ESI) calcd for $[M+Na]^+$ $C_{32}H_{30}O$: 453.2189, found 453.2187. dr > 19:1.



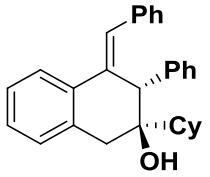
2-(4-methoxyphenyl)-4-(4-methylbenzylidene)-3-p-tolyl-1,2,3,4-tetrahydronaphthalen-2-ol **(3m)**

3m was obtained by silica gel chromatography eluted by (ethyl acetate/petroleum ether v/v= 1:10), 83.0 mg (93% yield), white solid. **^{1}H NMR** (400 MHz, acetone-d6) δ 7.97-7.95 (m, 1H), 7.39 (s, 1H), 7.35-7.23 (m, 3H), 7.14-7.07 (m, 6H), 6.83 (d, *J* = 8.0 Hz, 2H) , 6.79-6.75 (m, 2H), 6.49 (d, *J* = 8.4 Hz, 2H) , 4.36 (d, *J* = 1.2 Hz, 1H), 3.97 (s, 1H), 3.77 (s, 3H), 3.60 (d, *J* = 16.8 Hz, 1H), 2.93 (dd, *J* = 16.8, 1.6 Hz, 1H), 2.30 (s, 3H), 2.19 (s, 3H) . **^{13}C NMR** (100 MHz, acetone-d6) δ 159.62, 139.58, 139.40, 138.50, 137.26, 137.20, 136.53, 136.17, 135.96, 131.02, 130.04, 129.81, 129.50, 129.22, 128.42, 128.27, 128.00, 127.34, 124.66, 113.52, 75.60, 56.18, 55.43, 38.14, 21.16, 20.98. **HRMS** (ESI) calcd for $[M+Na]^+$ $C_{32}H_{30}O_2$: 469.2138, found 469.2139. dr > 19:1.



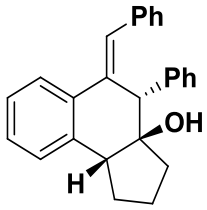
4-benzylidene-2-isopropyl-3-phenyl-1,2,3,4-tetrahydronaphthalen-2-ol **(3n)**

3n was obtained by silica gel chromatography eluted by (ethyl acetate/petroleum ether v/v= 1:10), 61.0 mg (86% yield), yellow oil. **^{1}H NMR** (400 MHz, acetone-d6) δ 7.85-7.83 (m, 1H), 7.36-7.13 (m, 11H), 7.12-7.11 (m, 3H), 4.53 (d, *J* = 1.2 Hz, 1H), 3.18 (s, 1H), 3.01 (dd, *J* = 17.5Hz, 1H), 2.88 (d, *J* = 17.5 Hz, 1H), 1.53 (dt, *J* = 13.4, 6.7 Hz, 1H), 1.00 (d, *J* = 6.6 Hz, 3H), 0.91 (d, *J* = 6.6 Hz, 3H). **^{13}C NMR** (100 MHz, acetone-d6) δ 142.97, 139.50, 138.93, 137.14, 136.51, 130.90, 130.03, 129.37, 129.31, 128.87, 128.51, 128.38, 127.57, 127.43, 127.34, 125.12, 75.33, 50.53, 38.20, 33.68, 17.00, 16.65. **HRMS** (ESI) calcd for $C_{26}H_{26}O$ $[M+Na]^+$: 377.1876, found 377.1875. dr > 19:1.



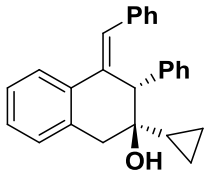
4-benzylidene-2-cyclohexyl-3-phenyl-1,2,3,4-tetrahydronaphthalen-2-ol **(3o)**

3o was obtained by silica gel chromatography eluted by (ethyl acetate/petroleum ether v/v= 1:10) 56.0 mg (71% yield), white solid. **^{1}H NMR** (400 MHz, acetone-d6) δ 7.85-7.83 (m, 1H), 7.36-7.18 (m, 12H), 7.13-7.11 (m, 2H), 4.58 (s, 1H), 3.14 (s, 1H), 3.00 (d, *J* = 17.6 Hz, 1H), 2.85 (d, *J* = 17.6 Hz, 1H), 1.74-1.72 (m, 3H), 1.29-1.06 (m, 8H). **^{13}C NMR** (100 MHz, acetone-d6) δ 143.10, 139.42, 138.92, 137.25, 136.48, 130.96, 130.02, 129.37, 129.33, 128.88, 128.50, 128.41, 127.57, 127.43, 127.33, 125.08, 75.38, 49.88, 43.86, 37.86, 27.43, 27.25, 27.11, 26.91, 26.56. **HRMS** (ESI) calcd for $C_{29}H_{30}O$ $[M+Na]^+$: 417.2189, found 417.2188. dr > 19:1.



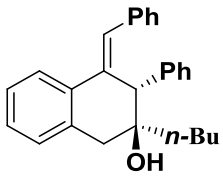
5-benzylidene-4-phenyl-2,3,3a,4,5,9b-hexahydro-1H-cyclopenta[a]naphthalen-3a-ol **(3p)**

3p was obtained by silica gel chromatography eluted by (ethyl acetate/petroleum ether v/v= 1:10) 61.3 mg (87% yield), yellow oil. **^{1}H NMR** (400 MHz, acetone-d6) δ 7.72-7.70 (m, 1H), 7.35-7.17 (m, 11H), 7.14-7.11 (m, 3H), 4.42 (s, 1H), 3.81 (s, 1H), 3.21 (t, *J* = 6.0 Hz, 1H) 2.29-2.26 (m, 1H), 1.96-1.88 (m, 1H), 1.79-1.72 (m, 1H), 1.60-1.57 (m, 1H), 1.43-1.38 (m, 1H), 0.84-0.0.81 (m, 1H). **^{13}C NMR** (100 MHz, acetone-d6) δ 143.61, 140.60, 139.74, 138.84, 138.17, 130.49, 129.96, 129.25, 129.16, 128.94, 128.86, 128.83, 127.56, 127.35, 127.24, 126.17, 82.99, 53.67, 50.75, 39.21, 33.10, 22.58. **HRMS** (ESI) calcd for $[M+Na]^+$ $C_{26}H_{24}O$: 375.1719, found 375.1719. d.r. > 19:1.



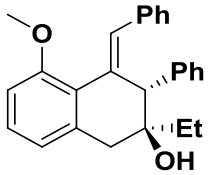
4-benzylidene-2-cyclopropyl-3-phenyl-1,2,3,4-tetrahydronaphthalen-2-ol **(3q)**

3q was obtained by silica gel chromatography eluted by (ethyl acetate/petroleum ether v/v= 1:10), 63.4 mg (90% yield), yellow oil. **^{1}H NMR** (400 MHz, acetone-d6) δ 7.90 (d, *J* = 6.8 Hz, 1H), 7.35-7.16(m, 14H), 4.22 (s, 1H), 3.19 (s, 1H), 2.94 (d, *J* = 17.6 Hz, 1H), 2.76 (d, *J* = 17.2 Hz, 1H), 0.67-0.62 (m, 1H), 0.50-0.49 (m, 2H), 0.32-0.28 (m, 2H). **^{13}C NMR** (101 MHz, acetone-d6) δ 143.30, 139.11, 138.80, 137.37, 136.21, 130.65, 130.03, 129.81, 129.14, 128.79, 128.40, 128.33, 127.56, 127.45, 127.29, 124.94, 71.77, 54.80, 39.56, 20.21, 0.80, -0.12. dr > 19:1. **HRMS** (ESI) calcd for $[M-H]^-$ $C_{26}H_{24}O$: 351.1754, found 351.1754.



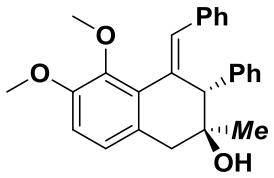
4-benzylidene-2-butyl-3-phenyl-1,2,3,4-tetrahydronaphthalen-2-ol **(3r)**

3r was obtained by silica gel chromatography eluted by (ethyl acetate/petroleum ether v/v= 1:10) 67.1 mg (91% yield), yellow oil. **^{1}H NMR** (400 MHz, acetone-d6) δ 7.87-7.86 (m, 1H), 7.32-7.14 (m, 14H), 4.22 (s, 1H), 3.36 (s, 1H), 2.88 (d, *J* = 17.2 Hz, 1H), 2.81 (d, *J* = 17.2 Hz, 1H), 1.60-1.21 (m, 6H), 0.84 (t, *J* = 7.6 Hz, 3H). **^{13}C NMR** (101 MHz, acetone-d6) δ 143.42, 139.40, 138.92, 137.50, 136.37, 130.69, 130.04, 129.57, 129.25, 128.82, 128.49, 128.47, 127.57, 127.48, 127.32, 125.10, 73.71, 54.48, 40.85, 38.76, 25.48, 23.92, 14.40. dr > 19:1. **HRMS** (ESI) calcd for $[M-H]^-$ $C_{27}H_{28}O$: 367.2067, found 367.2064.



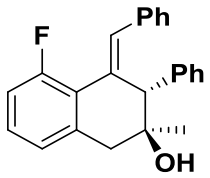
4-benzylidene-2-ethyl-5-methoxy-3-phenyl-1,2,3,4-tetrahydronaphthalen-2-ol **(3s)**

3s was obtained by silica gel chromatography eluted by (ethyl acetate/petroleum ether v/v= 1:10), 63.0 mg (85% yield), white solid. **^{1}H NMR** (400 MHz, acetone-d6) δ 7.75 (s, 1H), 7.32-7.28 (m, 2H) ,7.24-7.18 (m, 7H), 7.14-7.12 (m, 2H), 7.00 (d, *J* = 8.0 Hz, 1H), 6.83 (dd, *J* = 7.6, 0.8 Hz, 1H), 4.26 (s, 1H), 3.87 (s, 3H), 3.27 (s, 1H), 2.86 (d, *J* = 16.8 Hz, 1H), 2.81 (d, *J* = 16.8 Hz, 1H), 1.33-1.16 (m, 2H), 0.87 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR** (100 MHz, acetone-d6) δ 158.69, 143.49, 139.70, 138.61, 134.99, 134.11, 134.07, 129.84, 129.46, 129.14, 128.70, 128.49, 127.26, 127.16, 126.73, 122.91, 110.86, 73.61, 56.05, 55.27, 39.51, 32.90, 7.29 . **HRMS** (ESI) calcd for $[M+Na]^+$ $C_{26}H_{26}O_2$: 393.1825, found 393.1824. dr > 19:1.



4-benzylidene-5,6-dimethoxy-2-methyl-3-phenyl-1,2,3,4-tetrahydronaphthalen-2-ol **(3t)**

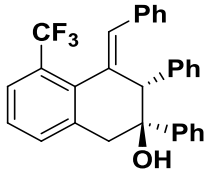
3t was obtained by silica gel chromatography eluted by (ethyl acetate/petroleum ether v/v= 1:10), 64.9 mg (84% yield), white solid. **^{1}H NMR** (400 MHz, acetone-d6) δ 7.79 (s, 1H), 7.32-7.18 (m, 10H), 6.98 (d, *J* = 8.4 Hz, 1H), 6.88 (d, *J* = 8.4 Hz, 1H), 4.20 (s, 1H), 3.90 (s, 3H), 3.70 (s, 3H), 3.49 (s, 1H), 2.79-2.72 (m, 2H), 1.00 (s, 3H). **^{13}C NMR** (100 MHz, acetone-d6) δ 153.05, 148.34, 143.91, 139.47, 135.32, 134.23, 131.42, 130.23, 129.86, 129.45, 129.19, 128.79, 127.39, 127.35, 125.22, 113.01, 72.29, 59.90, 56.39, 56.21, 41.41, 28.41. **HRMS** (ESI) calcd for $[M+Na]^+$ $C_{26}H_{26}O_3$: 409.1774, found 409.1774. dr > 19:1.



4-benzylidene-5-fluoro-2-methyl-3-phenyl-1,2,3,4-tetrahydronaphthalen-2-ol **(3u)**

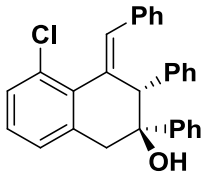
3u was obtained by silica gel chromatography eluted by (ethyl acetate/petroleum ether v/v= 1:10) 55.8 mg (81% yield), white solid. **^{1}H NMR** (400 MHz, MeOH-d3) δ 7.56 (s, 1H), 7.29-7.22 (m, 7H), 7.16-7.14 (m, 2H), 7.10-7.07 (m, 3H), 7.01 (d, *J* = 7.2 Hz , 1H), 4.12 (s, 1H), 2.86 (d, *J* = 15.6 Hz, 1H), 2.80 (d, *J* = 15.6 Hz, 1H), 1.08 (s, 3H) . **^{13}C NMR** (101 MHz, MeOH-d3) δ 162.28 (d, *J* = 251 Hz) , 143.70, 139.56 (d, *J* = 2.0 Hz), 139.27, 135.04, 134.86, 134.18 (d, *J* = 4 Hz), 130.13, 129.74, 129.54, 129.14, 129.02 (d, *J* = 7.0 Hz), 127.93, 126.47 (d, *J* = 4.0 Hz), 125.81 (d, *J* = 9.0 Hz), 115.38 (d, *J* = 25 Hz), 72.52, 56.10, 40.85, 28.43. dr > 19:1. **HRMS** (ESI) calcd for $[M-H]^-$ $C_{24}H_{21}FO$: 343.1504, found

343.1504.



4-benzylidene-2,3-diphenyl-5-(trifluoromethyl)-1,2,3,4-tetrahydronaphthalen-2-ol **(3v)**

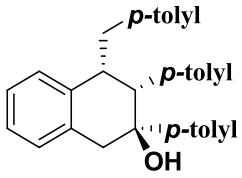
3v was obtained by silica gel chromatography eluted by (ethyl acetate/petroleum ether v/v= 1:10), 80.3 mg (88% yield), white solid. **^{1}H NMR** (400 MHz, acetone-d6) δ 7.82-7.80 (m, 1H), 7.54-7.52 (m, 2H), 7.32-7.30 (m, 2H), 7.27-7.22 (m, 6H), 7.17-7.14 (m, 3H), 7.11-7.09 (m, 2H), 6.87-6.83 (m, 3H), 4.64 (s, 1H), 3.46 (d, *J* = 14.8 Hz, 1H), 3.25 (s, 1H), 3.05(d, *J* = 14.4 Hz, 1H) . **^{13}C NMR** (101 MHz, acetone-d6) δ 149.14, 141.11, 140.71, 140.04, 140.02, 137.64, 137.54, 134.89 (q, *J* = 3.7 Hz), 133.01, 130.89, 129.82, 128.86, 128.65, 128.46, 128.24, 128.13, 127.49, 127.29, 126.77 (q, *J* = 5.4 Hz), 126.28, 123.57 (q, *J* = 251 Hz), 76.34, 58.99, 45.17. dr > 19:1. **HRMS** (ESI) calcd for $[M-H]^-$ $C_{30}H_{23}F_3O$: 455.1628, found 455.1624.



4-benzylidene-5-chloro-2,3-diphenyl-1,2,3,4-tetrahydronaphthalen-2-ol **(3w)**

3w was obtained by silica gel chromatography eluted by (ethyl acetate/petroleum ether v/v= 1:10), 66.8 mg (79% yield), white solid. **^{1}H NMR** (400 MHz, acetone-d6) δ 7.49 (d, *J* = 8.0 Hz, 1H), 7.37-7.35 (m, 2H), 7.29-7.19 (m, 10H), 7.09-6.97 (m, 6H), 4.74 (s, 1H), 3.39 (d, *J* = 14.4 Hz, 1H), 3.16 (s, 1H), 2.95 (d, *J* = 14.8 Hz, 1H) . **^{13}C NMR** (101 MHz, acetone-d6) δ 149.21, 141.88, 140.74, 138.27, 137.42, 136.22, 134.65, 131.15, 130.26, 129.78, 128.88, 128.83, 128.72, 128.23, 129.09, 127.50,

127.36, 126.40, 76.65, 57.92, 44.91. dr > 19:1. **HRMS** (ESI) calcd for $[M-H]^-$ $C_{29}H_{23}ClO$: 421.1365, found 421.1362.



4-(4-methylbenzyl)-2,3-dip-tolyl-1,2,3,4-tetrahydronaphthalen-2-ol **(4)**

4 was obtained by silica gel chromatography eluted by (ethyl acetate/petroleum ether v/v= 1:10) 8.2 mg (95% yield), white solid. **^{1}H NMR** (400 MHz, acetone-d6) δ 7.64 (d, *J* = 7.6 Hz, 1H), 7.28-7.21 (m, 3H), 7.02-6.98 (m, 4H), 6.92 (d, *J* = 8.0 Hz, 2H), 6.81 (d, *J* = 8.0 Hz, 2H), 6.77 (d, *J* = 8.0 Hz, 2H), 6.32 (d, *J* = 6.8 Hz, 2H), 4.31-4.27 (m, 1H), 4.23 (s, 1H), 3.69 (d, *J* = 17.2 Hz, 1H), 3.50 (dd, *J* = 13.6, 5.2 Hz, 1H), 3.00 (d, *J* = 5.2 Hz, 1H), 2.91 (d, *J* = 17.2 Hz, 1H), 2.47 (dd, *J* = 13.6, 10.8 Hz, 1H), 2.27 (s, 3H), 2.22 (s, 3H), 2.19 (s, 3H) . **^{13}C NMR** (101 MHz, acetone-d6) δ 145.40, 140.88, 138.63, 137.17, 136.97, 136.47, 136.31, 135.72, 131.36, 130.55, 128.78, 129.44, 128.68, 128.59, 127.04, 126.78, 126.49, 126.40, 74.93, 55.12, 40.41, 38.29, 36.80, 21.05, 21.01, 20.93. **HRMS** (ESI) calcd for $[M+Na]^+$ $C_{32}H_{32}O$: 455.2345, found 455.2344.dr > 19:1.

8 X-ray Diffraction Data of Compound 3l

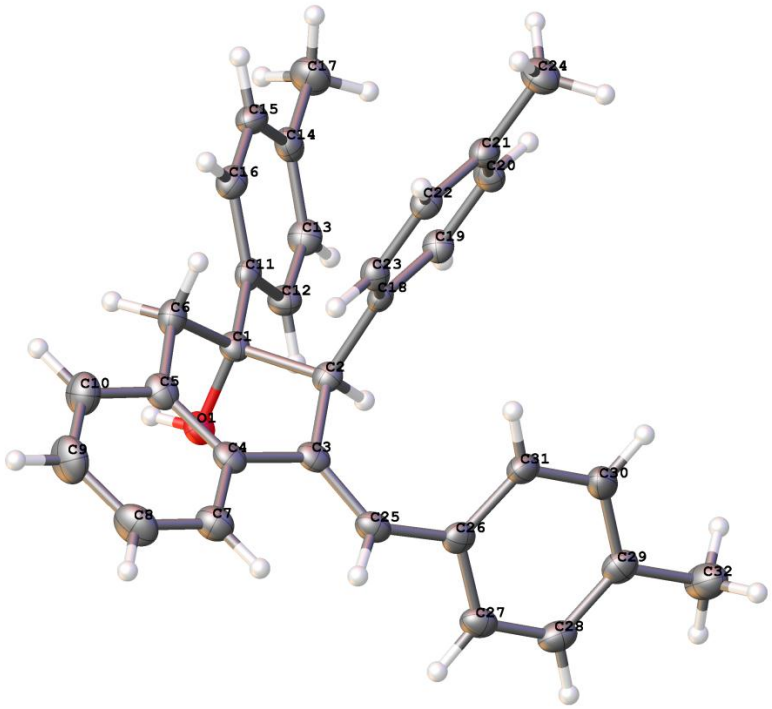


Table 1: Crystal data and structure refinement for exp_3015

Identification code exp_3015

Empirical formula C32H30O

Formula weight 430.56

Temperature / K 101.3

Crystal system monoclinic

Space group P21/n

a / Å, b / Å, c / Å 12.7452(15), 13.2920(9), 14.5536(14)

α/°, β/°, γ/° 90.00, 105.079(12), 90.00

Volume / Å3 2380.6(4)

Z 4

ρcalc / mg mm-3 1.201

μ / mm‑10.070

F(000) 920

Crystal size / mm3 0.50 × 0.25 × 0.09

2Θ range for data collection 6.14 to 52°

Index ranges -15 ≤ h ≤ 15, -15 ≤ k ≤ 16, -17 ≤ l ≤ 17

Reflections collected 12967

Independent reflections 4676[R(int) = 0.0478 (inf-0.9Å)]

Data/restraints/parameters 4676/0/302

Goodness-of-fit on F2 1.026

Final R indexes [I>2σ (I) i.e. Fo>4σ (Fo)] R1 = 0.0501, wR2 = 0.1009

Final R indexes [all data] R1 = 0.0742, wR2 = 0.1119

Largest diff. peak/hole / e Å-3 0.210/-0.186

Flack Parameters N

Completeness 0.998

Table 2 Fractional Atomic Coordinates (×104) and Equivalent Isotropic Displacement

Parameters (Å2×103) for exp_3015.

Ueq is defined as 1/3 of of the trace of the orthogonalised UIJ tensor.

Atom	x	y	z	U(eq)
O1	9926.2(9)	2944.4(8)	576.2(8)	25.0(3)
C19	13595.4(14)	3048.8(12)	1299.2(11)	22.8(4)
C23	13269.2(14)	2649.3(12)	2794.6(11)	22.6(4)
C11	11335.3(14)	4166.4(12)	587.3(11)	21.5(4)
C16	11849.5(14)	5039.6(12)	996.0(12)	25.1(4)

C12	11236.1(15)	4016.0(12)	-380.3(12)	25.0(4)
C14	12175.8(14)	5568.1(13)	-500.9(12)	26.1(4)
C21	15054.8(14)	3209.7(12)	2729.9(12)	23.6(4)
C18	12876.5(14)	2718.3(11)	1811.2(11)	19.1(4)
C2	11719.8(14)	2428.2(12)	1293.5(11)	20.8(4)
C25	11324.5(14)	607.6(12)	1468.3(12)	25.6(4)
C22	14339.8(14)	2893.9(12)	3240.9(12)	23.4(4)
C30	13407.2(15)	132.2(13)	61.0(12)	29.2(4)
C13	11649.7(15)	4695.9(13)	-908.6(12)	27.4(4)
C1	10938.8(14)	3346.3(12)	1140.4(11)	21.3(4)
C27	11376.9(15)	-523.3(12)	126.4(12)	27.7(4)
C20	14659.4(15)	3285.7(12)	1748.8(12)	25.1(4)
C15	12257.2(15)	5723.8(13)	456.8(12)	27.3(4)
C26	11887.6(15)	217.0(12)	774.2(12)	24.4(4)
C29	12879.6(16)	-585.3(12)	-593.6(12)	28.6(4)
C3	11244.4(14)	1565.2(12)	1747.0(11)	22.3(4)
C4	10635.5(14)	1828.7(12)	2459.1(11)	24.2(4)
C24	16222.5(15)	3461.1(14)	3223.7(13)	34.5(5)
C10	9831.8(16)	3069.6(15)	3287.5(13)	34.7(5)
C17	12617.4(17)	6315.5(14)	-1076.7(14)	38.2(5)
C32	13412.6(18)	-1002.4(14)	-1331.4(14)	41.8(5)
C6	10799.4(15)	3685.0(12)	2102.8(11)	25.4(4)

C5	10412.6(14)	2837.9(13)	2625.5(11)	26.5(4)
C28	11862.1(16)	-910.8(13)	-543.1(12)	29.8(4)
C8	9670.4(17)	1332.4(16)	3629.8(13)	39.6(5)
C31	12923.8(15)	522.9(12)	735.0(12)	27.1(4)
C9	9456.9(17)	2327.4(16)	3786.8(14)	41.4(5)
C7	10253.7(15)	1090.7(14)	2982.7(12)	31.5(4)

Table 3 Anisotropic Displacement Parameters (Å2×103) for exp_3015. The Anisotropic displacement factor exponent takes the form: -2π2[h2a*2U11+...+2hka×b×U12]

Atom	U11	U22	U33	U23	U13	U12
O1	18.6(7)	27.5(6)	26.4(6)	1.0(5)	1.3(6)	2.2(5)
C19	24(1)	26.4(9)	17.6(8)	-0.3(7)	4.7(8)	1.5(8)
C23	22.2(10)	23.5(9)	22.8(9)	3.1(7)	6.8(8)	3.1(8)
C11	19.2(9)	22.4(9)	21.5(8)	0.3(7)	2.7(8)	5.7(7)
C16	24.7(10)	25.9(9)	22.8(9)	-1.0(7)	2.4(8)	3.0(8)
C12	24.6(10)	24.9(9)	24.0(9)	-1.7(7)	3.7(8)	-2.2(8)
C14	20.3(10)	27.7(10)	30.8(10)	3.8(8)	7.7(9)	3.4(8)
C21	21.9(10)	21.9(9)	25.3(9)	-3.0(7)	3.2(8)	0.2(7)
C18	20.5(9)	15.8(8)	20.9(8)	-1.5(7)	5.1(8)	2.8(7)
C2	22.9(10)	21.6(9)	17.0(8)	-1.0(7)	3.8(8)	0.8(7)
C25	23.3(10)	25.5(9)	26.9(9)	5.1(8)	4.6(8)	-3.4(8)
C22	25.6(10)	23.3(9)	19.1(8)	0.1(7)	1.8(8)	3.1(8)

C30	23.9(10)	23.8(9)	41.0(11)	1.9(8)	10.3(9)	1.7(8)
C13	29.6(11)	30.9(10)	21.2(9)	-0.6(8)	5.8(8)	1.8(8)
C1	18.6(9)	24.6(9)	18.8(8)	-1.0(7)	1.6(8)	-0.3(7)
C27	27.5(11)	22.9(9)	31.1(10)	4.5(8)	4.7(9)	-3.9(8)
C20	23.3(10)	27.6(9)	26.3(9)	0.4(7)	10.0(9)	-2.0(8)
C15	23.8(10)	22.1(9)	33.9(10)	-4.2(8)	3.8(9)	-0.3(8)
C26	26.2(10)	18.3(9)	27.1(9)	4.6(7)	4.2(8)	2.3(8)
C29	34.8(12)	21.0(9)	29.9(10)	2.6(8)	8.4(9)	1.0(8)
C3	16.9(9)	27.1(9)	20.1(8)	2.7(7)	-0.4(8)	-2.3(8)
C4	17.7(9)	30.4(10)	21.9(9)	0.7(7)	0.5(8)	-2.3(8)
C24	28.1(11)	39.7(11)	33.1(10)	-1.8(9)	3.3(9)	-3.7(9)
C10	37.1(12)	39.3(11)	30.5(10)	0.5(9)	13.8(10)	5.7(9)
C17	37.4(13)	37.1(11)	43.8(11)	3.6(9)	17.2(10)	-4.9(9)
C32	51.3(14)	34.9(11)	45.1(12)	-7.3(9)	23.0(11)	-9.1(10)
C6	25.2(10)	27.0(9)	24.1(9)	0.2(7)	6.5(8)	6.1(8)
C5	22.6(10)	34.7(10)	20.8(9)	2.5(8)	3.0(8)	1.1(8)
C28	35.9(12)	21.9(9)	29(1)	-0.9(8)	4.1(9)	-2.3(8)
C8	39.6(13)	49.3(13)	33.4(11)	7.4(9)	15.8(10)	-7.4(10)
C31	25.7(10)	19.6(9)	34(1)	-2.4(8)	4.5(9)	0.5(8)
C9	41.6(13)	54.5(14)	34.6(11)	2.7(10)	21.9(10)	3.3(11)
C7	29.8(11)	34.5(10)	30.1(10)	2.1(8)	7.8(9)	-4.1(9)

Table 4 Bond Lengths for exp_3015.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C1	1.440(2)	C25	C26	1.477(2)
C19	C18	1.394(2)	C25	C3	1.348(2)
C19	C20	1.380(2)	C30	C29	1.391(2)
C23	C18	1.391(2)	C30	C31	1.388(2)
C23	C22	1.389(2)	C1	C6	1.525(2)
C11	C16	1.388(2)	C27	C26	1.401(2)
C11	C12	1.395(2)	C27	C28	1.382(2)
C11	C1	1.518(2)	C26	C31	1.397(2)
C16	C15	1.387(2)	C29	C32	1.517(2)
C12	C13	1.377(2)	C29	C28	1.387(3)
C14	C13	1.392(2)	C3	C4	1.489(2)
C14	C15	1.386(2)	C4	C5	1.405(2)
C14	C17	1.500(2)	C4	C7	1.404(2)
C21	C22	1.383(2)	C10	C5	1.394(2)
C21	C20	1.389(2)	C10	C9	1.382(3)
C21	C24	1.512(2)	C6	C5	1.511(2)
C18	C2	1.520(2)	C8	C9	1.381(3)
C2	C1	1.554(2)	C8	C7	1.381(2)
C2	C3	1.525(2)			

Table 5 Bond Angles for exp_3015.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚

C20	C19	C18	121.33(15)	C11	C1	C6	114.18(13)
C22	C23	C18	120.84(15)	C6	C1	C2	108.87(13)
C16	C11	C12	117.44(15)	C28	C27	C26	121.43(17)
C16	C11	C1	123.95(14)	C19	C20	C21	121.32(16)
C12	C11	C1	118.51(14)	C14	C15	C16	121.99(16)
C15	C16	C11	120.68(15)	C27	C26	C25	118.94(16)
C13	C12	C11	121.48(16)	C31	C26	C25	123.93(16)
C13	C14	C17	121.49(15)	C31	C26	C27	117.10(16)
C15	C14	C13	117.04(15)	C30	C29	C32	120.63(17)
C15	C14	C17	121.46(16)	C28	C29	C30	118.00(16)
C22	C21	C20	117.47(16)	C28	C29	C32	121.37(16)
C22	C21	C24	121.08(15)	C25	C3	C2	120.69(15)
C20	C21	C24	121.44(15)	C25	C3	C4	121.70(15)
C19	C18	C2	120.17(14)	C4	C3	C2	117.50(14)
C23	C18	C19	117.40(16)	C5	C4	C3	120.65(15)
C23	C18	C2	122.42(14)	C7	C4	C3	122.02(15)
C18	C2	C1	111.98(13)	C7	C4	C5	117.33(15)
C18	C2	C3	114.80(13)	C9	C10	C5	121.61(18)
C3	C2	C1	109.94(14)	C5	C6	C1	111.93(14)
C3	C25	C26	128.75(15)	C4	C5	C6	121.16(15)
C21	C22	C23	121.63(15)	C10	C5	C4	119.84(16)
C31	C30	C29	121.07(17)	C10	C5	C6	118.99(16)

C12	C13	C14	121.35(15)		C27	C28	C29	121.14(17)
O1	C1	C11	109.68(13)		C7	C8	C9	119.98(18)
O1	C1	C2	103.65(12)		C30	C31	C26	121.21(16)
O1	C1	C6	109.39(14)		C8	C9	C10	119.12(18)
C11	C1	C2	110.54(14)		C8	C7	C4	122.11(17)

Table 6 Torsion Angles for exp_3015.

A	B	C	D	Angle/˚
O1	C1	C6	C5	57.15(18)
C19	C18	C2	C1	-88.10(17)
C19	C18	C2	C3	145.63(15)
C23	C18	C2	C1	93.24(17)
C23	C18	C2	C3	-33.0(2)
C11	C16	C15	C14	-0.3(3)
C11	C12	C13	C14	-0.6(3)
C11	C1	C6	C5	-179.53(14)
C16	C11	C12	C13	1.2(3)
C16	C11	C1	O1	142.48(16)
C16	C11	C1	C2	-103.84(18)
C16	C11	C1	C6	19.3(2)
C12	C11	C16	C15	-0.8(3)
C12	C11	C1	O1	-41.3(2)
C12	C11	C1	C2	72.4(2)

C12 C11 C1 C6 -164.44(16)

C18 C19 C20 C21 -0.4(2)

C18 C23 C22 C21 -0.2(2)

C18 C2 C1 O1 175.12(11)

C18 C2 C1 C11 57.67(17)

C18 C2 C1 C6 -68.51(17)

C18 C2 C3 C25 -92.56(18)

C18 C2 C3 C4 91.11(17)

C2 C1 C6 C5 -55.48(19)

C2 C3 C4 C5 6.6(2)

C2 C3 C4 C7 -173.93(15)

C25 C26 C31 C30 -179.57(15)

C25 C3 C4 C5 -169.65(16)

C25 C3 C4 C7 9.8(3)

C22 C23 C18 C19 -0.5(2)

C22 C23 C18 C2 178.16(14)

C22 C21 C20 C19 -0.4(2)

C30 C29 C28 C27 1.1(3)

C13 C14 C15 C16 0.9(3)

C1 C11 C16 C15 175.50(16)

C1 C11 C12 C13 -175.25(15)

C1 C2 C3 C25 140.12(16)

C1 C2 C3 C4 -36.21(19)

C1 C6 C5 C4 26.5(2)

C1 C6 C5 C10 -153.95(16)

C27 C26 C31 C30 2.1(2)

C20 C19 C18 C23 0.8(2)

C20 C19 C18 C2 -177.89(14)

C20 C21 C22 C23 0.7(2)

C15 C14 C13 C12 -0.4(3)

C26 C25 C3 C2 3.6(3)

C26 C25 C3 C4 179.76(16)

C26 C27 C28 C29 0.5(3)

C29 C30 C31 C26 -0.6(3)

C3 C2 C1 O1 -56.01(15)

C3 C2 C1 C11 -173.46(13)

C3 C2 C1 C6 60.36(17)

C3 C25 C26 C27 -137.71(19)

C3 C25 C26 C31 44.0(3)

C3 C4 C5 C10 179.33(16)

C3 C4 C5 C6 -1.1(3)

C3 C4 C7 C8 -178.70(17)

C24 C21 C22 C23 -179.22(15)

C24 C21 C20 C19 179.52(16)

C17 C14 C13 C12 -179.37(17)

C17 C14 C15 C16 179.83(16)

C32 C29 C28 C27 -179.56(16)

C5 C4 C7 C8 0.8(3)

C5 C10 C9 C8 0.5(3)

C28 C27 C26 C25 179.53(15)

C28 C27 C26 C31 -2.1(2)

C31 C30 C29 C32 179.61(16)

C31 C30 C29 C28 -1.0(3)

C9 C10 C5 C4 -0.5(3)

C9 C10 C5 C6 179.96(18)

C9 C8 C7 C4 -0.8(3)

C7 C4 C5 C10 -0.1(3)

C7 C4 C5 C6 179.42(16)

C7 C8 C9 C10 0.2(3)

Table 7 Hydrogen Atom Coordinates (Å×104) and Isotropic Displacement Parameters (Å2×103) for exp_3015.

Atom x y z U(eq)

H1 94763414 408 38

H19 13348 3112 627 27

H23 12799 2432 3166 27

H16 11923 51701651 30

H12	10875	3432	-682	30
H2	11742	2193	646	25
H25	10971	118	175731	
H22	14587	2843	3914	28
H30	14110	358	46	35
H13	11575	4567	-1565	33
H27	10682	-764	148	33
H20	15131	3505	1380	30
H15	12603	6317	753	33
H24A	16309	3503	3912	52
H24B	16415	4109	2990	52
H24C	16700	2935	3090	52
H10	9690	37553398		42
H17A	12966	5957	-1507	57
H17B	13153	6747	-649	57
H17C	12022	6730	-1450	57
H32A	13788	-459	-1571	63
H32B	12856	-1294	-1859	63
H32C	13938	-1524	-1040	63
H6A	11502	3941	2497	30
H6B	10268	4243	2006	30
H28	11492	-1409	-976	36

H8 9416 814 3967 47

H31 13304 1007 1178 32

H9 9058 2499 4232 50

H7 10402 403 2889 38

[RSC Journal Format]

Experimental

Single crystals of C32H30O [exp_3015] were recrystallised from [solvents] mounted

in inert oil and

transferred to the cold gas stream of the diffractometer.

Crystal structure determination of [exp_3015]

Crystal Data. C32H30O, M =430.56, monoclinic, a = 12.7452(15) Å, b = 13.2920(9)

Å, c = 14.5536(14)

Å, β = 105.079(12)°, U = 2380.6(4) Å3, T = 101.3, space group P21/n (no. 14),

Z = 4, μ(Mo Kα) = 0.070,

12967 reflections measured, 4676 unique (Rint = 0.0478) which were used in all

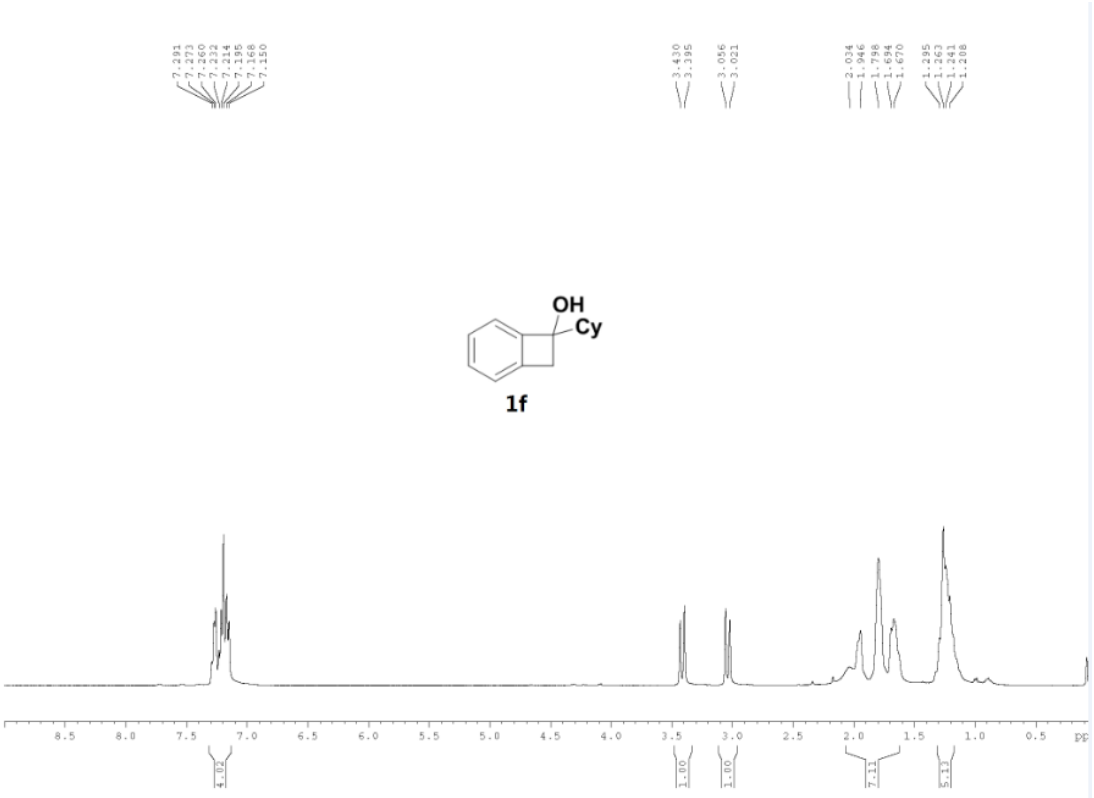
calculations. The final wR(F2) was 0.1119 (all data).

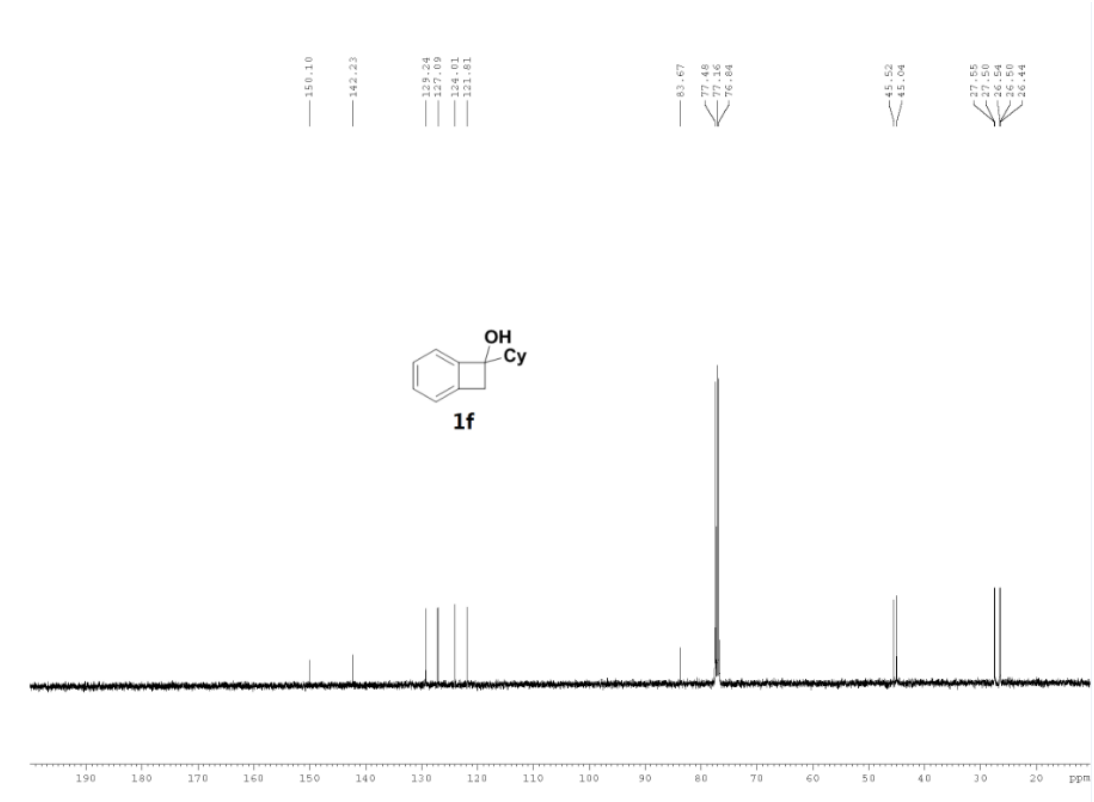
7 References

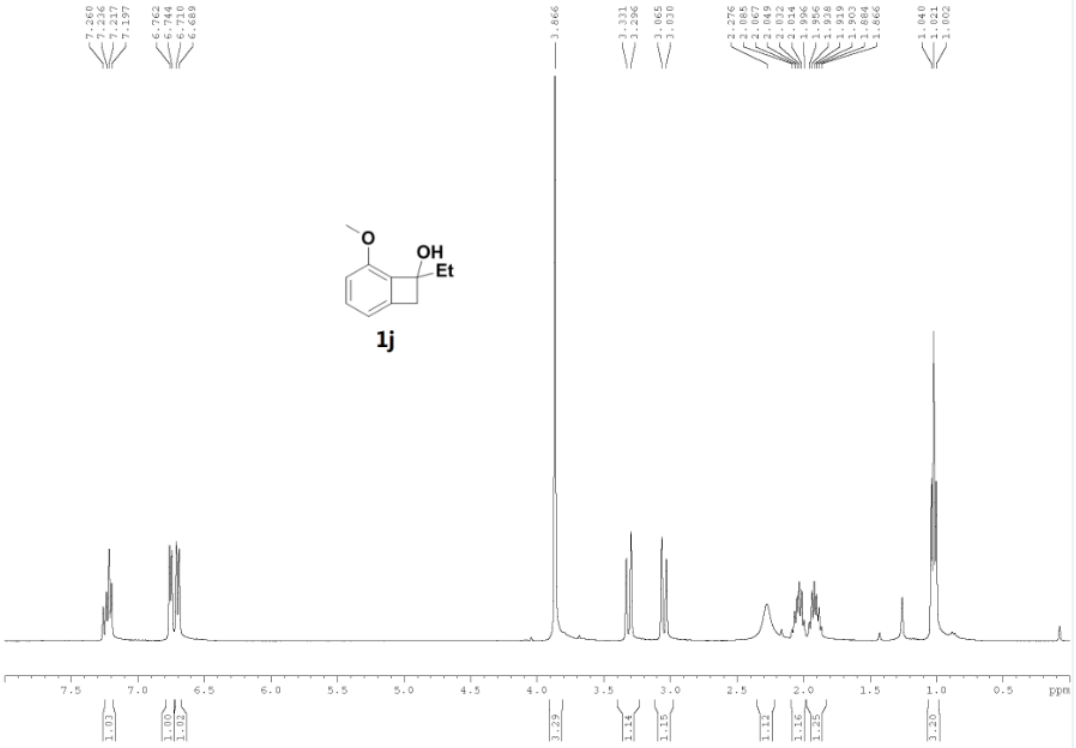
[1] Chen, P.-H.; Savage, N. A.; Dong, G., *Tetrahedron* **2014**, *70*, 4135-4146.

[2] Hossain, M. L.; Ye, F.; Zhang, Y.; Wang, J., *J. Org. Chem.* **2013**, *78*, 1236-1241.

8 Appendix: ^{1}H and ^{13}C NMR Spectra of Key Compounds



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O
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Et
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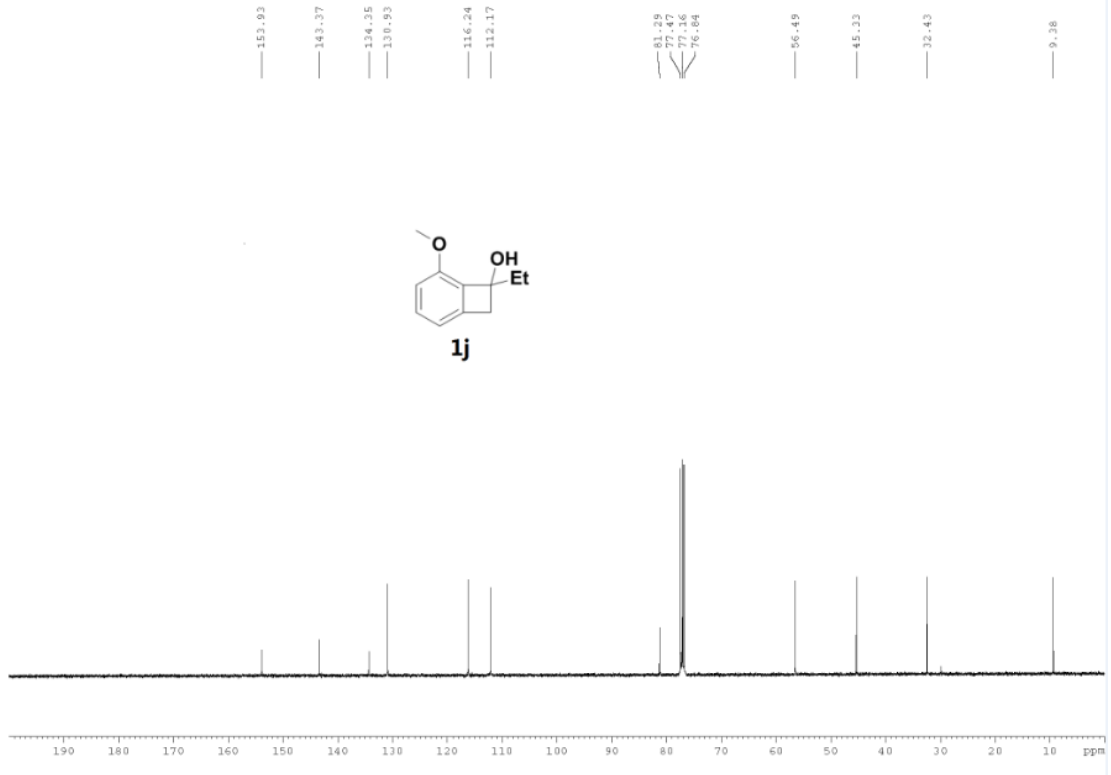
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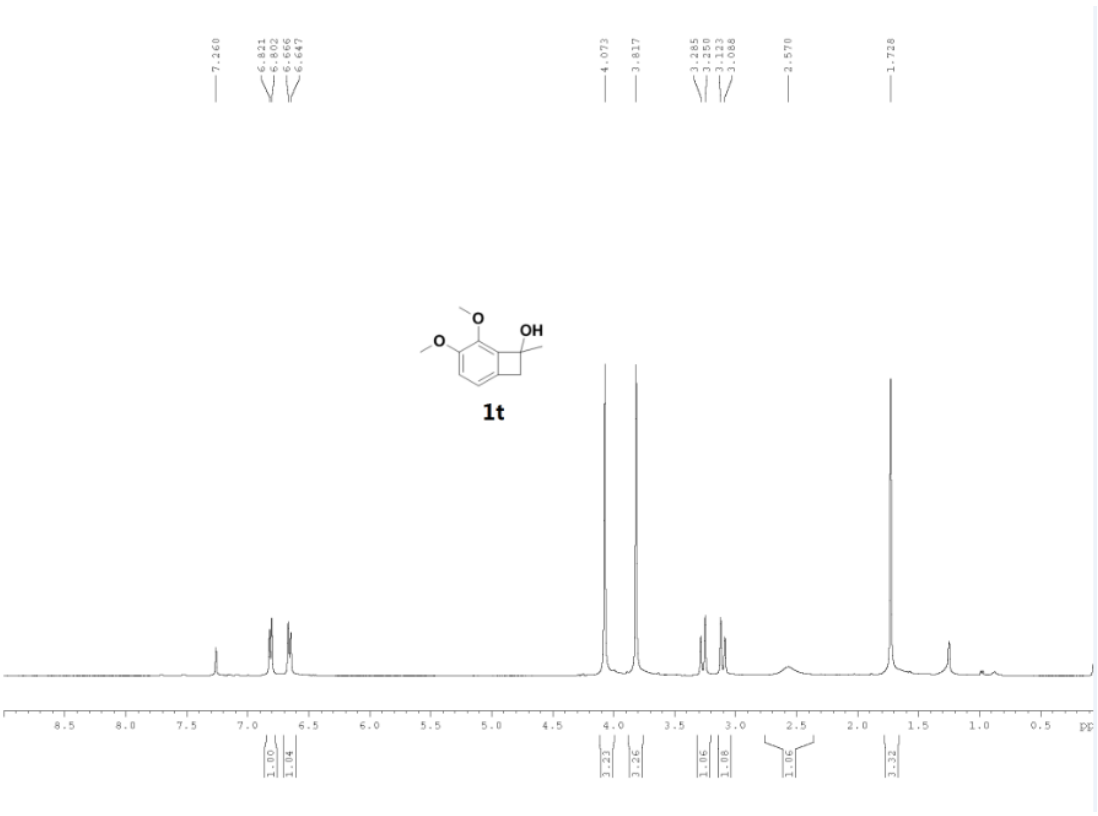
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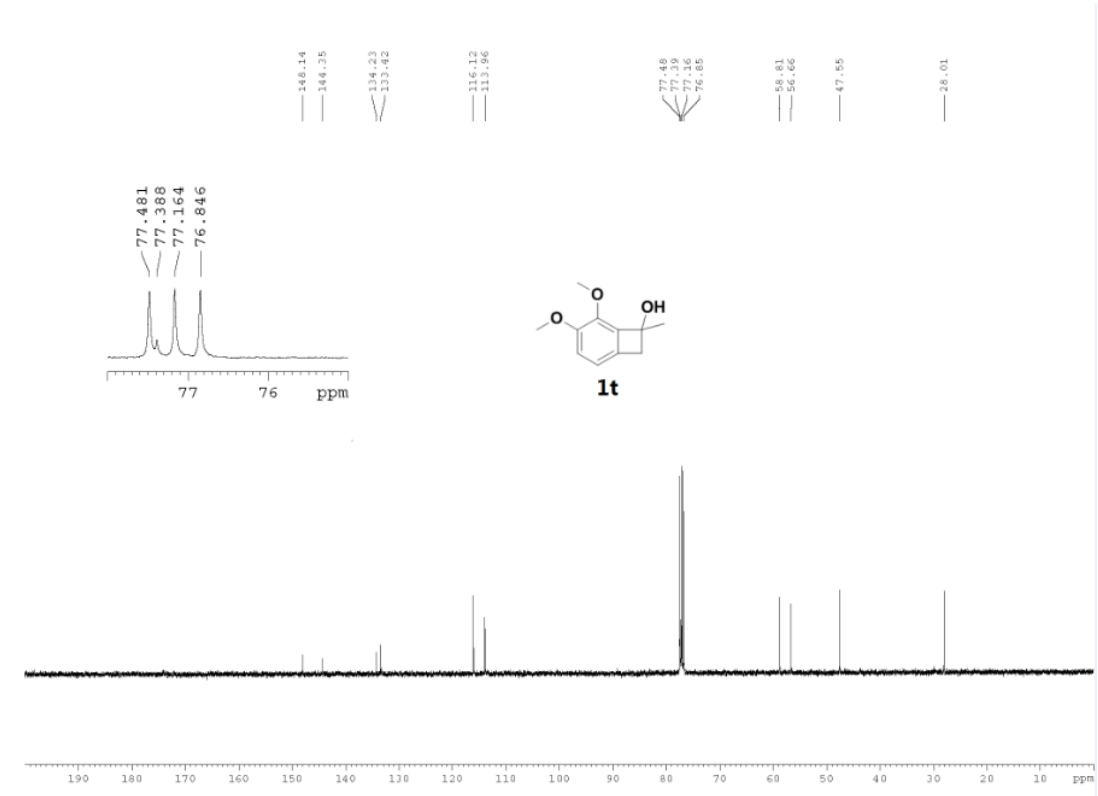
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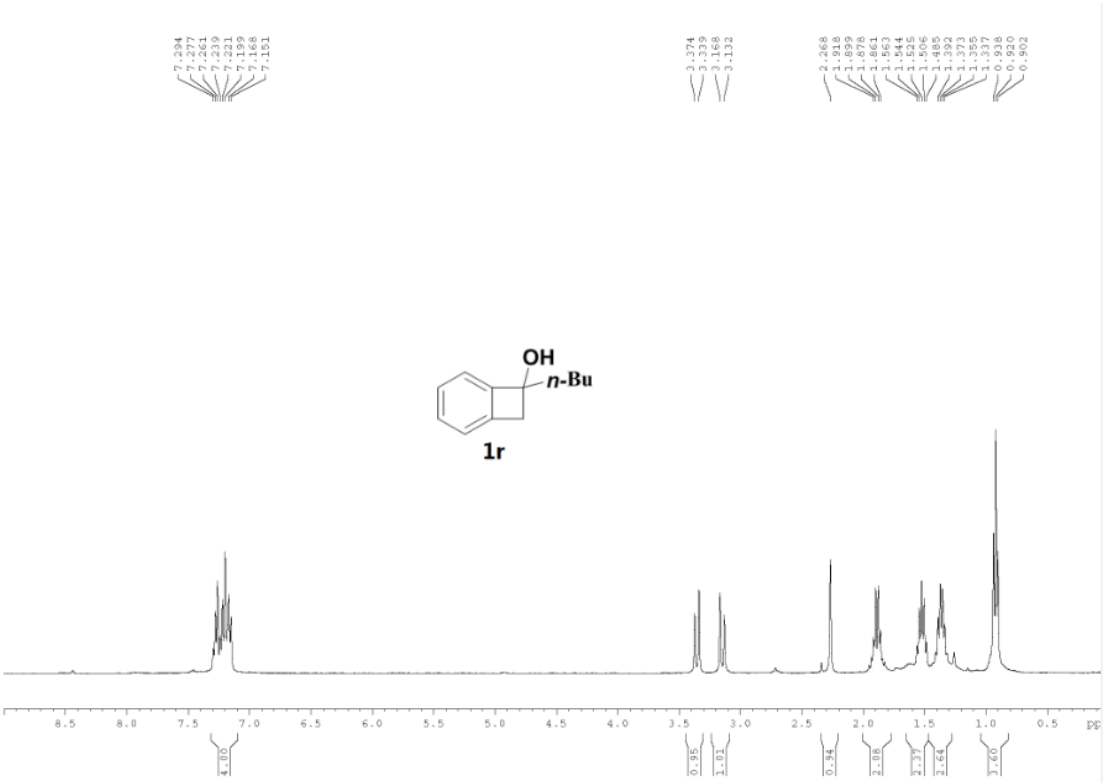
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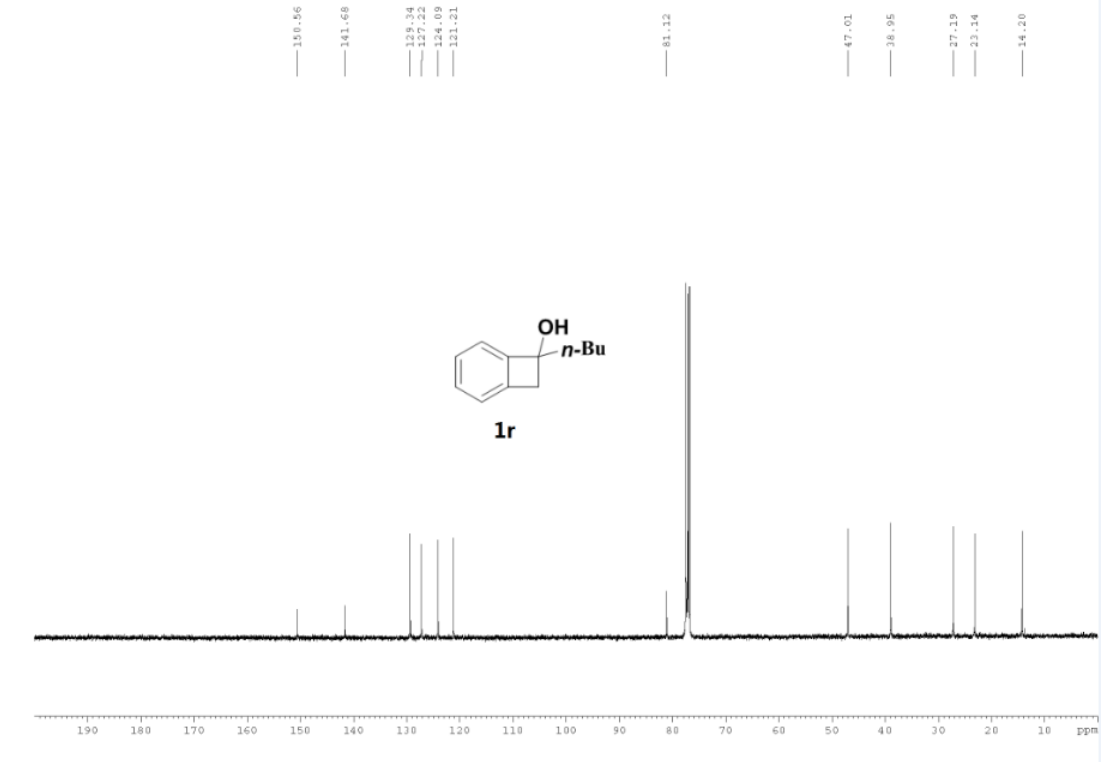
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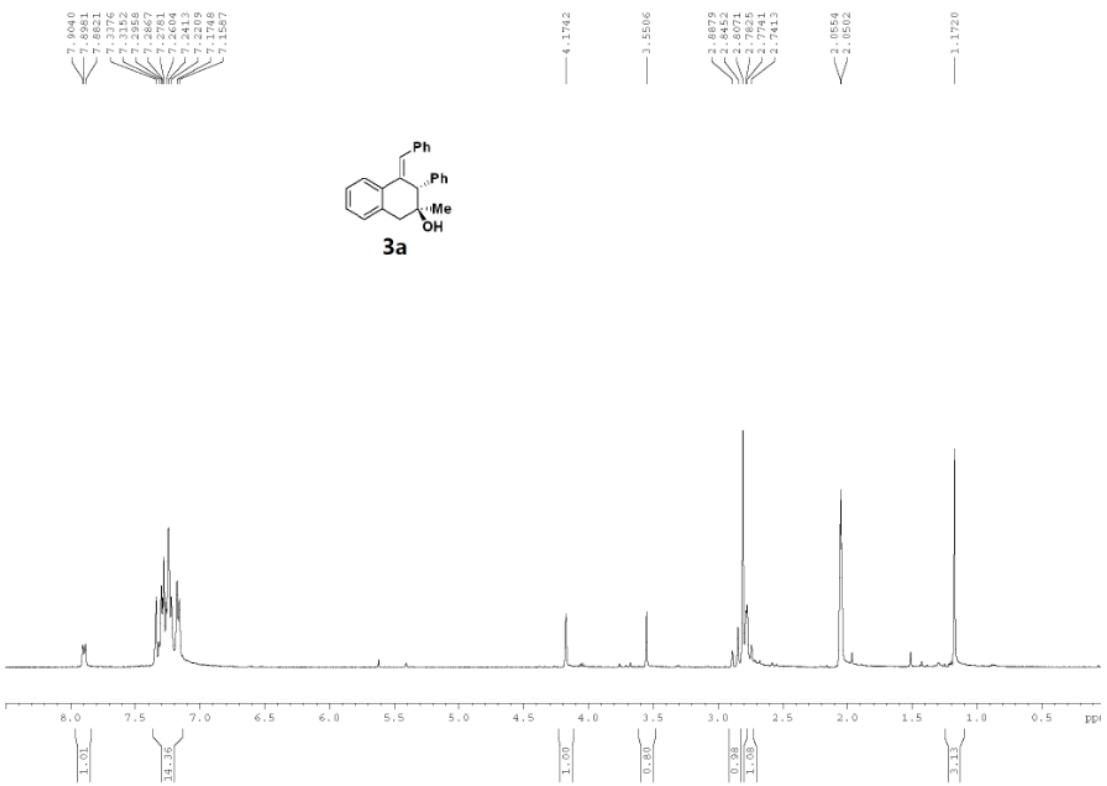
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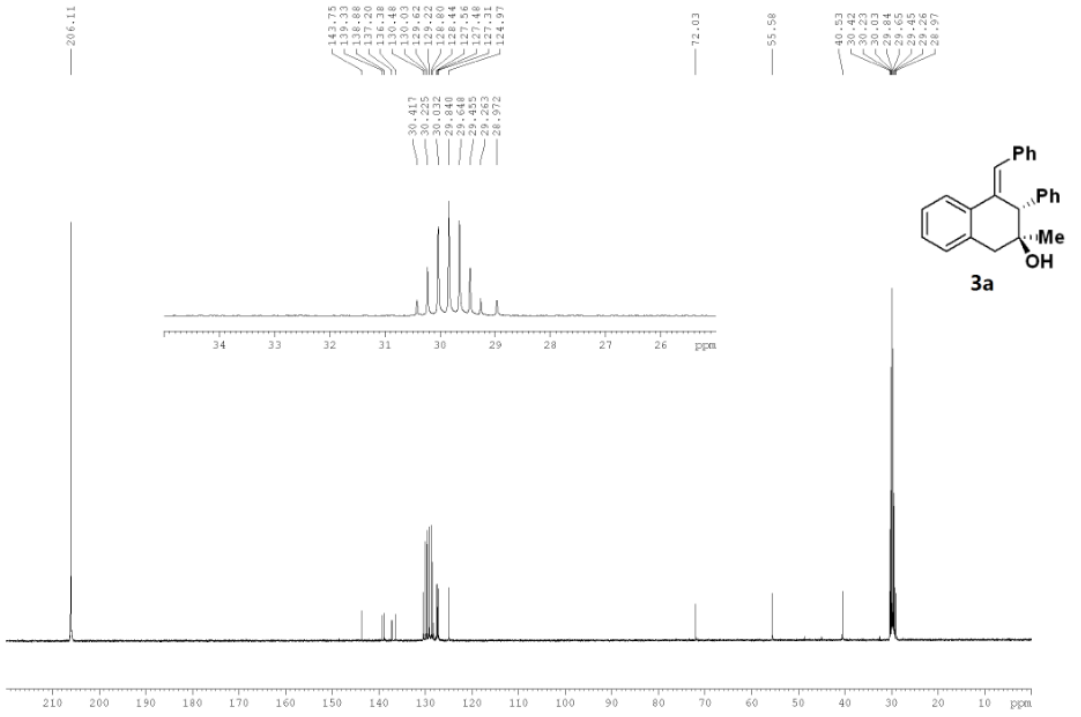
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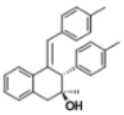
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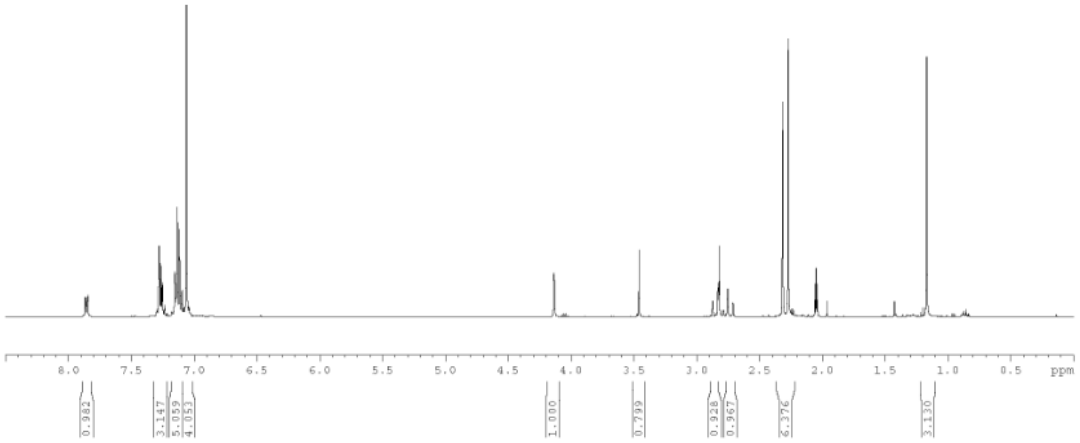
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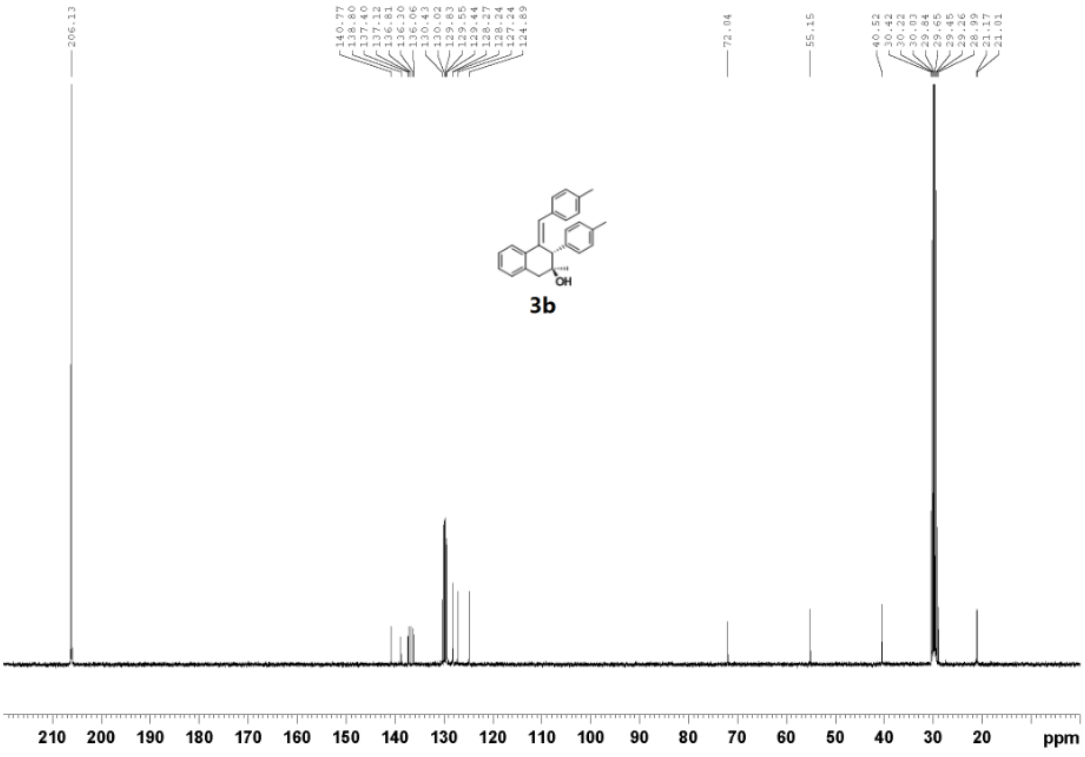
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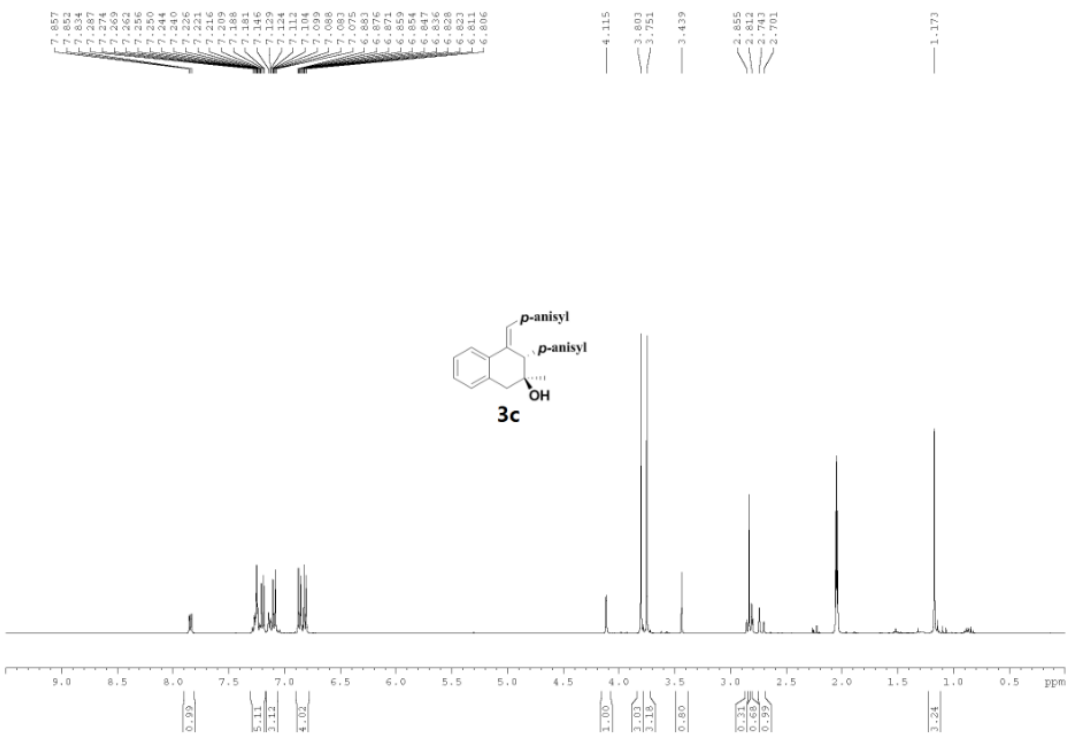
ppm

OH

3b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3.439
2.855
2.811
2.743
2.701
1.173
p-anisyl
p-anisyl
OH
3c
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 ppm
0.99
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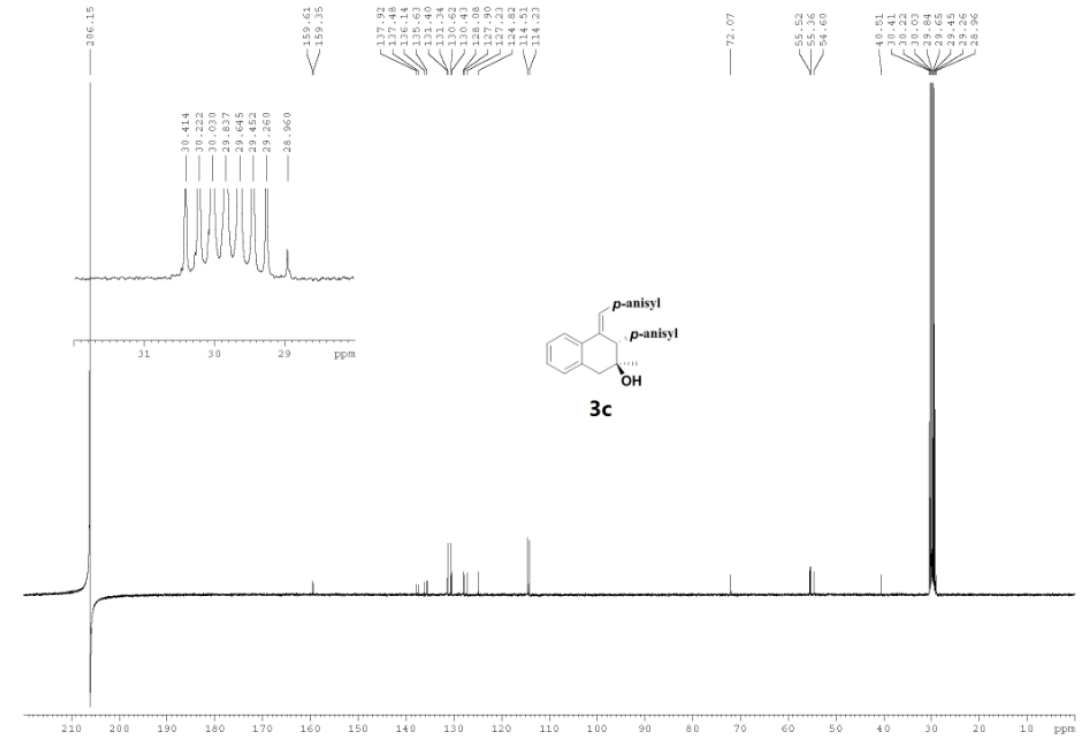
3.12
4.02
1.00
3.03
3.18
0.80
0.31
0.68
0.99
3.24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159.35
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135.63
131.40
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130.43
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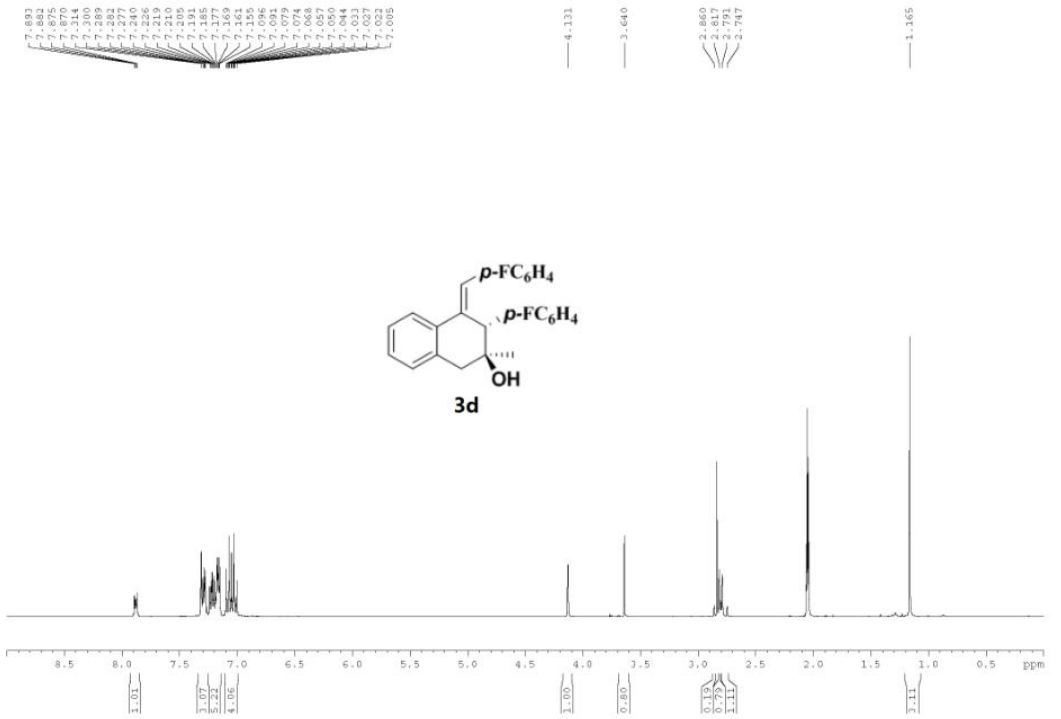
127.23
124.62
114.51
114.23
72.07
55.52
55.36
54.60
40.51
40.41
40.32
30.03
29.84
29.65
29.45
29.26
28.96
30.414
30.222
30.030
29.837
29.645
29.452
29.260
28.960
31 30 29 ppm
p-anisyl
p-anisyl
OH
3c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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7.875
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7.182
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7.240
7.226
7.219
7.210
7.205
7.191
7.185
7.177
7.169
7.161
7.155
7.096
7.091
7.079
7.074
7.066
7.057
7.050
7.044
7.033
7.027
7.022
7.005
4.131
3.640
2.860
2.817
2.791
2.747
1.165
p-FC6H4
p-FC6H4
OH
3d
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
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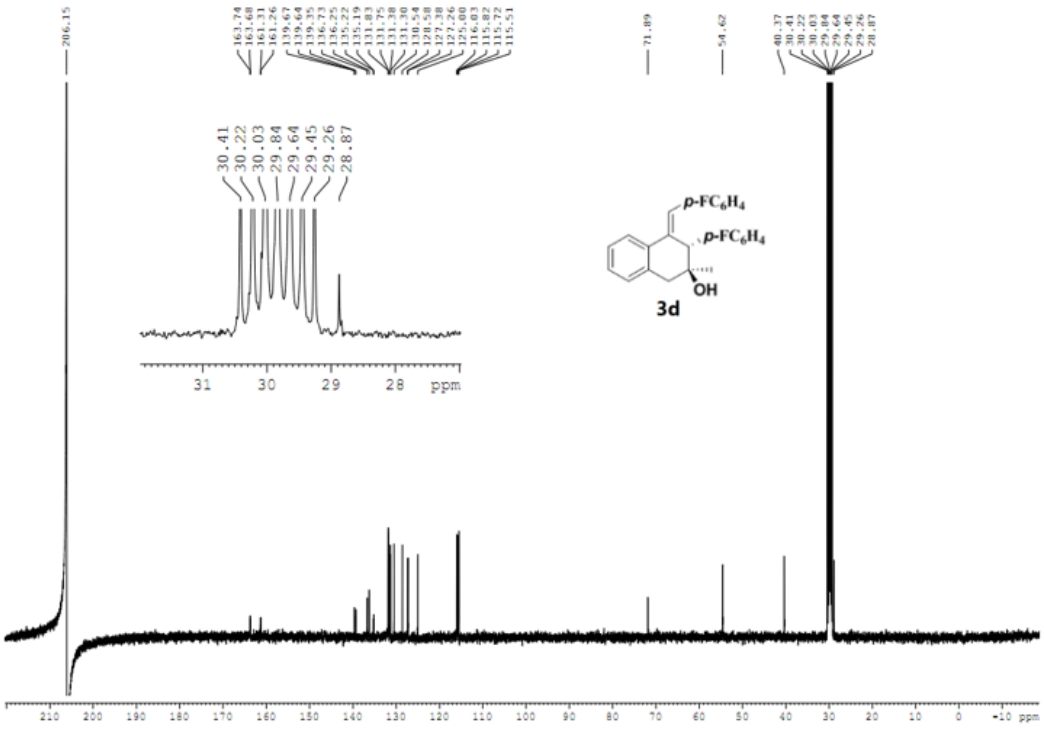
0.79
1.11
3.11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139.64
136.73
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135.19
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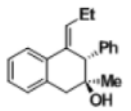
131.25
131.38
131.30
130.54
128.58
127.38
127.26
125.80
116.03
115.82
115.72
115.51
71.89
54.62
40.37
30.41
30.22
30.03
29.84
29.64
29.45
29.26
28.87
30.41
30.22
30.03
29.84
29.64
29.45
29.26
28.87
31
30
29
28
ppm
p-FC6H4
p-FC6H4
OH
3d
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10 ppm



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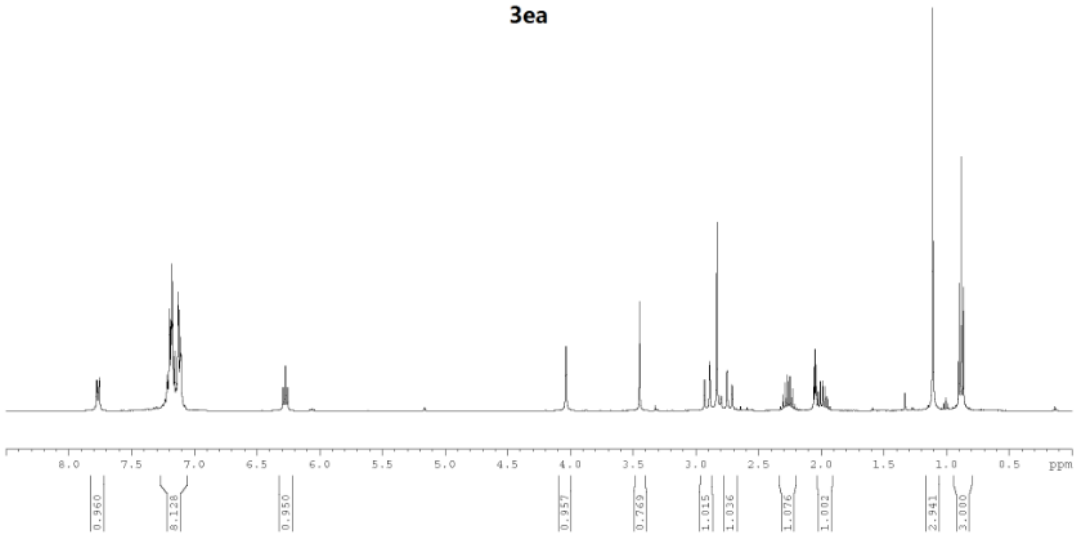

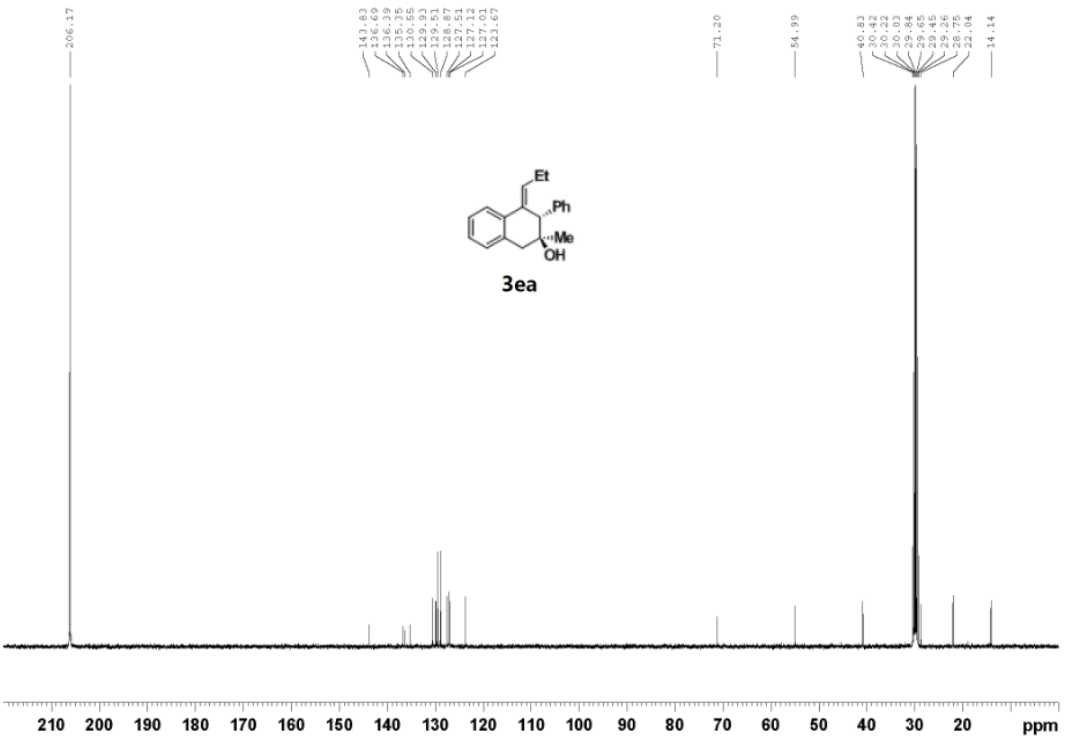

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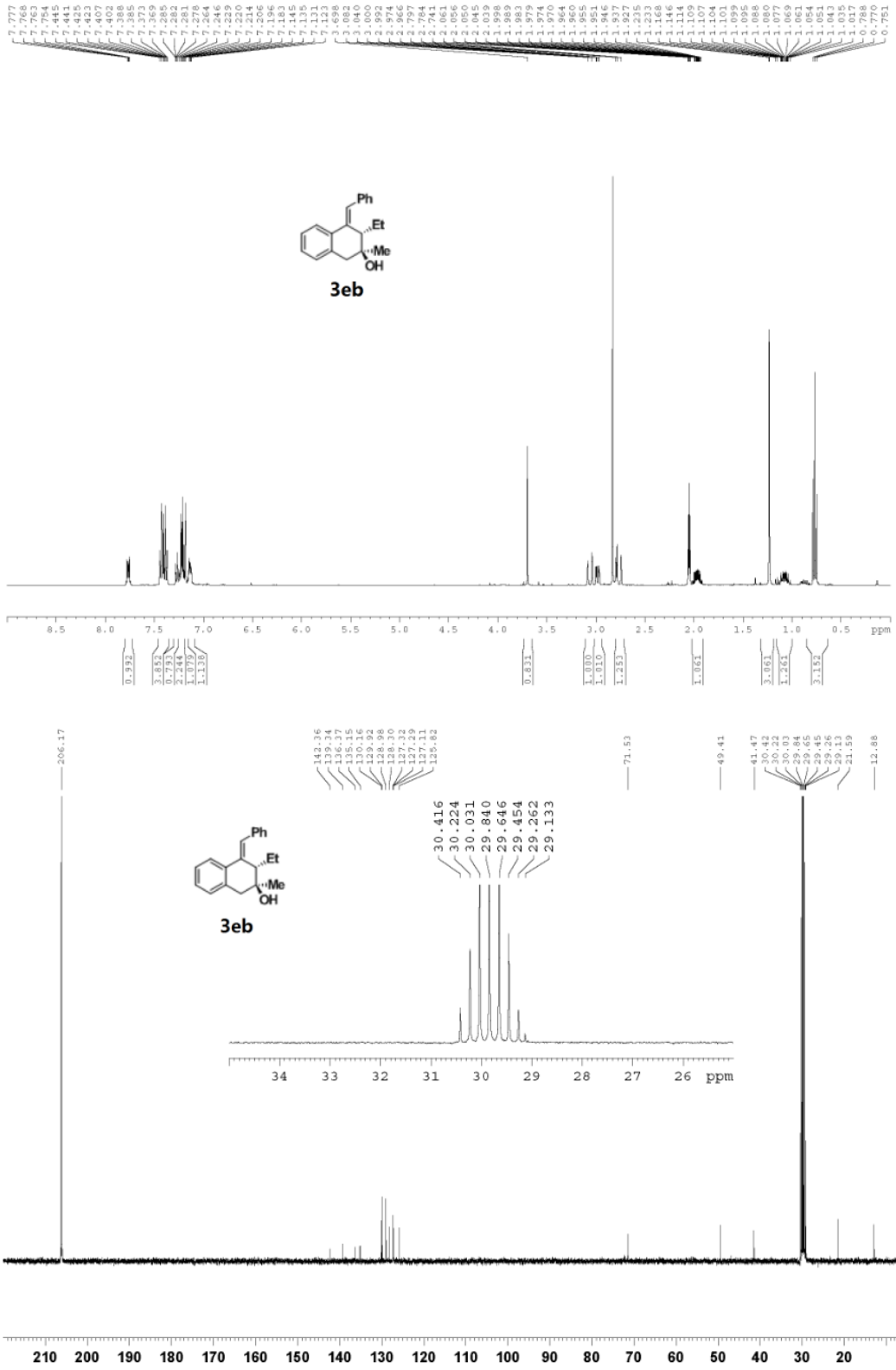
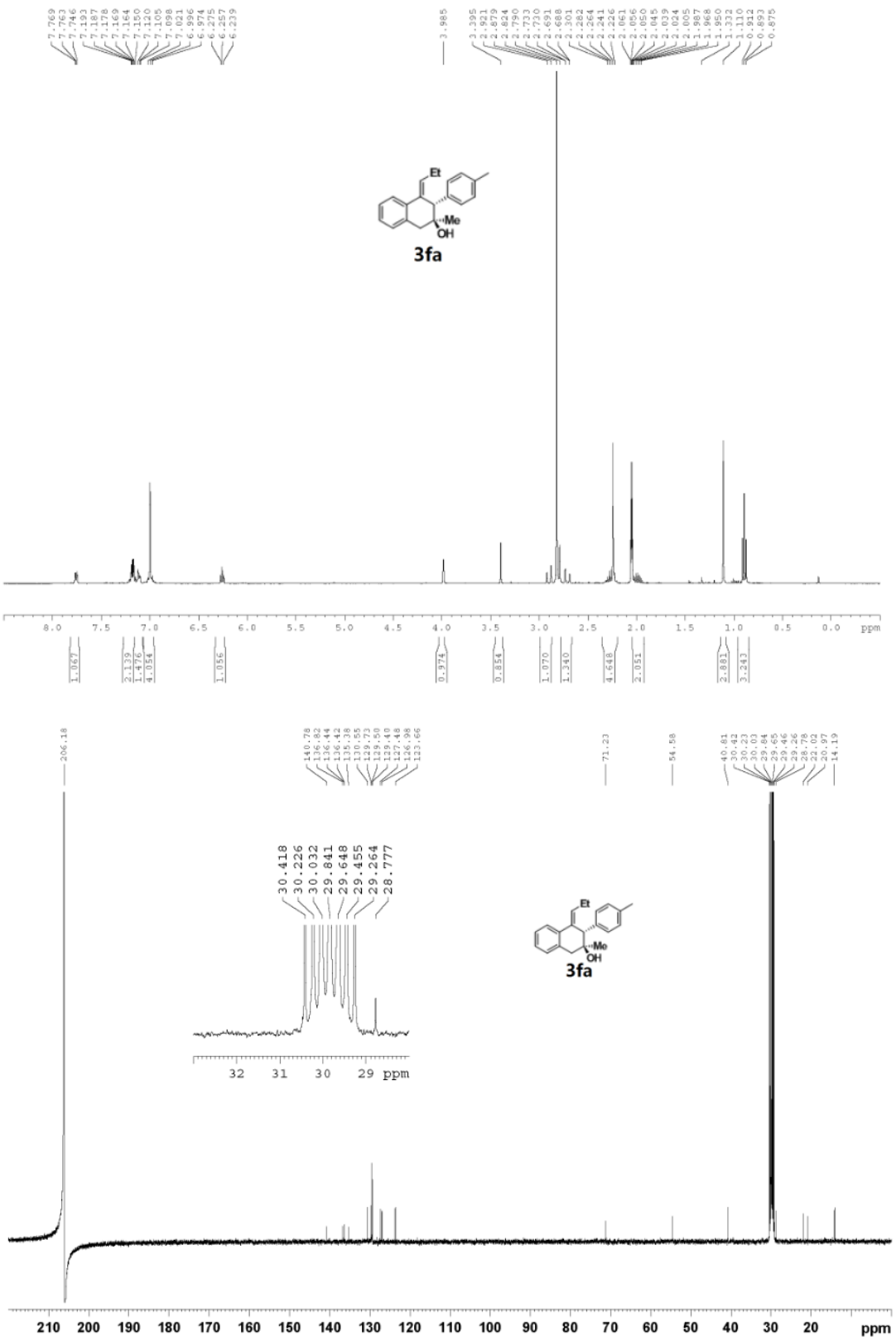

Ph
Et
Me
OH
3eb
ppm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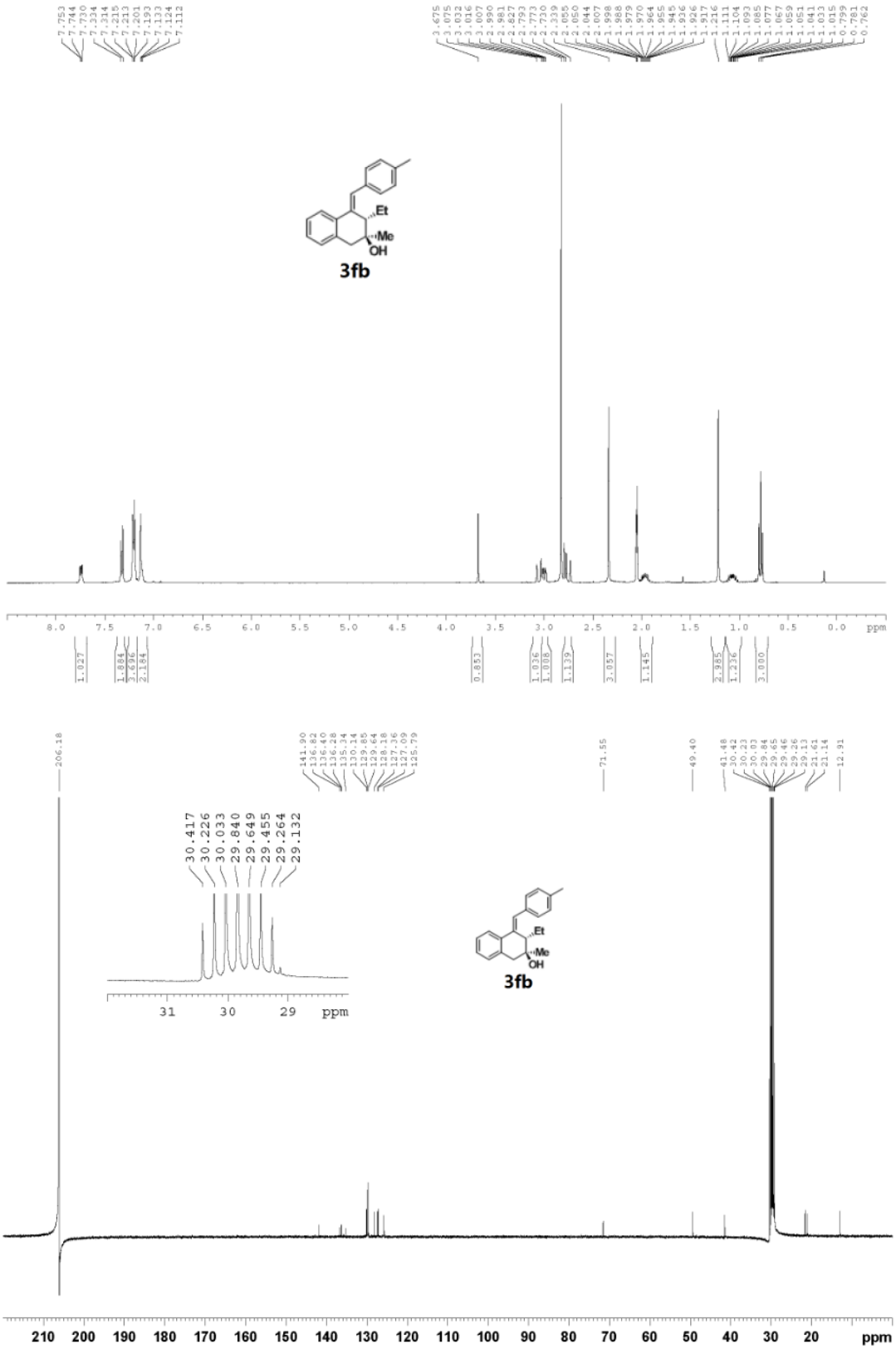
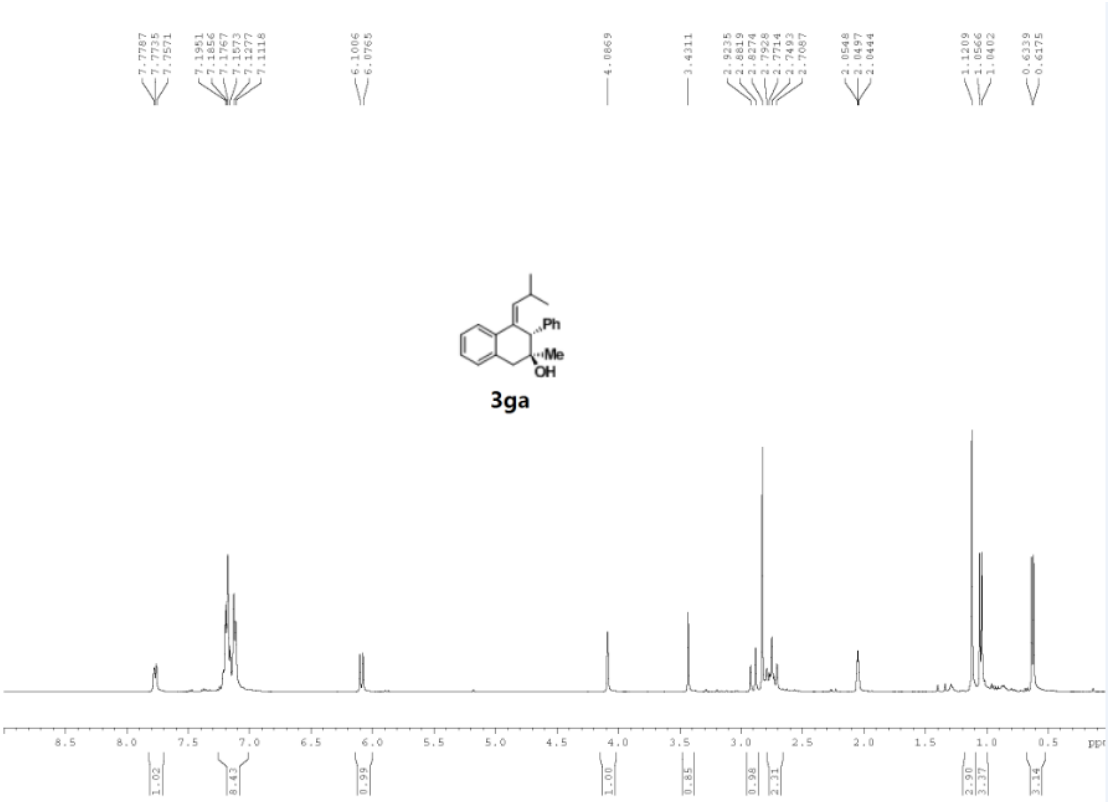
3fa


3fb
ppm
3fb
ppm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7.7571
7.1951
7.1856
7.1767
7.1677
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7.1277
7.1118
6.1006
6.0765
4.0869
3.4311
2.8235
2.8019
2.7874
2.7928
2.7714
2.7493
2.7087
2.0548
2.0497
2.0444
1.1269
1.0566
1.0402
0.6339
0.6175
Ph
Me
OH
3ga
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
ppm
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8.43
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1.00
0.85
0.98
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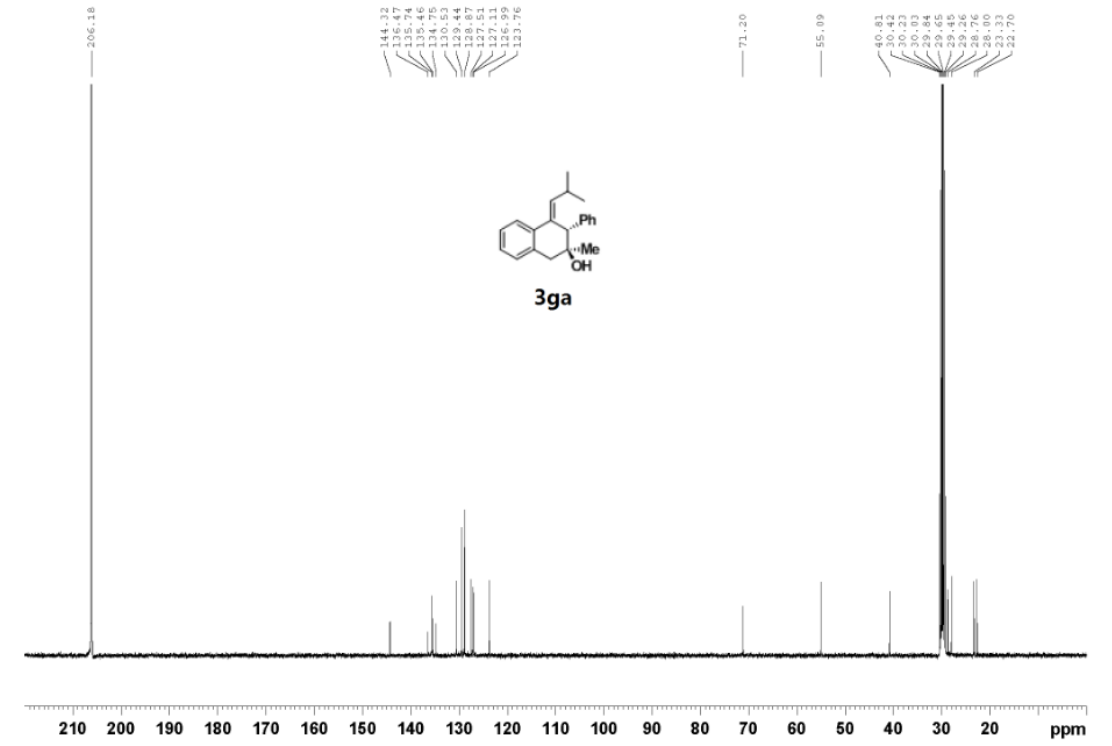
2.90
3.37
3.14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144.32
136.47
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135.46
134.75
134.53
129.44
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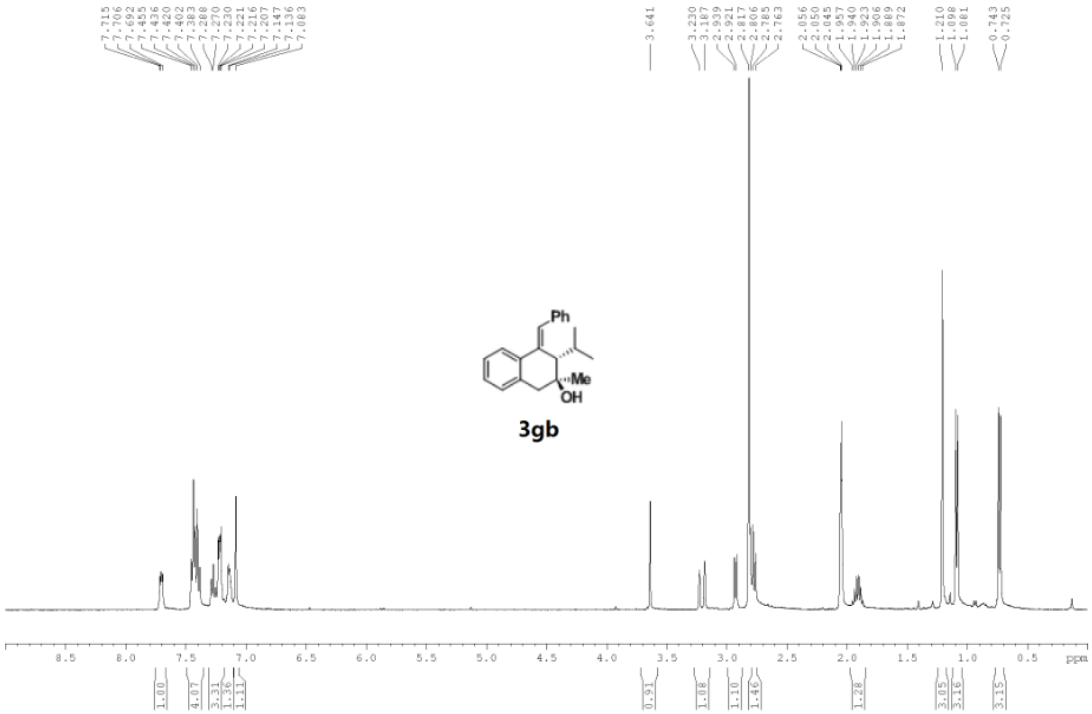
127.51
127.11
126.99
123.76
71.20
55.09
40.81
30.42
30.23
30.03
29.84
29.65
29.45
29.36
28.76
28.00
23.33
22.70
Ph
Me
OH
3ga
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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7.455
7.436
7.420
7.402
7.383
7.288
7.270
7.230
7.221
7.216
7.207
7.147
7.136
7.083
3.641
3.230
3.187
2.939
2.921
2.817
2.806
2.785
2.763
2.056
2.050
2.045
1.957
1.940
1.923
1.906
1.889
1.872
1.210
1.098
1.081
0.743
0.725
Ph
Me
OH
3gb
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
ppm
1.00
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1.08
1.10
1.46
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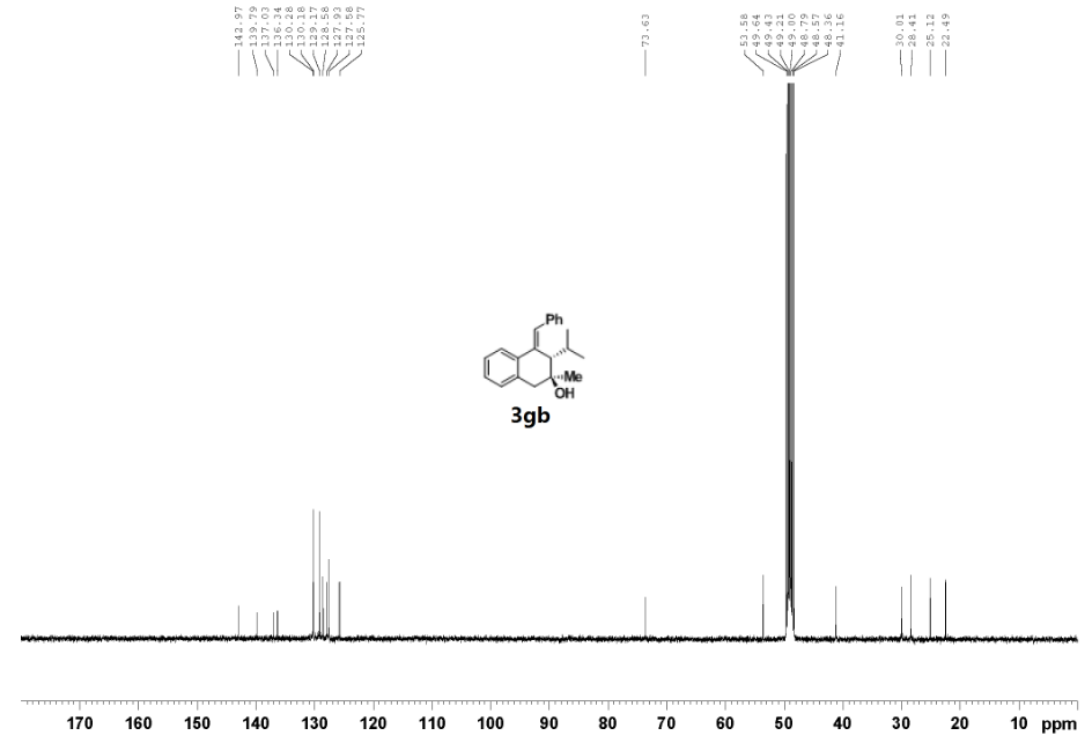
3.05
3.16
3.15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130.18
129.17
128.58
127.93
127.56
125.77
73.63
53.58
49.64
49.43
49.21
49.00
48.79
48.57
48.36
41.16
30.01
28.41
25.12
23.49
Ph
Me
OH
3gb
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150
140
130
120
110
100
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80
70
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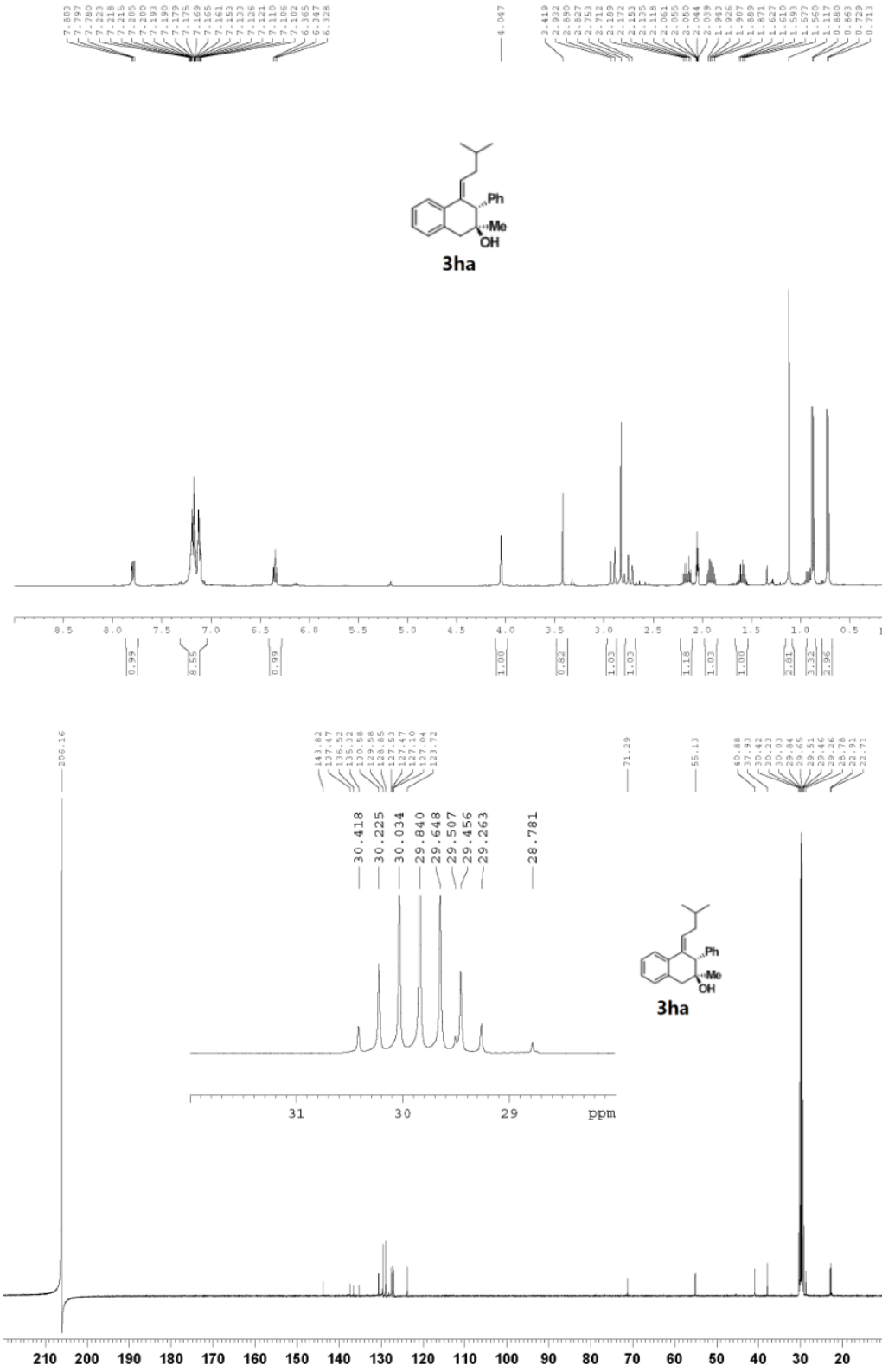
40
30
20
10
ppm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7.169
7.165
7.161
7.153
7.133
7.126
7.121
7.110
7.106
7.102
6.365
6.347
6.328
4.047
3.419
2.932
2.880
2.827
2.753
2.712
2.189
2.172
2.153
2.135
2.118
2.061
2.055
2.050
2.044
2.039
1.943
1.926
1.907
1.889
1.671
1.627
1.610
1.593
1.577
1.560
1.117
0.880
0.863
0.729
0.713
Ph
Me
OH
3ha
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
ppm
0.99
8.56
0.99
1.00
0.82
1.03
1.03
1.16
1.02
1.00
2.81
3.32
2.96
206.16
143.82
137.47
136.52
135.22
130.28
129.58
128.85
127.53
127.47
127.10
127.04
123.72
71.29
55.13
40.88
37.93
30.42
30.23
30.03
29.84
29.65
29.51
29.46
29.26
28.78
22.91
22.71
30.418
30.225
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29.648
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30
29
ppm
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200
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160
150
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80
70
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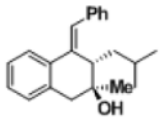
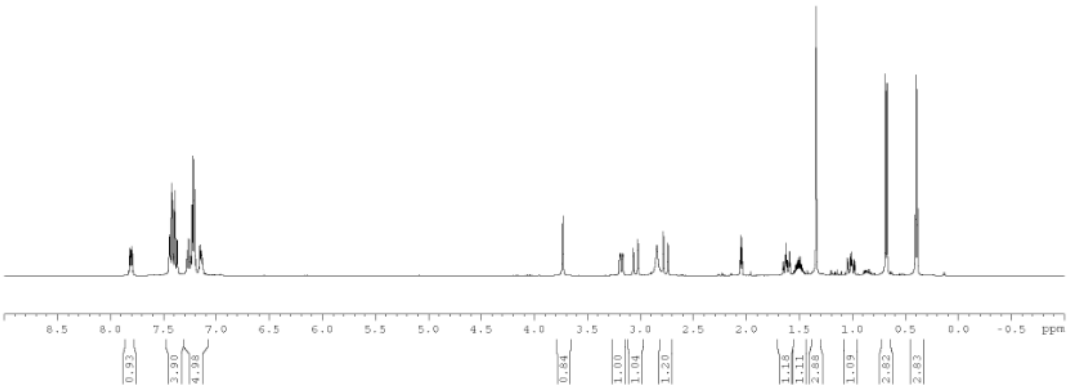
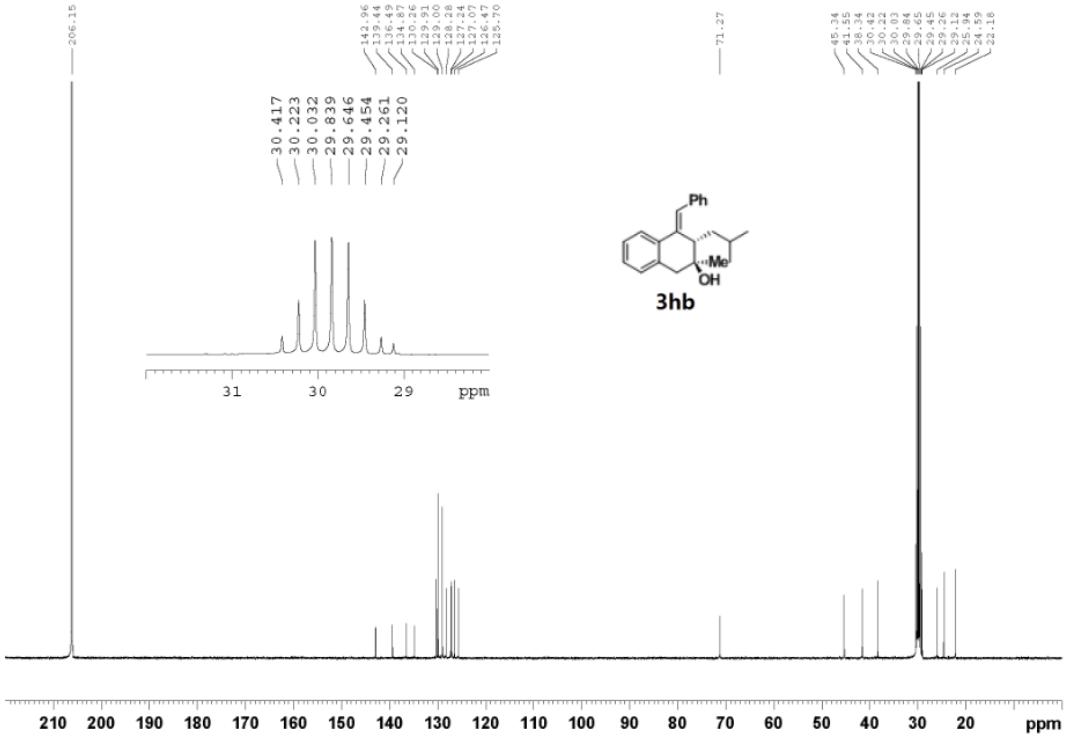
50
40
30
20
ppm


Ph
Me
OH

3hb

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29.839
29.646
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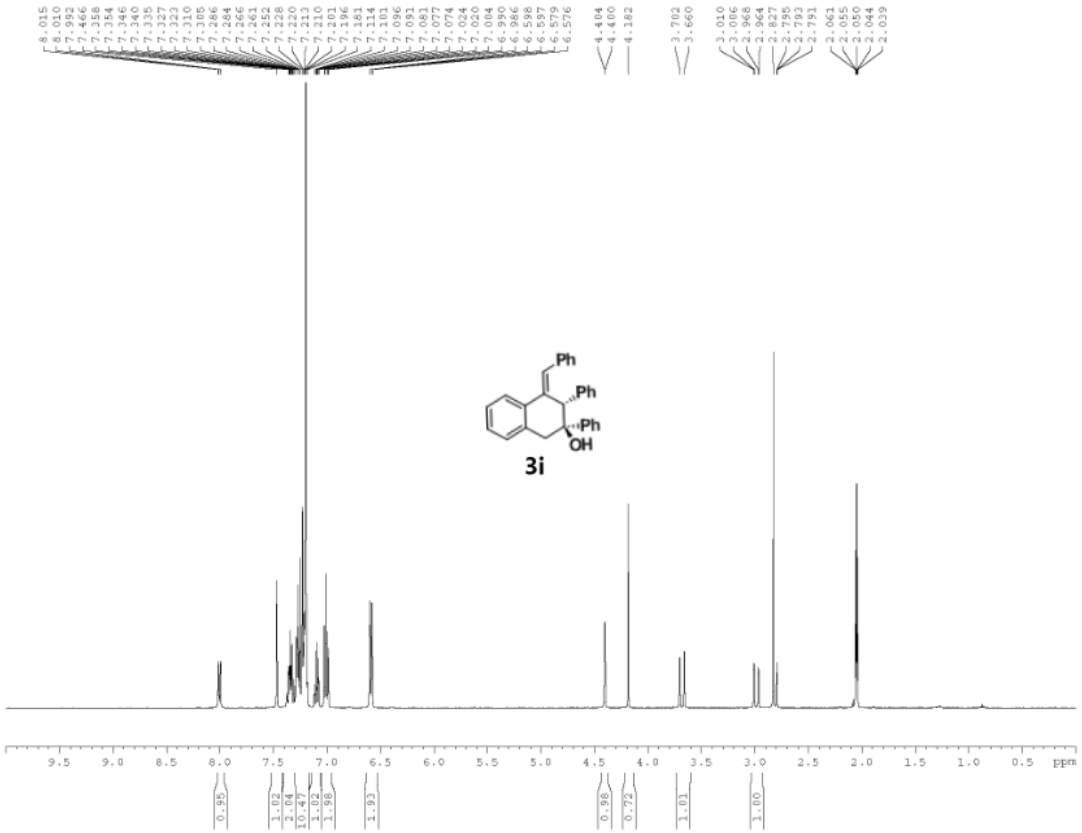
29.261
29.120
31
30
29
ppm
Ph
Me
OH
3hb
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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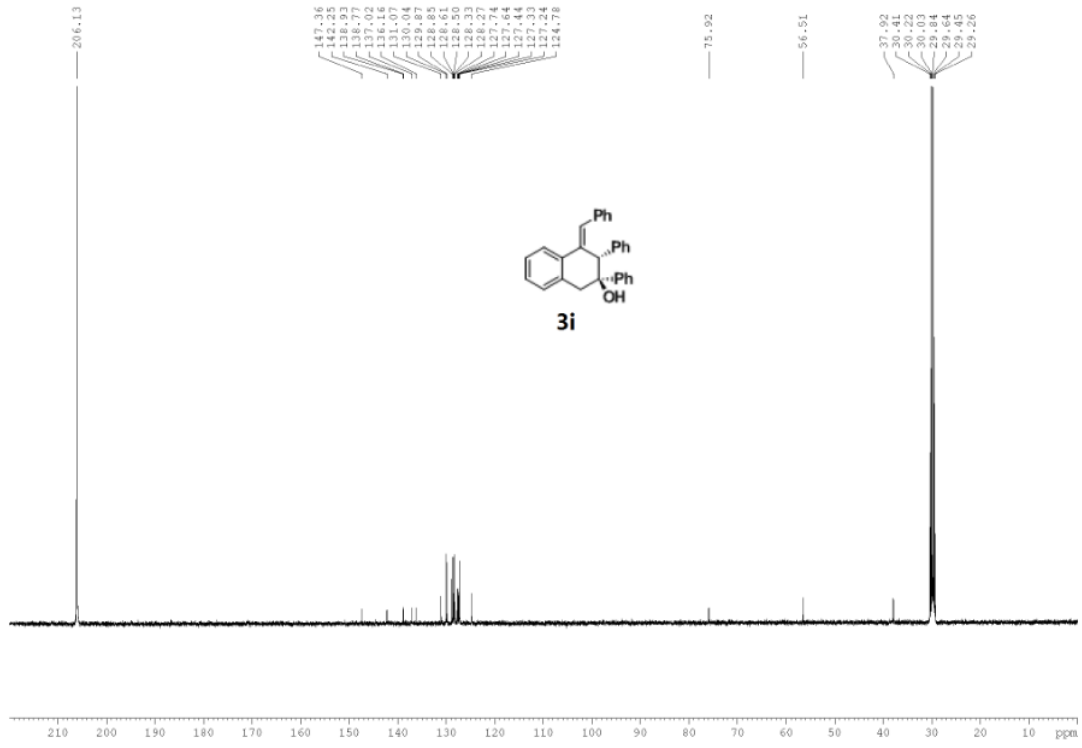
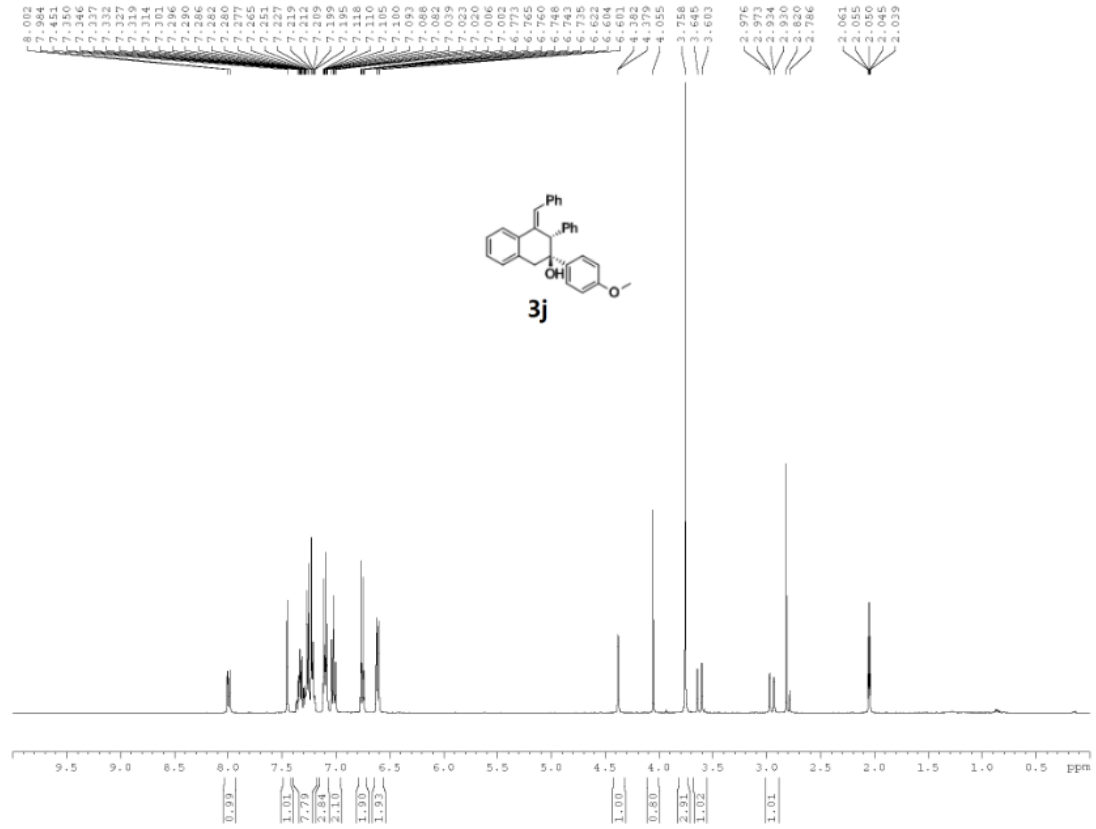
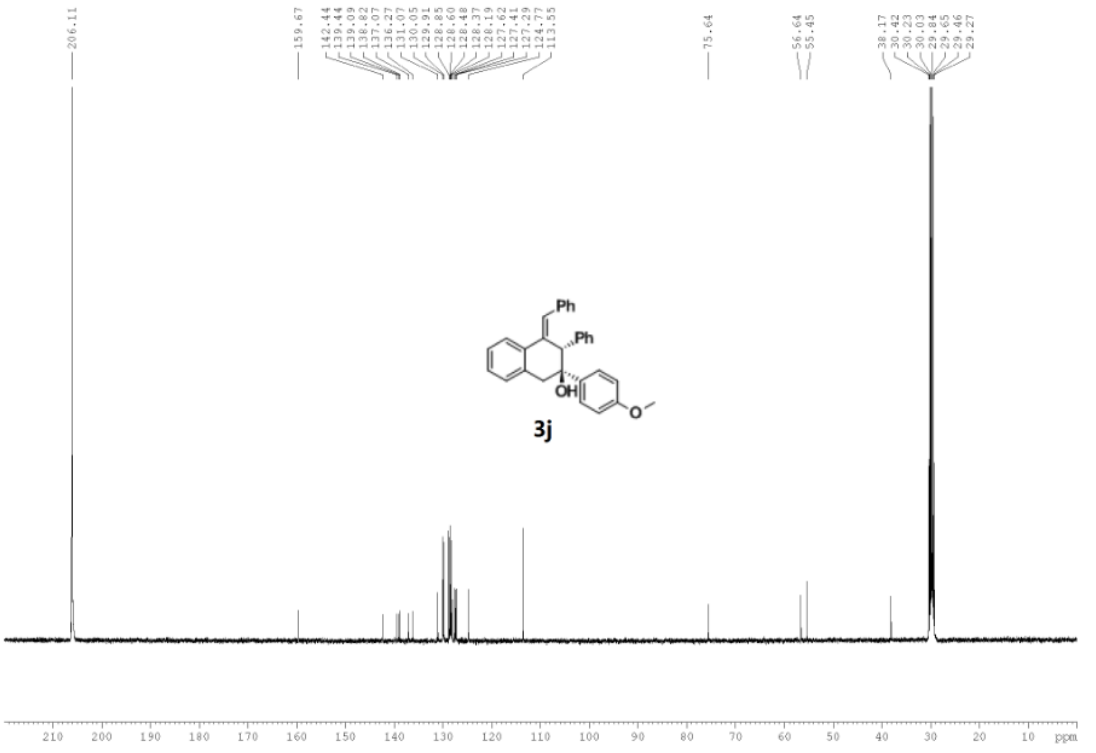
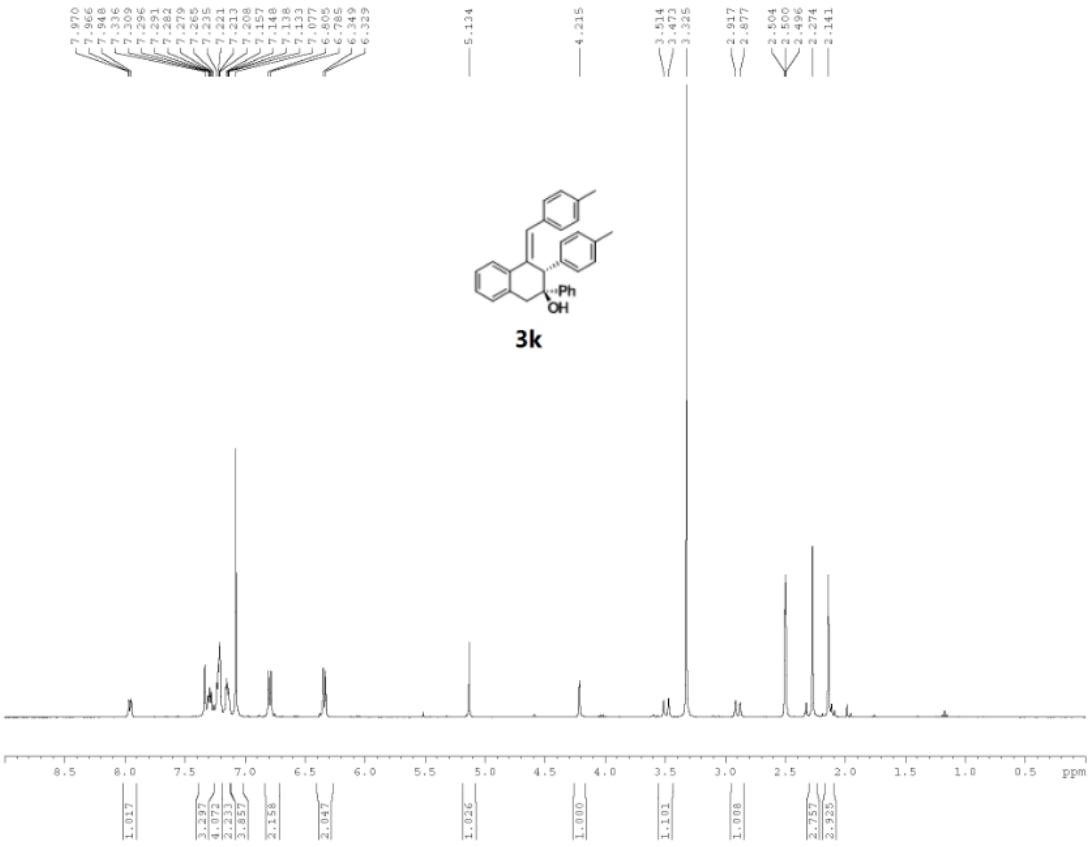
Ph
Ph
OH
3i


Ph
Ph
Ph
OH
3i


Ph
Ph
OH
O
3j


Ph
Ph
OH
O
3j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7.235
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7.213
7.208
7.157
7.148
7.138
7.133
7.077
6.805
6.785
6.349
6.329
5.134
4.215
3.614
3.473
3.325
2.917
2.877
2.504
2.500
2.496
2.274
2.141
Ph
OH
3k
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
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ppm
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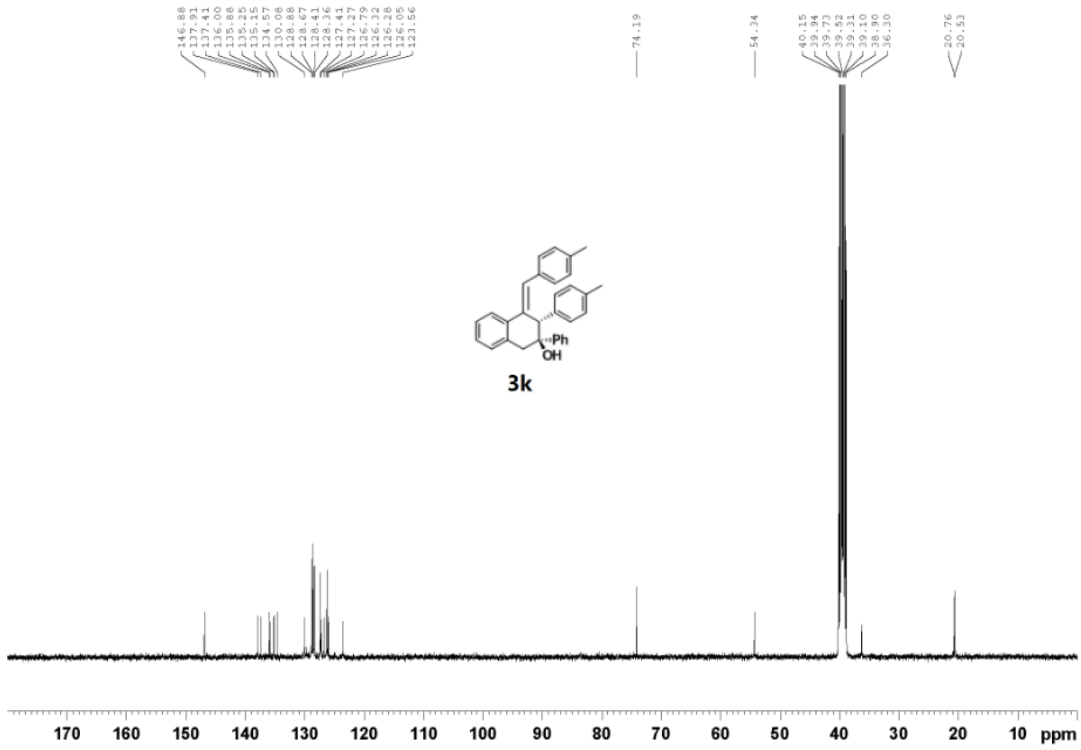
2.925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128.36
127.41
127.27
126.79
126.32
126.28
126.05
123.56
74.19
54.34
40.15
39.94
39.73
39.52
39.31
39.10
38.90
38.30
20.76
20.53
Ph
OH
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150
140
130
120
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100
90
80
70
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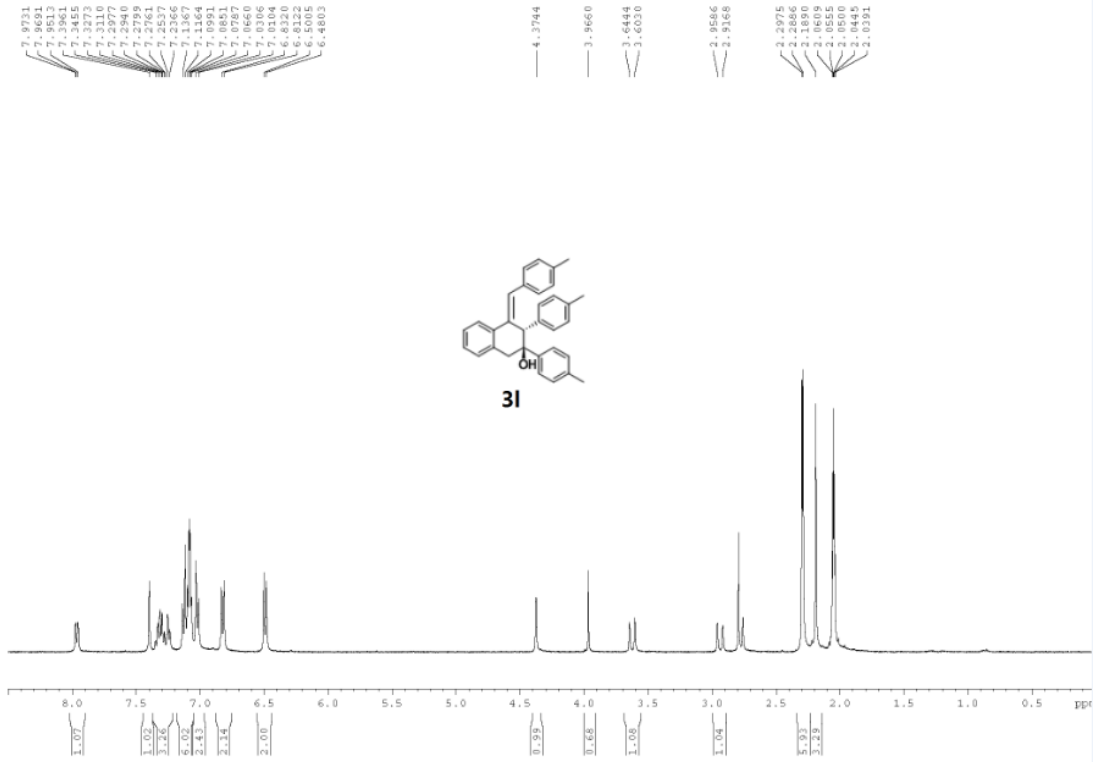
50
40
30
20
10
ppm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7.2761
7.2537
7.2366
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7.1164
7.0991
7.0851
7.0737
7.0660
7.0306
7.0104
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6.5005
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3.6444
3.6030
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2.9168
2.2975
2.2866
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2.0609
2.0555
2.0500
2.0445
2.0391
OH
3l
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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
1.07
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1.04
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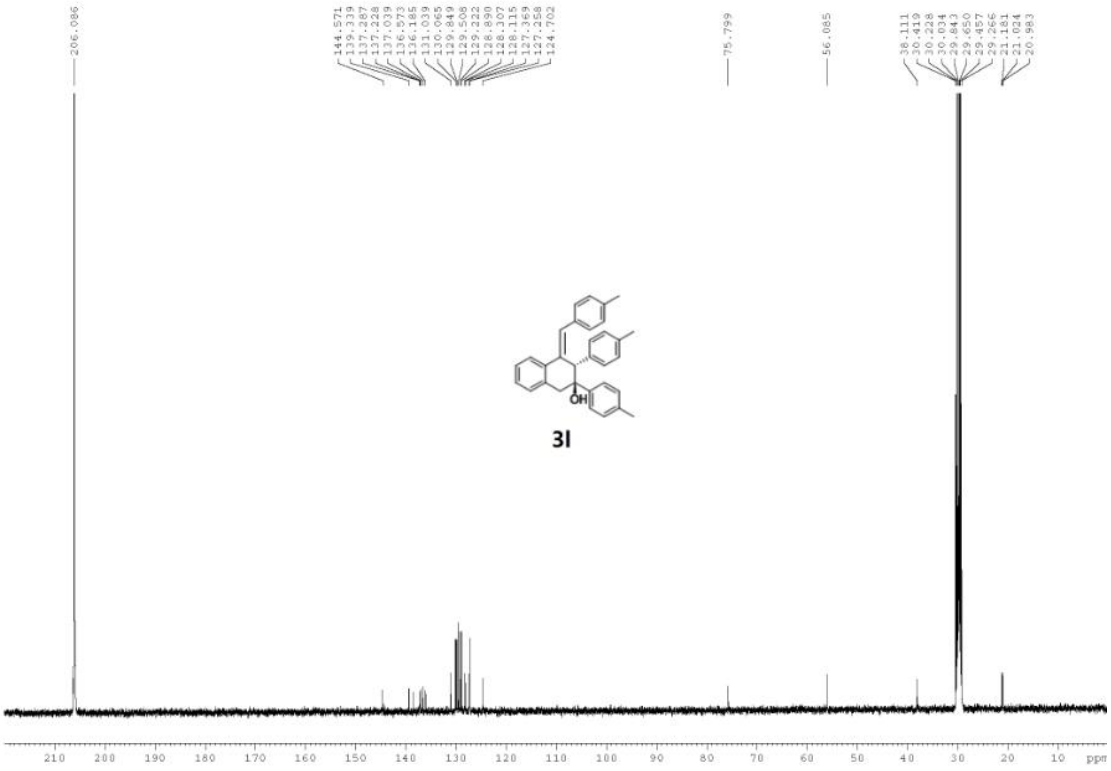
3.29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129.222
128.890
128.707
128.115
127.369
127.258
124.702
75.799
56.085
38.111
30.419
30.228
30.034
29.843
29.650
29.457
29.266
21.481
21.024
20.983
OH
3l
210
200
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180
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150
140
130
120
110
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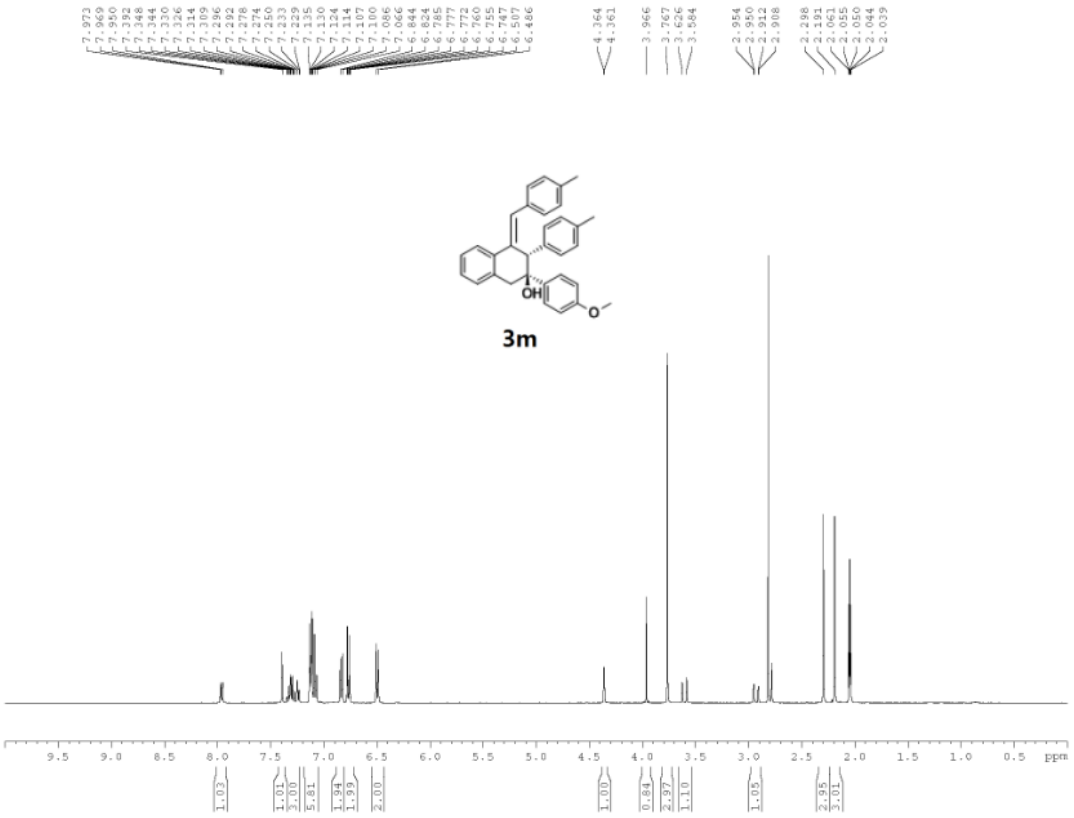
90
80
70
60
50
40
30
20
10
ppm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7.292
7.278
7.274
7.250
7.233
7.229
7.135
7.130
7.124
7.114
7.107
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7.086
7.066
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6.824
6.785
6.777
6.772
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6.486
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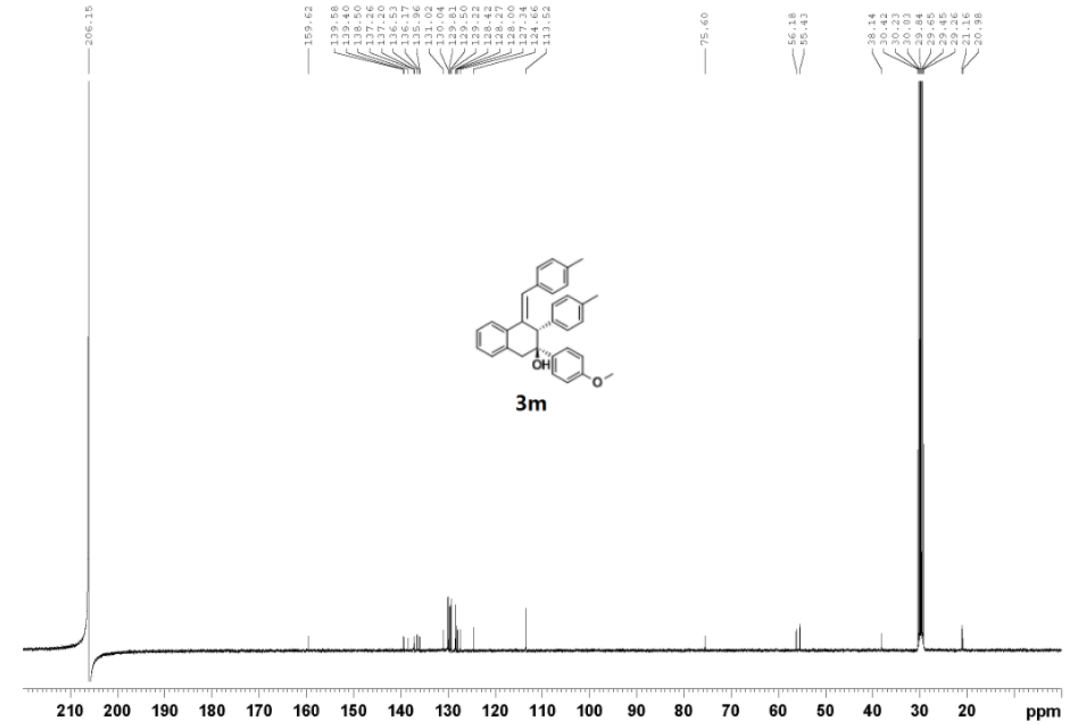
2.950
2.912
2.908
2.298
2.191
2.061
2.055
2.050
2.044
2.039
OH
O
3m
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.03
1.01
3.00
5.81
1.94
1.99
2.00
1.00
0.84
2.97
1.10
1.05
2.95
3.01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136.53
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128.42
128.27
128.00
127.34
124.66
113.52
75.60
56.18
55.43
38.14
30.42
30.23
30.03
29.84
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29.26
21.16
20.98
OH
O
3m
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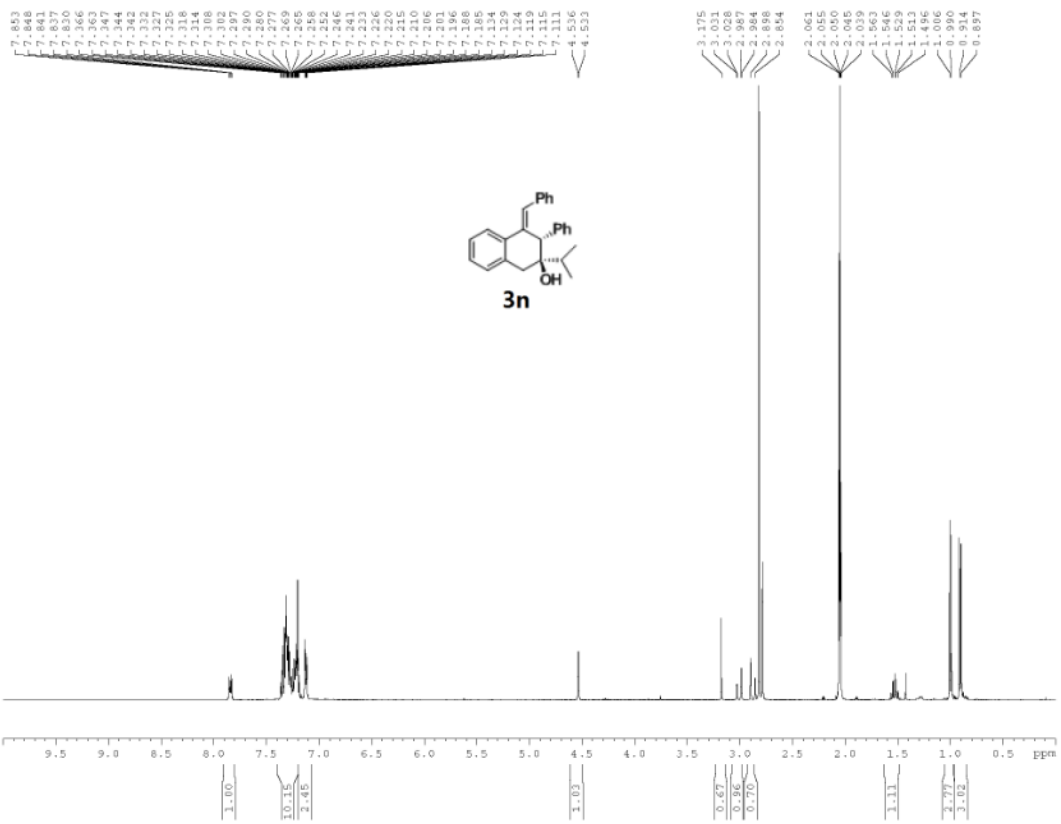
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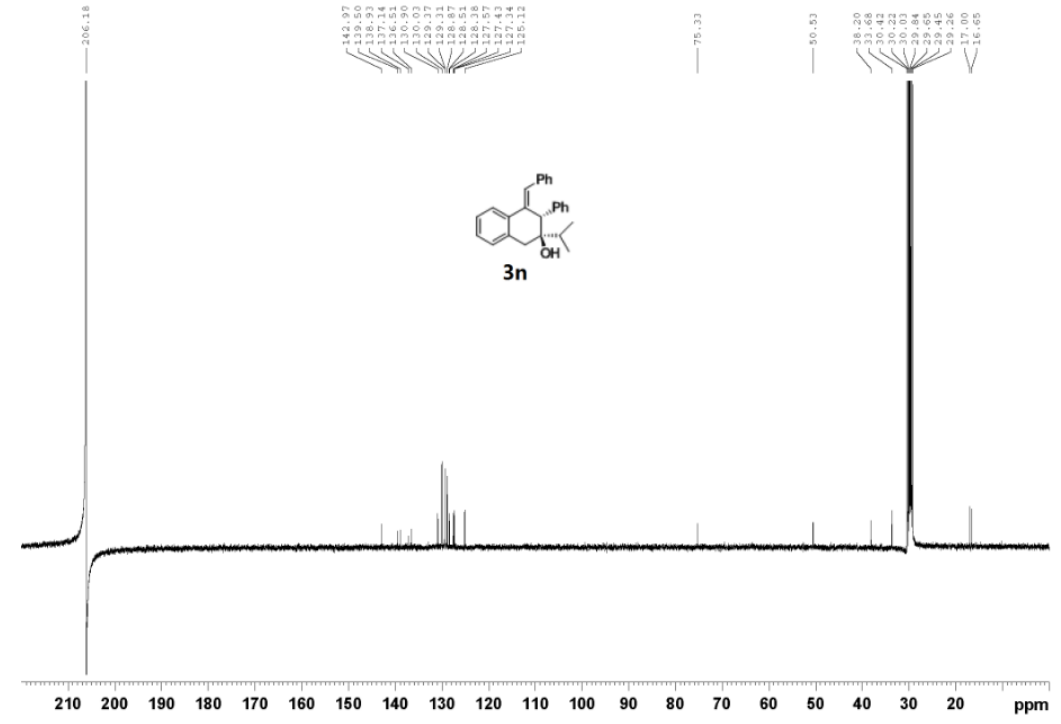
OH
3n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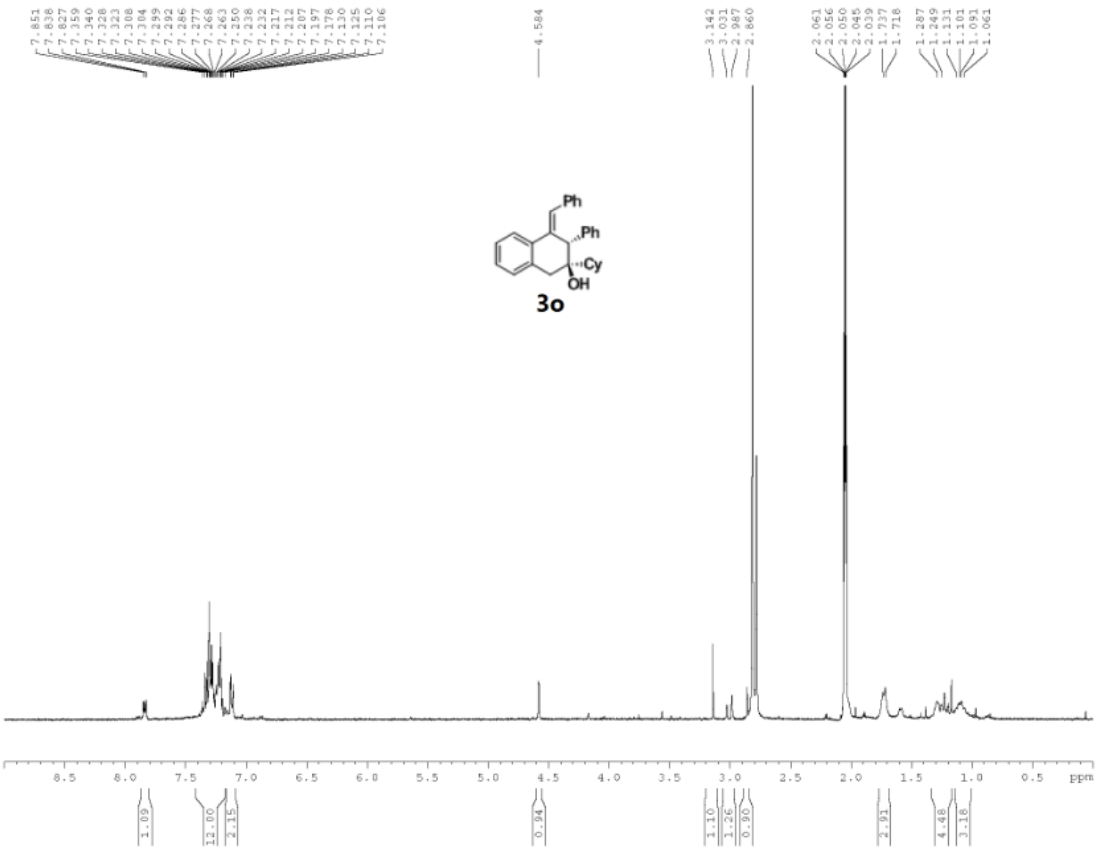
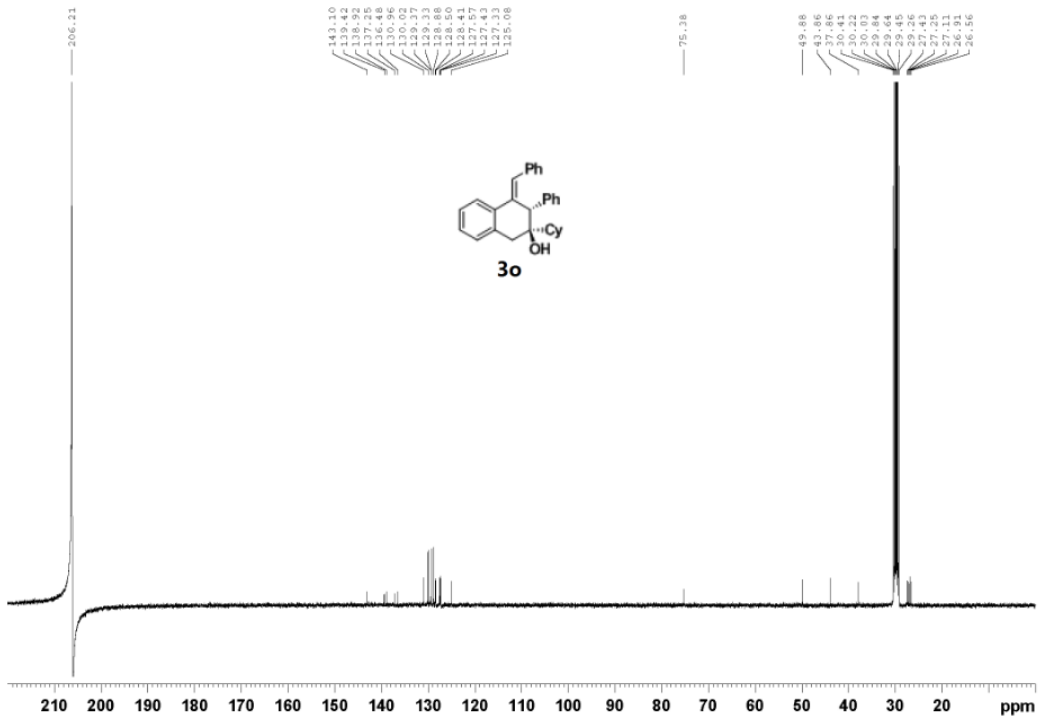
Ph
OH
3n
ppm


Ph
Ph
Cy
OH
3o
ppm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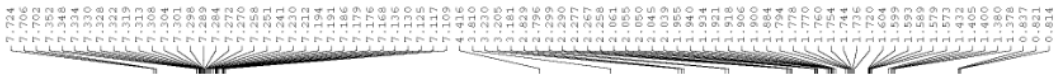
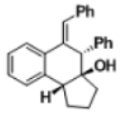
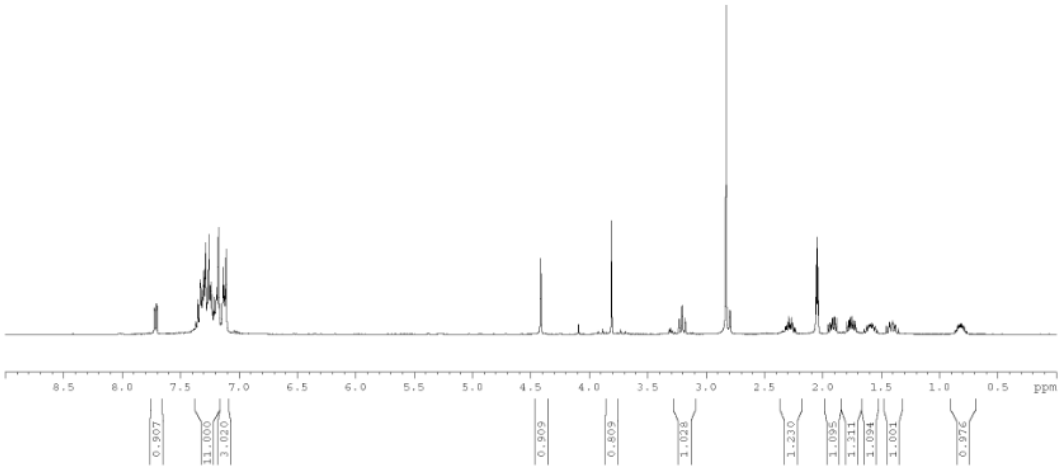
Ph
Cy
OH
3o
ppm




Ph
Ph
OH
H

3p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5.0
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4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
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0.909
0.809
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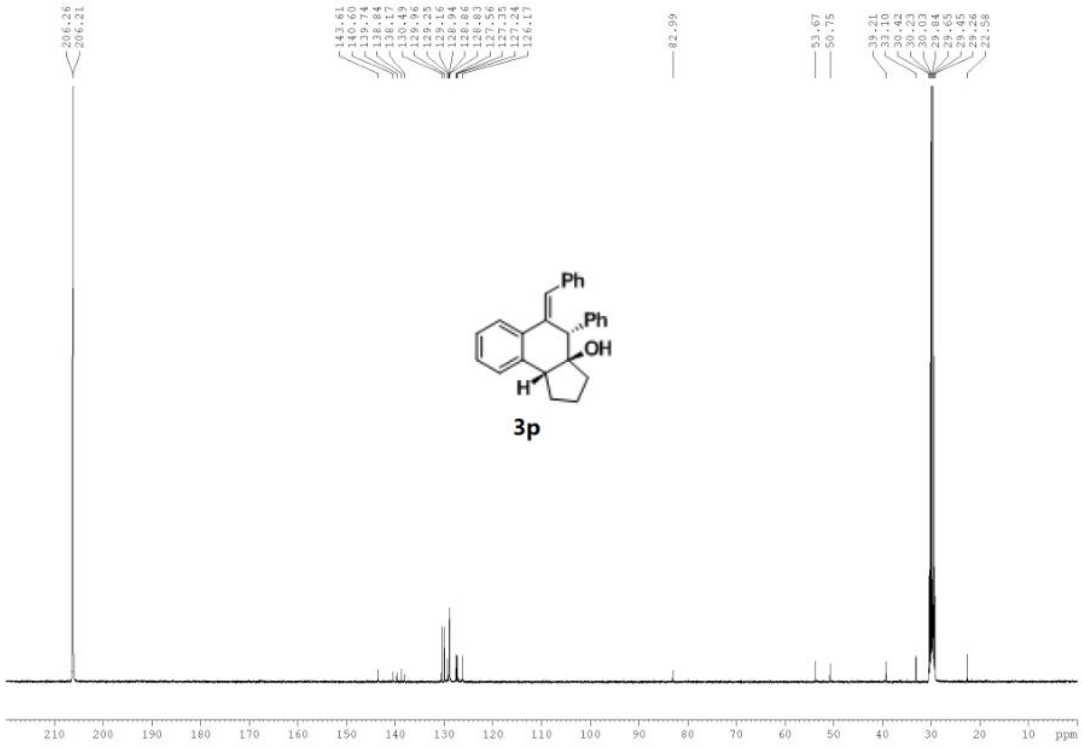
1.095
1.311
1.094
1.001
0.976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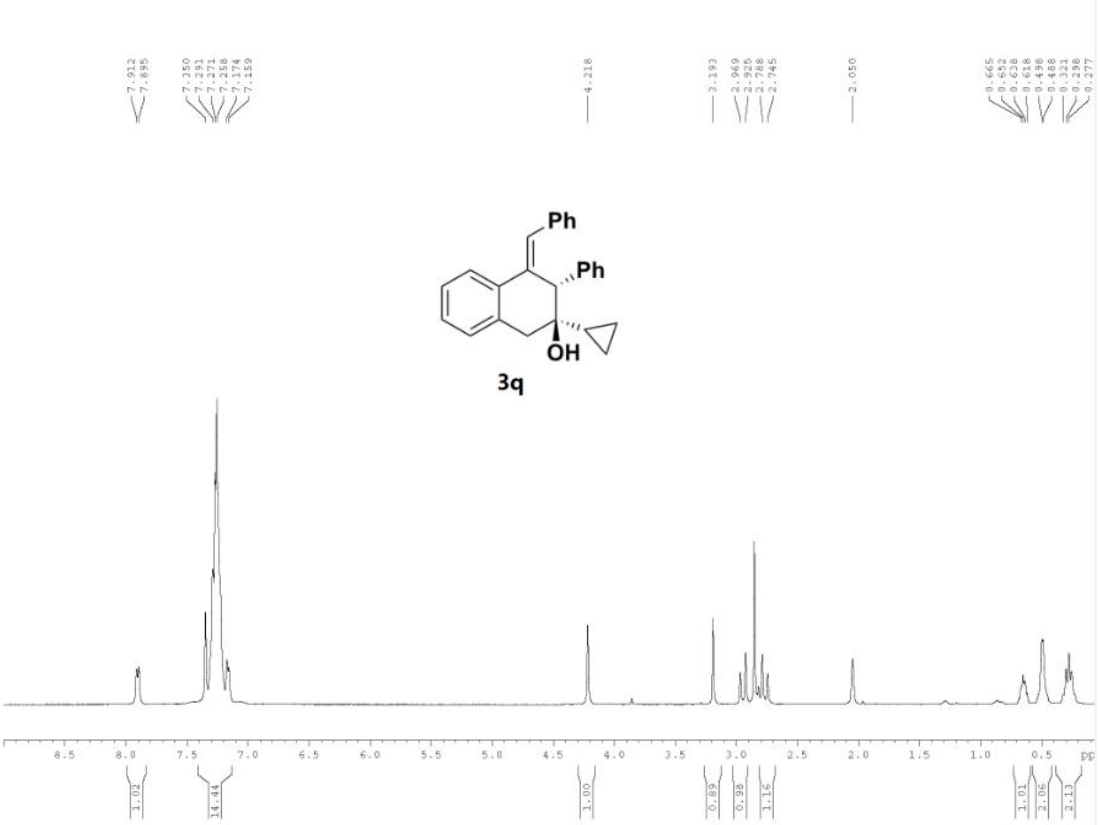
130.47
129.96
129.25
129.16
128.94
128.86
128.83
127.56
127.35
127.24
126.17
82.99
53.67
50.75
39.21
33.10
30.42
30.23
30.03
29.84
29.65
29.45
29.26
22.58
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

Ph
Ph
OH
H

3p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7.271
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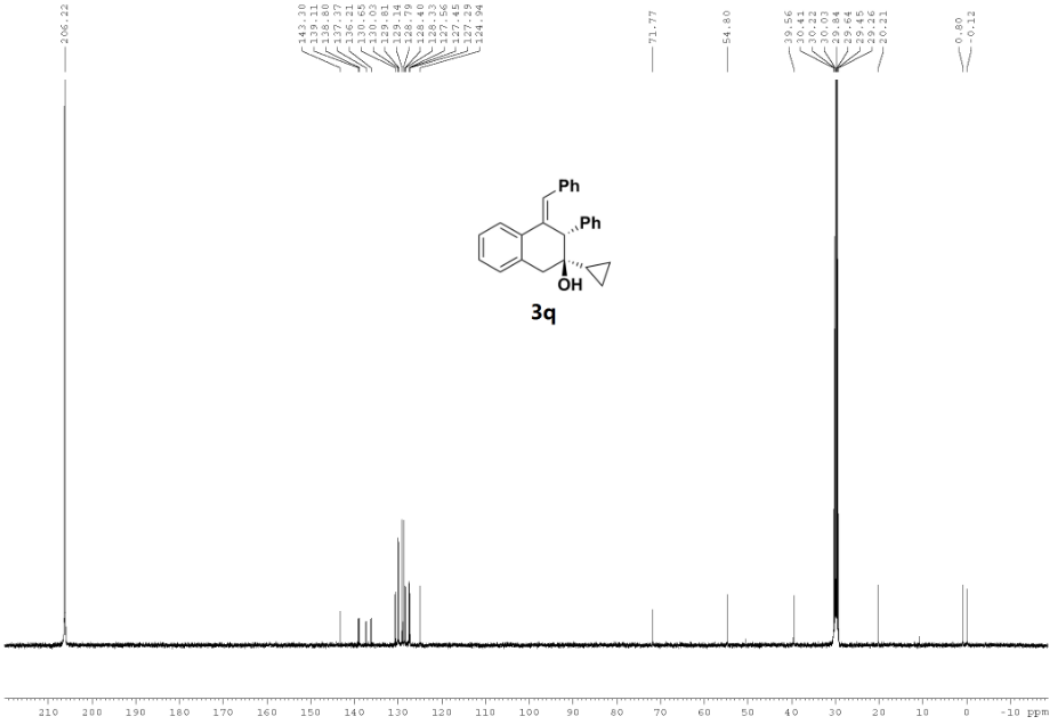
7.174
7.159
4.218
3.193
2.969
2.925
2.788
2.745
2.050
0.665
0.652
0.638
0.618
0.496
0.488
0.321
0.298
0.277
Ph
Ph
OH
3q
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.02
14.44
1.00
0.89
0.98
1.16
1.01
2.05
2.13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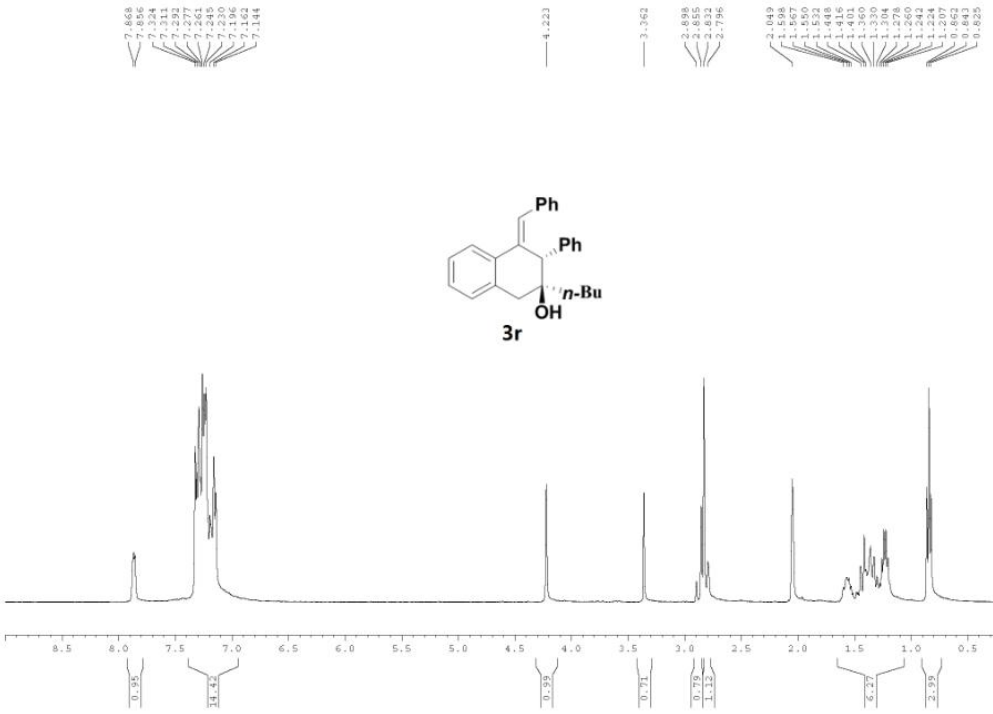
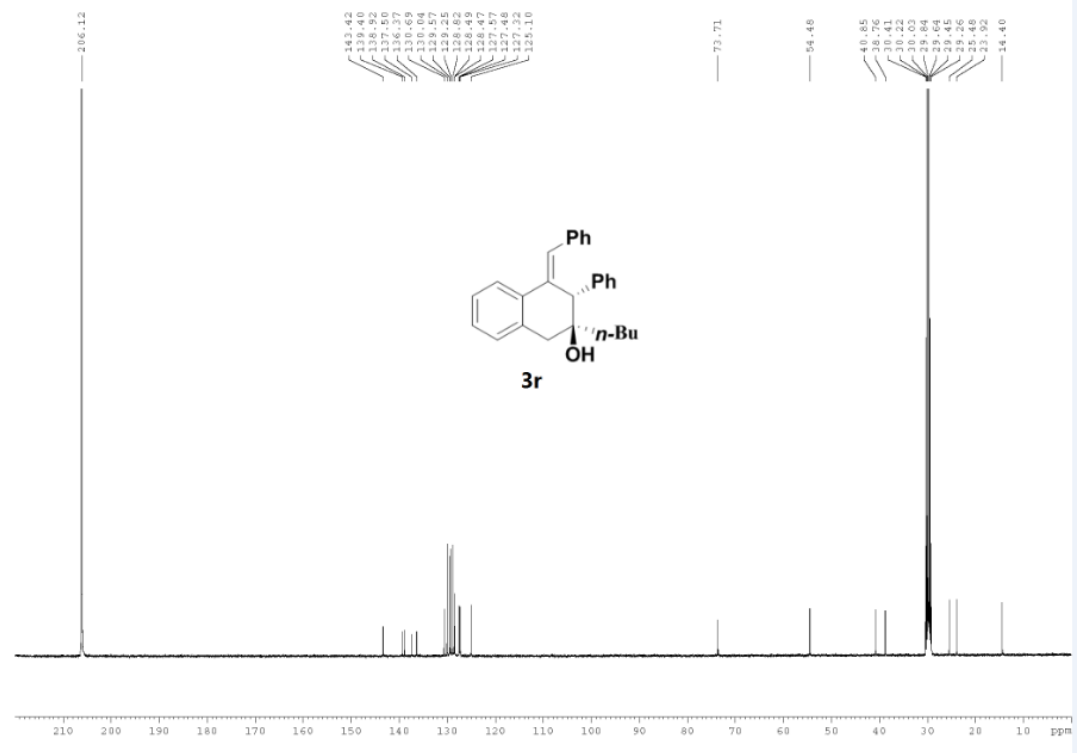
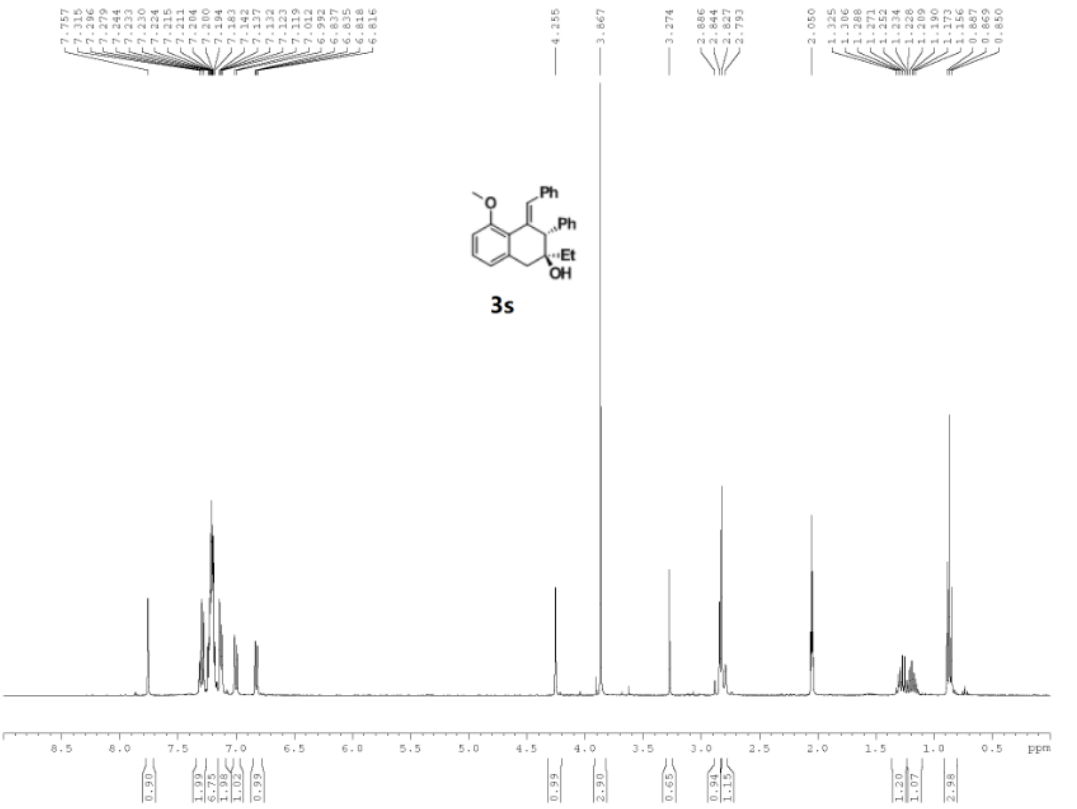
143.30
139.11
136.80
136.27
135.21
130.65
130.03
129.81
129.14
128.79
128.40
128.33
127.56
127.45
127.29
124.94
71.77
54.80
39.56
30.41
30.22
30.03
29.84
29.64
29.45
29.26
20.21
0.80
-0.12
Ph
Ph
OH
3q
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10 ppm


Ph
Ph
n-Bu
OH
3r
ppm


Ph
Ph
n-Bu
OH
3r
ppm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7.224
7.215
7.211
7.204
7.200
7.194
7.183
7.142
7.137
7.122
7.113
7.119
7.012
6.992
6.837
6.835
6.818
6.816
4.255
3.867
3.274
2.886
2.844
2.827
2.793
2.050
1.325
1.306
1.288
1.271
1.252
1.234
1.228
1.209
1.190
1.173
1.156
0.887
0.869
0.850
Ph
Ph
Et
OH
3s
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
ppm
0.90
1.99
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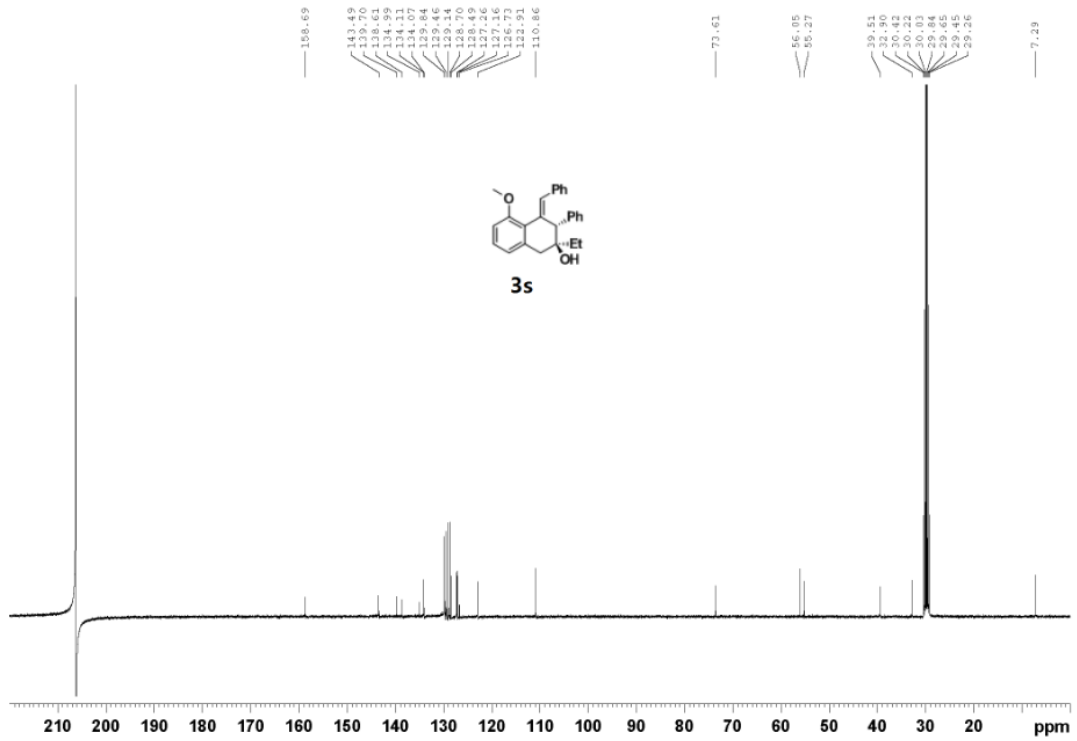
1.98
1.02
0.99
0.99
2.90
0.65
0.94
1.15
1.20
1.07
2.98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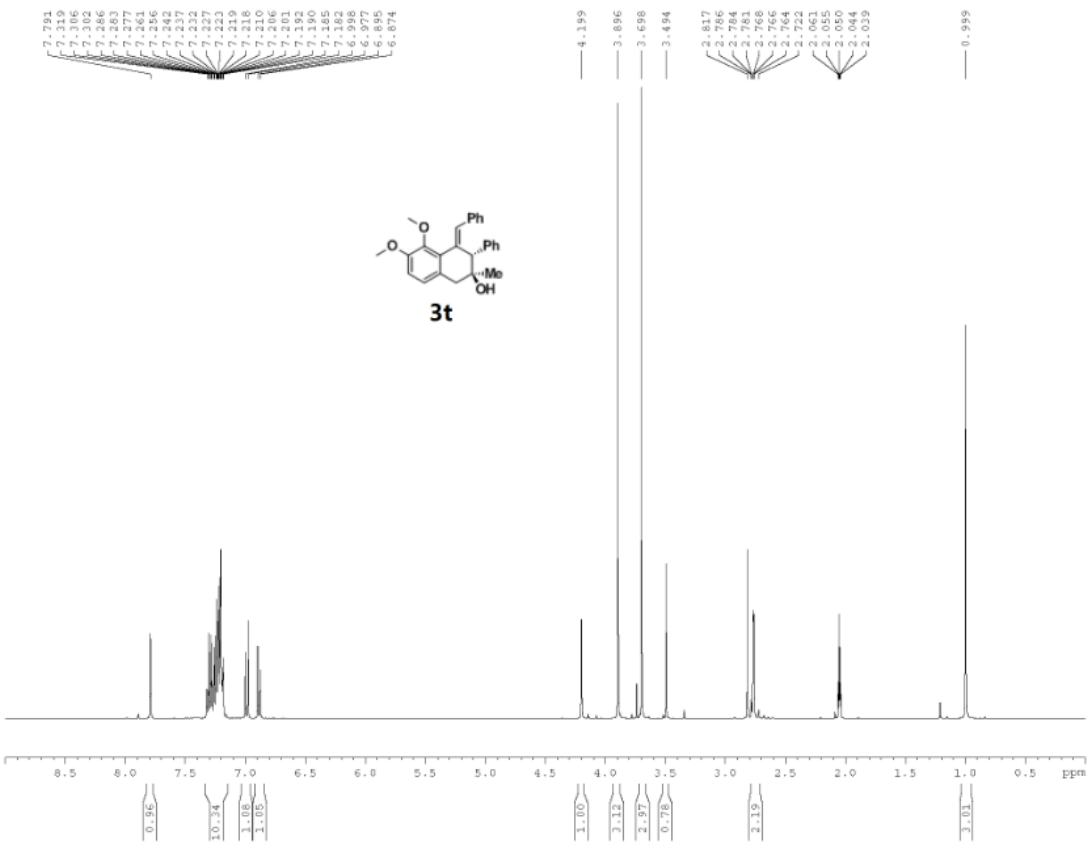
129.14
128.70
128.49
127.26
127.16
126.73
125.91
110.86
73.61
56.05
55.27
39.51
32.90
30.42
30.22
30.03
29.84
29.65
29.45
29.26
7.29
Ph
Ph
Et
OH
3s
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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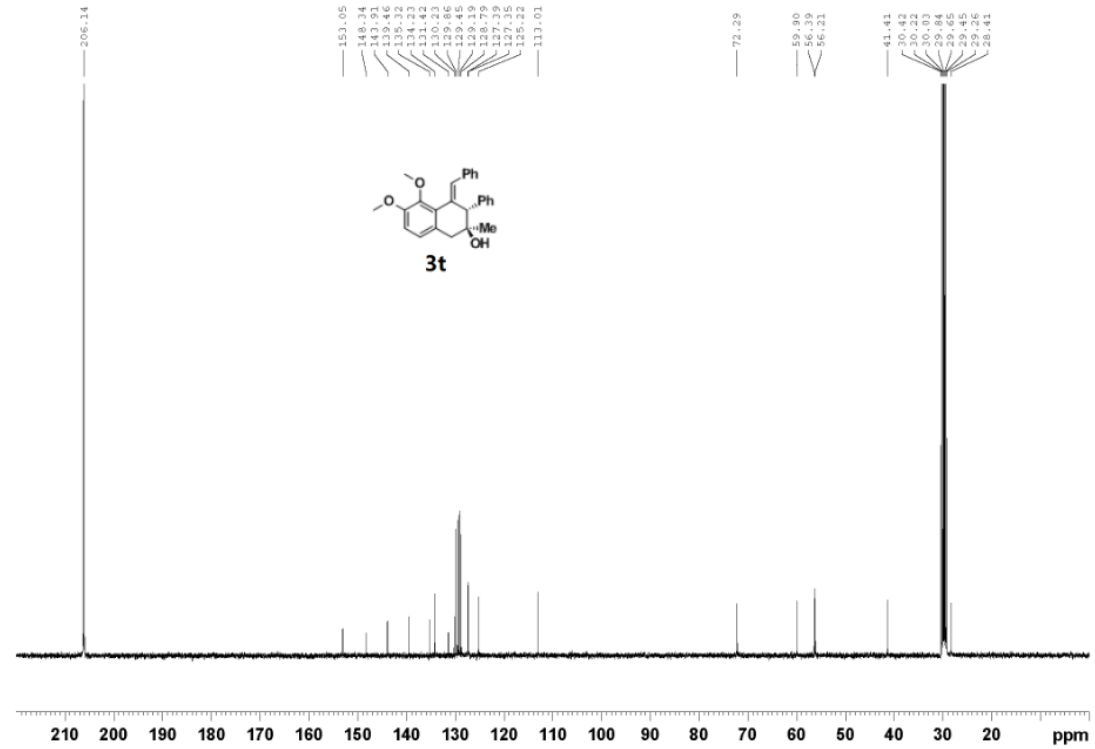
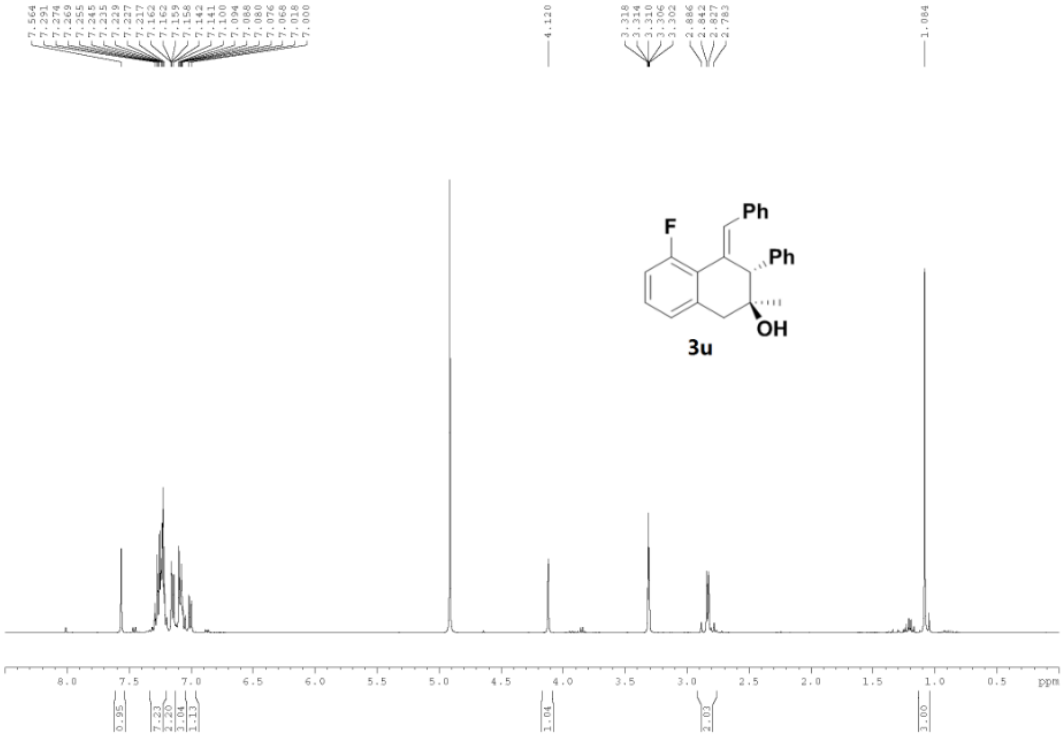

3t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7.269
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7.245
7.235
7.229
7.217
7.162
7.159
7.158
7.142
7.141
7.100
7.084
7.080
7.076
7.068
7.018
7.000
4.120
3.318
3.314
3.310
3.306
3.302
2.886
2.842
2.827
2.783
1.084
F
Ph
Ph
OH
3u
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
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0.5
ppm
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1.04
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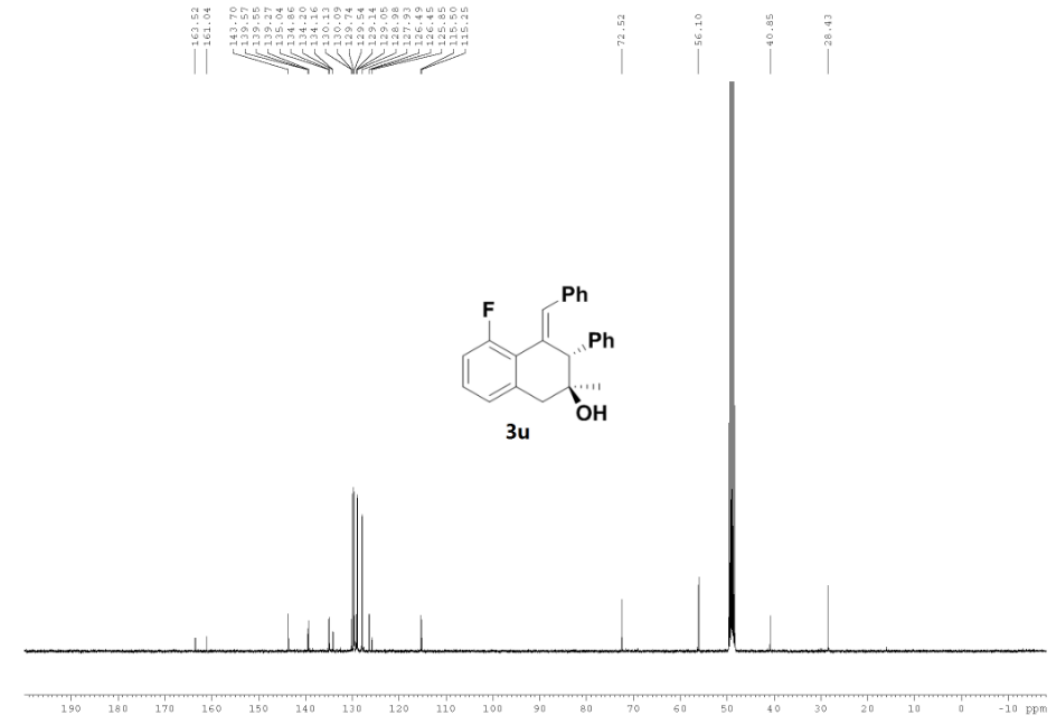
1.04
2.03
3.00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139.55
139.27
135.04
134.65
134.20
134.16
130.13
130.09
129.74
129.54
129.14
129.05
128.98
127.93
126.49
126.45
125.85
115.50
115.25
72.52
56.10
40.85
28.43
F
Ph
Ph
OH
3u
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10 ppm


7.821
7.813
7.797
7.536
7.526
7.521
7.323
7.318
7.313
7.307
7.300
7.299
7.269
7.261
7.256
7.247
7.243
7.237
7.231
7.227
7.221
7.169
7.164
7.156
7.152
7.142
7.109
7.100
7.088
7.085
6.869
6.864
6.855
6.845
6.829
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3.438
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3.070
3.034
2.061
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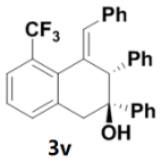
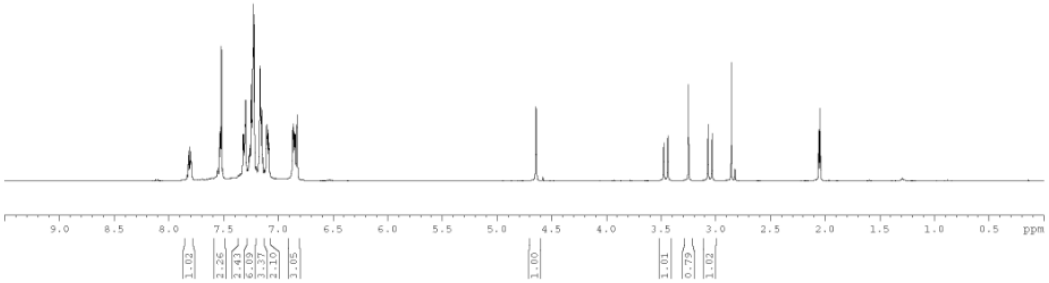
2.050
2.044
2.039


CF3
Ph
Ph
Ph
OH

3v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6.0
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5.0
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4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
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6.09
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3.05
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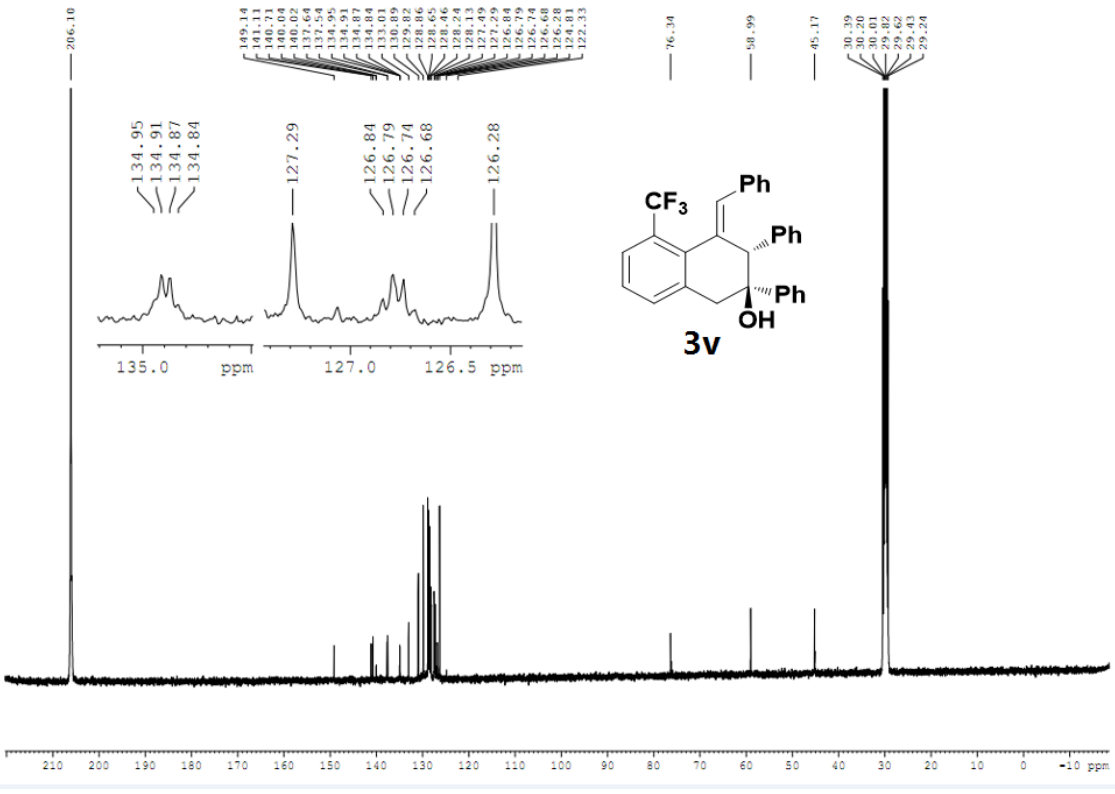
1.01
0.79
1.02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134.87
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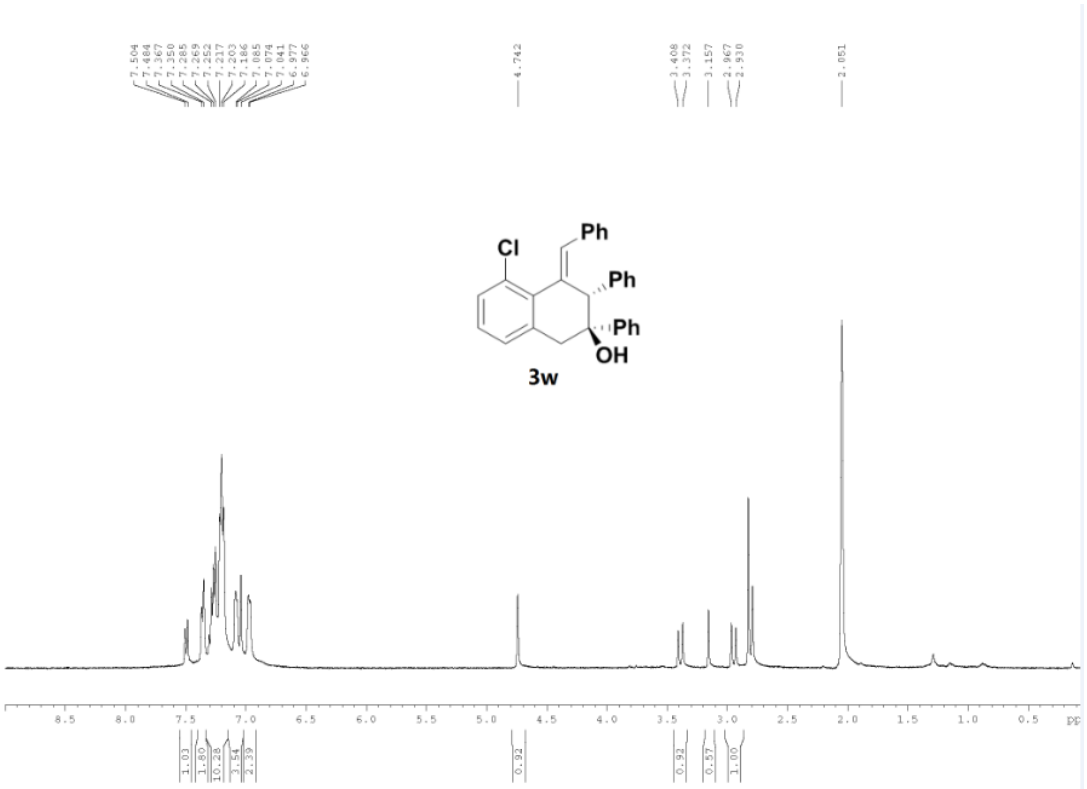
133.01
130.89
129.82
128.86
128.65
128.46
128.24
128.11
127.49
127.29
126.84
126.79
126.74
126.68
126.28
124.81
122.33
76.34
58.99
45.17
30.39
30.20
30.01
29.82
29.62
29.43
29.24
134.95
134.91
134.87
134.84
127.29
126.84
126.79
126.74
126.68
126.28
135.0
ppm
127.0
126.5
ppm
CF3
Ph
Ph
Ph
OH
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10 ppm

3v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7.041
6.977
6.966
4.742
3.408
3.372
3.157
2.967
2.930
2.051
Cl
Ph
Ph
Ph
OH
3w
1.03
1.80
10.28
3.54
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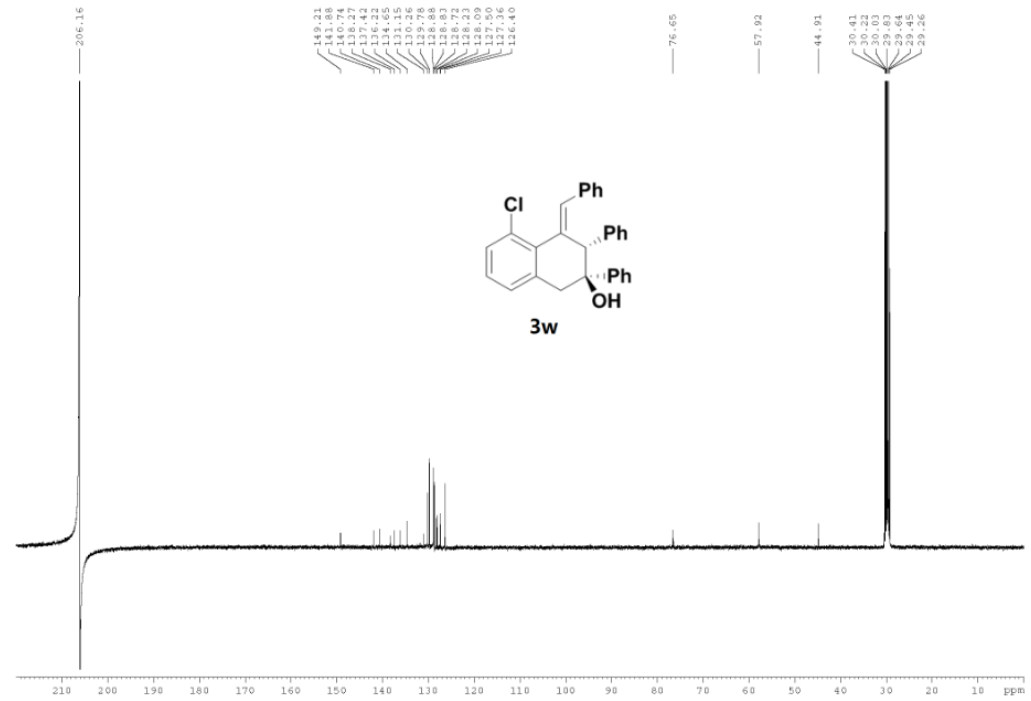
0.92
0.57
1.00
ppm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131.15
130.46
129.78
128.88
128.83
128.72
128.23
128.09
127.90
127.36
126.40
76.65
57.92
44.91
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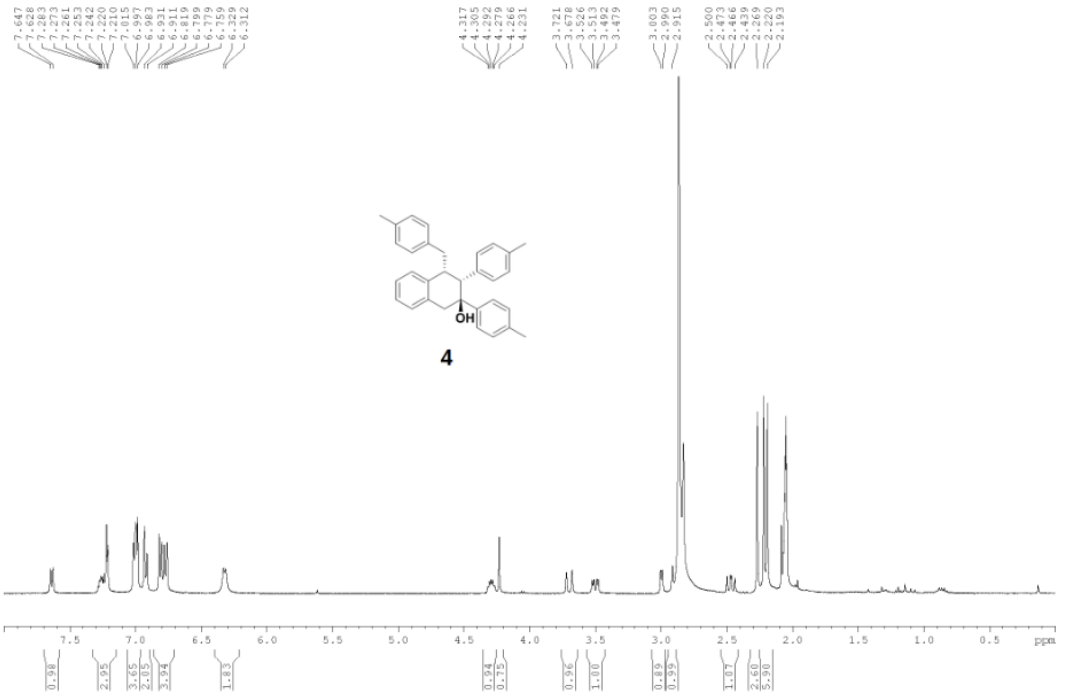
30.22
30.03
29.83
29.64
29.45
29.26
Cl
Ph
Ph
Ph
OH
3w
ppm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7.220
7.210
7.115
6.983
6.931
6.911
6.819
6.799
6.779
6.759
6.329
6.312
4.317
4.305
4.292
4.279
4.266
4.231
3.721
3.678
3.526
3.513
3.492
3.479
3.003
2.990
2.915
2.500
2.473
2.466
2.439
2.269
2.220
2.193
OH
4
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
ppm
0.98
2.95
3.65
2.05
3.94
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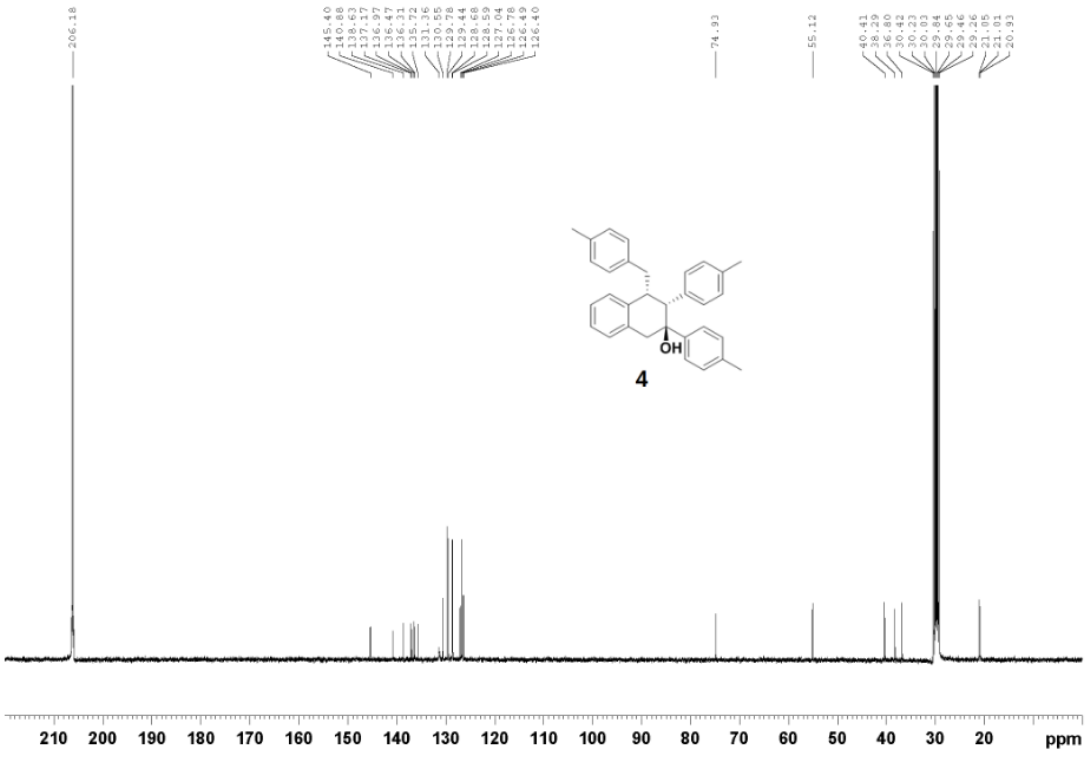
0.94
0.75
0.96
1.00
0.89
0.99
1.07
2.60
5.90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137.07
136.47
136.31
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131.36
130.55
129.78
129.44
128.86
128.59
127.04
126.78
126.49
126.40
74.93
55.12
40.41
38.29
36.80
30.42
30.23
30.03
29.84
29.65
29.46
29.26
21.05
21.01
20.93
OH
4
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm