Supporting Information for

Oxidative Cross-Dehydrogenative Coupling between *N*-aryl Tetrahydroisoquinolins and 5*H*-Oxazol-4-ones through Two Methodologies: Copper Catalysis or a Metal-Free Strategy

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Contents:

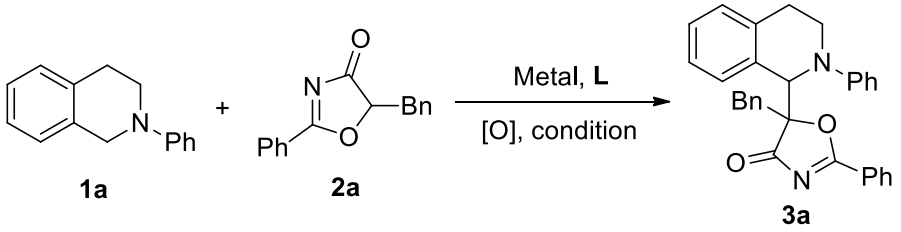
(A) General Information

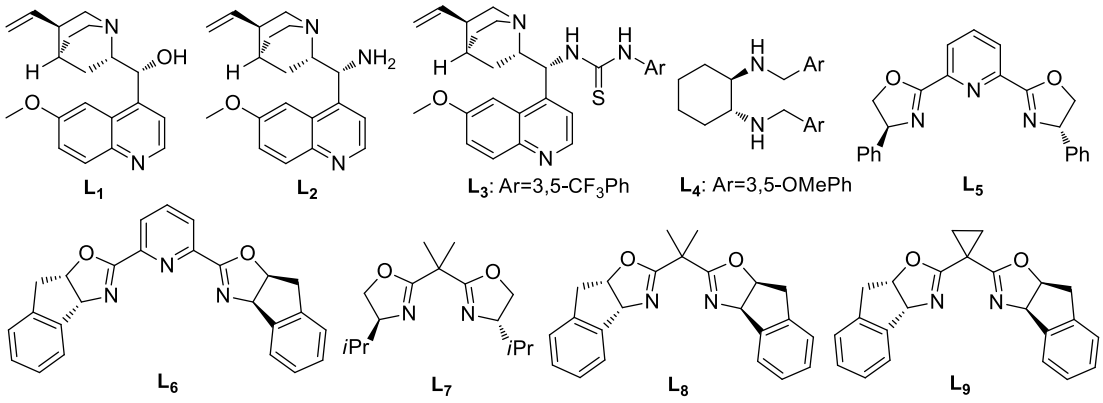
Unless stated otherwise, all reactions were carried out in flame dried glassware. All solvents were purified and dried according to standard methods prior to use. Reactions were monitored by thin layer chromatography (TLC), column chromatography purifications were carried out using silica gel. Proton nuclear resonance (^{1}H NMR) spectra were recorded on 300 MHz spectrometer in $CDCl_3$ and carbon nuclear magnetic resonance (^{13}C NMR) spectra were recorded on 75 MHz spectrometer in $CDCl_3$ using tetramethylsilane (TMS) as internal standard. Data for ^{1}H NMR are recorded as follows: chemical shift (δ, ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet, q = quartet or unresolved, coupling constant(s) in Hz, integration). Data for ^{13}C NMR are reported in terms of chemical shift (δ, ppm). IR spectra were recorded on a FT-IR spectrometer and only major peaks were reported in cm^{-1}. High resolution mass spectra (HRMS) were obtained by the ESI ionization sources. Substrates *N*-aryl tetrahydroisoquinolins **1**[1] and Oxazol-4(*5H*)-ones **2**[2] were prepared according to literature.

(B) Attempt at asymmetric aerobic oxidative coupling reaction between *N*-aryl Tetrahydroisoquinolins and 5*H*-Oxazol-4-ones

Typical experimental procedure: A solution of $Cu(OTf)_2$ (0.01 mmol) and chiral ligand in anhydrous DCM (0.3 mL) under Air (for **L$_1$** – **L$_3$**) or Ar (for **L$_4$** – **L$_9$**) atmosphere was stirred at room temperature for 1 h, and then a mixture of **1a** (0.15 mmol) and **2a** (0.10 mmol) in anhydrous DCM (0.2 mL) was added. The resultant reaction mixture was stirred at room temperature under air (O_2) atmosphere for 36 h.

Table 1. Optimizing reaction conditions[a]

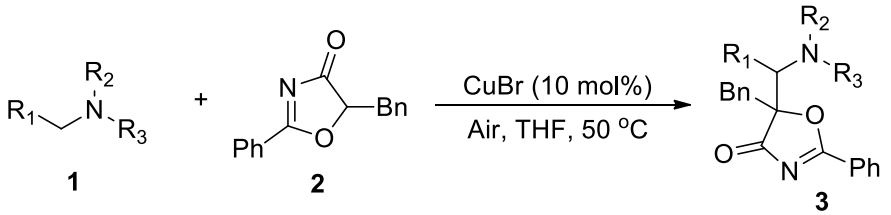


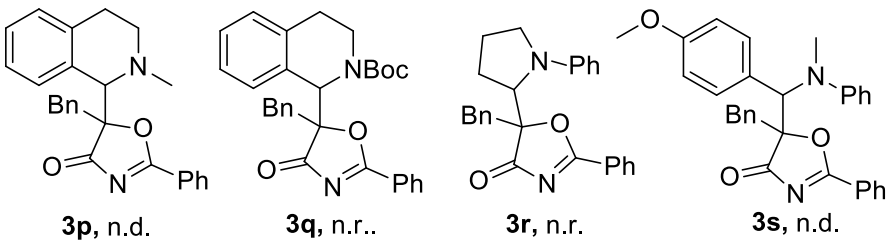


Entry	Metal (10 mol %)	**L** (mol %)	[O]	Ee (%)[b]	Conversion (%)[c]
1	$Cu(OTf)_2$	**L1** (20)	Air	0	67
2	$Cu(OTf)_2$	**L2** (20)	Air	-	trace
3	$Cu(OTf)_2$	**L3** (20)	Air	-	trace
4	$Cu(OTf)_2$	**L4** (12)	Air	0	46
5	$Cu(OTf)_2$	**L5** (12)	Air	-	trace
6	$Cu(OTf)_2$	**L6** (12)	Air	-	trace
7	$Cu(OTf)_2$	**L7** (12)	Air	0	88
8	$Cu(OTf)_2$	**L8** (12)	Air	0	47
9	$Cu(OTf)_2$	**L9** (12)	Air	0	35
10	$Mg(ClO_4)_2$	**L7** (12)	Air	-	trace

[a] Unless otherwise specified, the reaction was performed on a 0.1 mmol scale at room temperature. [b] Determined by HPLC on chiral stationary phase. [c] The conversion was determined by ^{1}H NMR spectroscopy of the crude mixture.

(C) Unsuccessful examples of aerobic oxidative coupling reaction of other amines and Oxazol-4(*5H*)-ones





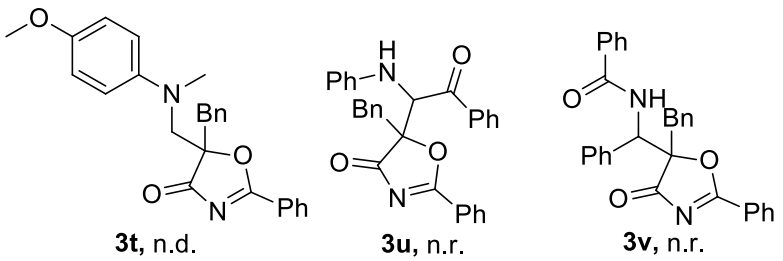
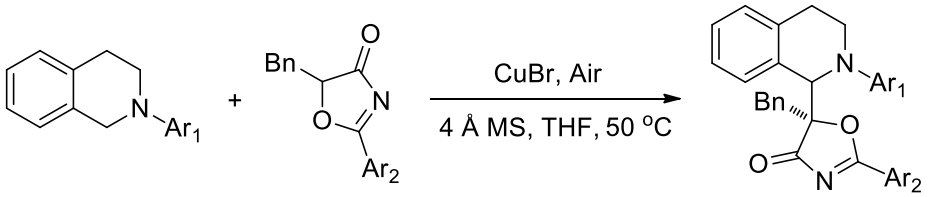


Figure 1. Unsuccessful examples

(D) General procedure of aerobic oxidative coupling reaction

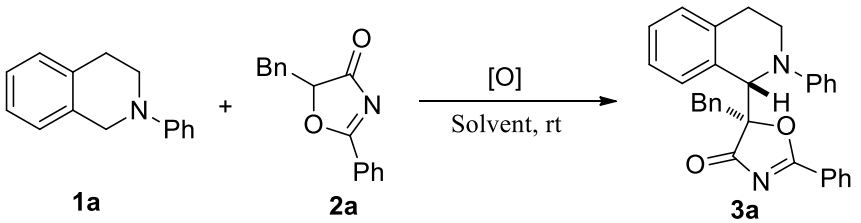


***Method A*:** The reaction mixture of aryl-substituted 1,2,3,4-tetrahydroisoquinolin (0.45 mmol, 1.5 equiv) , Oxazol-4(*5H*)-ones (0.30 mmol, 1.0 equiv), 4Å molecular sieves (100 mg) and CuBr (0.03mmol, 0.1 equiv) in anhydrous THF (0.6 mL) was stirred at 50 °C for the appropriate time under air atmosphere. After the reaction finished (monitored by TLC), the resulting mixture was concentrated under reduced pressure and the residue was purified by silica gel chromatography (eluent, ethyl acetate / hexane 1:7) to afford the desired coupling products, which can be further purified by recrystallization.

(E) General procedure of metal-free coupling reaction

1. The optimization of reaction conditions

Table 2. Optimizing reaction conditions [a]



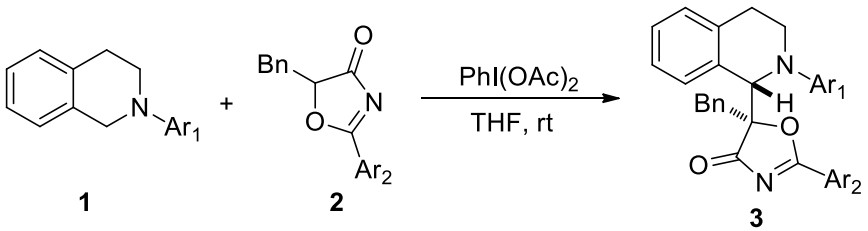
Entry	[O]	Solvent	Conversion (%)[b]
1	TBHP	CH_2Cl_2	60
2	*t*BuOO*t*Bu	CH_2Cl_2	38

3	DDQ	CH_2Cl_2	38
4	$PhI(OAc)_2$	CH_2Cl_2	90
5	$K_2S_2O_8$	CH_2Cl_2	43
6	$PhI(OAc)_2$	THF	98
7	$PhI(OAc)_2$	toluene	84

[a] Reactions were carried out with **1a** (0.12 mmol), **2a** (0.1 mmol), oxidant (0.12 mmol) in solvent (0.4 mL) for 24h. [b] The conversion was determined by ^{1}H NMR spectroscopy of the crude mixture.

Several oxidants were evaluated. As summarized in Table 1, excellent conversion could be obtained in the presence of $PhI(OAc)_2$ and subsequent screening of solvent displayed that THF gave the best result.

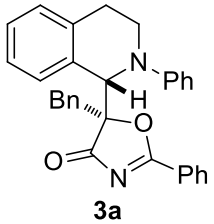
2. General Procedure for synthesis of compound 3



1 2 3

***Method B*:** The reaction mixture of aryl-substituted 1,2,3,4-tetrahydroisoquinolin (0.12 mmol, 1.2 equiv) , Oxazol-4(5*H*)-ones (0.10 mmol, 1.0 equiv) and $PhI(OAc)_2$ (0.12 mmol, 1.2 equiv) in anhydrous THF (0.4 mL) was stirred at room temperature for 24h. Then the resulting mixture was concentrated under reduced pressure and the residue was purified by silica gel chromatography (eluent, ethyl acetate / hexane 1:7) to afford the desired coupling products, which can be further purified by recrystallization.

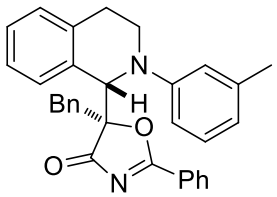
(F) Characterization of products



3a

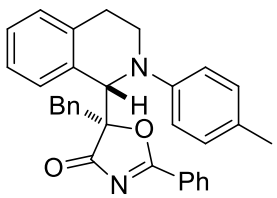
5-benzyl-2-phenyl-5-(2-phenyl-1,2,3,4-tetrahydroisoquinolin-1-yl)oxazol-4(5*H*)-one: yellow solid, m.p. 186 – 188 °C; 82% yield (method B: 87% yield); **^{1}H NMR** (300

MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.3 Hz, 2H), 7.60-7.42 (m, 1H), 7.43-7.20 (m, 4H), 7.21 – 7.01 (m, 8H), 6.96 (s, 3H), 6.83 (t, *J* = 6.7 Hz, 1H), 5.50 (s, 1H), 4.20 – 4.01 (m, 1H), 3.98 – 3.79 (m, 1H), 3.62 (d, *J* = 14.2 Hz, 1H), 3.36 (d, *J* = 14.2 Hz, 1H), 3.19 – 2.91 (m, 2H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.42, 185.42, 149.39, 135.53, 134.68, 133.22, 131.29, 130.01, 129.48, 129.28, 128.57, 128.25, 128.14, 127.69, 127.14, 127.06, 126.06, 125.11, 118.72, 114.76, 95.55, 63.31, 43.03, 39.86, 26.11; **IR:** 3464.6, 2924.7, 2158.2, 1738.4, 1536.4, 1359.9, 1177.0, 942.3, 751.9, 548.0 cm^{-1}. **HRMS (ESI):** calcd for $C_{31}H_{26}N_2O_2+Na^+$: 481.1886; found: 481.1885.



3b

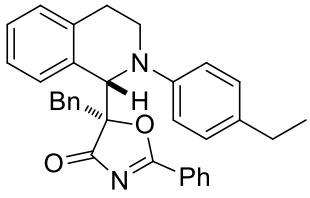
5-benzyl-2-phenyl-5-(2-(m-tolyl)-1,2,3,4-tetrahydroisoquinolin-1-yl)oxazol-4(5*H*)-one: yellow solid, m.p. 175 - 176 °C; 77% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.6 Hz, 2H), 7.51 (t, *J* = 7.2 Hz, 1H), 7.32 (t, *J* = 7.4 Hz, 2H), 7.27 – 7.01 (m, 7H), 6.94 (d, *J* = 8.8 Hz, 5H), 6.66 (d, *J* = 7.2 Hz, 1H), 5.49 (s, 1H), 4.20 – 4.01 (m, 1H), 4.01 – 3.84 (m, 1H), 3.62 (d, *J* = 14.2 Hz, 1H), 3.36 (d, *J* = 14.2 Hz, 1H), 3.20 – 3.03 (m, 1H), 3.00-2.93 (m, 1H), 2.35 (s, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.46, 185.42, 149.46, 139.26, 135.50, 134.67, 133.25, 131.29, 130.00, 129.32, 129.27, 128.56, 128.30, 128.13, 127.63, 127.12, 127.05, 125.99, 125.10, 119.66, 115.53, 112.00, 95.67, 63.27, 42.89, 39.86, 26.02, 21.92; **IR:** 3382.0, 2923.6, 2370.7, 1886.7, 1746.5, 1602.2, 1450.9, 1261.3, 1115.4, 1026.9, 702.9, 603.5 cm^{-1}. **HRMS (ESI):** calcd for $C_{32}H_{28}N_2O_2+Na^+$: 495.2043; found: 495.2048.



3c

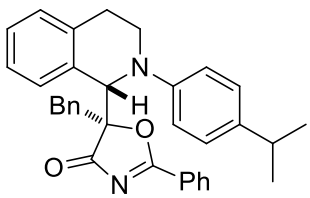
5-benzyl-2-phenyl-5-(2-(p-tolyl)-1,2,3,4-tetrahydroisoquinolin-1-yl)oxazol-4(5*H*)-

one: yellow solid, m.p. 181 - 183 °C; 71% yield (method B: 86% yield); **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.4 Hz, 2H), 7.50 (t, *J* = 7.4 Hz, 1H), 7.30 (t, *J* = 7.7 Hz, 2H), 7.16-6.97 (m, 10H), 6.94 (s, 3H), 5.42 (s, 1H), 4.19 – 4.01 (m, 1H), 3.94 – 3.76 (m, 1H), 3.64 (d, *J* = 14.2 Hz, 1H), 3.34 (d, *J* = 14.2 Hz, 1H), 3.16 – 2.87 (m, 2H), 2.26 (s, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.46, 185.39, 147.25, 135.56, 134.64, 133.30, 131.27, 129.98, 129.92, 129.23, 128.53, 128.26, 128.17, 128.09, 127.58, 127.07, 127.04, 125.96, 125.09, 115.22, 95.70, 63.40, 43.30, 39.83, 25.85, 20.25; **IR:** 3374.8, 2921.7, 2374.7, 1748.3, 1548.1, 1359.1, 1176.9, 941.6, 800.9, 703.6, 553.6 cm^{-1}. **HRMS (ESI):** calcd for $C_{32}H_{28}N_2O_2+Na^+$: 495.2043; found: 495.2045.



3d

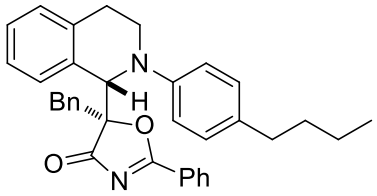
5-benzyl-5-(2-(4-ethylphenyl)-1,2,3,4-tetrahydroisoquinolin-1-yl)-2-phenyloxazol-4(5*H*)-one: yellow solid, m.p. 183 - 184 °C; 87% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.1 Hz, 2H), 7.54 – 7.43 (m, 1H), 7.36 – 7.24 (m, 2H), 7.20-7.00 (m, 10H), 6.93 (s, 3H), 5.44 (s, 1H), 4.20-4.00 (m, 1H), 3.89-3.75 (m, 1H), 3.65 (d, *J* = 14.2 Hz, 1H), 3.35 (d, *J* = 14.1 Hz, 1H), 3.20-2.85 (m, 2H), 2.66 – 2.44 (m, 2H), 1.19 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.45, 185.37, 147.41, 135.56, 134.61, 133.28, 131.28, 129.96, 129.20, 128.71, 128.51, 128.39, 128.24, 128.07, 127.55, 127.05, 127.01, 126.90, 125.93, 125.07, 115.12, 95.66, 63.45, 43.23, 39.83, 27.71, 25.88, 15.77; **IR:** 3360.1, 2962.1, 1961.1, 1748.6, 1548.1, 1359.4, 1177.5, 942.3, 703.6, 599.5 cm^{-1}. **HRMS (ESI):** calcd for $C_{33}H_{30}N_2O_2+Na^+$: 509.2199; found: 509.2208.



3e

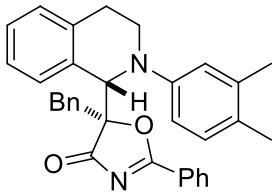
5-benzyl-5-(2-(4-isopropylphenyl)-1,2,3,4-tetrahydroisoquinolin-1-yl)-2-

phenyloxazol-4(5*H*)-one: yellow solid, m.p. 195 - 197 °C; 69% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.5 Hz, 2H), 7.50 (t, *J* = 7.4 Hz, 1H), 7.31 (t, *J* = 7.7 Hz, 2H), 7.21 – 6.99 (m, 10H), 6.99 – 6.87 (m, 3H), 5.44 (s, 1H), 4.18 – 4.01 (m, 1H), 3.94 – 3.79 (m, 1H), 3.65 (d, *J* = 14.2 Hz, 1H), 3.37 (d, *J* = 14.2 Hz, 1H), 3.15-2.70 (m, 3H), 1.23 (s, 3H), 1.21 (s, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.49, 185.39, 147.47, 139.26, 135.59, 134.63, 133.32, 131.34, 130.00, 129.25, 128.54, 128.25, 128.11, 127.58, 127.28, 127.09, 127.05, 125.97, 125.12, 114.98, 95.68, 63.53, 43.18, 39.87, 33.02, 25.94, 24.12; **IR:** 3342.6, 2958.3, 2370.0, 1748.7, 1548.4, 1451.5, 1359.1, 1176.9, 942.3, 748.0, 702.9, 546.0 cm^{-1}. **HRMS (ESI):** calcd for $C_{34}H_{32}N_2O_2+Na^+$: 523.2356; found: 523.2360.



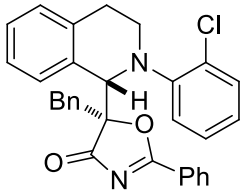
3f

5-benzyl-5-(2-(4-butylphenyl)-1,2,3,4-tetrahydroisoquinolin-1-yl)-2-phenyloxazol-4(5*H*)-one: yellow solid, m.p. 157 - 159 °C; 75% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.6 Hz, 2H), 7.51 (t, *J* = 7.2 Hz, 1H), 7.31 (t, *J* = 7.5 Hz, 2H), 7.21 – 6.99 (m, 10H), 6.95 (s, 3H), 5.43 (s, 1H), 4.19 – 4.00 (m, 1H), 3.94 – 3.78 (m, 1H), 3.65 (d, *J* = 14.3 Hz, 1H), 3.36 (d, *J* = 14.2 Hz, 1H), 3.17 – 3.01 (m, 1H), 3.01 – 2.86 (m, 1H), 2.53 (t, *J* = 7.5 Hz, 2H), 1.69 – 1.45 (m, 2H), 1.43-1.20 (m, 2H), 0.91 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.49, 185.40, 147.42, 135.61, 134.64, 133.36, 131.36, 130.02, 129.30, 128.55, 128.27, 128.12, 127.60, 127.09, 126.00, 125.16, 115.09, 95.73, 63.50, 43.27, 39.88, 34.55, 33.84, 25.95, 22.33, 13.96; **IR:** 3335.0, 2926.9, 2372.0, 1749.1, 1548.9, 1359.2, 1176.6, 942.0, 703.7, 548.3 cm^{-1}. **HRMS (ESI):** calcd for $C_{35}H_{34}N_2O_2+Na^+$: 537.2512; found: 537.2532.



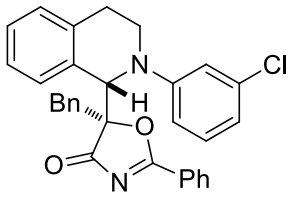
3g

5-benzyl-5-(2-(3,4-dimethylphenyl)-1,2,3,4-tetrahydroisoquinolin-1-yl)-2-phenyloxazol-4(5*H*)-one: yellow solid, m.p. 151 - 153 °C; 84% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.70 (d, *J* = 7.5 Hz, 2H), 7.51 (t, *J* = 7.4 Hz, 1H), 7.32 (t, *J* = 7.7 Hz, 2H), 7.19 – 6.99 (m, 7H), 7.00-6.85 (m, 5H), 5.42 (s, 1H), 4.19 – 4.01 (m, 1H), 3.97 – 3.82 (m, 1H), 3.65 (d, *J* = 14.2 Hz, 1H), 3.34 (d, *J* = 14.2 Hz, 1H), 3.15-3.03 (m, 1H), 2.97-2.87 (m, 1H), 2.26 (s, 3H), 2.18 (s, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.50, 185.41, 147.69, 137.55, 135.57, 134.63, 133.38, 131.32, 130.45, 130.02, 129.27, 128.55, 128.33, 128.12, 127.55, 127.08, 125.95, 125.17, 116.83, 112.75, 95.84, 63.36, 43.18, 39.88, 25.84, 20.36, 18.65; **IR:** 3354.9, 2923.5, 1960.2, 1748.0, 1604.0, 1451.3, 1176.0, 1025.5, 703.2, 599.7 cm^{-1}. **HRMS (ESI):** calcd for $C_{33}H_{30}N_2O_2+Na^+$: 509.2199; found: 509.2203.



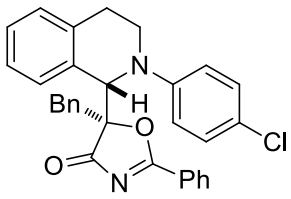
3h

5-benzyl-5-(2-(2-chlorophenyl)-1,2,3,4-tetrahydroisoquinolin-1-yl)-2-phenyloxazol-4(5*H*)-one: yellow solid, m.p. 154 - 156 °C; 49% yield (method B: 72% yield); **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.4 Hz, 2H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.32 (t, *J* = 7.7 Hz, 2H), 7.24 (d, *J* = 8.8 Hz, 2H), 7.12-7.01 (m, 8H), 6.98 (s, 3H), 5.41 (s, 1H), 4.17 – 4.00 (m, 1H), 3.92 – 3.73 (m, 1H), 3.56 (d, *J* = 14.1 Hz, 1H), 3.32 (d, *J* = 14.2 Hz, 1H), 3.19 – 2.91 (m, 2H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.23, 185.46, 148.00, 135.31, 134.78, 132.99, 130.94, 129.98, 129.26, 128.60, 128.26, 128.18, 127.88, 127.23, 127.05, 126.20, 125.00, 123.55, 115.99, 95.24, 63.36, 43.35, 39.80, 26.04; **IR:** 3341.9, 2925.5, 2371.5, 1748.4, 1547.7, 1359.0, 1177.7, 941.2, 809.4, 700.9, 549.6 cm^{-1}. **HRMS (ESI):** calcd for $C_{31}H_{25}ClN_2O_2+Na^+$: 515.1497; found: 515.1514.



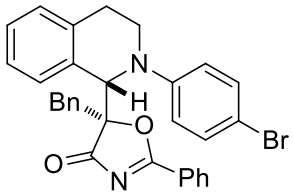
3i

5-benzyl-5-(2-(3-chlorophenyl)-1,2,3,4-tetrahydroisoquinolin-1-yl)-2-phenyloxazol-4(5*H*)-one: yellow solid, m.p. 141 - 143 °C; 68% yield (method B: 79% yield); **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.6 Hz, 2H), 7.53 (t, *J* = 7.2 Hz, 1H), 7.32 (t, *J* = 7.5 Hz, 2H), 7.26 – 7.19 (m, 1H), 7.11 – 6.98 (m, 11H), 6.79 (d, *J* = 7.5 Hz, 1H), 5.45 (s, 1H), 4.19 – 3.99 (m, 1H), 3.95 – 3.76 (m, 1H), 3.54 (d, *J* = 14.2 Hz, 1H), 3.33 (d, *J* = 14.1 Hz, 1H), 3.23 – 2.93 (m, 2H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.12, 185.46, 150.46, 135.35, 135.23, 134.79, 132.93, 130.86, 130.43, 130.00, 129.30, 128.61, 128.30, 128.19, 127.93, 127.25, 127.09, 126.22, 124.99, 118.56, 114.45, 112.75, 95.17, 63.20, 43.03, 39.81, 26.13; **IR:** 3366.4, 2925.7, 2371.6, 1748.7, 1547.7, 1358.8, 1177.8, 944.9, 701.0, 545.6 cm^{-1}. **HRMS (ESI):** calcd for $C_{31}H_{25}ClN_2O_2$+Na^+: 515.1497; found: 515.1512.



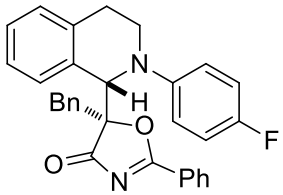
3j

5-benzyl-5-(2-(4-chlorophenyl)-1,2,3,4-tetrahydroisoquinolin-1-yl)-2-phenyloxazol-4(5*H*)-one: yellow solid, m.p. 138 - 140 °C ; 74% yield (method B: 85% yield); **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.4 Hz, 2H), 7.52 (t, *J* = 7.0 Hz, 1H), 7.32 (t, *J* = 7.4 Hz, 2H), 7.24 (d, *J* = 8.5 Hz, 2H), 7.20-6.80 (m, 11H), 5.41 (s, 1H), 4.20 – 3.98 (m, 1H), 3.91 – 3.72 (m, 1H), 3.57 (d, *J* = 14.1 Hz, 1H), 3.32 (d, *J* = 14.1 Hz, 1H), 3.19 – 2.90 (m, 2H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.23, 185.46, 148.00, 135.31, 134.78, 132.99, 130.93, 129.98, 129.26, 128.60, 128.27, 128.18, 127.88, 127.23, 127.05, 126.20, 125.00, 123.55, 115.99, 95.24, 63.36, 43.35, 39.81, 26.04; **IR:** 3339.7, 2925.5, 1748.4, 1547.4, 1494.3, 1358.9, 1177.6, 941.0, 808.8, 700.6, 549.3 cm^{-1}. **HRMS (ESI):** calcd for $C_{31}H_{25}ClN_2O_2$+Na^+: 515.1497; found: 515.1513.



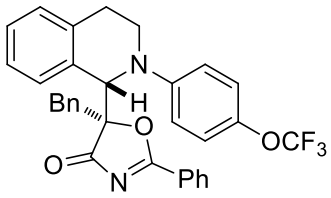
3k

5-benzyl-5-(2-(4-bromophenyl)-1,2,3,4-tetrahydroisoquinolin-1-yl)-2-phenyloxazol-4(5*H*)-one: yellow solid, m.p. 152 - 154 °C; 66% yield (method B: 77% yield); **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.68 (d, *J* = 7.3 Hz, 2H), 7.50-7.35 (m, 1H), 7.42 – 7.21 (m, 4H), 7.10-6.95 (m, 11H), 5.42 (s, 1H), 4.09-4.02 (m, 1H), 3.89 – 3.71 (m, 1H), 3.55 (d, *J* = 14.1 Hz, 1H), 3.31 (d, *J* = 14.1 Hz, 1H), 3.15-2.90 (m, 2H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.18, 185.42, 148.33, 135.26, 134.77, 132.89, 132.09, 130.85, 129.91, 129.22, 128.56, 128.21, 128.12, 127.85, 127.19, 126.95, 126.12, 124.87, 116.25, 110.59, 95.11, 63.22, 43.17, 39.73, 26.02; **IR:** 3337.2, 2925.5, 2370.8, 1747.9, 1547.5, 1358.8, 1177.5, 995.3, 806.1, 699.7, 503.4 cm^{-1}. **HRMS (ESI):** calcd for $C_{31}H_{25}BrN_2O_2+Na^+$: 559.0992; found: 559.1016.



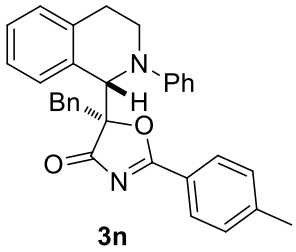
3l

5-benzyl-5-(2-(4-fluorophenyl)-1,2,3,4-tetrahydroisoquinolin-1-yl)-2-phenyloxazol-4(5*H*)-one: yellow solid, m.p. 74 - 76 °C; 55% yield (method B: 74% yield); **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.69 (d, *J* = 5.5 Hz, 2H), 7.60-7.43 (m, 1H), 7.44-7.20 (m, 2H), 7.21-6.80 (m, 13H), 5.32 (s, 1H), 4.20-3.98 (m, 1H), 3.90-3.70 (m, 1H), 3.65 (d, *J* = 13.9 Hz, 1H), 3.31 (d, *J* = 13.9 Hz, 1H), 3.15-2.80 (m, 2H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.32, 185.47, 146.10, 135.42, 134.72, 133.17, 130.98, 129.99, 129.26, 128.57, 128.36, 128.15, 127.74, 127.17, 127.06, 126.13, 125.05, 117.09, 117.00, 115.95, 115.65, 95.50, 63.74, 44.08, 39.84, 25.61; **IR:** 3479.7, 3062.2, 1965.0, 1748.5, 1603.8, 1359.5, 1177.8, 941.7, 822.2, 704.0, 554.1 cm^{-1}. **HRMS (ESI):** calcd for $C_{31}H_{25}FN_2O_2+Na^+$: 499.1792; found: 499.1796.



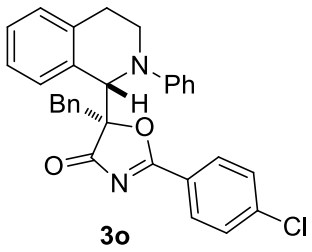
3m

5-benzyl-2-phenyl-5-(2-(4-(trifluoromethoxy)phenyl)-1,2,3,4-tetrahydroisoquinolin-1-yl)oxazol-4(5*H*)-one: yellow solid, m.p. 125 - 127 °C; 64% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.3 Hz, 2H), 7.60-7.43 (m, 1H), 7.33 (t, *J* = 7.7 Hz, 2H), 7.19 – 7.03 (m, 10H), 7.03 – 6.88 (m, 3H), 5.43 (s, 1H), 4.19 – 4.00 (m, 1H), 3.90 – 3.77 (m, 1H), 3.58 (d, *J* = 14.2 Hz, 1H), 3.33 (d, *J* = 14.2 Hz, 1H), 3.22 – 2.89 (m, 2H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.22, 185.50, 148.17, 135.30, 134.80, 132.99, 130.92, 130.01, 129.31, 128.62, 128.30, 128.21, 127.93, 127.27, 127.10, 126.96, 126.27, 125.03, 122.44, 115.95, 115.40, 95.19, 63.52, 43.49, 39.84, 26.04; **IR:** 3365.2, 2923.3, 2378.1, 1745.8, 1603.6, 1452.1, 1360.0, 1259.5, 1093.2, 801.2, 703.5 cm^{-1}. **HRMS (ESI):** calcd for $C_{32}H_{25}FN_2O_3$+Na^+: 565.1709; found: 565.1717.



3n

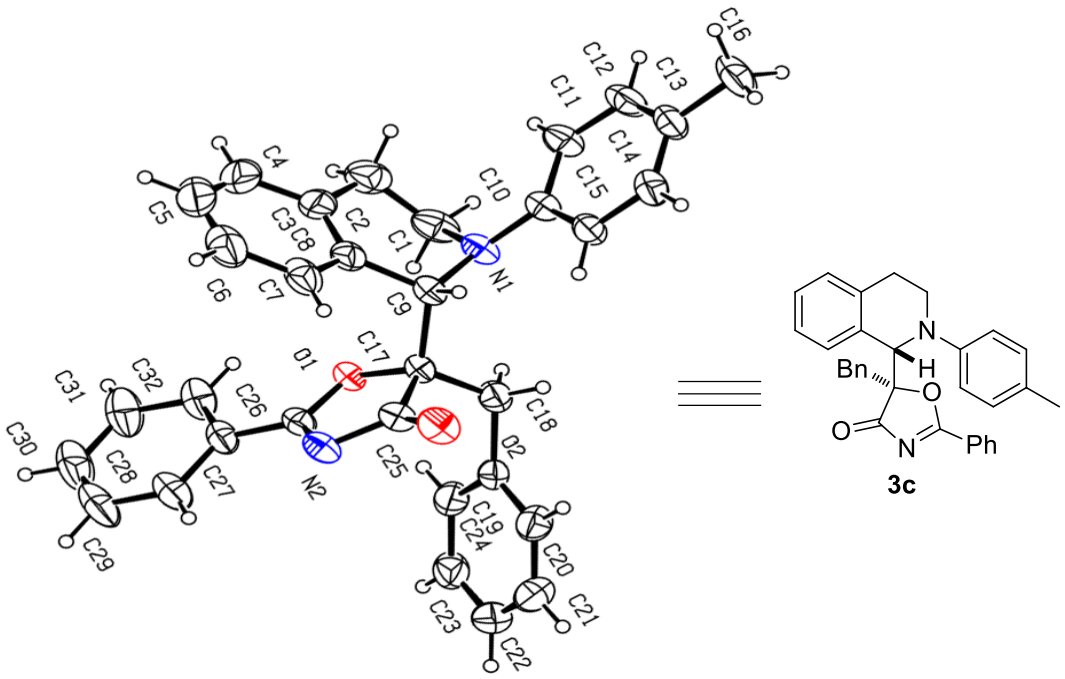
5-benzyl-5-(2-phenyl-1,2,3,4-tetrahydroisoquinolin-1-yl)-2-(p-tolyl)oxazol-4(5*H*)-one: yellow solid, m.p. 192 - 194 °C; 61% yield (method B: 90% yield); **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.2 Hz, 2H), 7.30 (t, *J* = 8.0 Hz, 2H), 7.18 – 7.08 (m, 6H), 7.08 – 7.00 (m, 4H), 7.00 – 6.88 (m, 3H), 6.82 (t, *J* = 7.2 Hz, 1H), 5.49 (s, 1H), 4.16 – 4.02 (m, 1H), 3.96 – 3.81 (m, 1H), 3.60 (d, *J* = 14.2 Hz, 1H), 3.35 (d, *J* = 14.2 Hz, 1H), 3.17 – 2.90 (m, 2H), 2.33 (s, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.40, 185.38, 149.39, 146.01, 135.51, 133.30, 131.34, 130.00, 129.45, 129.36, 128.20, 128.09, 127.64, 127.07, 126.00, 122.27, 118.63, 114.70, 95.32, 63.26, 42.98, 39.82, 26.09, 21.88; **IR:** 3463.3, 2927.0, 2365.4, 1921.7, 1744.2, 1548.0, 1358.1, 1183.8, 943.4, 736.6, 601.5, 483.3 cm^{-1}. **HRMS (ESI):** calcd for $C_{32}H_{28}N_2O_2$+Na^+: 495.2043; found: 495.2055.



3o

5-benzyl-2-(4-chlorophenyl)-5-(2-phenyl-1,2,3,4-tetrahydroisoquinolin-1-yl)oxazol-4(5*H*)-one: yellow solid, m.p. 196 - 198 ºC; 57% yield (method B: 81% yield); **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.4 Hz, 2H), 7.31 (t, *J* = 8.1 Hz, 4H), 7.18 – 7.01 (m, 8H), 6.96 (d, *J* = 9.4 Hz, 3H), 6.84 (t, *J* = 7.1 Hz, 1H), 5.49 (s, 1H), 4.26 – 3.97 (m, 1H), 3.97 – 3.81 (m, 1H), 3.61 (d, *J* = 14.2 Hz, 1H), 3.36 (d, *J* = 14.2 Hz, 1H), 3.22 – 3.04 (m, 1H), 3.04 – 2.89 (m, 1H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.15, 184.37, 149.33, 141.35, 135.51, 133.11, 131.20, 130.47, 129.96, 129.50, 129.12, 128.27, 128.18, 127.78, 127.22, 127.01, 126.10, 123.50, 118.82, 114.78, 95.84, 63.34, 43.09, 39.83, 26.14; **IR:** 3366.2, 2923.3, 2368.1, 1739.0, 1597.3, 1260.5, 1085.6, 942.8, 742.3, 604.4 cm^{-1}. **HRMS (ESI):** calcd for $C_{31}H_{25}ClN_2O_2+Na^+$: 515.1497; found: 515.1502.

(G) X-ray single crystal data for 3c



3c

Bond precision: C-C=0.0045 A Wavelength=0.71073

Cell: a = 6.5198 (3) b = 16.3244 (7) c = 24.2413 (9)

alpha = 90 beta = 94.884 (4) gamma = 90

Temperature: 293 K

	Calculated	Reported
Volume	2570.68(19)	2570.66(18)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C32 H28 N2 O2	C32 H28 N2 O2
Sum formula	C32 H28 N2 O2	C32 H28 N2 O2
Mr	472.56	472.56
Dx, g cm-3	1.221	1.221
Z	4	4
Mu (mm-1)	0.076	0.076
F000	1000.0	1000.0
F000'	1000.40	
h, k, lmax	8, 21, 32	8, 21, 30
Nref	6508	5764
Tmin, Tmax	0.973, 0.981	0.566, 1.000
Tmin'	0.973	

Correction method = MULTI-SCAN

Data completeness = 0.886 Theta (max) = 28.477

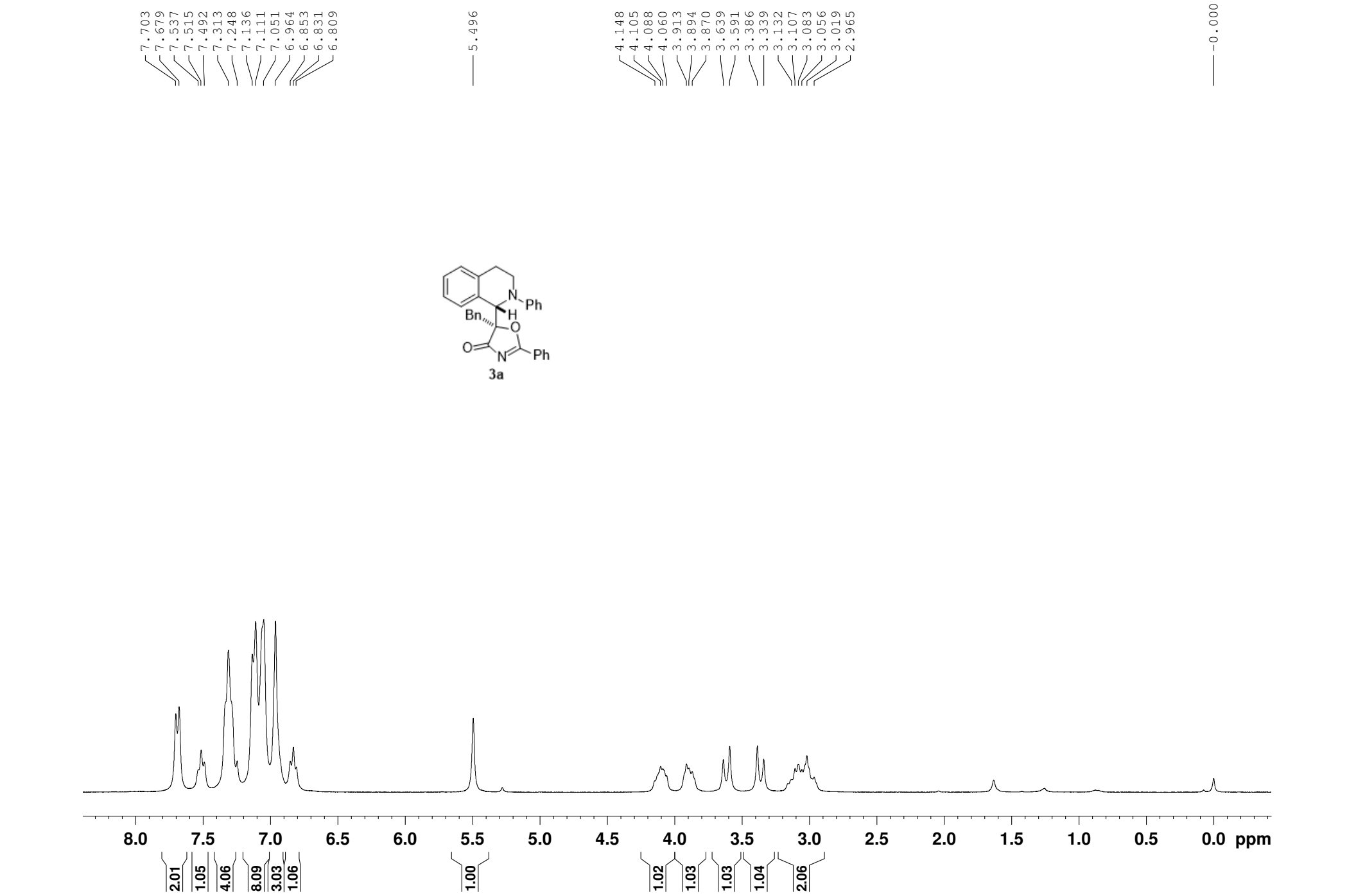
R (reflections) = 0.0667 (3293) wR2 (reflections)= 0.1843 (5764)

S = 1.073 Npar = 373

(H) References

[1] X.-Z. Shu, X.-F. Xia, K.-G. Ji, X.-Y. Liu and Y.-M. Liang, *J. Org. Chem.*, 2009, **74**, 7464.

[2] T. Misaki, G. Takimoto and T. Sugimura, *J. Am. Chem. Soc.*, 2010, **132**, 6286.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1.04
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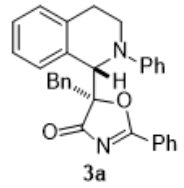
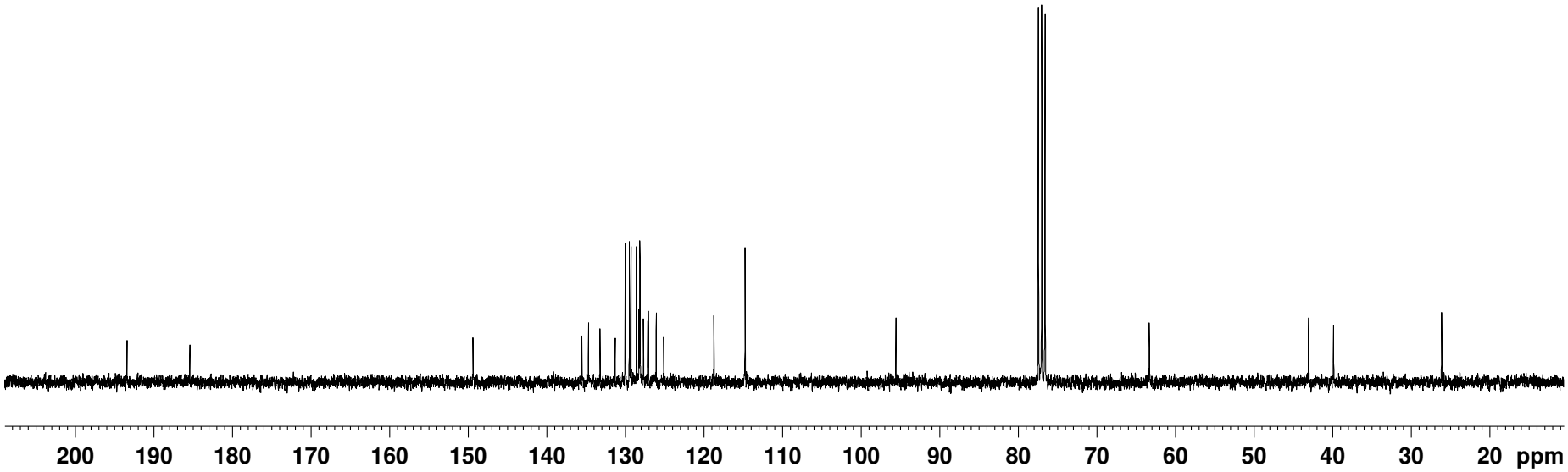
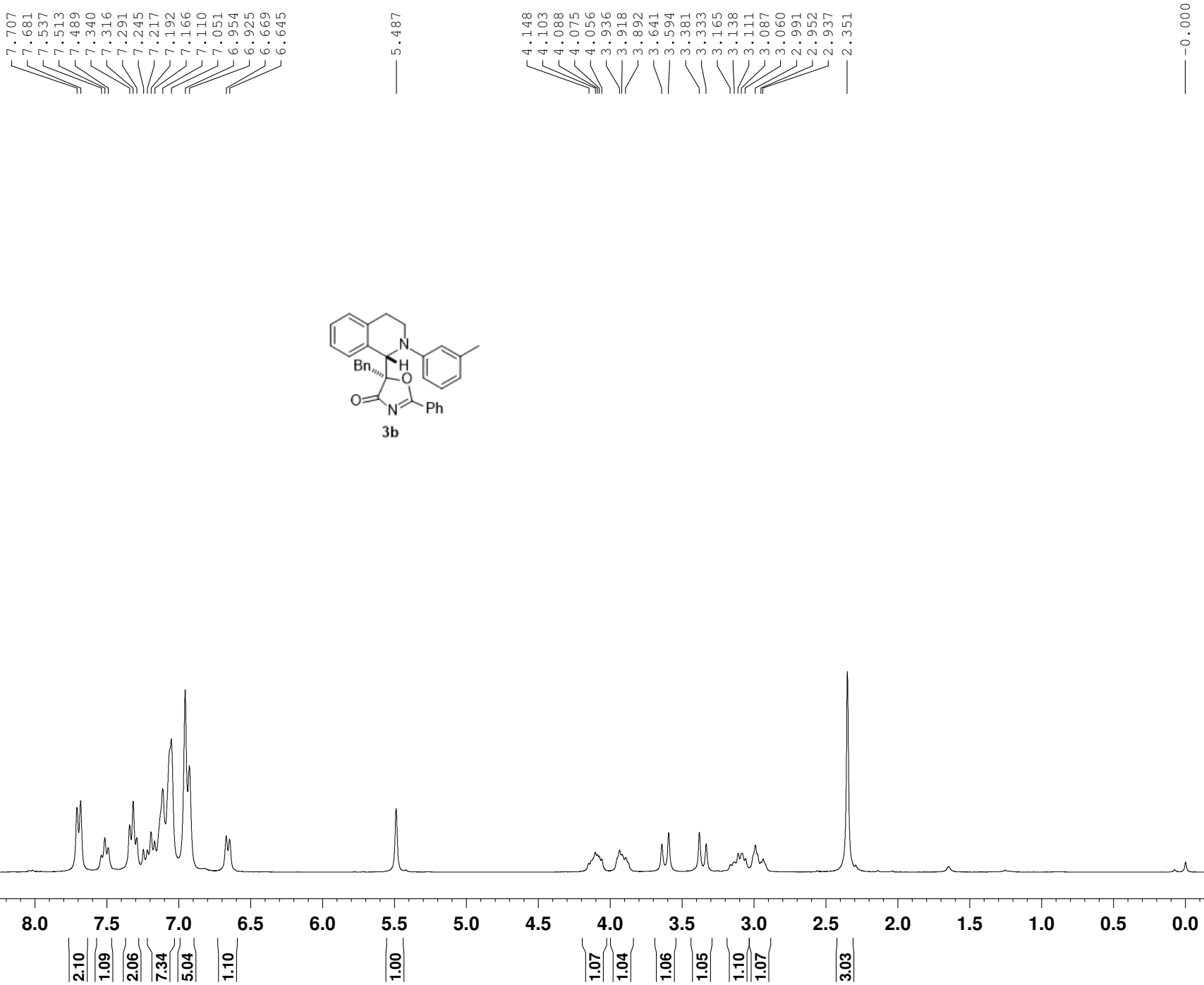
26.10



3a

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3.03

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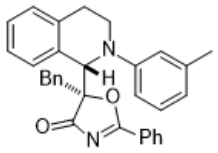
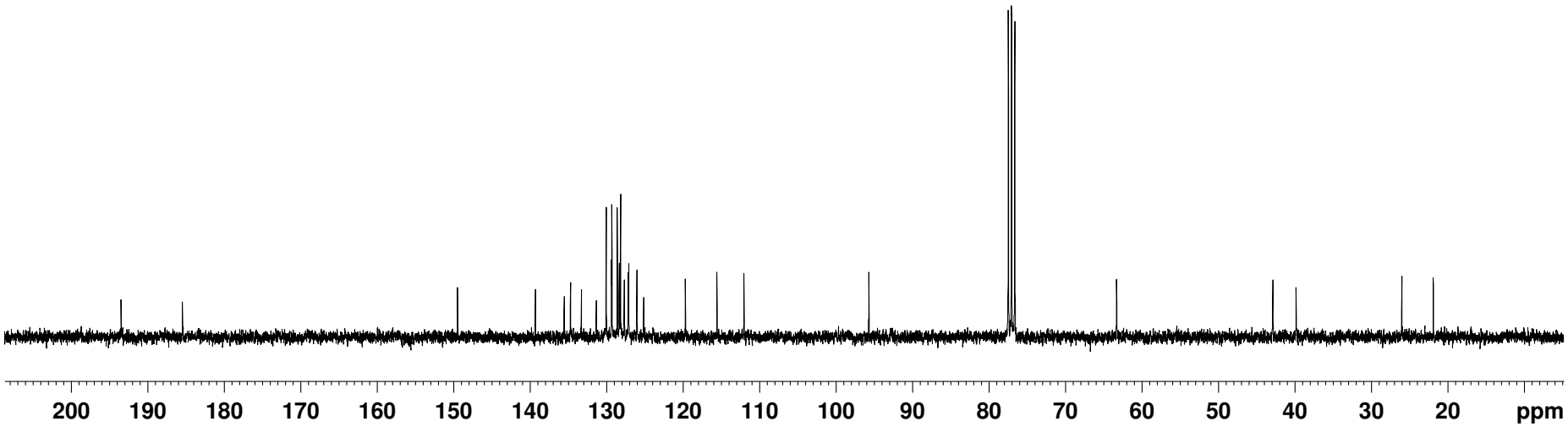
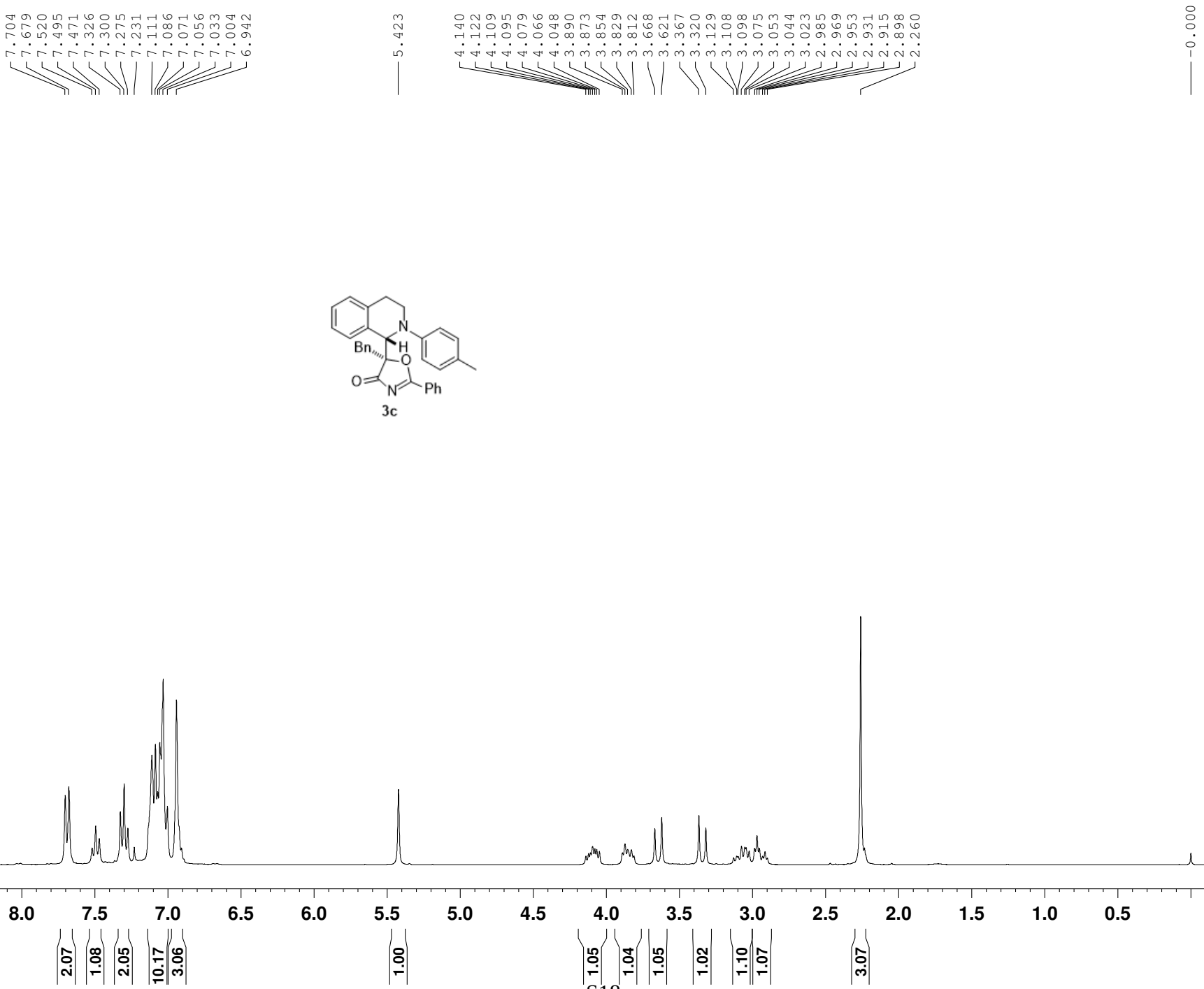


3b

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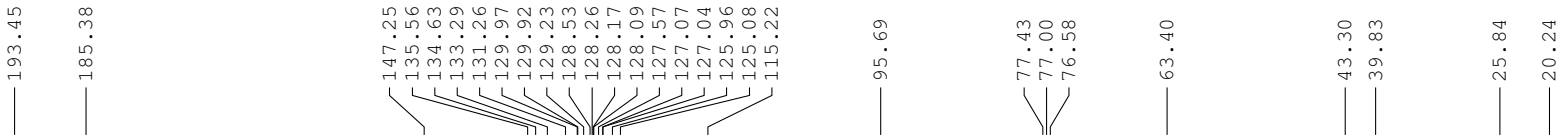
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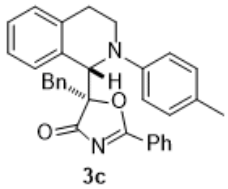
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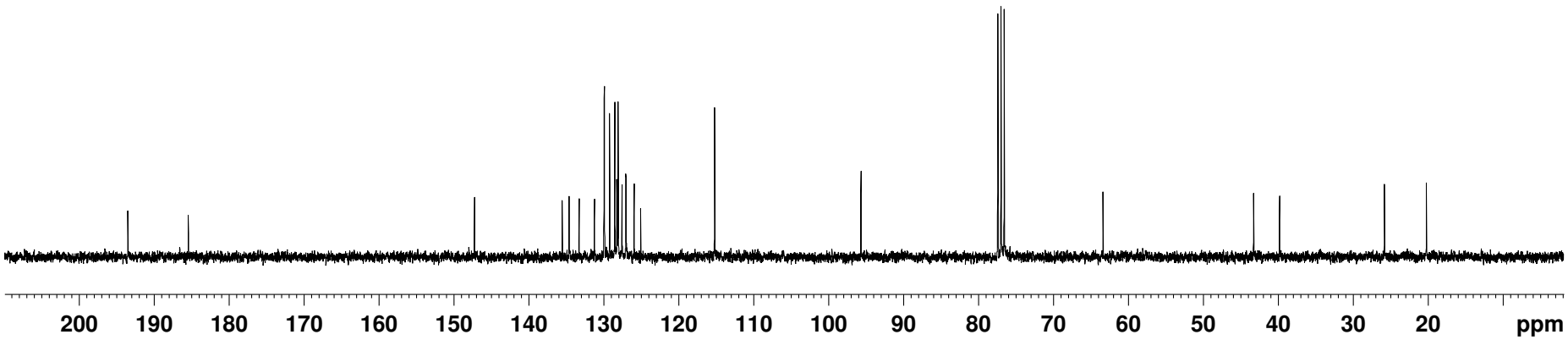
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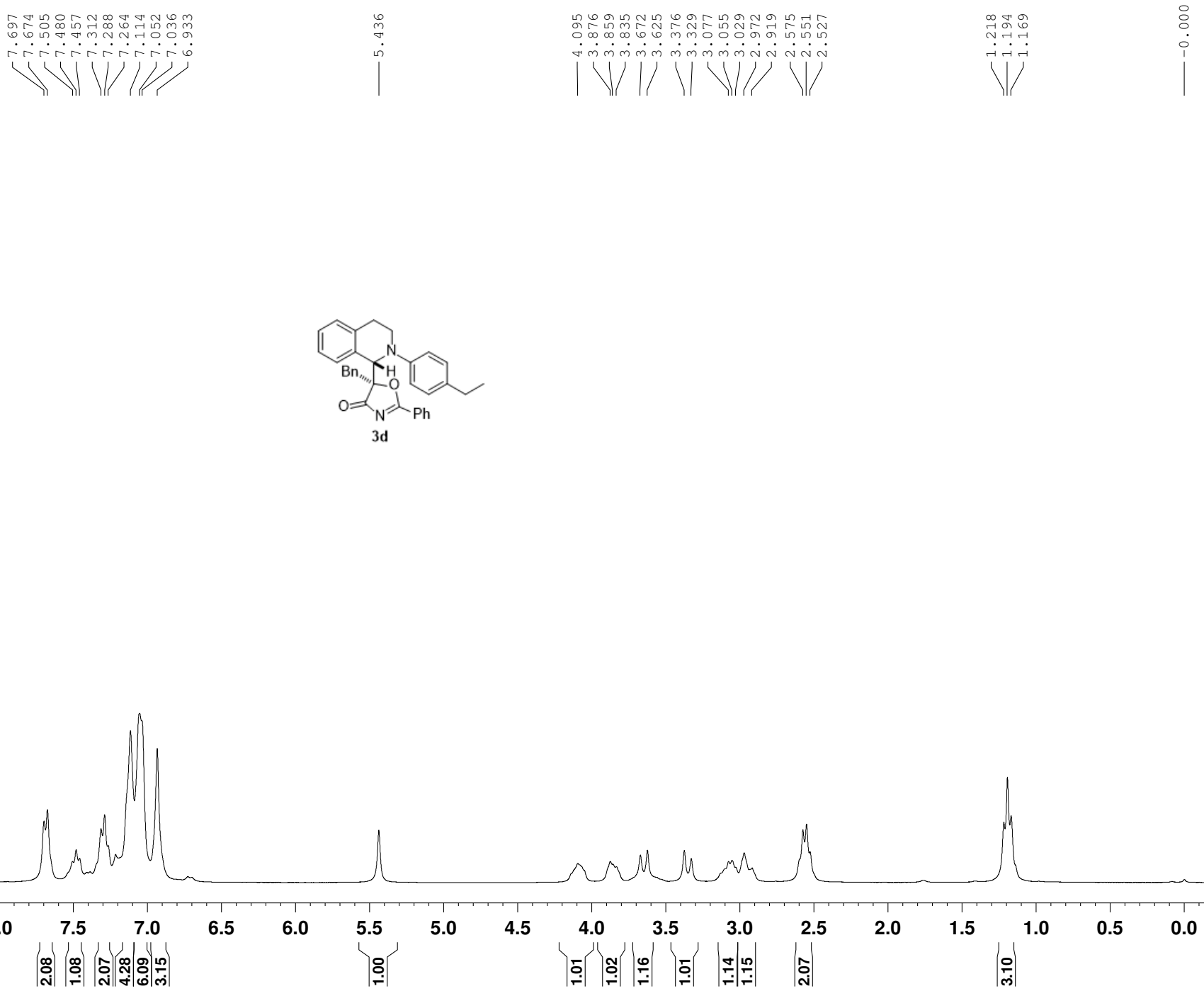
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Bn
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Ph
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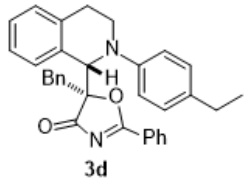

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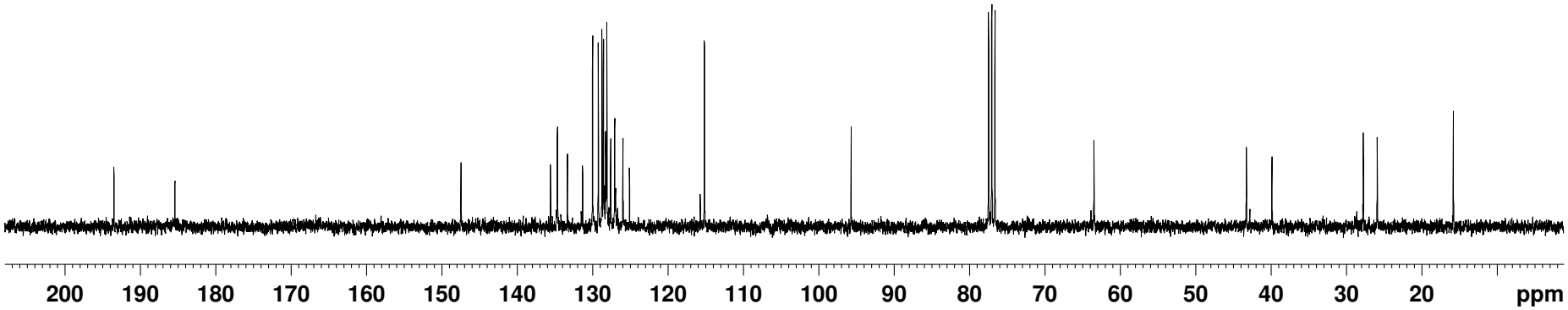

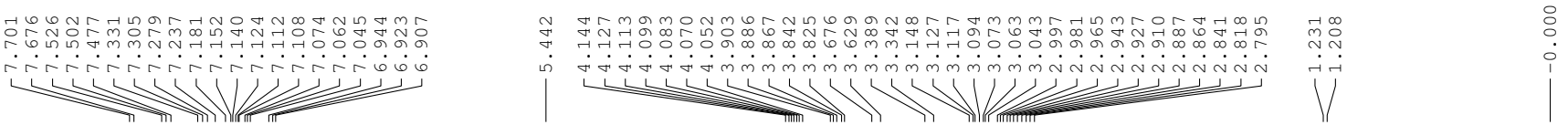
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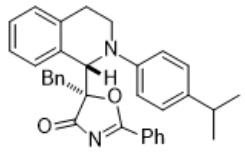
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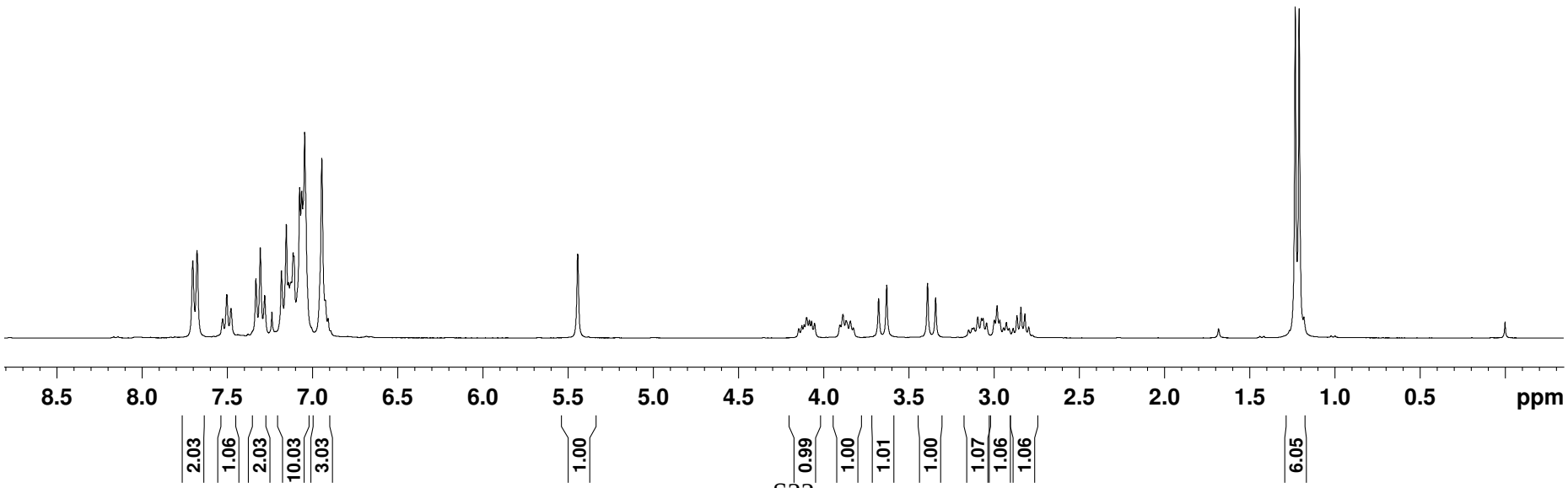
3e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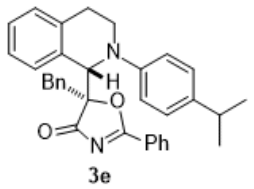

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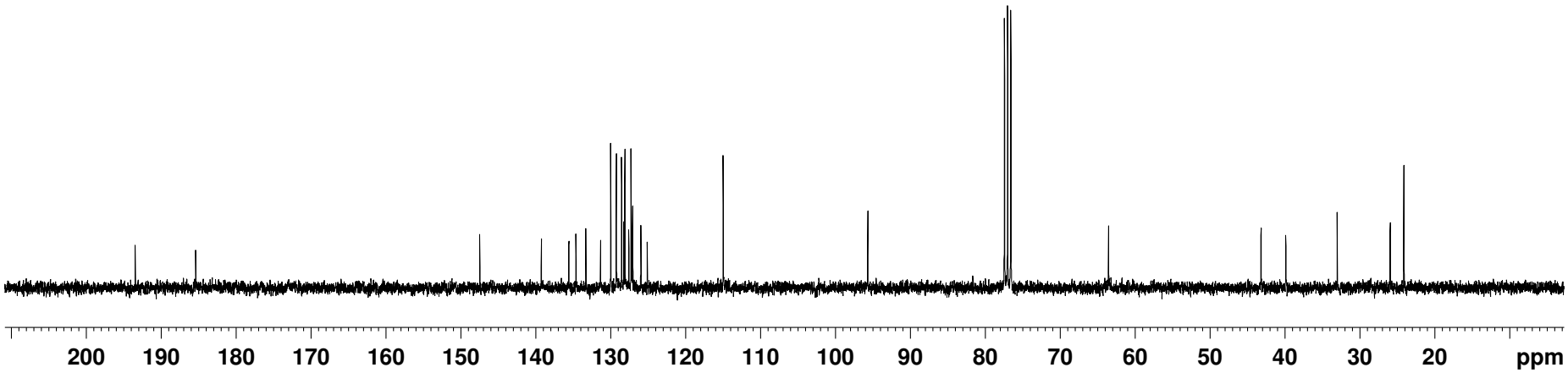

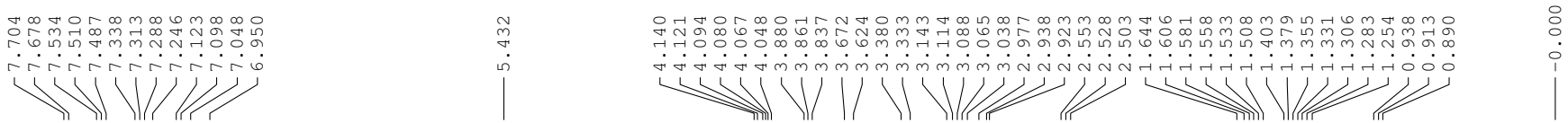
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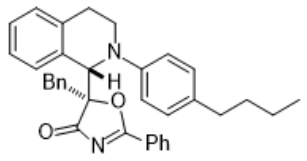
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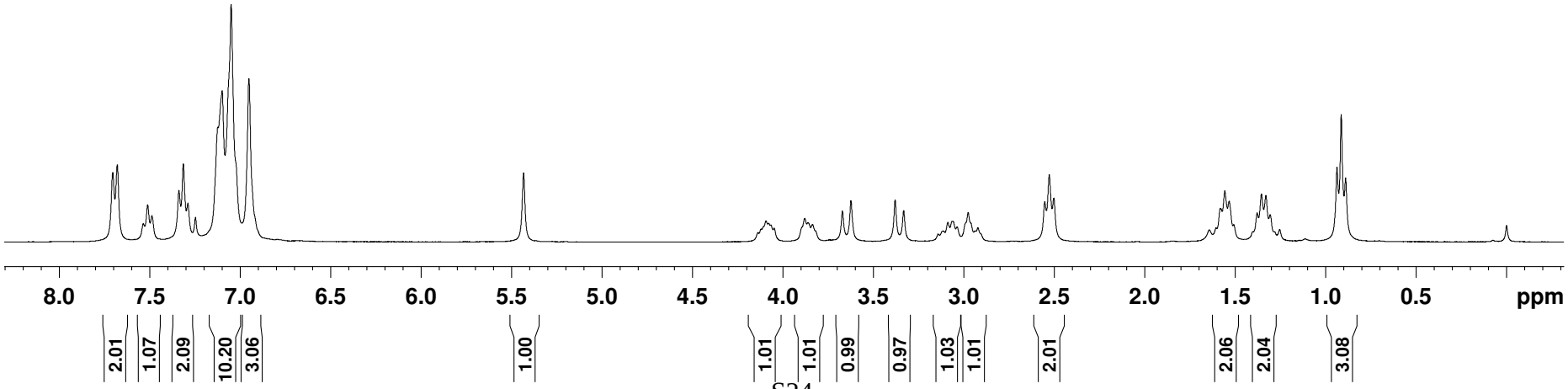
3f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2.04
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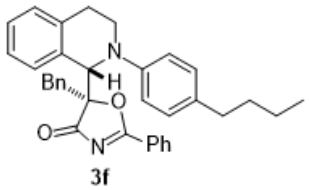

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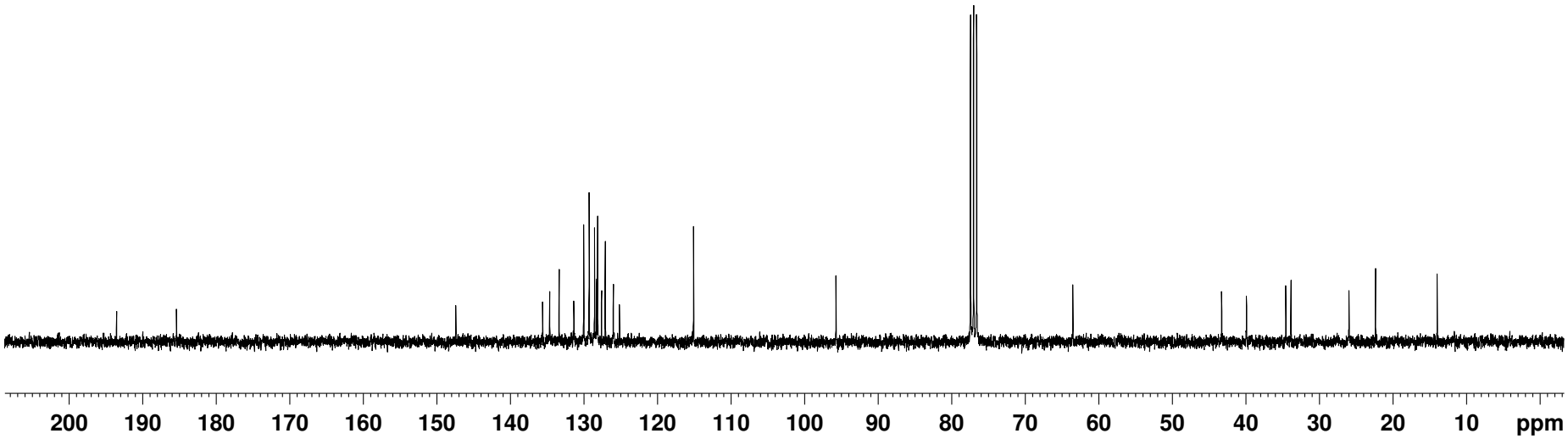

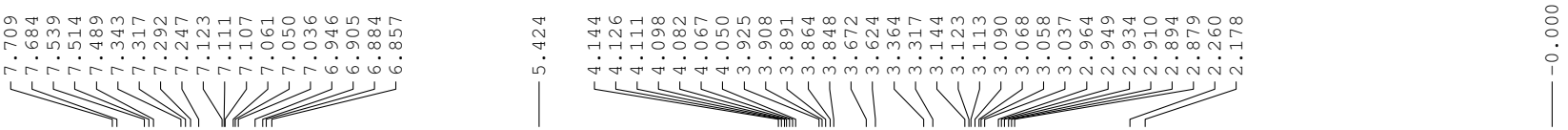
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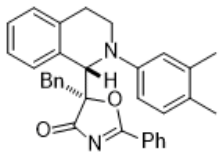
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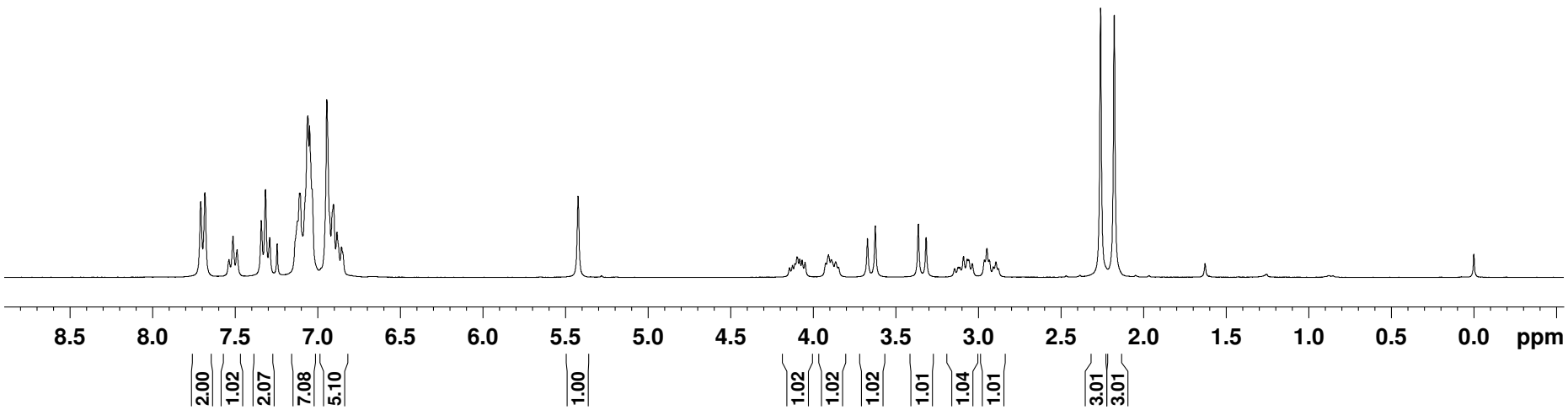
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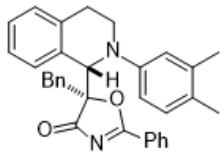

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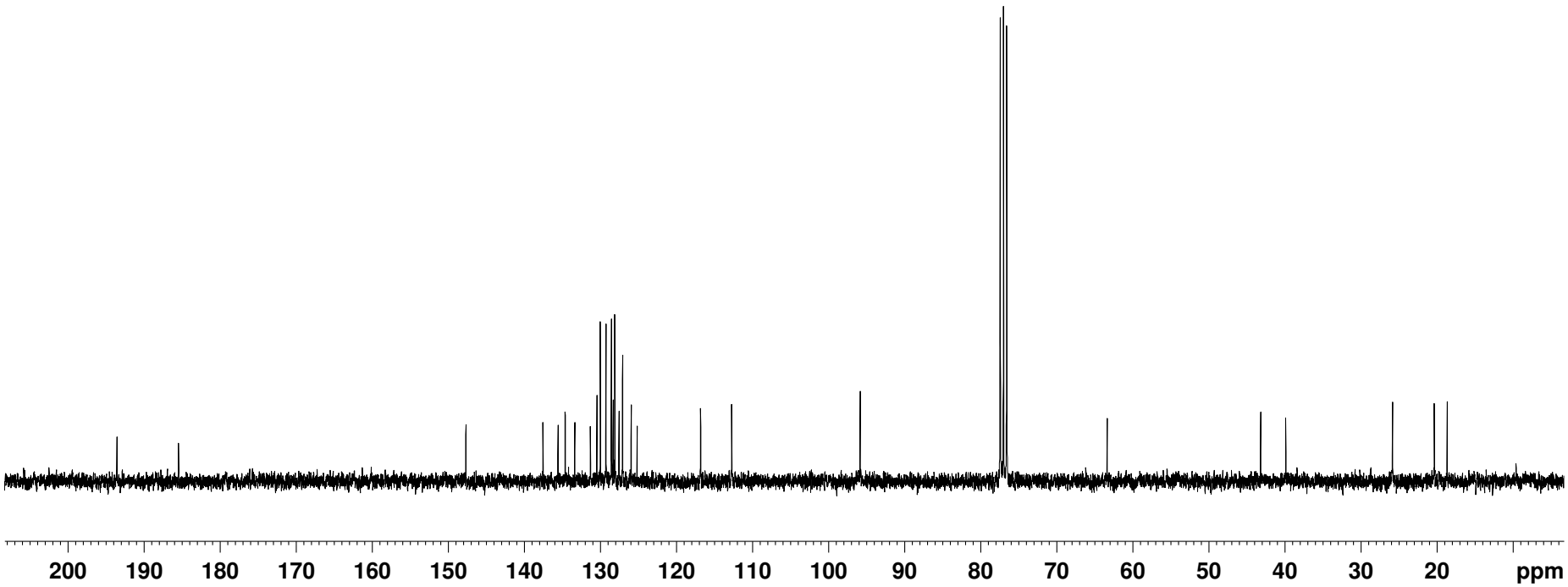

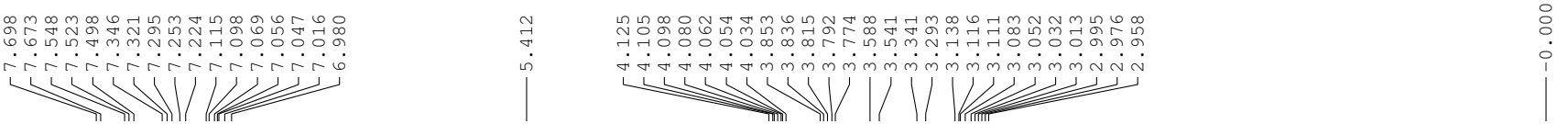
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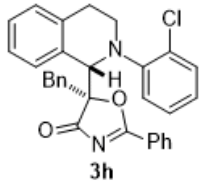
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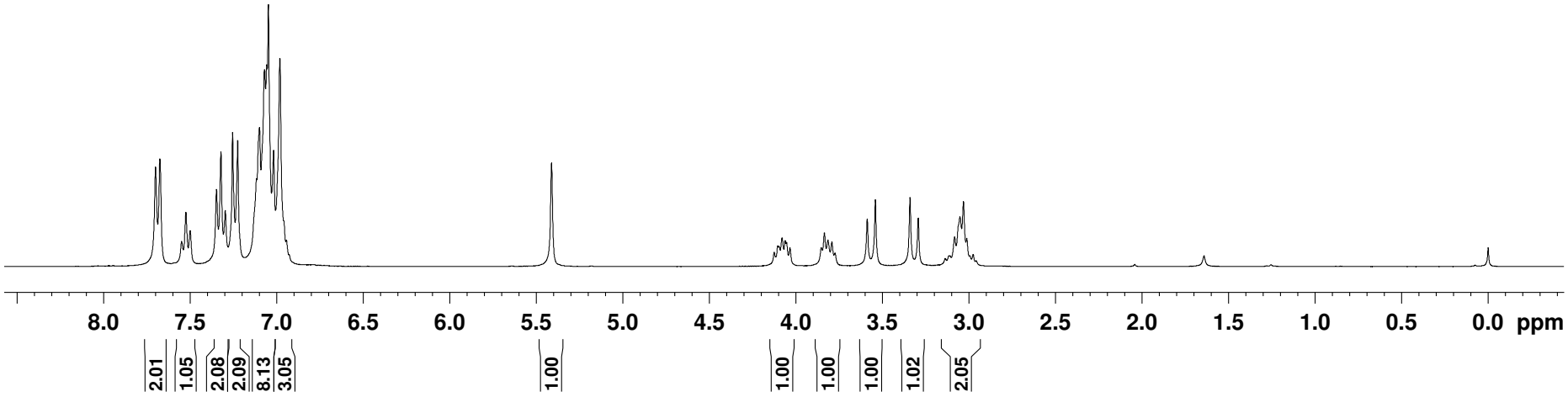
3h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2.05

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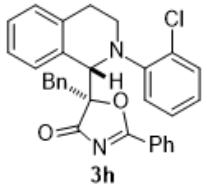

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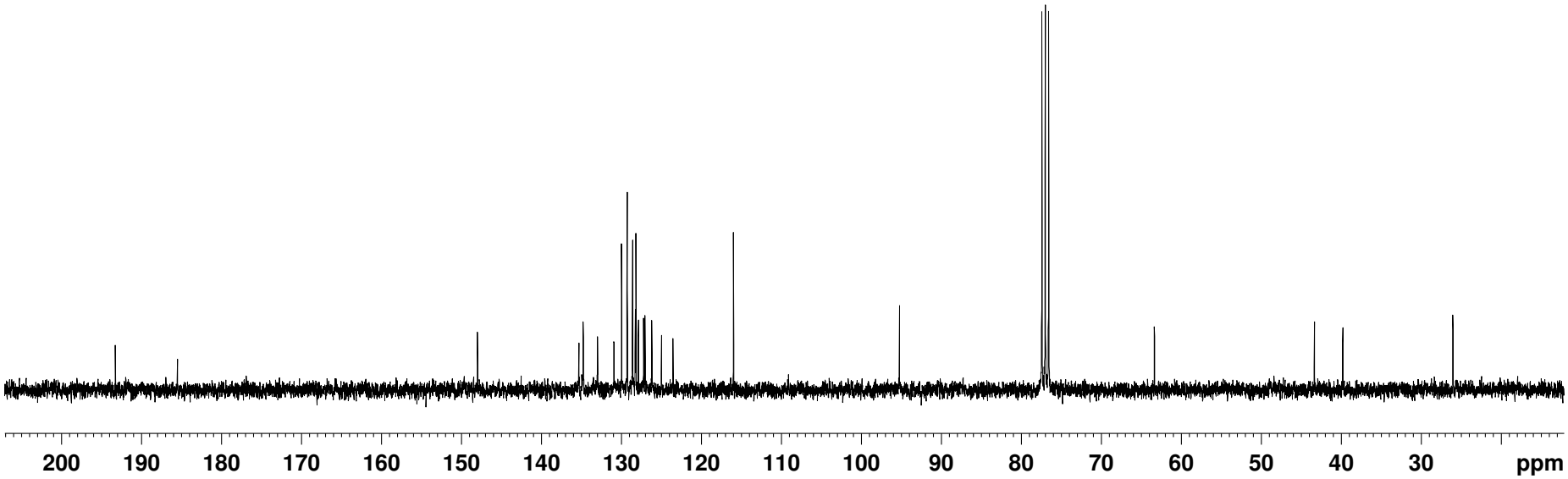

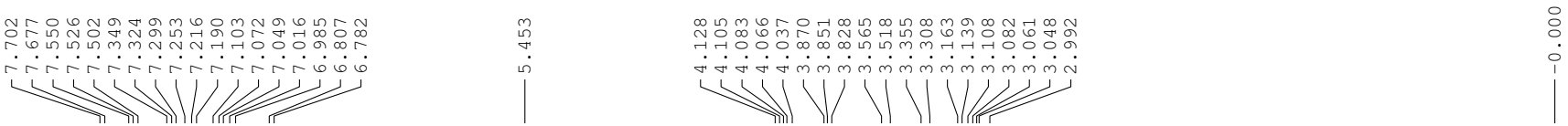
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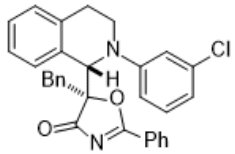
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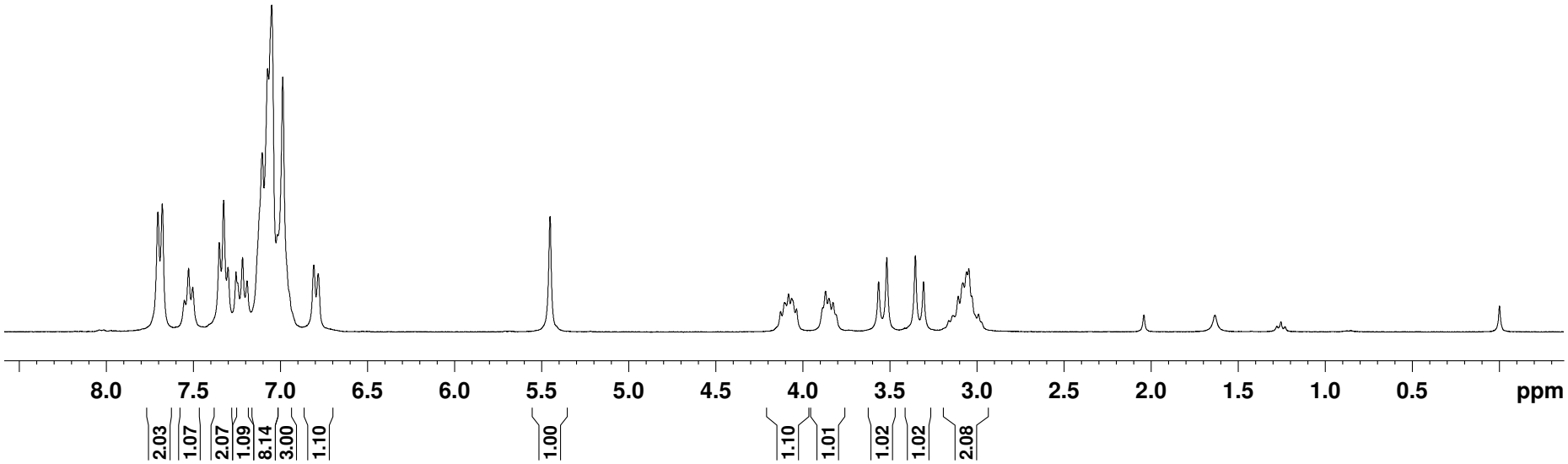
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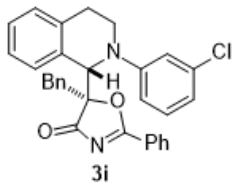

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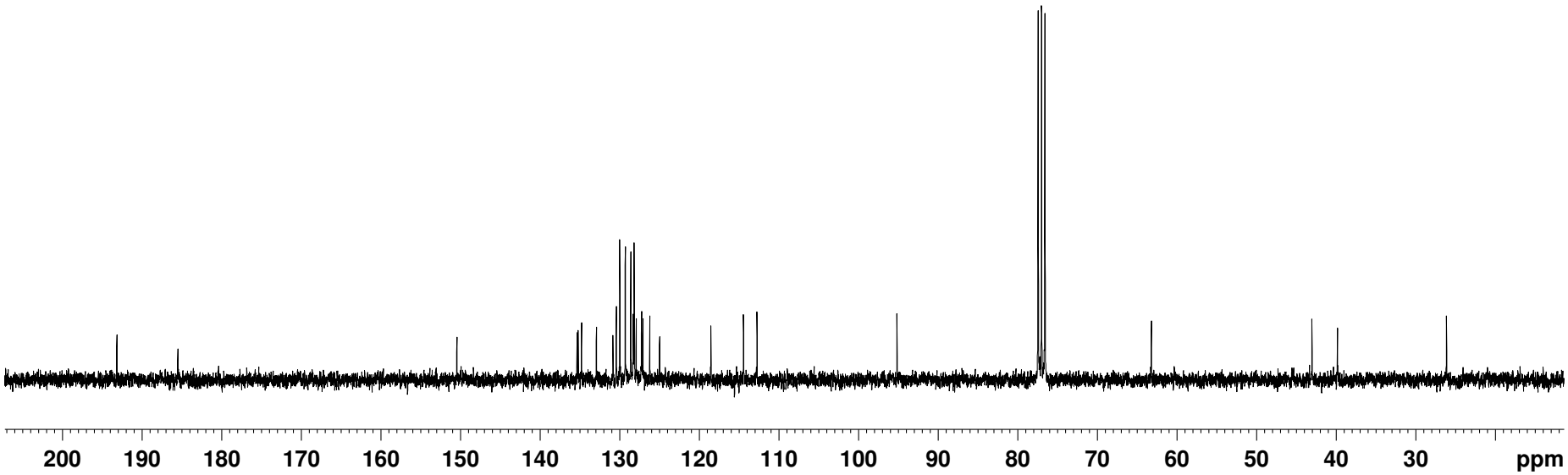

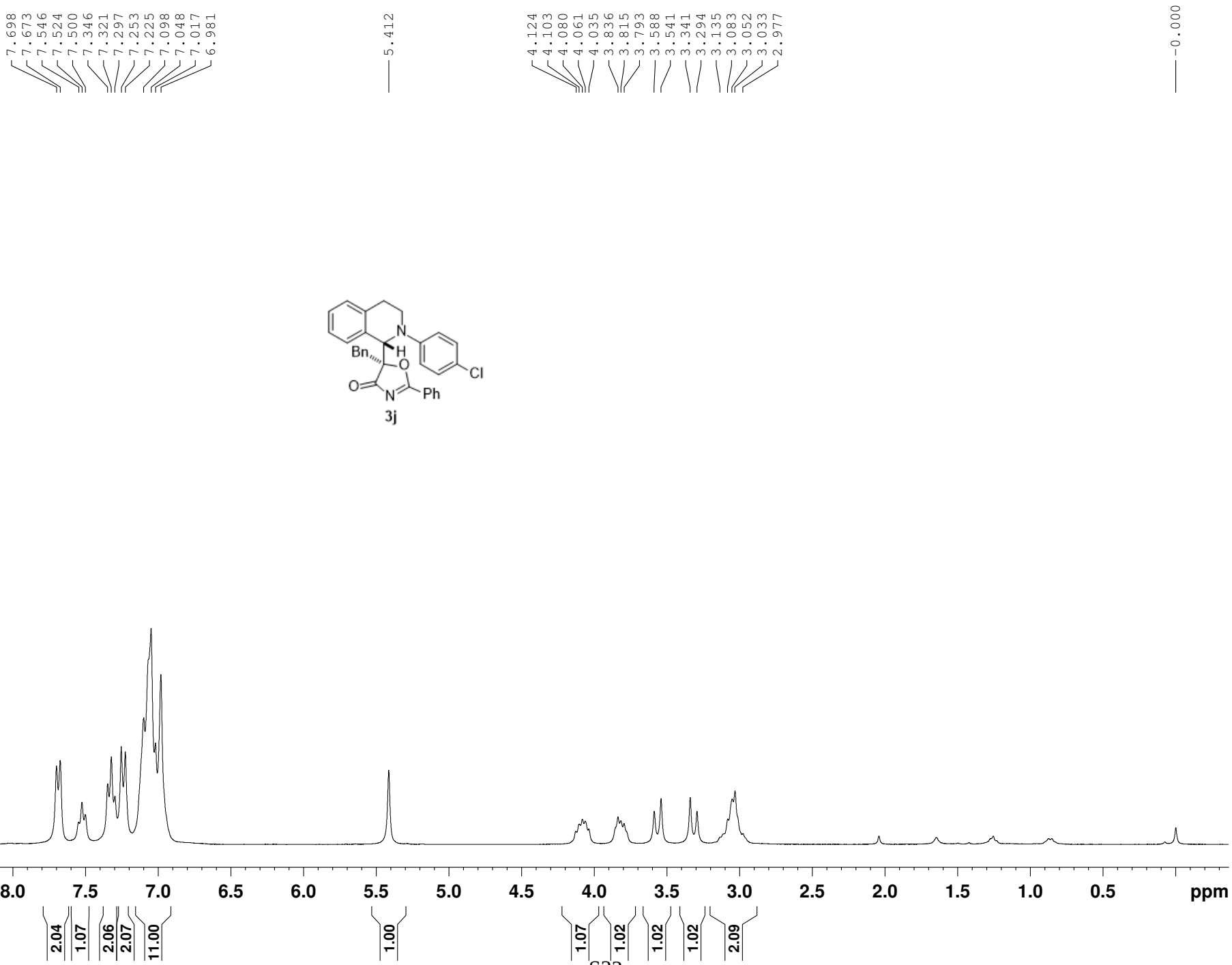
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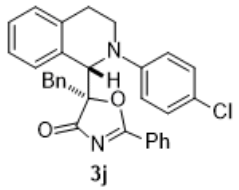

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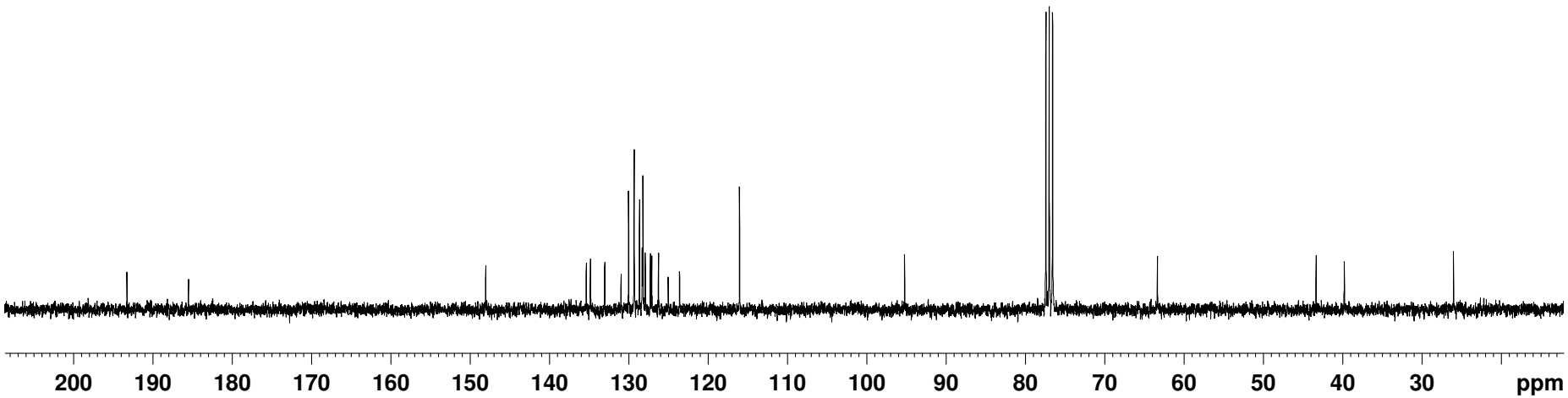

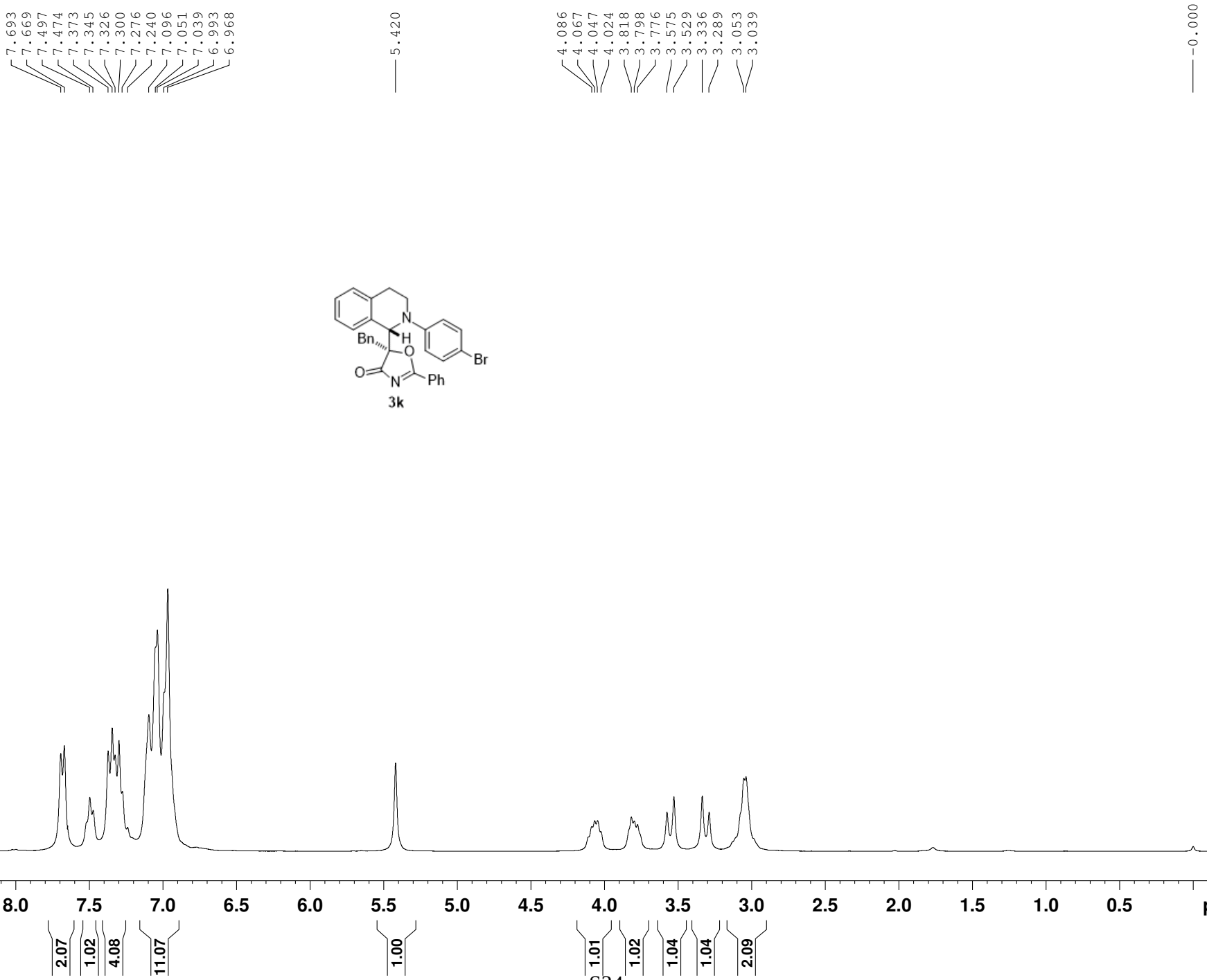
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1.02
1.04
1.04
2.09

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185.42
148.33
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132.09
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128.21
128.12
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127.18
126.94
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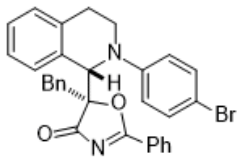

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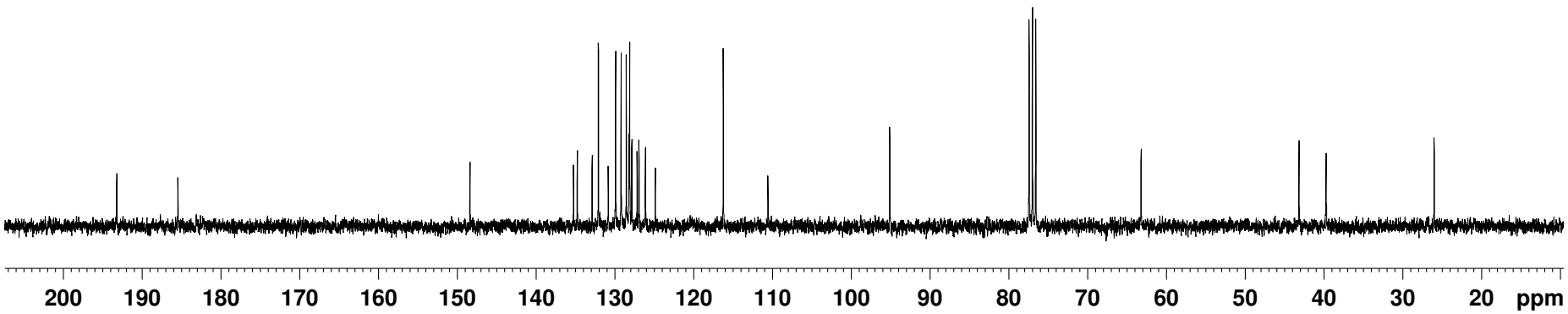

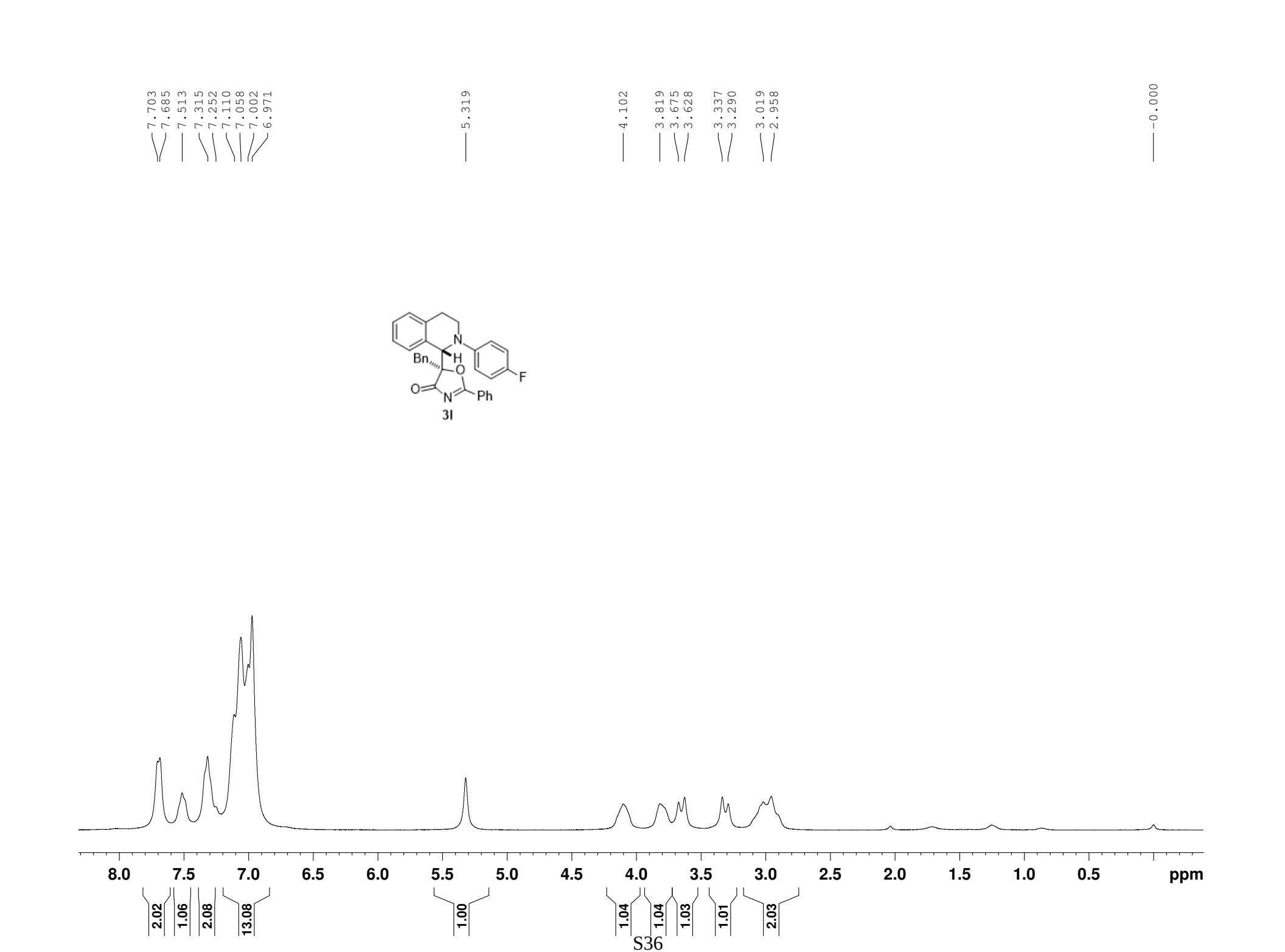
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3.628
3.337
3.290
3.019
2.958
0.000
Bn
H
O
N
O
N
Ph
F
3l
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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1.0
0.5
ppm
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1.06
2.08
13.08
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1.04
1.04
1.03
1.01
2.03

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129.98
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126.13
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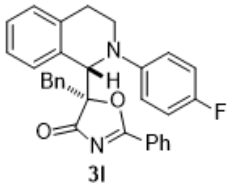

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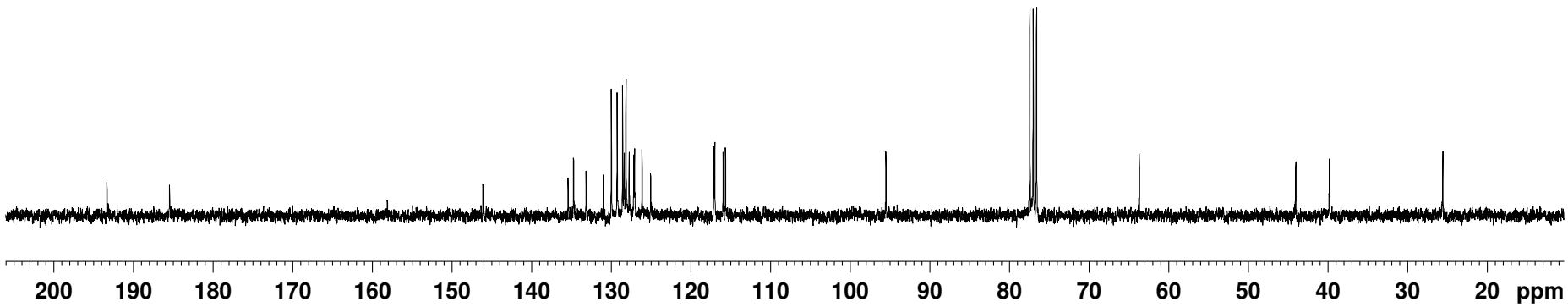

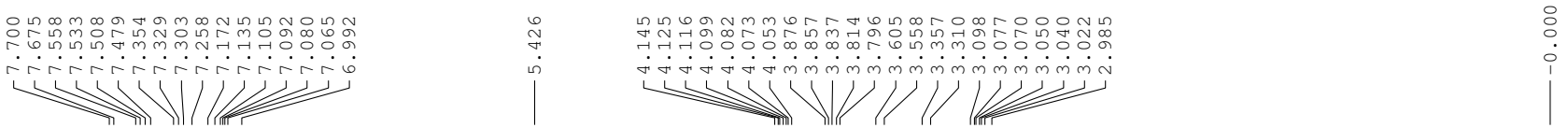
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7.080
7.065
6.992
5.426
4.145
4.125
4.116
4.099
4.082
4.073
4.053
3.876
3.857
3.837
3.814
3.796
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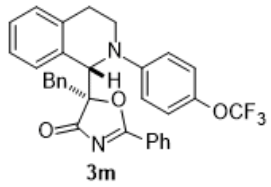
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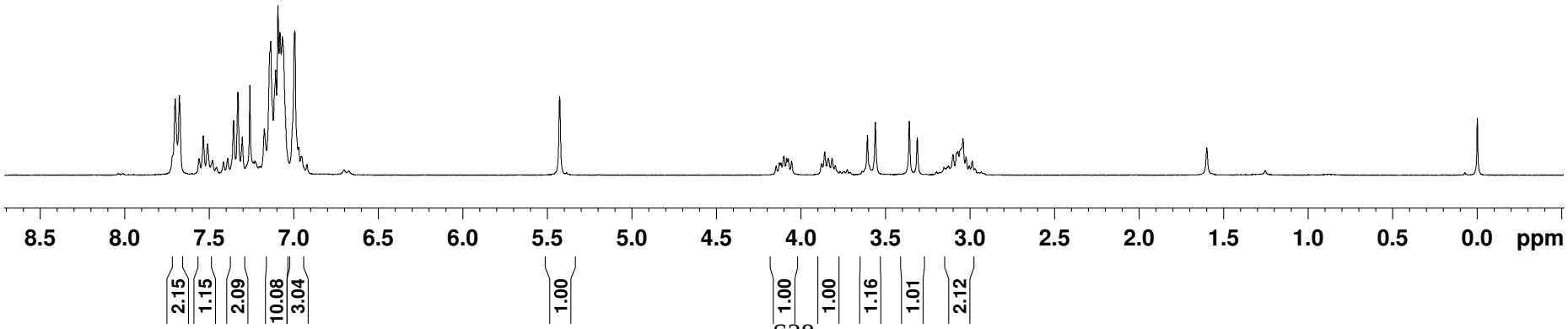
N
O
N
Ph
OCF3

3m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1.00
1.00
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1.01
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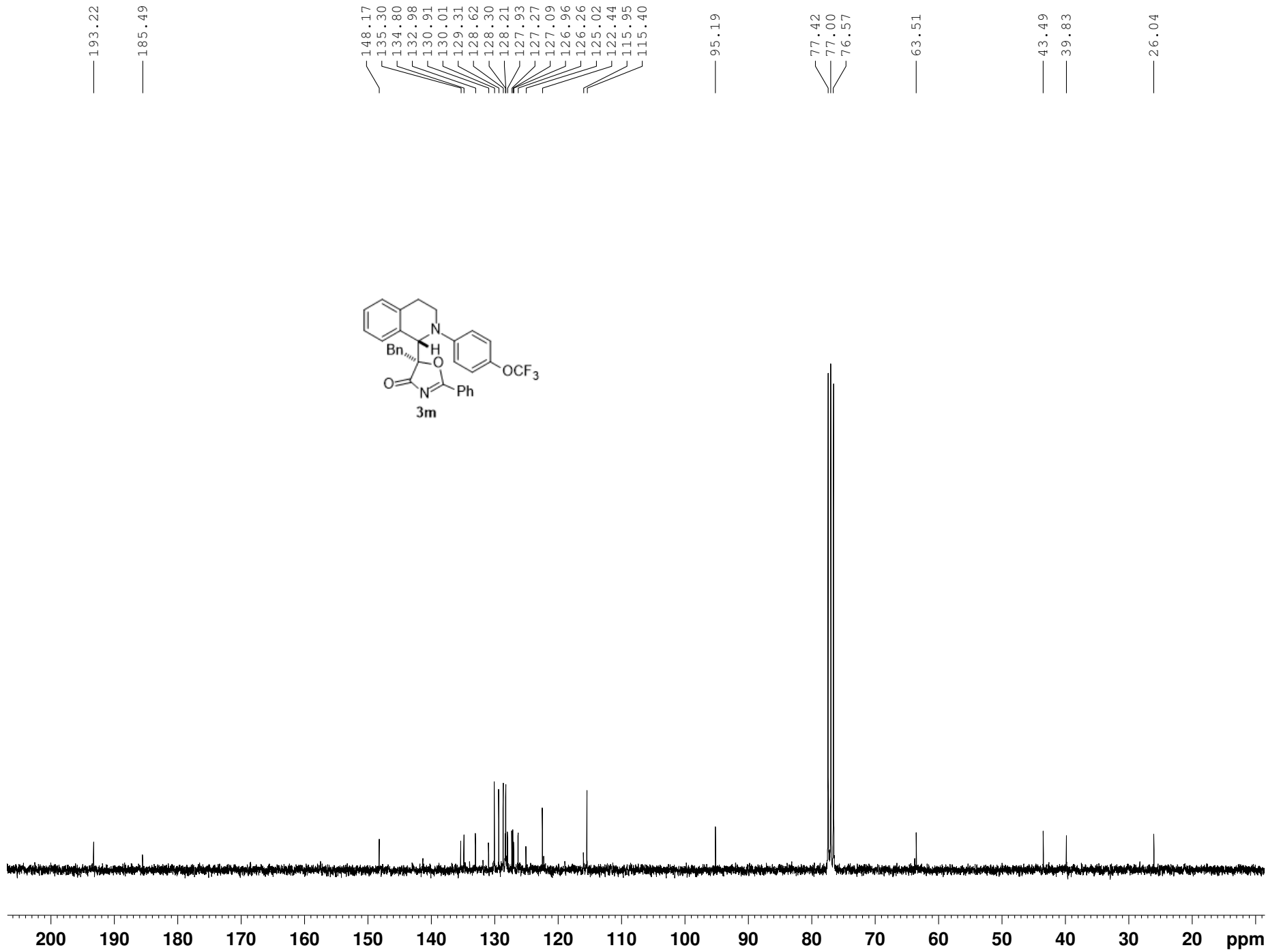
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127.27
127.09
126.96
126.26
125.02
122.44
115.95
115.40
95.19
77.42
77.00
76.57
63.51
43.49
39.83
26.04
Bn
H
N
O
O
N
Ph
OCF3
3m
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150
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80
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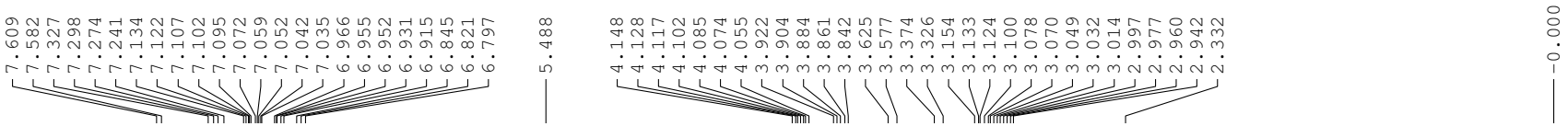
20
ppm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7.042
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6.955
6.952
6.931
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6.845
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5.488
4.148
4.128
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4.102
4.085
4.074
4.055
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3.904
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3.842
3.625
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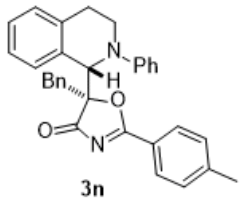
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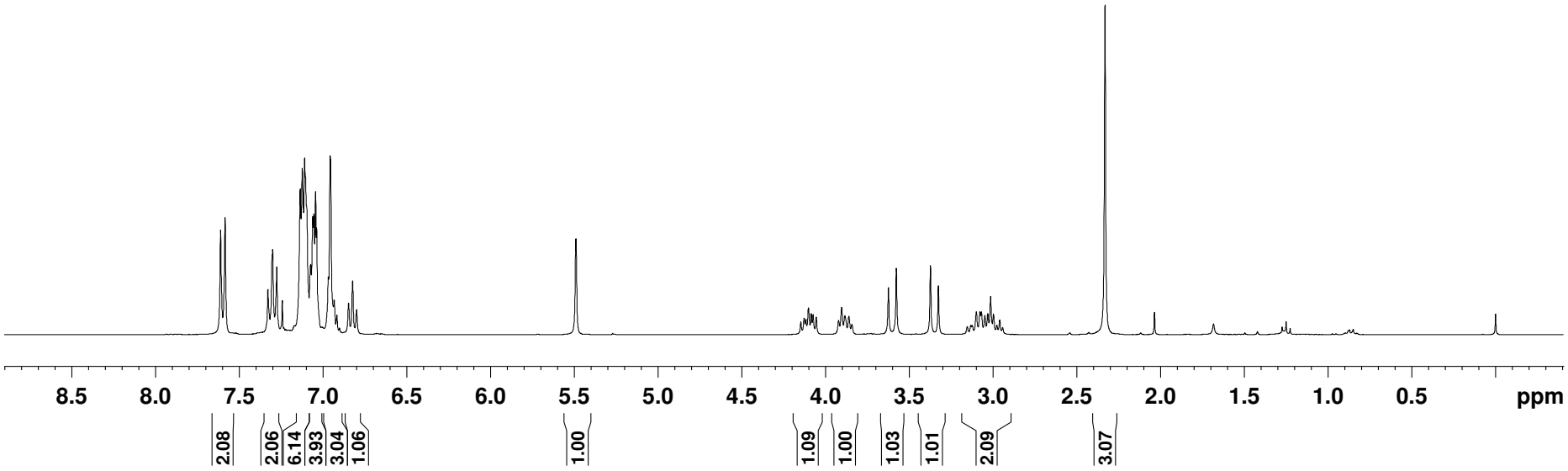
Ph
Bn
H
O
O
N

3n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2.0
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1.0
0.5
ppm
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2.06
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3.93
3.04
1.06
1.00
1.09
1.00
1.03
1.01
2.09
3.07

193.40
185.38
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146.01
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133.29
131.34
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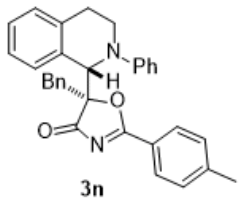

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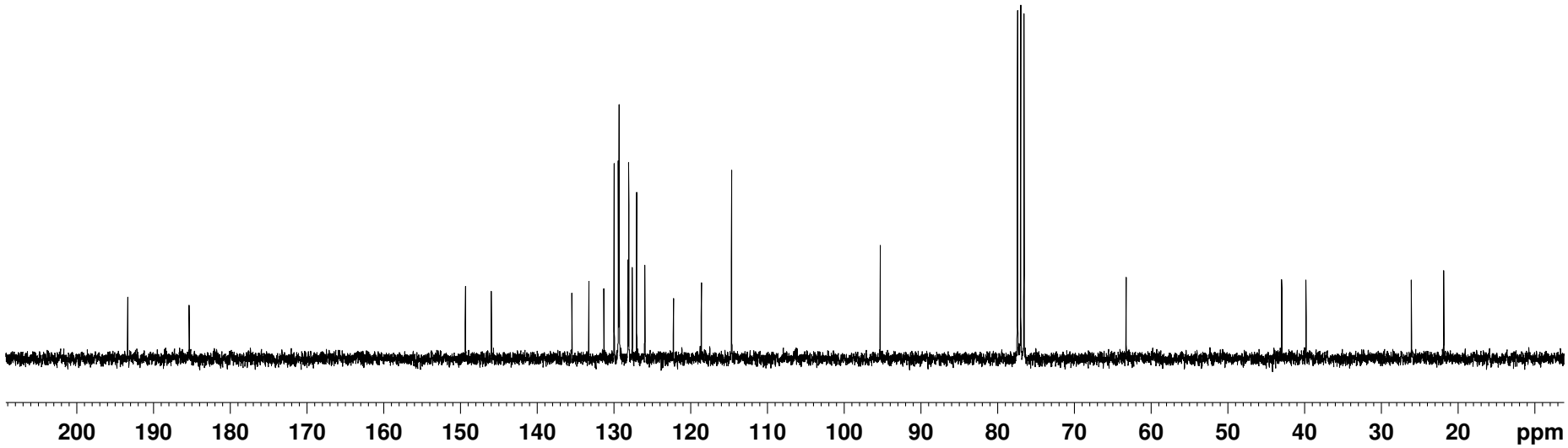

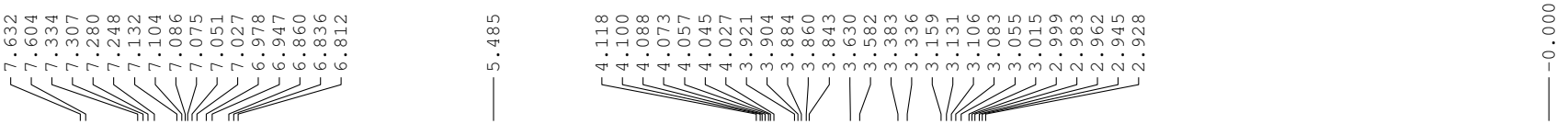
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6.860
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4.045
4.027
3.921
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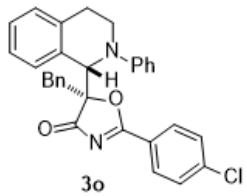
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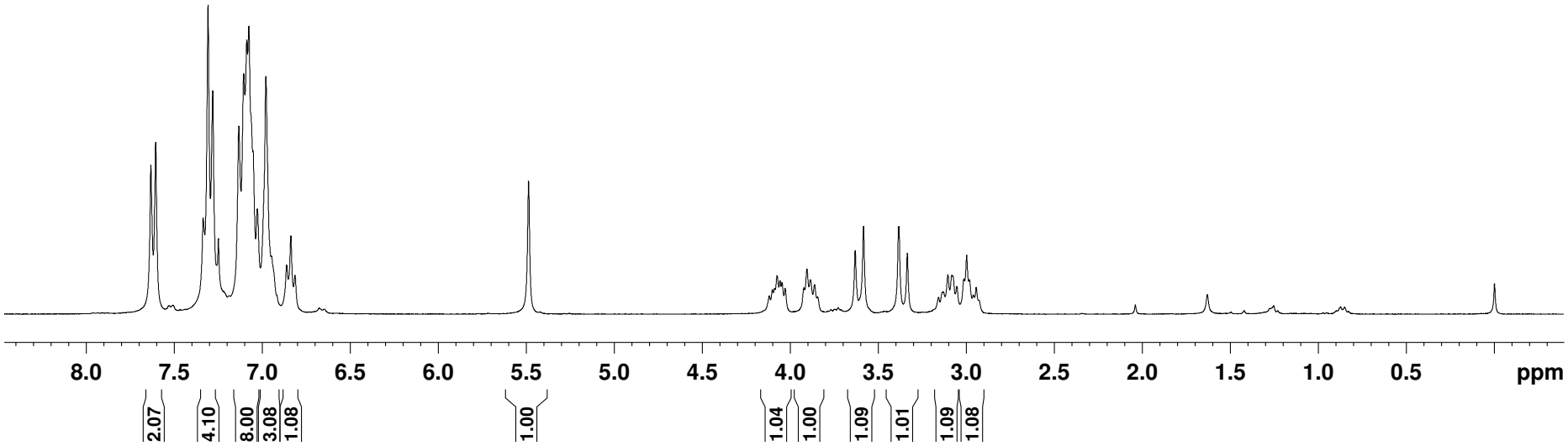
Bn
H
O
O
N
Cl

3o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1.5
1.0
0.5
ppm
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4.10
8.00
3.08
1.08
1.00
1.04
1.00
1.09
1.01
1.09
1.08

193.15
184.37
149.33
141.35
135.50
133.11
131.20
130.47
129.96
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129.11
128.27
128.18
127.78
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127.00
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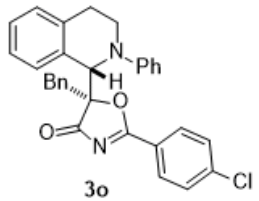

3o