Supporting Information

Iron-Catalyzed Synthesis of Benzoxazoles by Oxidative Coupling/Cyclization of Phenol Derivatives with Benzoyl Aldehyde Oximes

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1. General Information

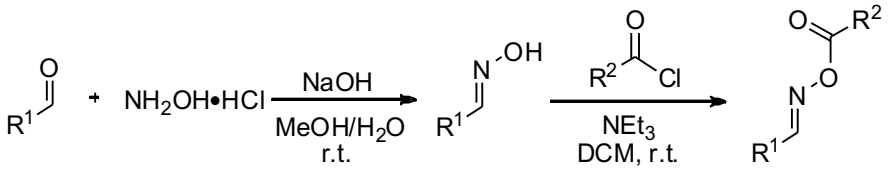
All glassware was oven dried at 100 ºC for more than 2 hours prior to use. Column chromatography was performed with silica gel (200-300 mesh). High-resolution mass spectra (HRMS) were obtained with a Waters-Q-TOF-Premier (ESI). ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker 400 MHz and 100 MHz instrument. ^{1}H NMR spectra are reported relative to Me_4Si (δ 0.0 ppm) and $CDCl_3$ (δ 7.26 ppm). ^{13}C NMR spectra are reported relative to $CDCl_3$ (δ 77.0 ppm). Splitting patterns are designated as follows: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet. Compounds were characterized by ^{1}H NMR, ^{13}C NMR and HRMS. Known products were characterized by comparison of ^{1}H and ^{13}C NMR spectroscopic data with those available in the literature. Melting points were determined on a melting point apparatus and uncorrected. GC-MS were obtained with Agilent Technologies 6890-5973N instrument.

2. Materials

Unless otherwise noted, all reagents were obtained from commercial suppliers and used without further purification. Toluene was dried and distilled from sodium/benzophenone ketyl under nitrogen atmosphere. 7-Methoxy-2-naphthol,[1] 6-methyl-2-naphthol,[2] ethyl 6-hydroxy-2-naphthoate,[3] hydrazone,[4] oxime ether,[5] *N*-benzylideneaniline,[6] *N*-(1-phenylethylidene)aniline,[7] were prepared according to the literature procedures.

Oxime esters **2** were prepared according to the reported methods.[8]

Method **I** for the preparation of oxime esters **2**:



Method **II** for the preparation of oxime esters **2**:

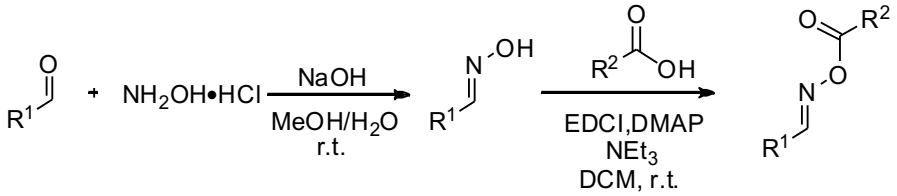
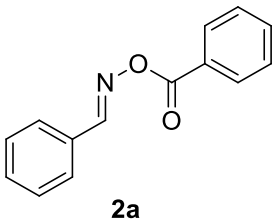
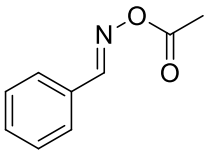
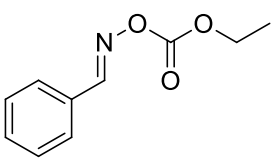
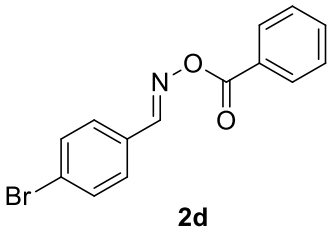
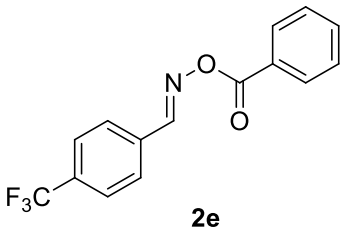
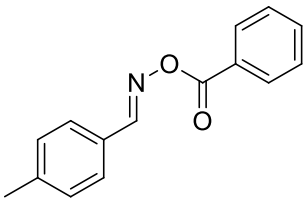
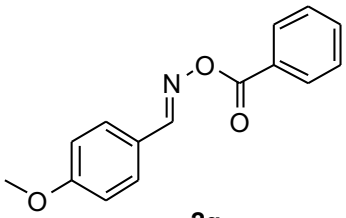
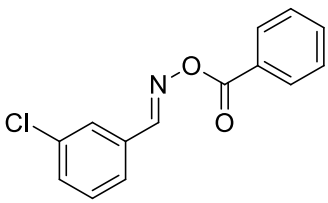
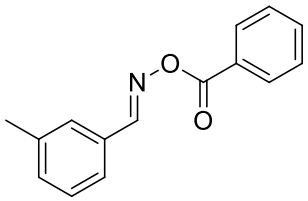


Table S1. Methods for the preparation of aldoxime carboxylates **2**

Aldoxime carboxylate	Method	Aldoxime carboxylate	Method
 **2a**	**I**	 **2b**	**I**
 **2c**	**I**	 **2d**	**I**
 **2e**	**I**	 **2f**	**I**
 **2g**	**I**	 **2h**	**I**



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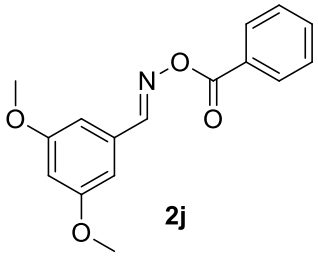

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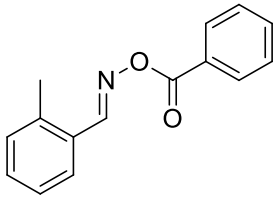

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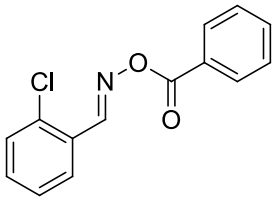

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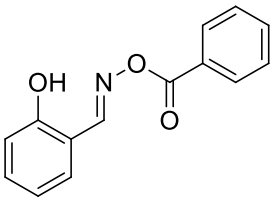

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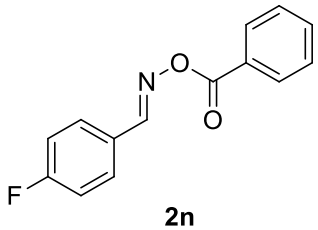

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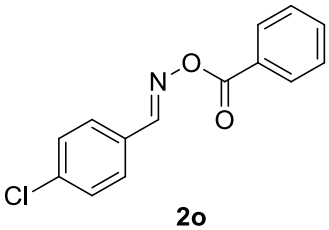

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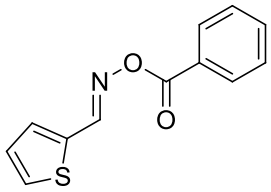

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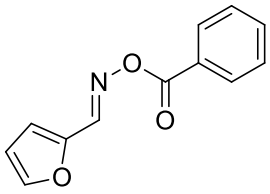

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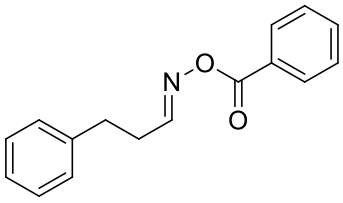

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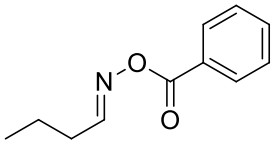

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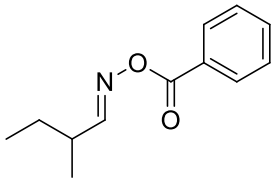

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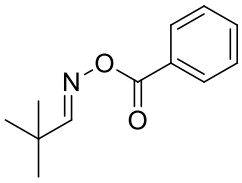
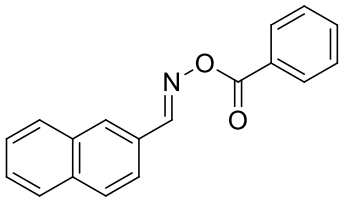


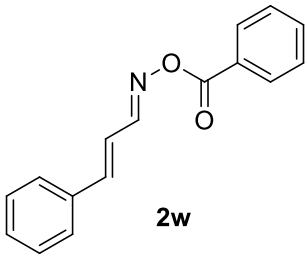
2u

II



2v

II

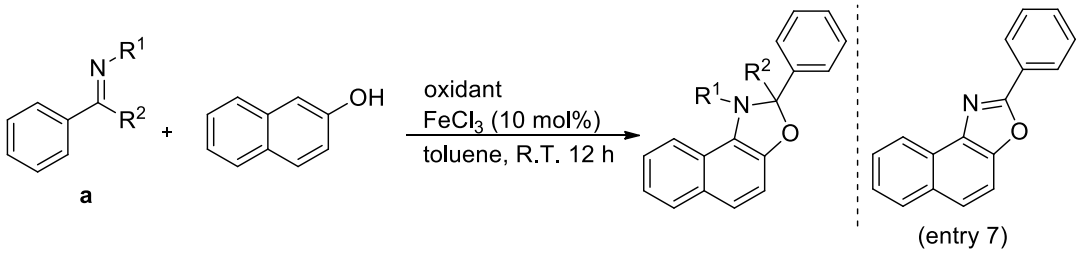


2w

II

3. Optimizing Reaction Conditions

Table S2. Oxidative cross-coupling/cyclization reaction of 2-naphthol with different compounds containing C=N scaffolds.[a]



Entry	R^1	R^2	Oxidant[b]	Product yield (%)[c]
1	NH_2	H	A/ B/ C/ D/ -	- / - / - / - / -
2	NH_2	Me	A/ B/ C/ D/ -	- / - / - / - / -
3	OH	H	A/ B/ C/ D/ -	- / - / - / - / -
4	OH	Me	A/ B/ C/ D/ -	- / - / - / - / -
5	OMe	H	A/ B/ C/ D/ -	- / - / - / - / -

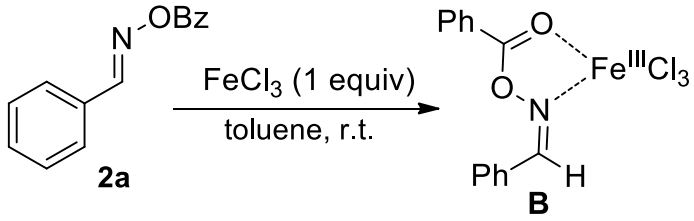
6	OMe	Me	A/ B/ C/ D/ -	- / - / - / - / -
7	**OBz**	**H**	**A/ B/ C/ D/ -**	**- / 27 / 10 / - / 35**
8	OBz	Me	A/ B/ C/ D/ -	- / - / - / - / -
9	Ph	Me	A/ B/ C/ D/ -	- / - / - / - / -
10	Ph	H	A/ B/ C/ D/ -	- / - / - / - / -

[a]The reaction was performed using naphthol (0.4 mmol), **a** (0.8 mmol), $FeCl_3$ (10 mol %), and oxidant (0.5 mmol) in 8 mL of toluene in Schlenk tubes at room temperature for 12 h under argon. [b]Oxidant: A = DDQ (dichlorodicyano benzoquinone), B = DTBP (di-*t*-butyl peroxide), C = TBHP (*tert*-butyl hydroperoxide), D = PIDA (phenyliodine diacetate). [c]Isolated yields are given for the related cases of using oxidants of A, B, C and D.

4. Procedure for Iron-Catalyzed Synthesis of Benzoxazole Derivatives

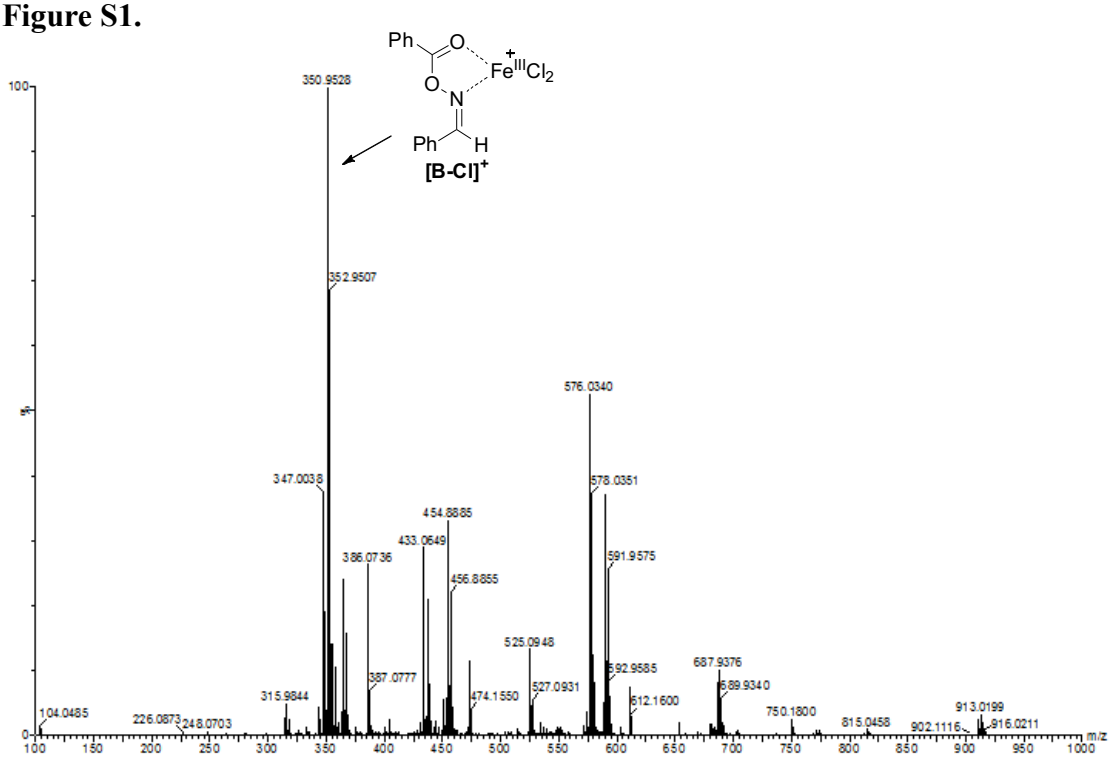
$FeCl_3$ (0.12 mmol) and phenol **1** (0.4 mmol) were added to an oven dried Schlenk tube. The tube was evacuated and filled with oxygen for three times, and then toluene (2 mL) was added. A solution of aldoxime carboxylate **2** (1.4 mmol) in 6 mL of toluene was added by a syringe pump over 3 hours at room temperature. After the addition completed, the reaction mixture was allowed to stir for additional 8 h at room temperature. After evaporation of the solvent, the residue was dissolved in ethyl acetate (20 mL), washed with saturated sodium bicarbonate solution (3 × 15 mL) and water (3 × 15 mL). The aqueous layer was extracted with ethyl acetate (2 × 15 mL). All organic fractions were combined and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel with petroleum ether/ethyl acetate (v/v) as the eluent to afford the desired products.

5. Mass Spectra of the Reaction Mixture



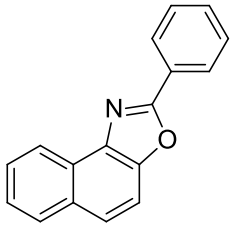
An oven dried Schlenk tube was charged with $FeCl_3$ (0.4 mmol), **2a** (0.8 mmol), and toluene (6 mL). The content of sealed tube was stirred at room temperature for 2 hours. The reaction mixture was directly analyzed by high-resolution mass spectrum measurement.

Figure S1.



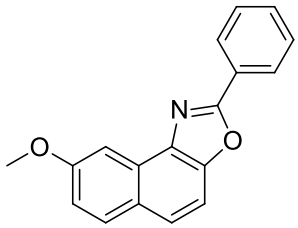
6. The Spectra Data of Products

2-Phenylnaphtho[1,2-*d*]oxazole **3a**[9]



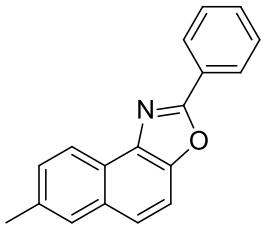
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 200/1, v/v) afforded **3a** as a white solid; mp = 132–133 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.61 (d, *J* = 8.4 Hz, 1H), 8.37–8.32 (m, 2H), 7.98 (d, *J* = 8.0 Hz, 1H), 7.82 (d, *J* = 8.8 Hz, 1H), 7.75 (d, *J* = 8.8 Hz, 1H), 7.68 (t, *J* = 8.0 Hz, 1H), 7.58–7.53 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 162.4, 148.1, 137.6, 131.3, 131.1, 128.9, 128.6, 127.6, 127.4, 127.0, 126.6, 126.0, 125.4, 122.3, 110.9. HRMS (ESI): *m*/*z* calcd for $C_{17}H_{12}NO$ $[M+H]^+$: 246.0913, found: 246.0912.

8-Methoxy-2-phenylnaphtho[1,2-*d*]oxazole **3b**



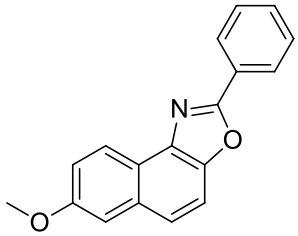
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 200/1, v/v) afforded **3b** as a white solid; mp = 135–137 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.34–8.32 (m, 2H), 7.89 (d, *J* = 2.8 Hz, 1H), 7.85 (d, *J* = 9.2 Hz, 1H), 7.73 (d, *J* = 8.8 Hz, 1H), 7.59–7.52 (m, 4H), 7.19 (dd, *J* = 8.8, 2.8 Hz, 1H), 4.05 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 162.0, 158.9, 148.6, 137.0, 131.0, 130.2, 128.9, 127.9, 127.6, 127.3, 126.4, 125.8, 118.0, 108.2, 100.8, 55.7. HRMS (ESI): *m*/*z* calcd for $C_{18}H_{14}NO_2$ $[M+H]^+$: 276.1019, found: 276.1017.

7-Methyl-2-phenylnaphtho[1,2-*d*]oxazole **3c**



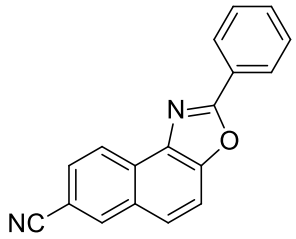
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 200/1, v/v) afforded **3c** as a white solid; mp = 140–141 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.48 (d, *J* = 8.4 Hz, 1H), 8.34–8.29 (m, 2H), 7.73–7.66 (m, 3H), 7.56–7.49 (m, 4H), 2.55 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 162.2, 147.7, 137.6, 135.0, 131.5, 131.0, 129.1, 128.9, 127.7, 127.6, 127.3, 125.4, 124.7, 122.1, 110.8, 21.7. HRMS (ESI): *m*/*z* calcd for $C_{18}H_{14}NO$ $[M+H]^+$: 260.1070, found: 260.1065.

7-Methoxy-2-phenylnaphtho[1,2-*d*]oxazole **3d**[9]



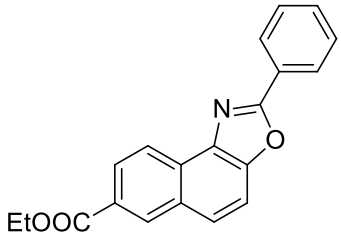
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 200/1, v/v) afforded **3d** as a white solid; mp = 128–129 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.48 (d, *J* = 8.8 Hz, 1H), 8.32–8.30 (m, 2H), 7.70–7.65 (m, 2H), 7.55–7.49 (m, 3H), 7.33 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.25 (d, *J* = 9.2 Hz, 1H), 3.94 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 162.3, 157.4, 146.9, 137.9, 132.5, 131.0, 128.9, 127.6, 127.3, 124.7, 123.8, 121.6, 119.1, 111.2, 107.3, 55.4. HRMS (ESI): *m*/*z* calcd for $C_{18}H_{14}NO_2$ $[M+H]^+$: 276.1019, found: 276.1020.

2-Phenylnaphtho[1,2-*d*]oxazole-7-carbonitrile **3e**



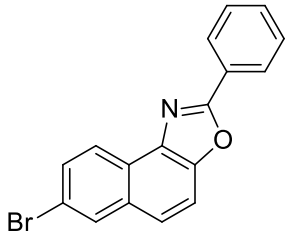
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 200/1, v/v) afforded **3e** as a white solid; mp > 250 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.67 (d, *J* = 8.4 Hz, 1H), 8.36–8.33 (m, 3H), 7.89–7.84 (m, 2H), 7.81 (d, *J* = 8.8 Hz,1H), 7.58–7.57 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 163.4, 149.7, 137.8, 134.6, 131.7, 130.1, 129.1, 128.1, 127.7, 127.6, 126.9, 126.2, 123.8, 119.2, 112.9, 109.0. HRMS (ESI): *m*/*z* calcd for $C_{18}H_{11}N_2O$ $[M+H]^+$: 271.0866, found: 271.0867.

Ethyl 2-phenylnaphtho[1,2-*d*]oxazole-7-carboxylate **3f**



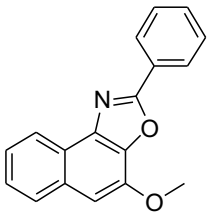
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **3f** as a white solid; mp = 166–168 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.71 (s, 1H), 8.59 (d, *J* = 8.4 Hz, 1H), 8.32–8.30 (m, 2H), 8.25 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.89 (d, *J* = 9.2 Hz, 1H), 7.76 (d, *J* = 9.2 Hz, 1H), 7.55–7.52 (m, 3H), 4.46 (q, *J* = 7.2 Hz, 2H), 1.47 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.7, 162.8, 149.4, 137.6, 131.5, 131.3, 130.3, 129.0, 128.8, 127.4, 127.3, 127.3, 127.2, 126.5, 122.5, 111.7, 61.2, 14.4. HRMS (ESI): *m*/*z* calcd for $C_{20}H_{16}NO_3$ $[M+H]^+$: 318.1125, found: 318.1129.

7-Bromo-2-phenylnaphtho[1,2-*d*]oxazole **3g**



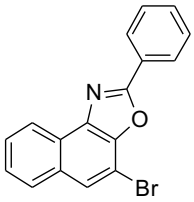
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 200/1, v/v) afforded **3g** as a white solid; mp = 172–173 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.45 (d, *J* = 8.8 Hz, 1H), 8.32–8.29 (m, 2H), 8.11 (d, *J* = 1.6 Hz, 1H), 7.75–7.72 (m, 2H), 7.68 (d, *J* = 8.8 Hz, 1H), 7.55–7.53 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 162.8, 148.1, 137.8, 132.3, 131.3, 130.6, 130.2, 129.0, 127.4, 127.3, 125.0, 124.9, 124.1, 119.3, 112.0. HRMS (ESI): *m*/*z* calcd for $C_{17}H_{11}BrNO$ $[M+H]^+$: 324.0019, found: 324.0027.

4-Methoxy-2-phenylnaphtho[1,2-*d*]oxazole **3h**



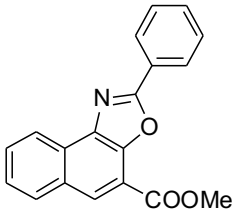
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **3h** as a white solid; mp = 123–124 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.51 (d, *J* = 7.2 Hz, 1H), 8.38–8.35 (m, 2H), 7.85 (d, *J* = 7.2 Hz, 1H), 7.56–7.51 (m, 5H), 7.14 (s, 1H), 4.15 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 161.5, 143.9, 138.8, 138.3, 131.2, 130.1, 127.8, 126.5, 126.3, 124.9, 123.6, 121.3, 121.2, 103.0, 55.1. HRMS (ESI): *m*/*z* calcd for $C_{18}H_{14}NO_2$ $[M+H]^+$: 276.1019, found: 276.1021.

4-Bromo-2-phenylnaphtho[1,2-*d*]oxazole **3i**



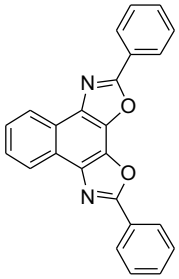
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **3i** as a slight yellow solid; mp = 139–140 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.52 (d, *J* = 8.4 Hz, 1H), 8.35–8.32 (m, 2H), 7.95 (s, 1H), 7.87–7.85 (d, *J* = 8.4 Hz, 1H), 7.66 (t, *J* = 8.0 Hz 1H), 7.56–7.52 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 162.5, 145.9, 138.2, 132.2, 131.5, 128.9, 127.9, 127.7, 127.6, 127.2, 127.0, 126.2, 125.6, 122.5, 102.6. HRMS (ESI): *m*/*z* calcd for $C_{17}H_{11}BrNO$ $[M+H]^+$: 324.0019, found: 324.0025.

Methyl 2-phenylnaphtho[1,2-*d*]oxazole-4-carboxylate **3j**



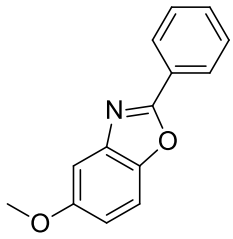
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **3j** as a white solid; mp = 152–153 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.59 (d, *J* = 8.4 Hz, 1H), 8.51 (s, 1H), 8.39–8.37 (m, 2H), 8.04 (d, *J* = 8.4 Hz, 1H), 7.76 (t, *J* = 8.0 Hz 1H), 7.61–7.55 (m, 4H), 4.11 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 164.8, 163.3, 145.7, 139.1, 131.4, 130.2, 129.9, 129.5, 129.3, 128.9, 128.7, 127.6, 127.2, 126.2, 122.4, 114.9, 52.5. HRMS (ESI): *m*/*z* calcd for $C_{19}H_{14}NO_3$ $[M+H]^+$: 304.0968, found: 304.0973.

2,5-Diphenylnaphtho[1,2-*d*:4,3-*d'*]bis(oxazole) **3k**



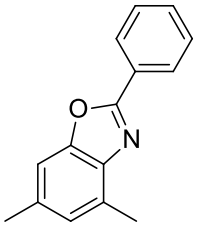
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 200/1, v/v) afforded **3k** as a white solid; mp > 220 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.67 (dd, *J* = 6.4, 3.2 Hz, 2H), 8.40–8.38 (m, 4H), 7.72 (dd, *J* = 6.4, 3.2 Hz, 2H), 7.61–7.56 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 162.2, 137.4, 133.9, 131.3, 129.0, 127.4, 127.1, 126.5, 124.1, 123.1. HRMS (ESI): *m*/*z* calcd for $C_{24}H_{15}N_2O_2$ $[M+H]^+$: 363.1128, found: 363.1130.

5-Methoxy-2-phenylbenzo[*d*]oxazole **3l**



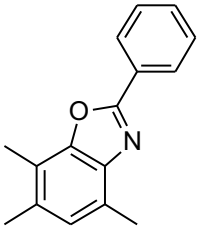
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 50/1, v/v) afforded **3l** as a white solid; mp = 78–79 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.25–8.22 (m, 2H), 7.53–7.51 (m, 3H), 7.47 (d, *J* = 8.8 Hz, 1H), 7.27 (s, 1H), 6.95 (dd, *J* = 8.8, 2.4 Hz, 1H), 3.88 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 163.8, 157.4, 145.4, 142.9, 131.5, 128.9, 127.5, 127.3, 113.7, 110.8, 102.8, 55.9. HRMS (ESI): *m*/*z* calcd for $C_{14}H_{12}NO_2$ $[M+H]^+$: 226.0863, found: 226.0867.

4,6-Dimethyl-2-phenylbenzo[*d*]oxazole **3m**



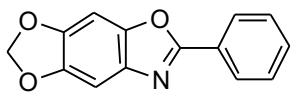
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **3m** as a white solid; mp = 130–131 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.26–8.23 (m, 2H), 7.52–7.50 (m, 3H), 7.20 (s, 1H), 6.98 (s, 1H), 2.64 (s, 3H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 161.8, 150.9, 139.3, 135.1, 131.0, 129.8, 128.8, 127.6, 127.4, 126.4, 108.0, 21.8, 16.5. HRMS (ESI): *m*/*z* calcd for $C_{15}H_{14}NO$ $[M+H]^+$: 224.1070, found :224.1074.

4,6,7-Trimethyl-2-phenylbenzo[*d*]oxazole **3n**



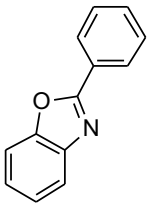
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 200/1, v/v) afforded **3n** as colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.28–8.26 (m, 2H), 7.53–7.50 (m, 3H), 6.96 (s, 1H), 2.61 (s, 3H), 2.46 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 161.7, 150.2, 138.9, 133.4, 130.9, 128.8, 127.8, 127.4, 126.9, 126.6, 116.3, 19.2, 16.2, 12.1. HRMS (ESI): *m*/*z* calcd for $C_{16}H_{16}NO$ $[M+H]^+$: 238.1226, found: 238.1231.

6-Phenyl-[1,3]dioxolo[4',5':4,5]benzo[1,2-*d*]oxazole **3o**



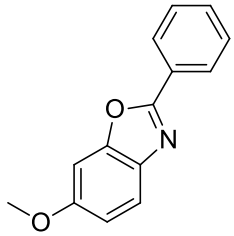
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **3o** as a white solid; mp = 147–148 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ =8.17–8.14 (m, 2H), 7.50–7.48 (m, 3H), 7.17 (s, 1H), 7.06 (s, 1H), 6.03 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 162.6, 146.4, 145.8, 145.7, 136.1, 130.9, 128.9, 127.4, 127.0, 101.7, 99.5, 92.6. HRMS (ESI): *m*/*z* calcd for $C_{14}H_{10}NO_3$ $[M+H]^+$: 240.0655, found: 240.0652.

2-Phenylbenzo[d]oxazole **3p**



Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **3p** as white solid; mp = 101–102 ^{o}C ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.26 (d, *J* = 5.2 Hz, 2H), 7.80–7.78 (m, 1H), 7.60–7.57 (m, 1H), 7.54–7.50 (m, 3H), 7.38–7.34 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 163.1, 150.8, 142.1, 131.5, 128.9, 127.6, 127.2, 125.1, 124.6, 120.0, 110.6. HRMS (ESI): *m*/*z* calcd for $C_{13}H_{10}NO$ $[M+H]^+$: 196.0757, found: 196.0763.

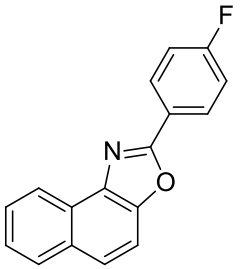
6-Methoxy-2-phenylbenzo[*d*]oxazole **3q**



Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 50/1, v/v) afforded **3q** as colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.21–8.19 (m, 2H), 7.64 (d, *J* = 8.8 Hz, 1H), 7.51–7.49 (m, 3H), 7.11 (d, *J* = 2.4 Hz, 1H), 6.95 (dd, *J*

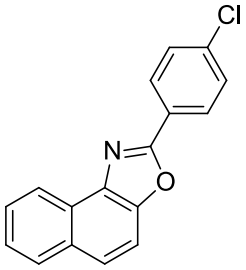
= 8.8, 2.4 Hz, 1H), 3.88 (s, 3H) ; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 162.3, 158.3, 151.7, 135.9, 131.1, 128.9, 127.4, 127.2, 120.0, 112.8, 95.5, 56.0. HRMS (ESI): *m*/*z* calcd for $C_{14}H_{12}NO_2$ $[M+H]^+$: 226.0863, found: 226.0870.

2-(4-Fluorophenyl)naphtho[1,2-*d*]oxazole **3r**[9]



Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 200/1, v/v) afforded **3r** as a white solid; mp = 166–167 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.56 (d, *J* = 8.4 Hz, 1H), 8.31–8.28 (m, 2H), 7.95 (d, *J* = 8.4 Hz, 1H), 7.78 (d, *J* = 8.8 Hz, 1H), 7.68–7.64 (m, 2H), 7.54 (t, *J* = 7.2 Hz, 1H), 7.21 (t, *J* = 8.8, 2H), ; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 164.5 (d, *J* = 250.5 Hz) 161.5, 148.1, 137.6, 131.3, 129.5 (d, *J* = 8.7 Hz), 128.6, 127.0, 126.5, 126.1, 125.4, 123.8 (d, *J* = 3.2 Hz), 122.2, 116.2 (d, *J* = 22.1 Hz), 110.8; ^{19}F NMR (377 MHz, $CDCl_3$): δ = –108.2. HRMS (ESI): *m*/*z* calcd for $C_{17}H_{11}FNO$ $[M+H]^+$: 264.0819, found: 264.0816.

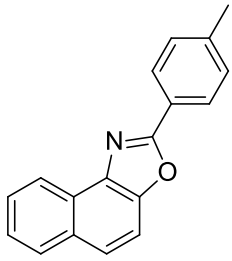
2-(4-Chlorophenyl)naphtho[1,2-*d*]oxazole **3s**[9]



Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 200/1, v/v) afforded **3s** as a white solid; mp = 189–190 °C; ^{1}H NMR (400 MHz, $CDCl_3$):

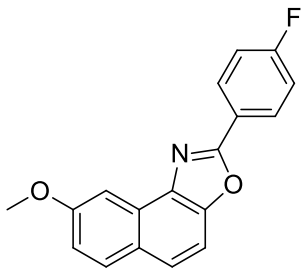
δ = 8.57 (d, *J* = 8.0 Hz, 1H), 8.28–8.24 (m, 2H), 7.98 (d, *J* = 8.4 Hz, 1H), 7.82 (d, *J* = 9.2 Hz, 1H), 7.72 (d, *J* = 9.2 Hz, 1H), 7.68 (dt, *J* = 8.0, 1.2 Hz, 1H), 7.56 (dt, *J* = 8.0, 1.2 Hz, 1H), 7.53–7.50 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 161.3, 148.1, 137.6, 137.2, 131.2, 129.2, 128.6, 128.5, 127.1, 126.5, 126.3, 126.0, 125.5, 122.2, 110.7. HRMS (ESI): *m*/*z* calcd for $C_{17}H_{11}ClNO$ $[M+H]^+$: 280.0524, found: 280.0525.

2-(*p*-Tolyl)naphtho[1,2-*d*]oxazole **3t**[9]



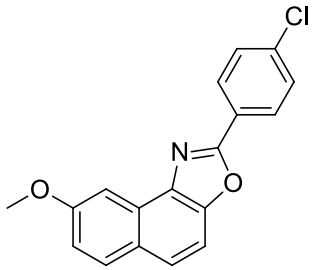
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 200/1, v/v) afforded **3t** as a white solid; mp = 167–168 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.60 (d, *J* = 8.4 Hz, 1H), 8.23 (d, *J* = 8.4 Hz, 2H), 7.97 (d, *J* = 8.0 Hz, 1H), 7.80 (d, *J* = 8.8 Hz, 1H), 7.73 (d, *J* = 8.8 Hz, 1H), 7.67 (dt, *J* = 8.4, 1.2 Hz, 1H), 7.55 (dt, *J* = 8.0, 1.2 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 2H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 161.6, 146.8, 140.5, 136.6, 130.1, 128.6, 127.5, 126.3, 125.8, 125.5, 124.7, 124.2, 123.7, 121.2, 109.7, 20.6. HRMS (ESI): *m*/*z* calcd for $C_{18}H_{14}NO$ $[M+H]^+$: 260.1070, found: 260.1075.

2-(4-Fluorophenyl)-8-methoxynaphtho[1,2-*d*]oxazole **3u**



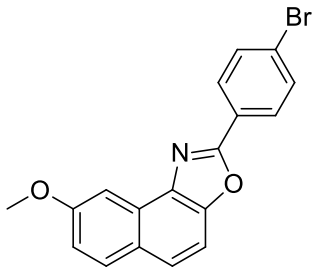
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **3u** as a white solid; mp = 153–154 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.33–8.28 (m, 2H), 7.85–7.83 (m, 2H), 7.71 (d, *J* = 8.8 Hz, 1H), 7.55 (d, *J* = 8.8 Hz, 1H), 7.25–7.20 (m, 2H), 7.18 (dd, *J* = 8.8, 2.4 Hz, 1H), 4.04 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 164.5 (d, *J* = 250.5 Hz), 161.1, 158.9, 148.6, 136.9, 130.2, 129.5 (d, *J* = 8.7 Hz), 127.9, 126.4, 125.9, 123.9 (d, *J* = 3.1 Hz), 118.1, 116.2 (d, *J* = 22.1 Hz), 108.1, 100.8, 55.6; ^{19}F NMR (377 MHz, $CDCl_3$): δ = –108.3. HRMS (ESI): *m*/*z* calcd for $C_{18}H_{13}FNO_2$ $[M+H]^+$: 294.0925, found: 294.0927.

2-(4-Chlorophenyl)-8-methoxynaphtho[1,2-*d*]oxazole **3v**



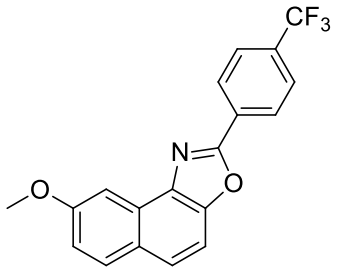
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **3v** as a white solid; mp = 173–174 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.24 (d, *J* = 8.4 Hz, 2H), 7.86–7.84 (m, 2H), 7.73 (d, *J* = 8.8 Hz, 1H), 7.55 (d, *J* = 8.8 Hz, 1H), 7.51 (d, *J* = 8.4 Hz, 2H), 7.19 (dd, *J* = 8.8, 2.4 Hz, 1H), 4.04 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 161.0, 158.9, 148.7, 137.2, 137.0, 130.2, 129.3, 128.5, 127.9, 126.4, 126.1, 118.1, 108.1, 100.8, 55.6. HRMS (ESI): *m*/*z* calcd for $C_{18}H_{13}ClNO_2$ $[M+H]^+$: 310.0629, found: 310.0622.

2-(4-Bromophenyl)-8-methoxynaphtho[1,2-*d*]oxazole **3w**



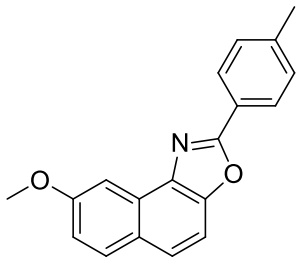
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **3w** as a white solid; mp = 186–187 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.17–8.13 (m, 2H), 7.84–7.82 (m, 2H), 7.71 (d, *J* = 8.8 Hz, 1H),7.67–7.64 (m, 2H), 7.53 (d, *J* = 8.8 Hz, 1H), 7.17 (dd, *J* = 8.8, 2.4 Hz, 1H), 4.03 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 161.0, 158.9, 148.6, 136.9, 132.2, 130.2, 128.7, 127.9, 126.5, 126.4, 126.1, 125.6, 118.1, 108.1, 100.8, 55.6. HRMS (ESI): *m*/*z* calcd for $C_{18}H_{13}BrNO_2$ $[M+H]^+$: 354.0124, found: 354.0128.

8-Methoxy-2-(4-(trifluoromethyl)phenyl)naphtho[1,2-*d*]oxazole **3x**



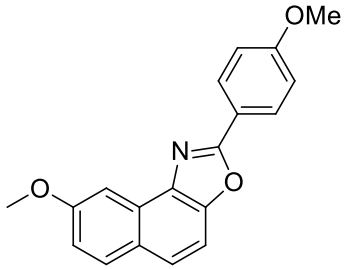
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **3x** as a white solid; mp = 145–146 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.38 (d, *J* = 8.4 Hz, 2H), 7.86–7.82 (m, 2H), 7.77 (d, *J* = 8.0 Hz, 2H), 7.73 (d, *J* = 8.8 Hz, 1H), 7.54 (d, *J* = 8.8 Hz, 1H), 7.19 (dd, *J* = 8.8, 2.4 Hz, 1H), 4.04 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 160.3, 159.0, 148.8, 136.9, 132.4 (q, *J* = 32.6 Hz), 130.7, 130.2, 127.9, 127.4, 126.6, 126.4, 125.8 (q, *J* = 3.7Hz), 123.8 (q, *J* = 270.7 Hz), 118.1, 108.0, 100.8, 55.6; ^{19}F NMR (377 MHz, $CDCl_3$): δ = –62.8. HRMS (ESI): *m*/*z* calcd for $C_{19}H_{13}F_3NO_2$ $[M+H]^+$: 344.0893, found: 344.0890.

8-Methoxy-2-(p-tolyl)naphtho[1,2-*d*]oxazole **3y**



Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **3y** as a white solid; mp = 165–166 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.21 (d, *J* = 8.0 Hz, 2H), 7.87 (d, *J* = 2.4 Hz, 1H), 7.84 (d, *J* = 9.2 Hz, 1H), 7.71 (d, *J* = 8.8 Hz, 1H), 7.57 (d, *J* = 8.8 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 2H), 7.17 (dd, *J* = 8.8, 2.4 Hz, 1H), 4.05 (s, 3H), 2.45 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 162.3, 158.8, 148.5, 141.5, 137.0, 130.2, 129.7, 127.9, 127.3, 126.4, 125.6, 124.9, 117.9, 108.1, 100.8, 55.6, 21.6. HRMS (ESI): *m*/*z* calcd for $C_{19}H_{16}NO_2$ $[M+H]^+$: 290.1176, found: 290.1175.

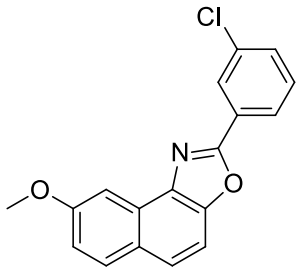
8-Methoxy-2-(4-methoxyphenyl)naphtho[1,2-*d*]oxazole **3z**



Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **3z** as a white solid; mp = 109–110 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.27–8.23 (m, 2H), 7.86–7.82 (m, 2H), 7.69 (d, *J* = 8.8 Hz, 1H), 7.55 (d, *J* = 8.8 Hz, 1H), 7.16 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.06–7.02 (m, 2H), 4.03 (s, 3H), 3.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 162.2, 162.0, 158.7, 148.4, 137.1, 130.2, 129.1, 127.8,

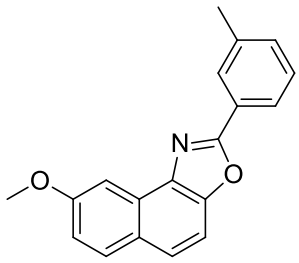
126.4, 125.3, 120.2, 117.9, 114.4, 108.1, 100.8, 55.6, 55.5. HRMS (ESI): *m*/*z* calcd for $C_{19}H_{16}NO_3$ $[M+H]^+$: 306.1125, found: 306.1122.

2-(3-Chlorophenyl)-8-methoxynaphtho[1,2-*d*]oxazole **3aa**



Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **3aa** as a white solid; mp = 139–141 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.29 (s, 1H), 8.16 (d, *J* = 6.8 Hz, 1H), 7.84–7.82 (m, 2H), 7.71 (d, *J* = 8.8 Hz, 1H), 7.53 (d, *J* = 8.8 Hz, 1H), 7.49–7.42 (m, 2H), 7.17 (dd, *J* = 8.8, 2.4 Hz, 1H), 4.03 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 160.5, 158.9, 148.7, 136.9, 135.0, 130.9, 130.2, 129.2, 127.9, 127.3, 126.4, 126.3, 125.3, 118.1, 108.1, 100.8, 55.6. HRMS (ESI): *m*/*z* calcd for $C_{18}H_{13}ClNO_2$ $[M+H]^+$: 310.0629, found: 310.0628.

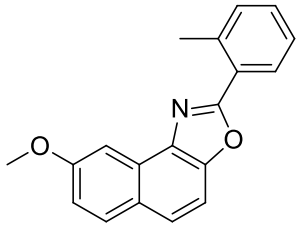
8-Methoxy-2-(m-tolyl)naphtho[1,2-*d*]oxazole **3ab**



Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **3ab** as a white solid; mp = 118–119 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.15 (s, 1H), 8.11 (d, *J* = 7.6 Hz, 1H), 7.88 (d, *J* = 2.4 Hz, 1H), 7.84 (d, *J* = 8.8 Hz, 1H), 7.71 (d, *J* = 8.8 Hz, 1H), 7.56 (d, *J* = 8.8 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 1H),

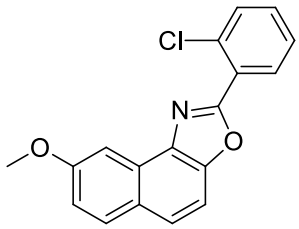
7.33 (d, J = 7.6 Hz, 1H), 7.17 (dd, J = 8.8, 2.4 Hz, 1H), 4.04 (s, 3H), 2.48 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 162.2, 158.8, 148.6, 138.7, 137.0, 131.9, 130.2, 128.9, 127.9, 127.4, 126.4, 125.8, 124.5, 118.0, 108.2, 100.8, 55.7, 21.4. HRMS (ESI): *m*/*z* calcd for $C_{19}H_{16}NO_2$ $[M+H]^+$: 290.1176, found: 290.1178.

8-Methoxy-2-(*o*-tolyl)naphtho[1,2-*d*]oxazole **3ac**



Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **3ac** as a white solid; mp = 84–85 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.23–8.21 (m, 1H), 7.87–7.84 (m, 2H), 7.72 (d, J = 8.8 Hz, 1H), 7.57 (d, J = 8.8 Hz, 1H), 7.43–7.34 (m, 3H), 7.18 (dd, J = 8.8, 2.4 Hz, 1H), 4.03 (s, 3H), 2.87 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 162.4, 158.8, 148.2, 138.4, 136.8, 131.8, 130.5, 130.2, 129.8, 128.0, 126.7, 126.1, 125.7, 117.8, 108.2, 100.9, 55.6, 22.2. HRMS (ESI): *m*/*z* calcd for $C_{19}H_{16}NO_2$ $[M+H]^+$: 290.1176, found: 290.1173.

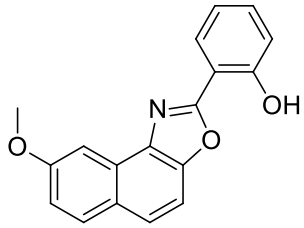
2-(2-Chlorophenyl)-8-methoxynaphtho[1,2-*d*]oxazole **3ad**



Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **3ad** as a white solid; mp = 116–117 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.22–8.18 (m, 1H), 7.88–7.85 (m, 2H), 7.76 (d, J = 8.8 Hz, 1H), 7.60 (d, J

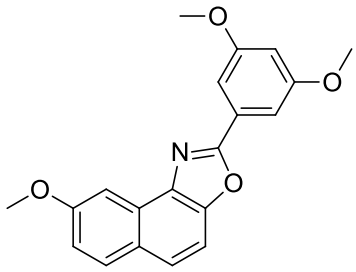
= 8.8 Hz, 1H), 7.59–7.56 (m, 1H), 7.47–7.41 (m, 2H), 7.20 (dd, *J* = 8.8, 2.4 Hz, 1H), 4.03(s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 159.9, 159.0, 148.7, 136.6, 133.3, 131.8, 131.6, 131.3, 130.2, 128.0, 127.0, 126.8, 126.4, 118.1, 108.2, 100.9, 55.7. HRMS (ESI): *m*/*z* calcd for $C_{18}H_{13}ClNO_2$ $[M+H]^+$: 310.0629, found: 310.0630.

2-(8-Methoxynaphtho[1,2-*d*]oxazol-2-yl)phenol **3ae**



Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **3ae** as a white solid; mp = 195–196 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 11.58 (br, 1H), 8.04 (dd, *J* = 7.6, 1.6 Hz 1H), 7.84 (d, *J* = 8.8 Hz, 1H), 7.73 (d, *J* = 8.8 Hz, 1H), 7.68 (d, *J* = 2.4 Hz, 1H), 7.57 (d, *J* = 8.8, Hz, 1H), 7.44 (ddd, *J* = 8.8, 7.6, 1.6 Hz, 1H), 7.20–7.15 (m, 2H), 7.03 (td, *J* = 8.0, 1.2 Hz, 1H), 4.02 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 161.6, 159.0, 158.1, 147.0, 134.8, 133.1, 130.3, 126.9, 126.8, 126.5, 126.2, 119.7, 118.2, 117.3, 111.0, 107.9, 100.7, 55.7. HRMS (ESI): *m*/*z* calcd for $C_{18}H_{14}NO_3$ $[M+H]^+$: 292.0968, found: 292.0961.

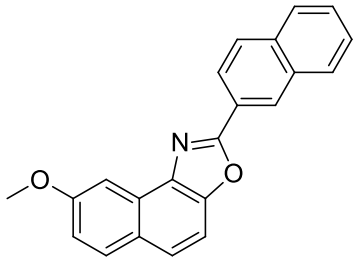
2-(3,5-Dimethoxyphenyl)-8-methoxynaphtho[1,2-*d*]oxazole **3af**



Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **3af** as a white solid; mp = 161–162 °C; ^{1}H NMR (400 MHz,

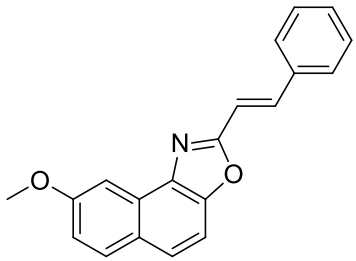
$CDCl_3$): δ = 7.87 (d, *J* = 2.4 Hz, 1H), 7.84 (d, *J* = 8.8 Hz, 1H), 7.72 (d, *J* = 8.8 Hz, 1H), 7.56 (d, *J* = 8.8 Hz, 1H), 7.48 (d, *J* = 2.4 Hz, 2H), 7.18 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.63 (t, *J* = 2.4 Hz, 1H), 4.05 (s, 3H), 3.93 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 161.9, 161.1, 158.8, 148.6, 136.9, 130.2, 129.2, 127.9, 126.4, 126.0, 118.0, 108.1, 105.0, 104.1, 100.8, 55.7, 55.6. HRMS (ESI): *m*/*z* calcd for $C_{20}H_{18}NO_4$ $[M+H]^+$: 336.1230, found: 336.1223.

8-Methoxy-2-(naphthalen-2-yl)naphtho[1,2-*d*]oxazole **3ag**



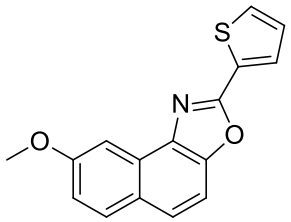
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **3ag** as a white solid; mp = 169–170 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.76 (s, 1H), 8.36 (dd, *J* = 8.8, 1.6 Hz, 1H), 7.98–7.94 (m, 2H), 7.88–7.85 (m, 2H), 7.82 (d, *J* = 8.8 Hz, 1H), 7.69 (d, *J* = 8.8 Hz, 1H), 7.57–7.51 (m, 3H), 7.17 (dd, *J* = 8.8, 2.4 Hz, 1H), 4.03 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 162.1, 158.9, 148.7, 137.1, 134.5, 133.1, 130.2, 128.9, 128.7, 128.0, 127.9, 127.6, 127.5, 126.9, 126.4, 125.9, 124.8, 124.0, 118.0, 108.1, 100.8, 55.7. HRMS (ESI): *m*/*z* calcd for $C_{22}H_{16}NO_2$ $[M+H]^+$: 326.1176, found: 326.1175.

8-Methoxy-2-styrylnaphtho[1,2-*d*]oxazole **3ah**



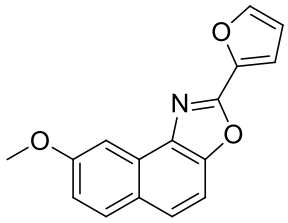
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **3ah** as a white solid; mp = 123–124 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.83 (d, *J* = 8.8 Hz, 1H), 7.80–7.76 (m, 2H), 7.71 (d, *J* = 8.8 Hz, 1H), 7.61 (d, *J* = 7.2 Hz, 2H), 7.52 (d, *J* = 8.8 Hz, 1H), 7.44–7.35 (m, 3H), 7.21–7.16 (m, 2H), 4.01 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 161.8, 158.9, 148.3, 138.2, 137.0, 135.4, 130.2, 129.6, 129.0, 127.7, 127.4, 126.3, 126.1, 118.1, 114.1, 107.9, 100.6, 55.7. HRMS (ESI): *m*/*z* calcd for $C_{20}H_{16}NO_2$ $[M+H]^+$: 302.1176, found: 302.1180.

8-Methoxy-2-(thiophen-2-yl)naphtho[1,2-*d*]oxazole **3ai**



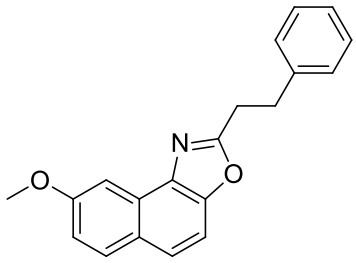
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 50/1, v/v) afforded **3ai** as a white solid; mp = 180–181 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.93 (dd, *J* = 3.6, 1.2 Hz, 1H), 7.85–7.82 (m, 2H), 7.71 (d, *J* = 8.8 Hz, 1H), 7.55–7.53 (m, 2H), 7.21–7.16 (m, 2H), 4.04 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 158.8, 158.0, 148.2, 136.8, 130.2, 130.1, 129.5, 129.2, 128.2, 127.7, 126.5, 125.8, 118.1, 107.9, 100.9, 55.7. HRMS (ESI): *m*/*z* calcd for $C_{16}H_{12}NO_2S$ $[M+H]^+$: 282.0583, found: 282.0575.

2-(Furan-2-yl)-8-methoxynaphtho[1,2-*d*]oxazole **3aj**



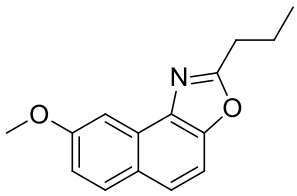
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 50/1, v/v) afforded **3aj** as a white solid; mp = 106–107 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.87 (d, *J* = 2.4 Hz, 1H), 7.83 (d, *J* = 8.8 Hz, 1H), 7.72–7.68 (m, 2H), 7.53 (d, *J* = 8.8 Hz, 1H), 7.25 (s, 1H), 7.17 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.63–6.61 (m, 1H), 4.00 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 158.9, 154.3, 148.0, 145.3, 142.9, 136.5, 130.1, 127.8, 126.5, 126.1, 118.3, 113.3, 112.2, 107.9, 100.8, 55.7. HRMS (ESI): *m*/*z* calcd for $C_{16}H_{12}NO_3$ $[M+H]^+$: 266.0812, found: 266.0806.

8-Methoxy-2-phenethylnaphtho[1,2-*d*]oxazole **3ak**



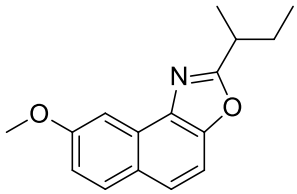
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **3ak** as a colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.80 (d, *J* = 8.8 Hz, 1H), 7.74 (d, *J* = 2.4 Hz, 1H), 7.65 (d, *J* = 8.8 Hz, 1H), 7.47 (d, *J* = 8.8 Hz, 1H), 7.31–7.25 (m, 4H), 7.24–7.19 (m, 1H), 7.14 (dd, *J* = 8.8, 2.4 Hz, 1H), 3.98 (s, 3H), 3.37–3.30 (m, 2H), 3.27–3.22 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.0, 158.8, 148.6, 140.3, 135.8, 130.1, 128.7, 128.4, 127.7, 126.5, 126.2, 125.2, 117.9 108.1, 100.5, 55.6, 33.5, 30.9. HRMS (ESI): *m*/*z* calcd for $C_{20}H_{18}NO_2$ $[M+H]^+$: 304.1332, found: 304.1329.

8-Methoxy-2-propylnaphtho[1,2-*d*]oxazole **3al**



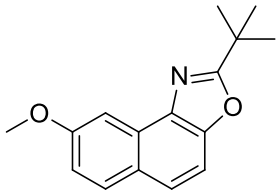
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **3al** as a colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.82 (d, *J* = 8.8 Hz, 1H), 7.74 (d, *J* = 2.4 Hz, 1H), 7.66 (d, *J* = 8.8 Hz, 1H), 7.48 (d, *J* = 8.8 Hz, 1H) 7.14 (dd, *J* = 8.8, 2.4 Hz, 1H), 3.99 (s, 3H), 3.01 (t, *J* = 7.2 Hz, 2H), 2.01–1.92 (m, 2H), 1.08 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.9, 158.7, 148.5, 135.8, 130.1, 127.6, 126.1, 125.0, 117.8, 108.1, 100.4, 55.6, 30.8, 20.9, 13.8. HRMS (ESI): *m*/*z* calcd for $C_{15}H_{16}NO_2$ $[M+H]^+$: 242.1176, found: 242.1177.

2-(2-Butyl)-8-methoxynaphtho[1,2-*d*]oxazole **3am**



Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **3am** as a colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.82 (d, *J* = 8.8 Hz, 1H), 7.76 (d, *J* = 2.4 Hz, 1H), 7.66 (d, *J* = 8.8 Hz, 1H), 7.50 (d, *J* = 8.8 Hz, 1H), 7.14 (dd, *J* = 8.8, 2.4 Hz, 1H), 4.00 (s, 3H), 3.22-3.13 (m, 1H), 2.05–1.94 (m, 1H), 1.86–1.75 (m, 1H), 1.48 (d, *J* = 7.2 Hz, 3H), 0.98 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 169.4, 158.7, 148.4, 135.7, 130.1, 127.7, 126.1, 124.9, 117.8, 108.1, 100.5, 55.6, 36.2, 28.4, 18.3, 11.9. HRMS (ESI): *m*/*z* calcd for $C_{16}H_{18}NO_2$ $[M+H]^+$: 256.1332, found: 256.1335.

2-(tert-Butyl)-8-methoxynaphtho[1,2-*d*]oxazole **3an**



Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **3an** as a colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.81 (d, *J* = 8.8 Hz, 1H), 7.78 (d, *J* = 2.4 Hz, 1H), 7.66 (d, *J* = 8.8 Hz, 1H), 7.49 (d, *J* = 8.8 Hz, 1H), 7.14 (dd, *J* = 8.8, 2.4 Hz, 1H), 4.02 (s, 3H), 1.56 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 172.2, 158.6, 148.5, 135.8, 130.1, 127.8, 126.1, 124.9, 117.7, 108.1, 100.7, 55.6, 34.4, 28.8. HRMS (ESI): *m*/*z* calcd for $C_{16}H_{18}NO_2$ $[M+H]^+$: 256.1332, found: 256.1331.

7. References

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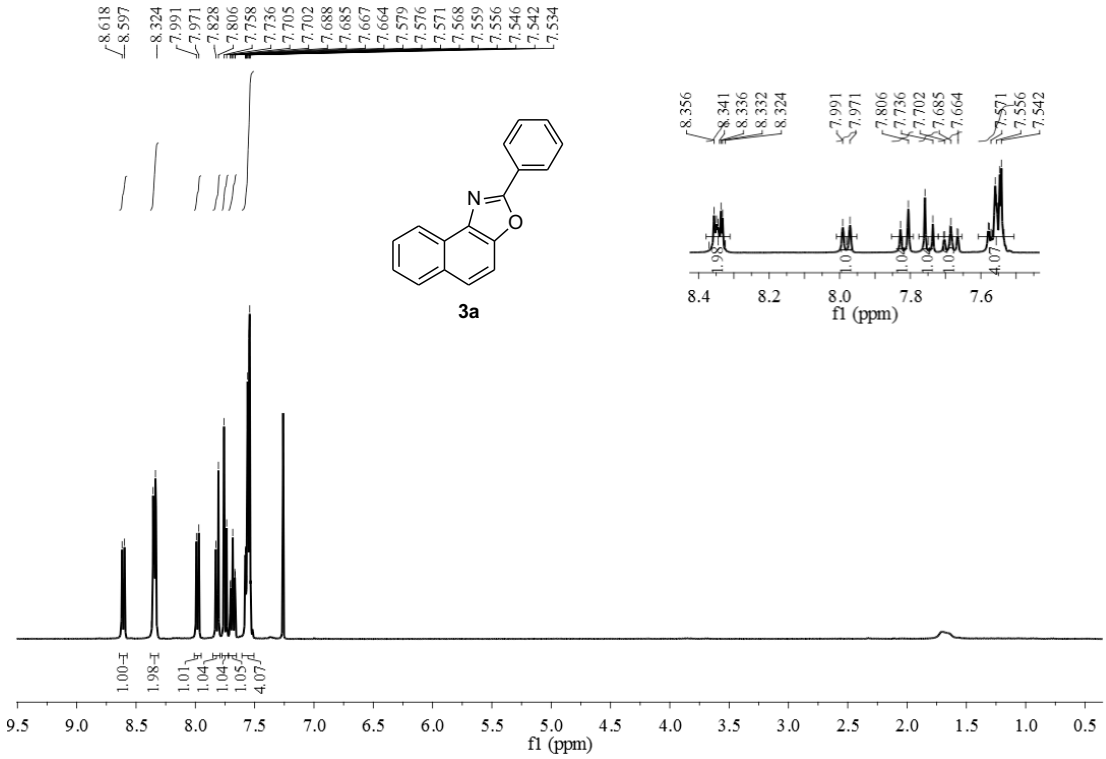
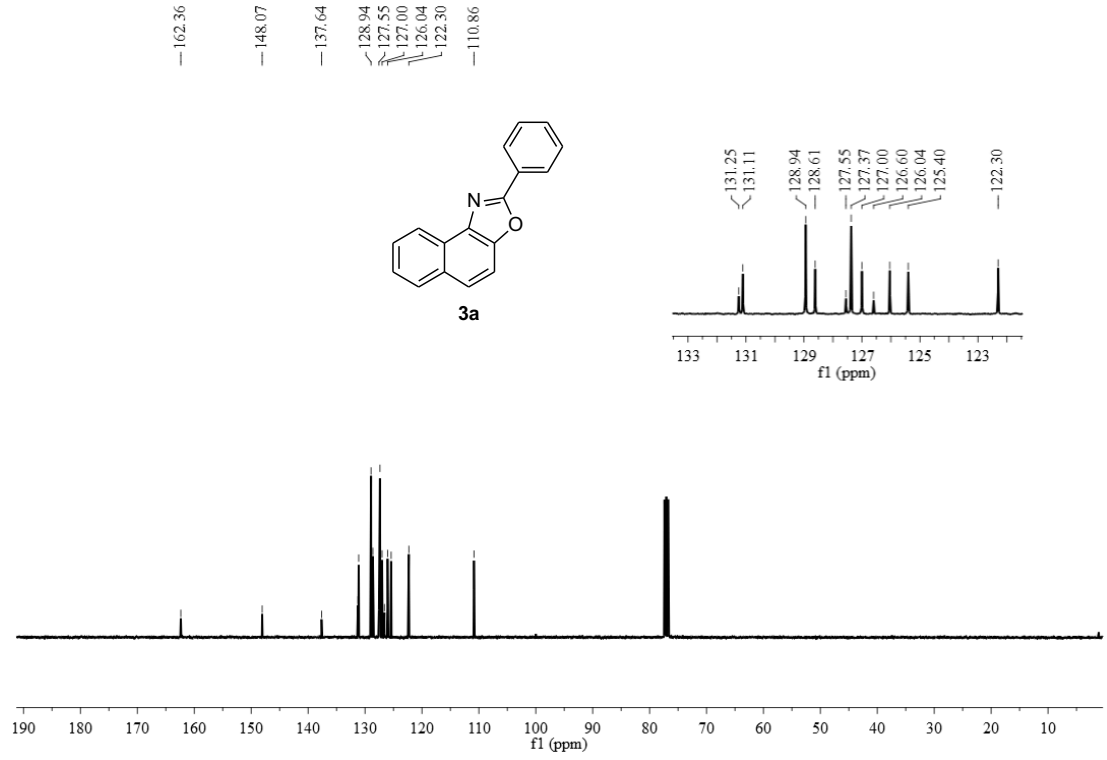
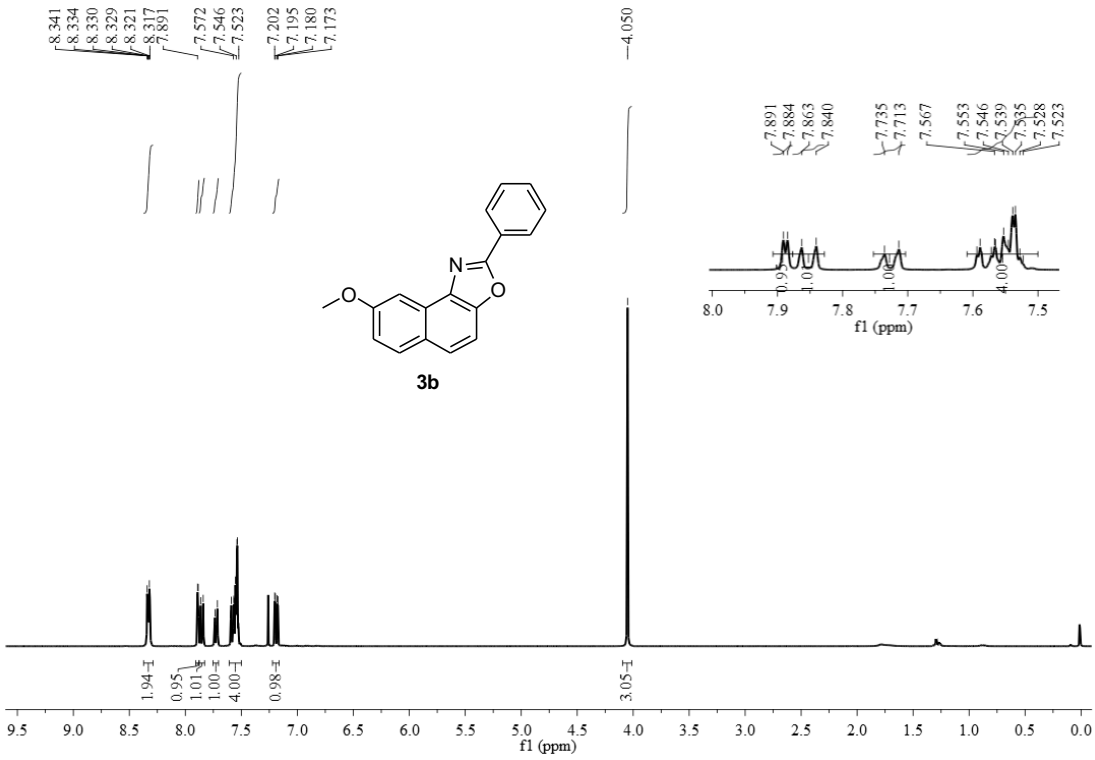
8. ^{1}H, ^{13}C and ^{19}F NMR Spectra



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8.321
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7.572
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7.523
7.202
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7.173
4.050
7.891
7.884
7.863
7.840
7.735
7.713
7.567
7.553
7.546
7.539
7.535
7.528
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N
O
O
3b
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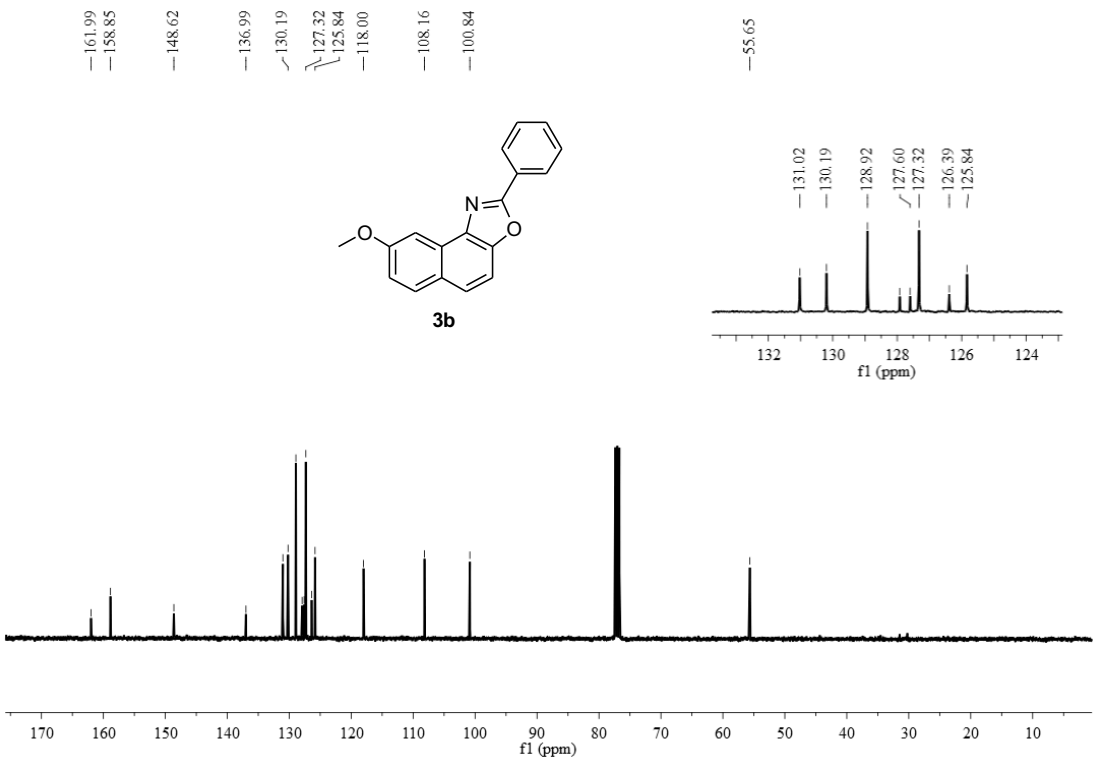
0.95
1.01
1.00
4.00
0.98
3.05
f1 (ppm)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148.62
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130.19
127.32
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118.00
108.16
100.84
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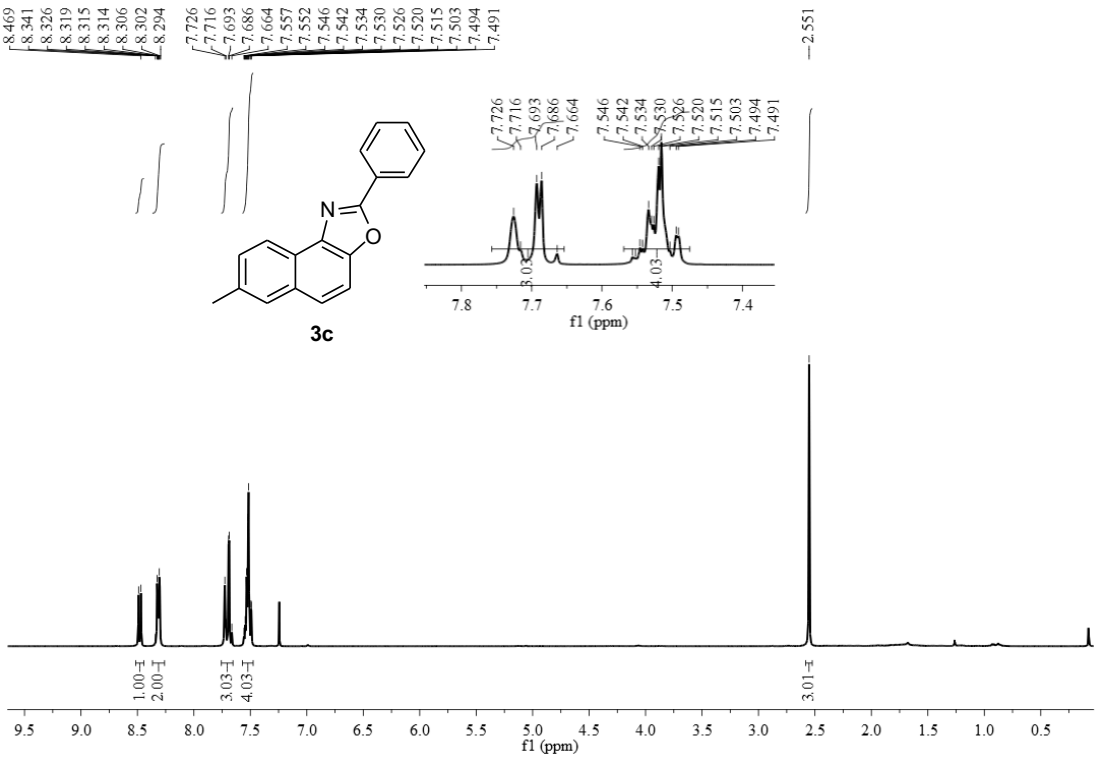
130.19
128.92
127.60
127.32
126.39
125.84
N
O
O
3b
f1 (ppm)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8.315
8.314
8.306
8.302
8.294
7.726
7.716
7.693
7.686
7.664
7.557
7.552
7.546
7.542
7.534
7.530
7.526
7.520
7.515
7.503
7.494
7.491
2.551
N
O
3c
3.03
4.03
7.8
7.7
7.6
7.5
7.4
f1 (ppm)
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2.00
3.03
4.03
3.01
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
3.5
3.0
2.5
2.0
1.5
1.0
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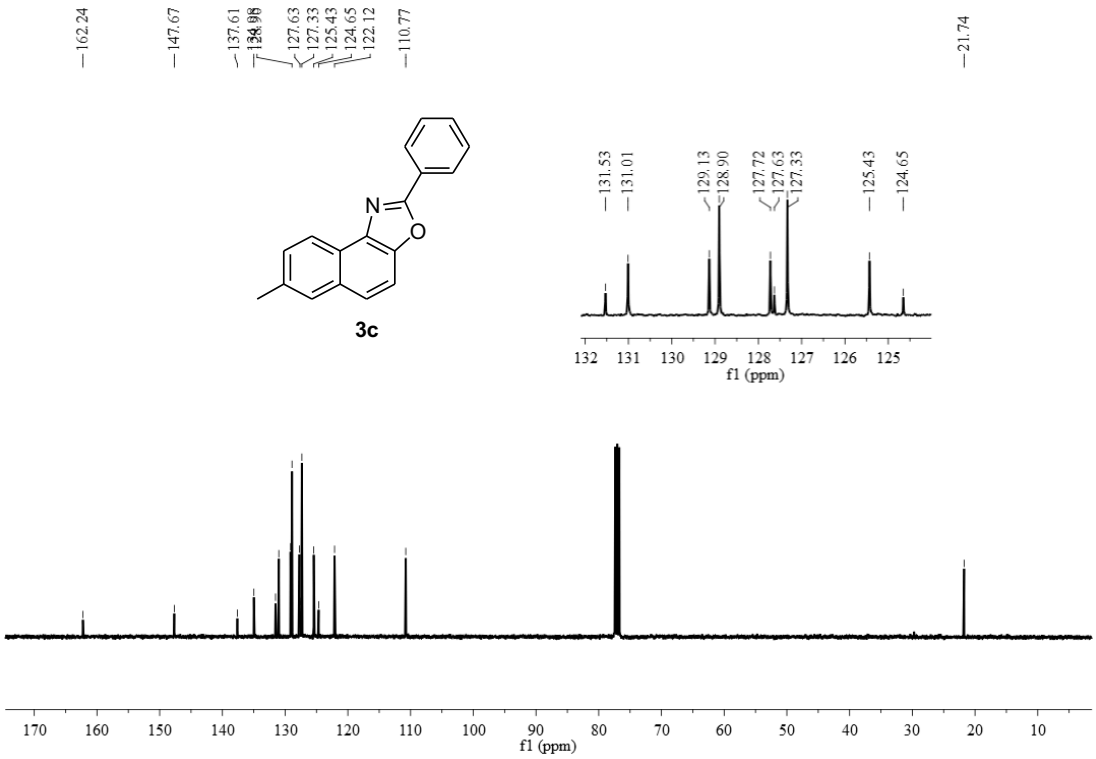
f1 (ppm)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127.33
125.43
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122.12
110.77
21.74
N
O
3c
131.53
131.01
129.13
128.90
127.72
127.63
127.33
125.43
124.65
132
131
130
129
128
127
126
125
f1 (ppm)
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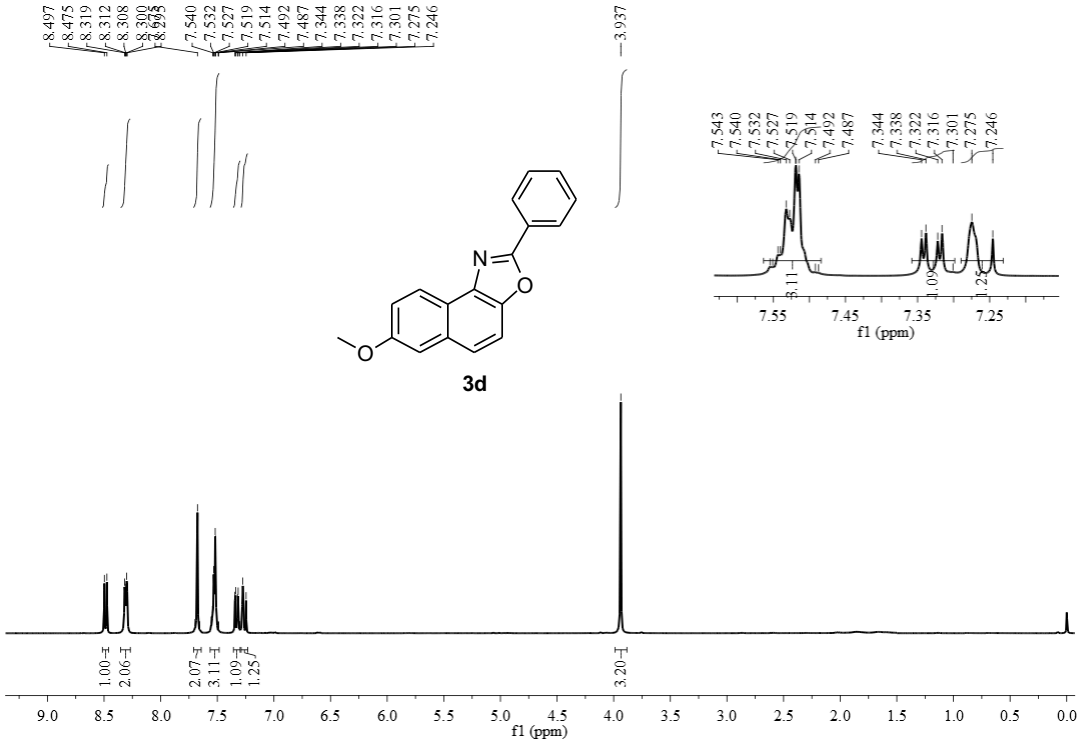
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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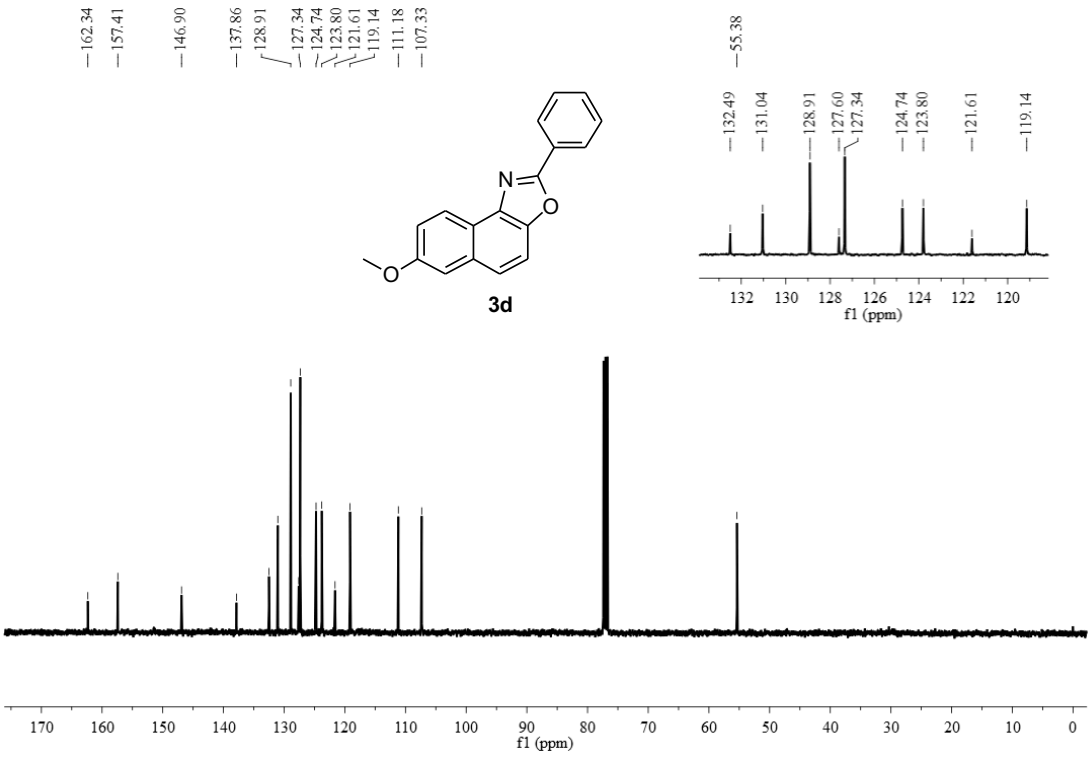
f1 (ppm)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127.34
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123.80
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119.14
111.18
107.33
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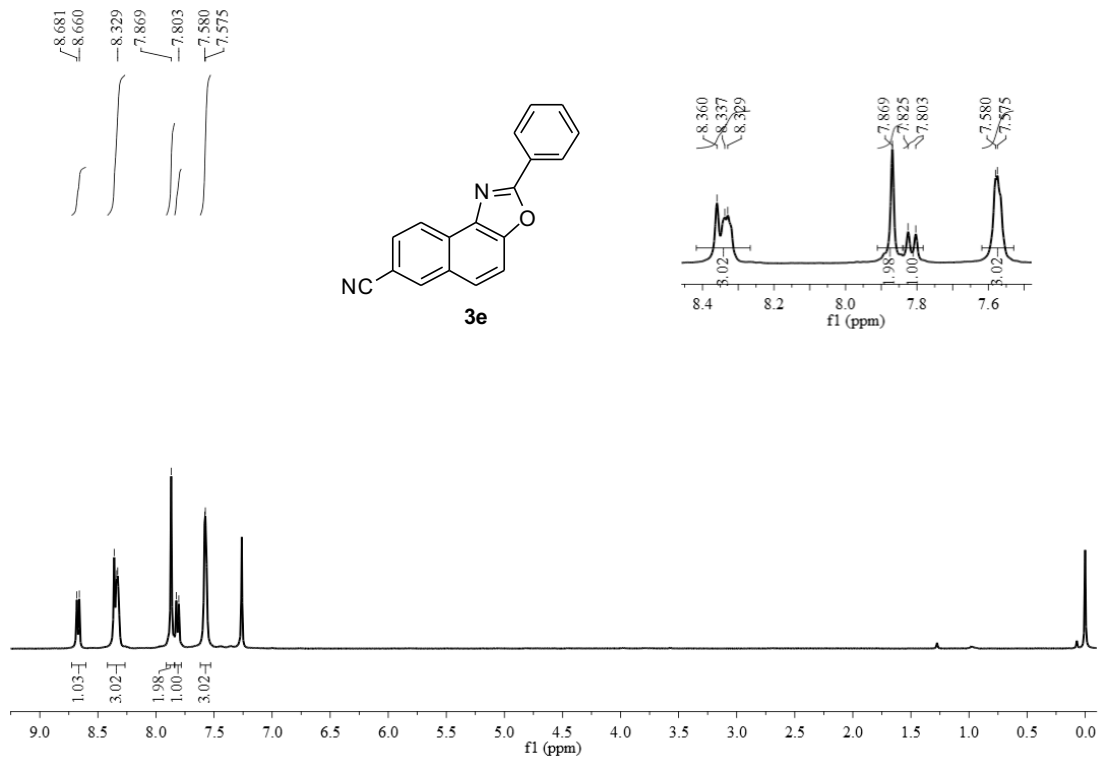
123.80
121.61
119.14
3d
f1 (ppm)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8.329
7.869
7.825
7.803
7.580
7.575
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1.98
1.00
3.02
8.4
8.2
8.0
7.8
7.6
f1 (ppm)
1.03
3.02
1.98
1.00
3.02
9.0
8.5
8.0
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7.0
6.5
6.0
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4.5
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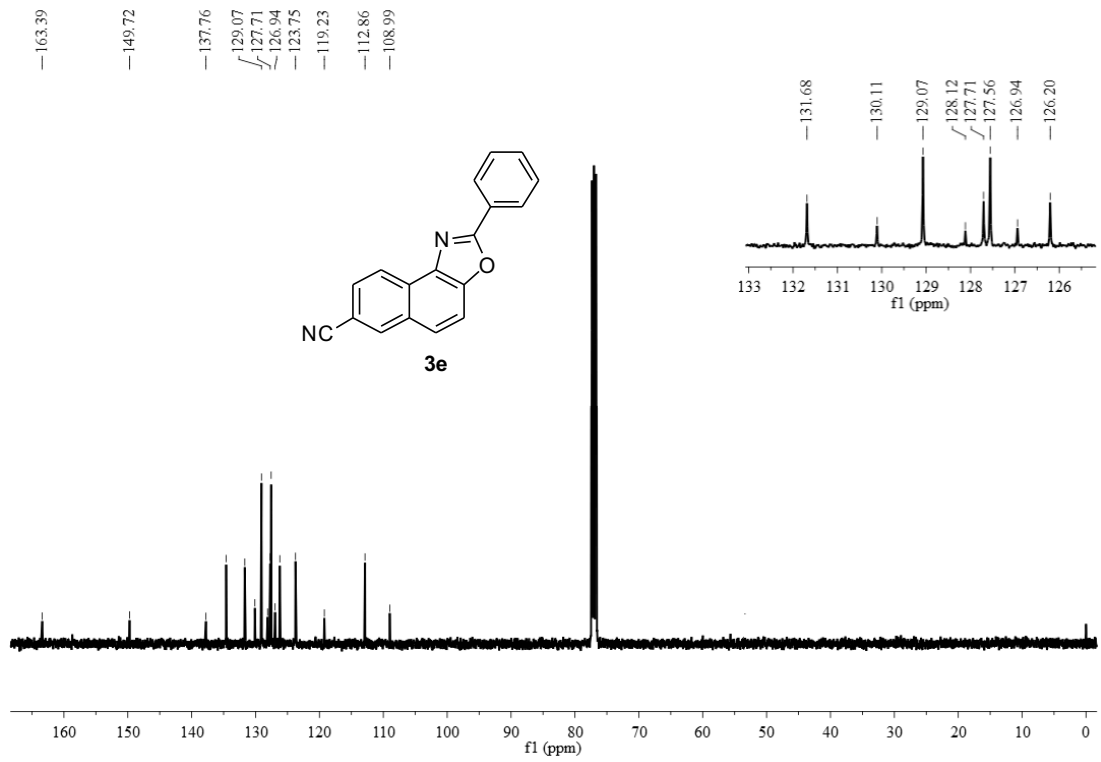
0.0
f1 (ppm)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3e
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130.11
129.07
128.12
127.71
127.56
126.94
126.20
133
132
131
130
129
128
127
126
f1 (ppm)
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140
130
120
110
100
90
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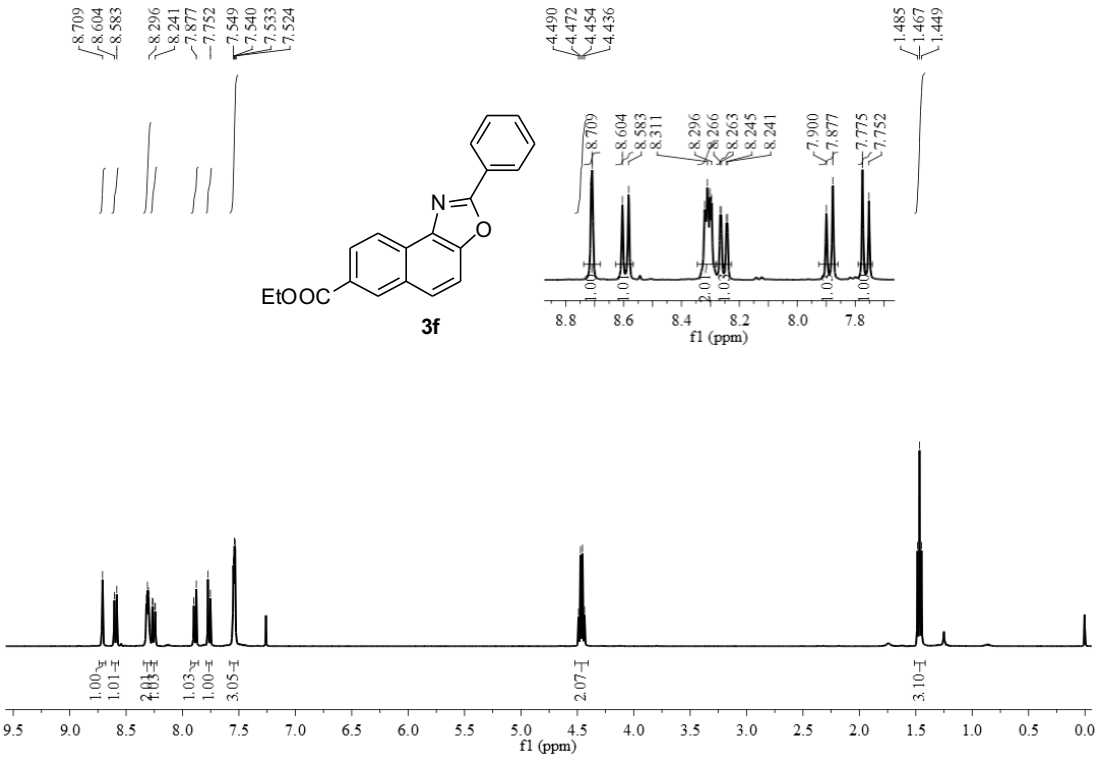
50
40
30
20
10
0
f1 (ppm)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4.472
4.454
4.436
1.485
1.467
1.449
N
O
EtOOC
3f
f1 (ppm)

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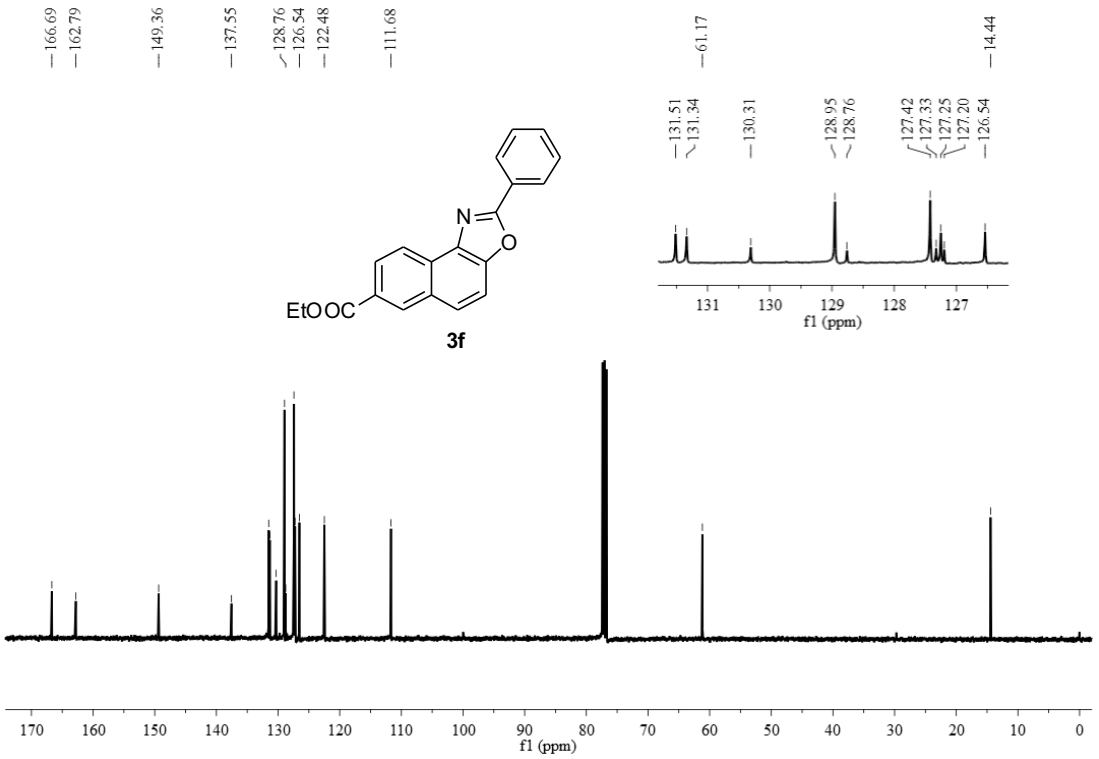
2.01
1.03
1.00
3.05
2.07
3.10
f1 (ppm)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128.95
128.76
127.42
127.33
127.25
127.20
126.54
N
O
EtOOC
3f
f1 (ppm)


8.457
8.435
8.318
8.313
8.309
8.306
8.300
8.294
8.110
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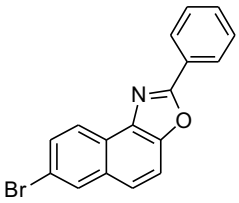
7.554
7.545
7.538
7.529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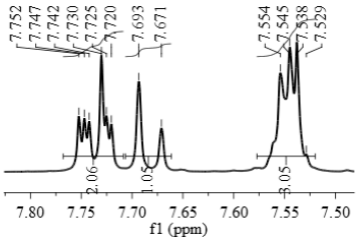
Br

3g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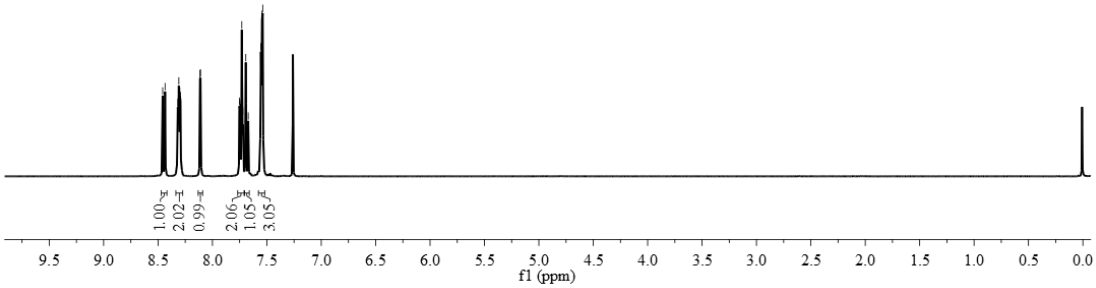
f1 (ppm)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6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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f1 (ppm)


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124.08
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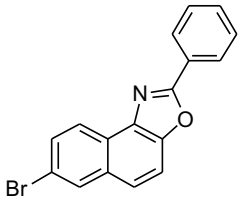
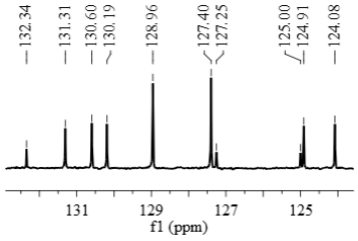

N
O
Br

3g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124.08
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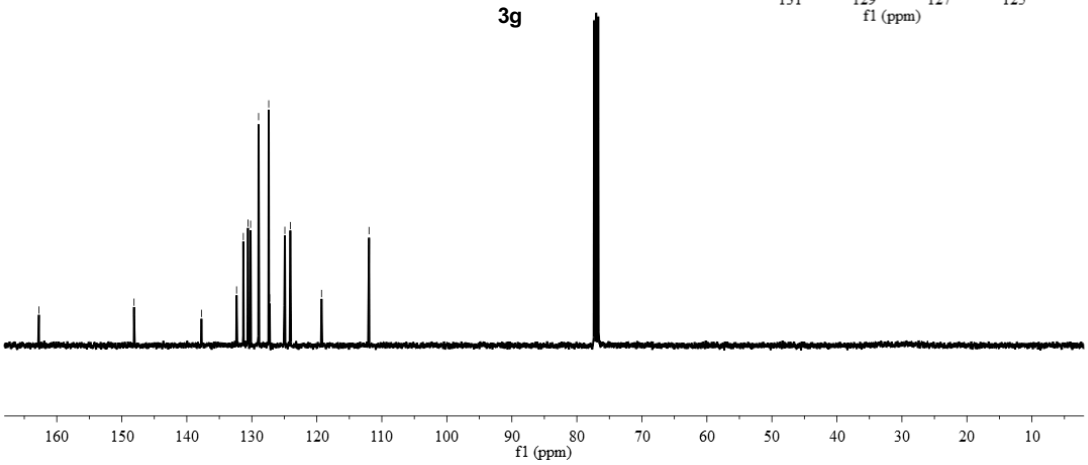
129
127
125
f1 (ppm)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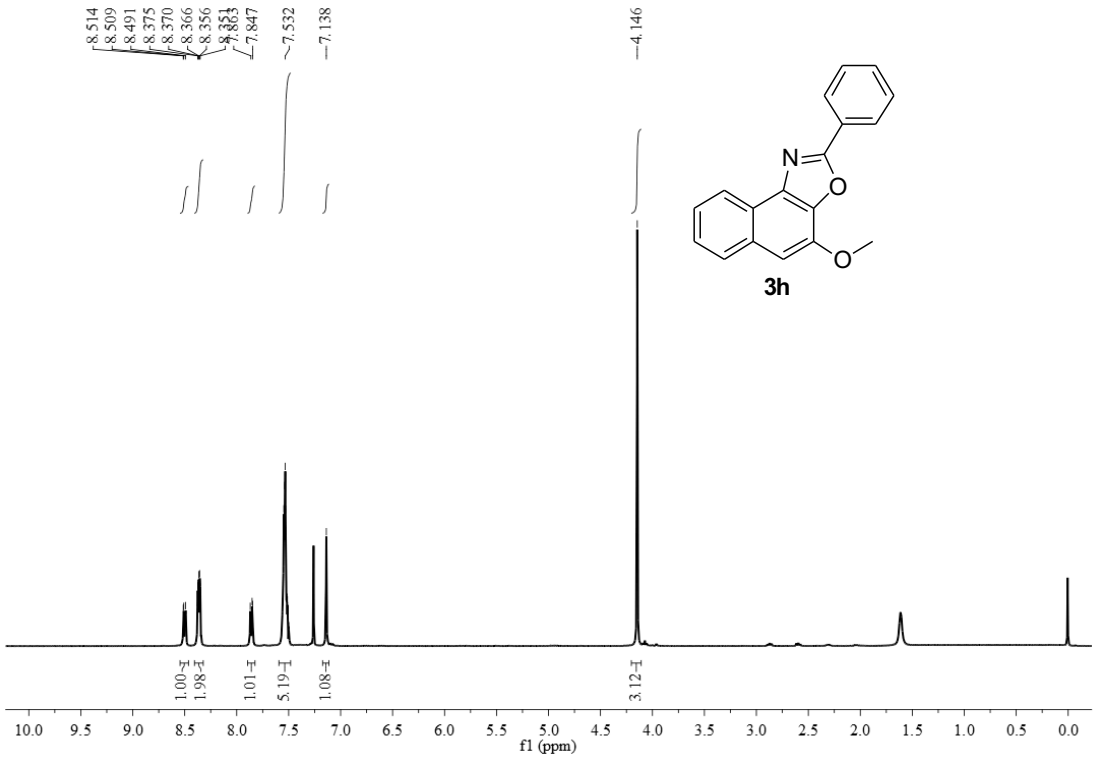
50
40
30
20
10
f1 (ppm)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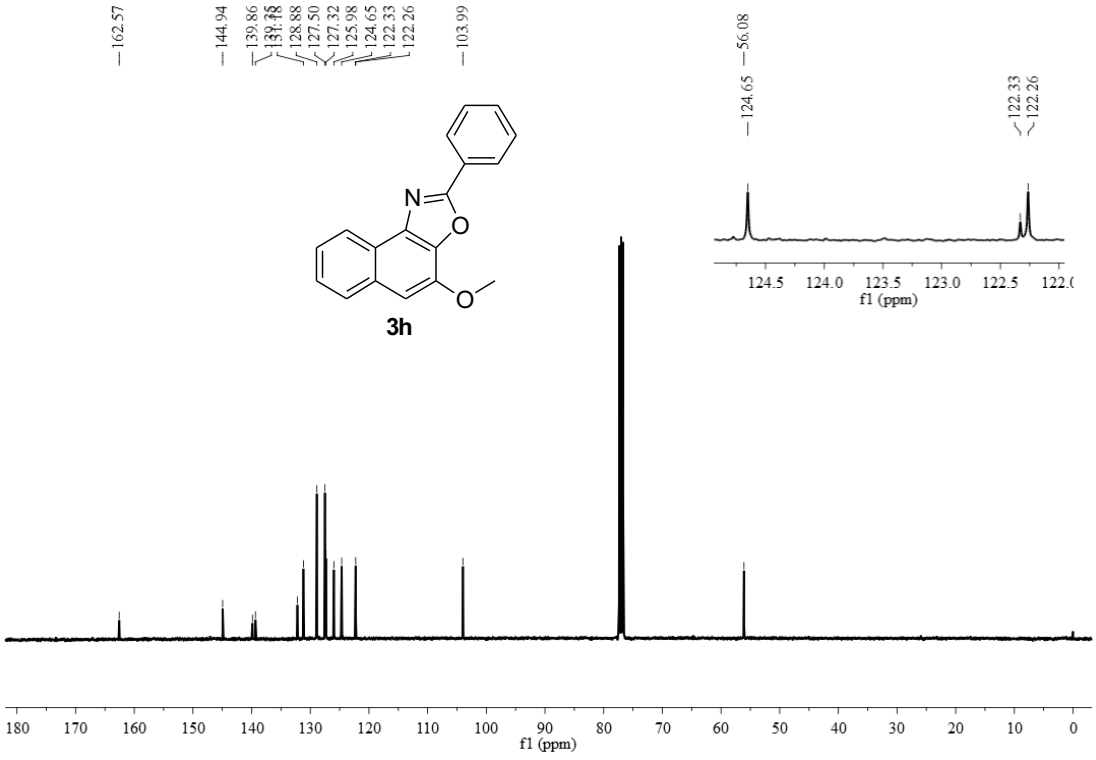
1.08
3.12
f1 (ppm)
3h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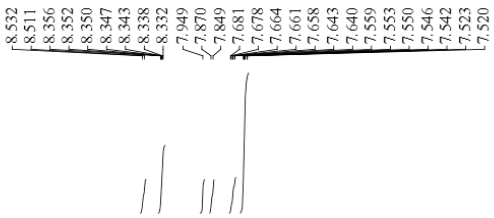
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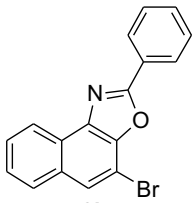
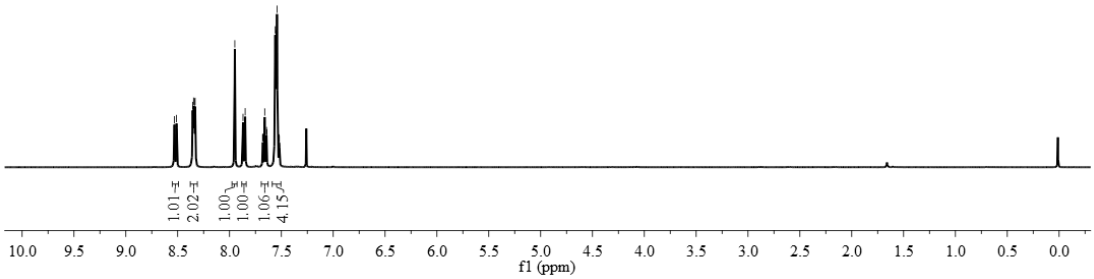

N
O
Br

3i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1.00
1.06
4.15
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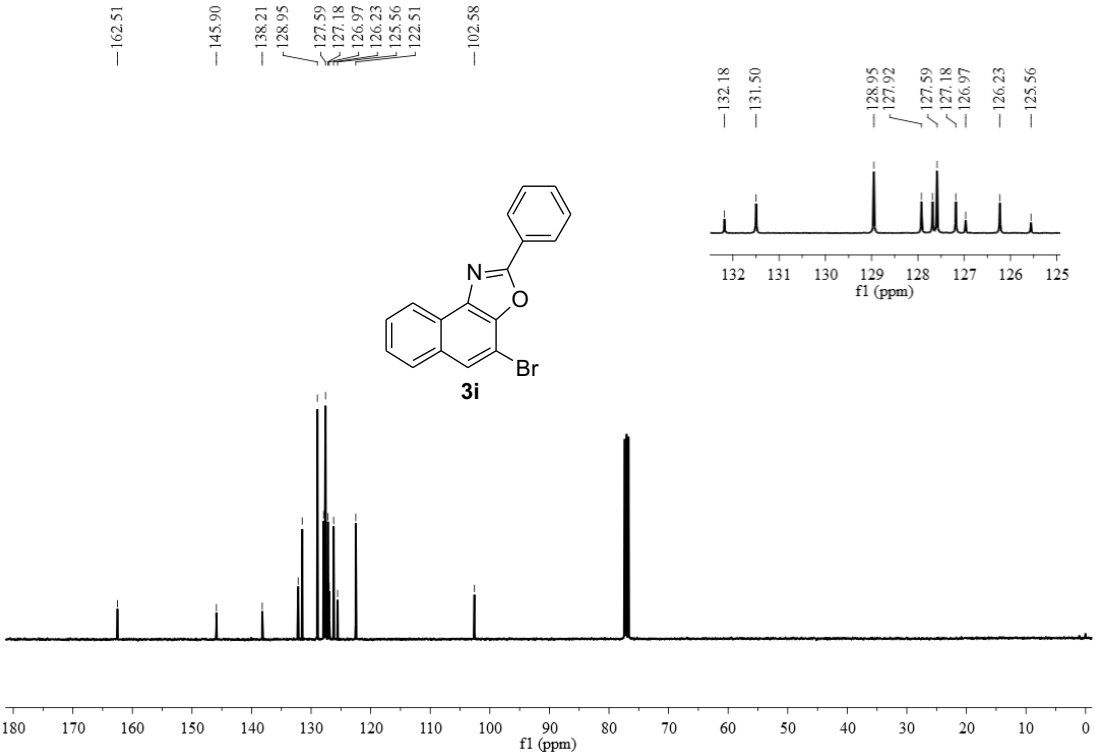
f1 (ppm)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131.50
128.95
127.92
127.59
127.18
126.97
126.23
125.56
N
O
Br
132 131 130 129 128 127 126 125
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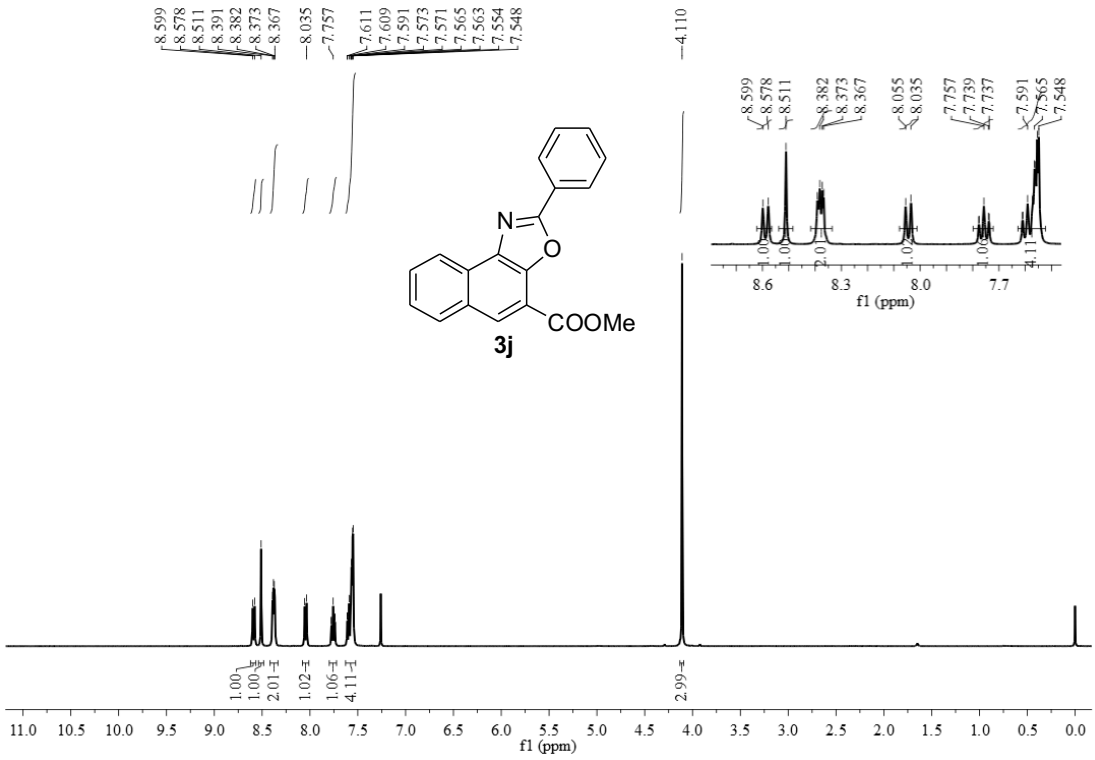
f1 (ppm)

3i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7.563
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7.548
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COOMe
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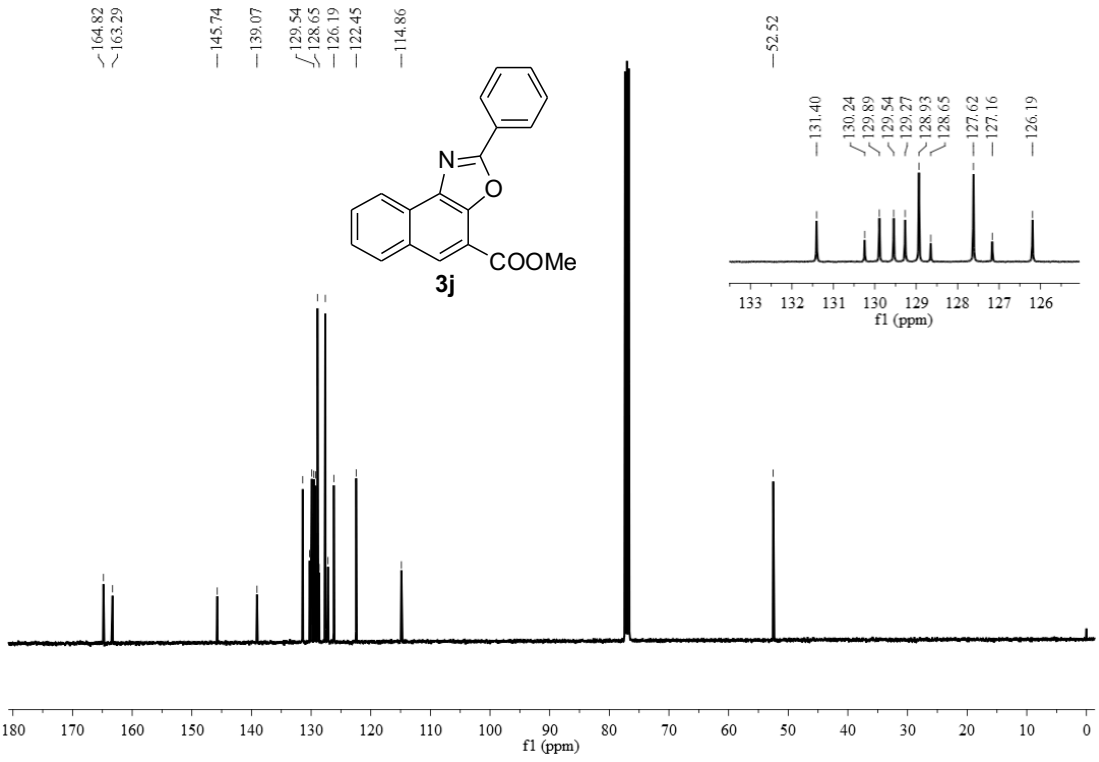
1.06
4.11
2.99
f1 (ppm)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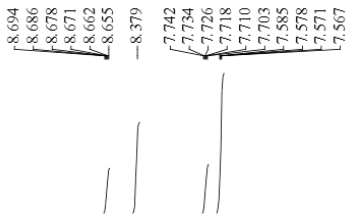
N
O
COOMe
3j
f1 (ppm)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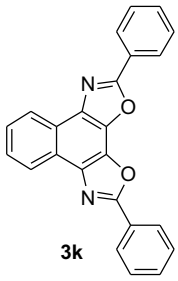
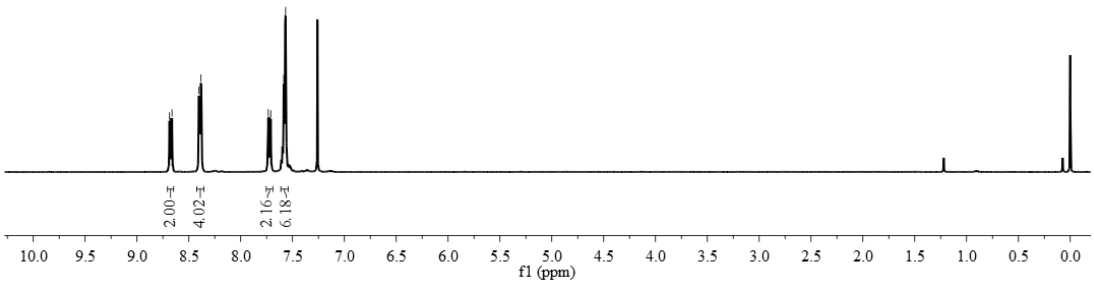


3k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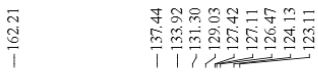
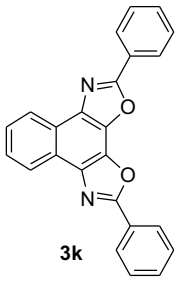
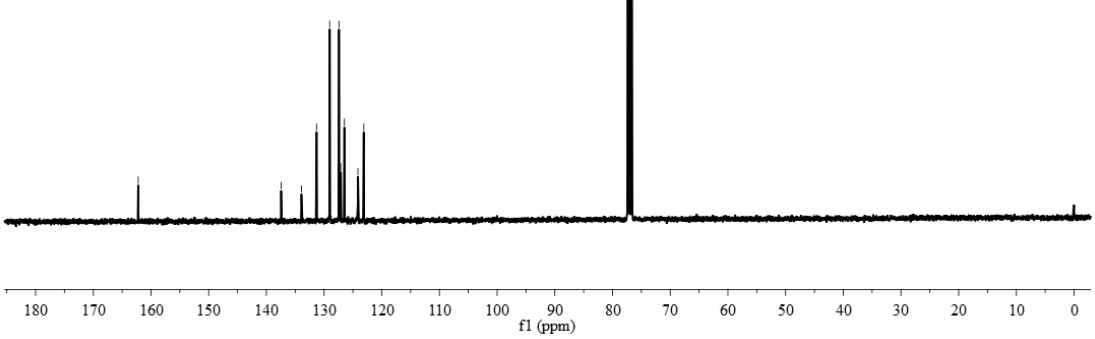
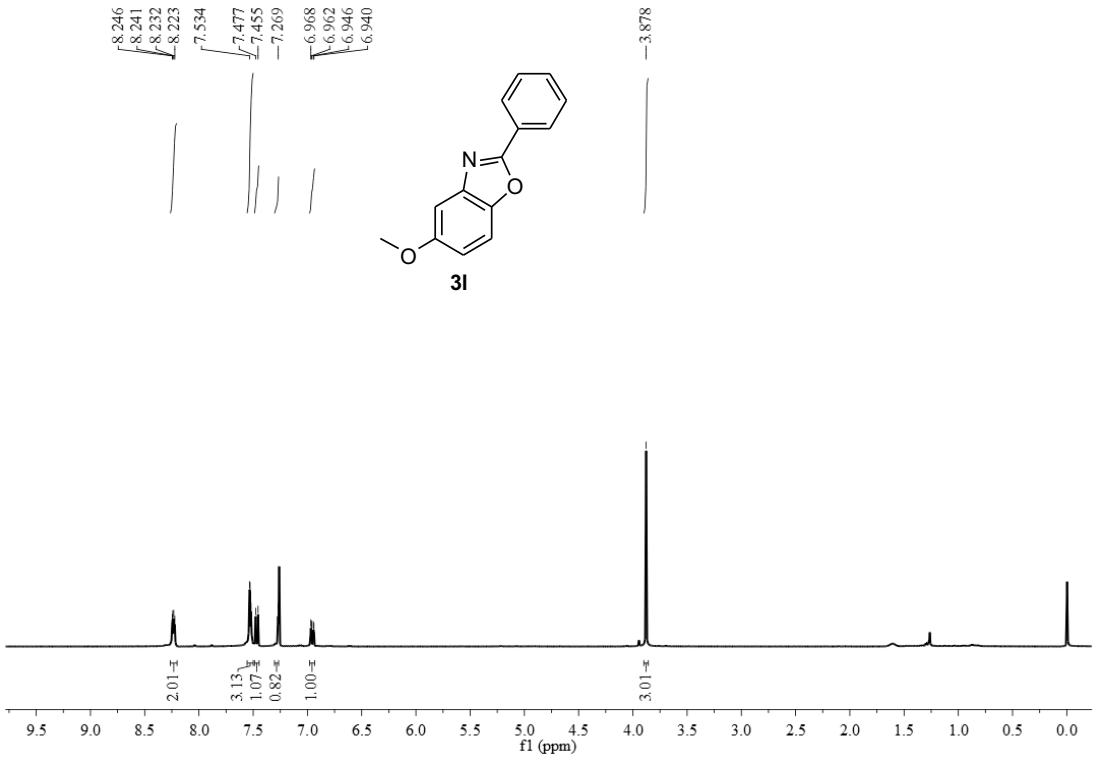
2.16
6.18
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

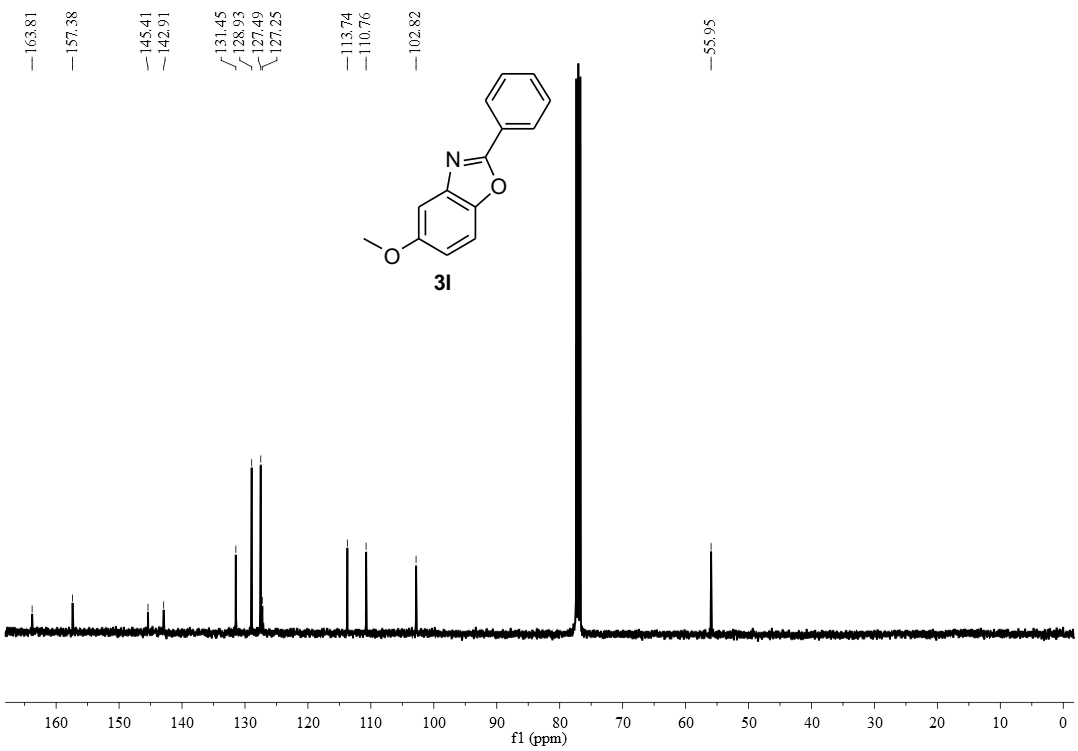

162.21
137.44
133.92
131.30
129.03
127.42
127.11
126.47
124.13
123.11

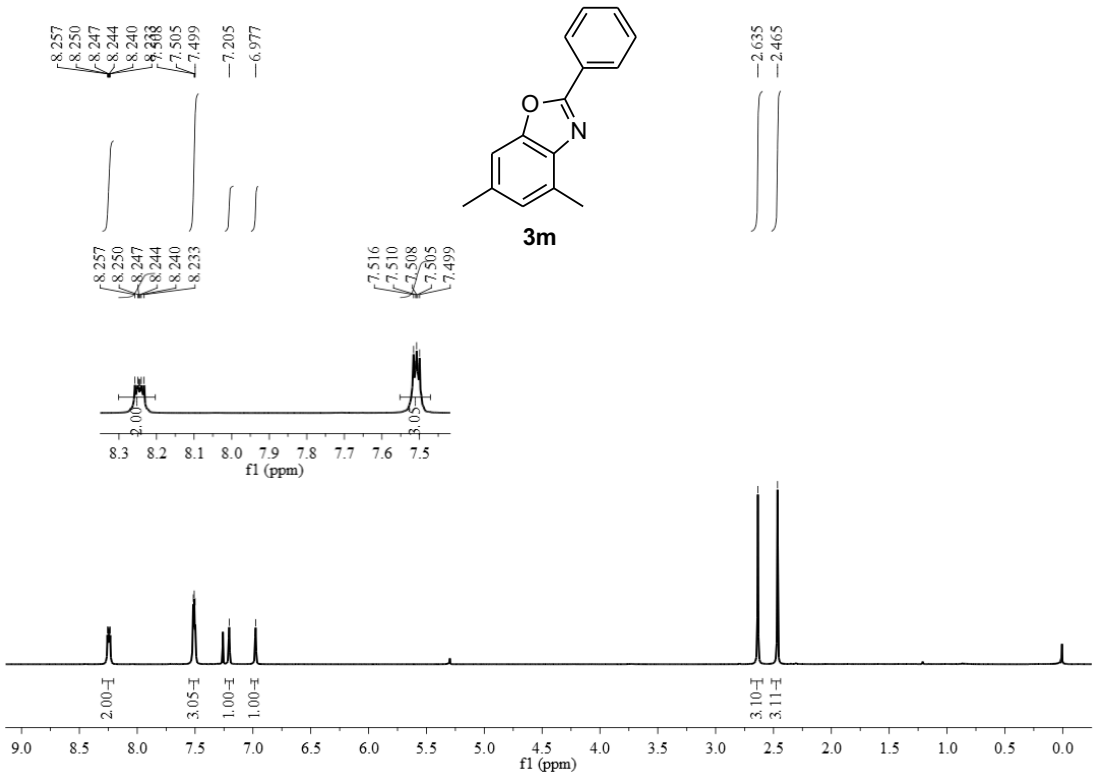


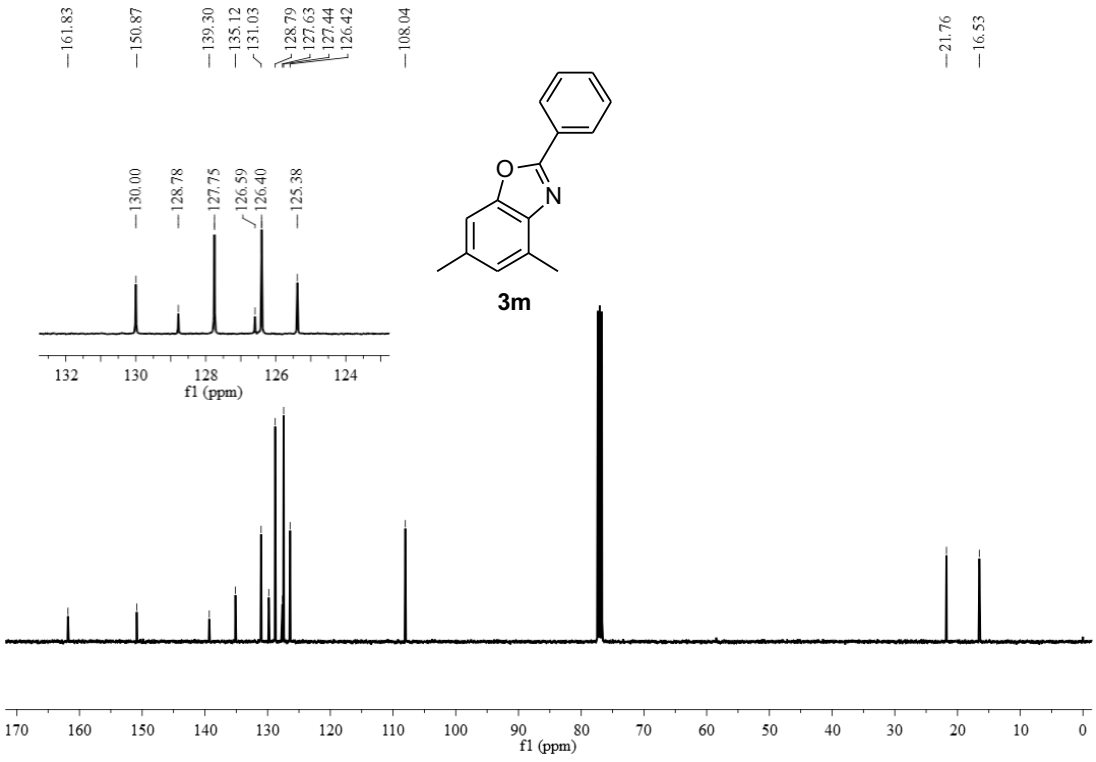
3k

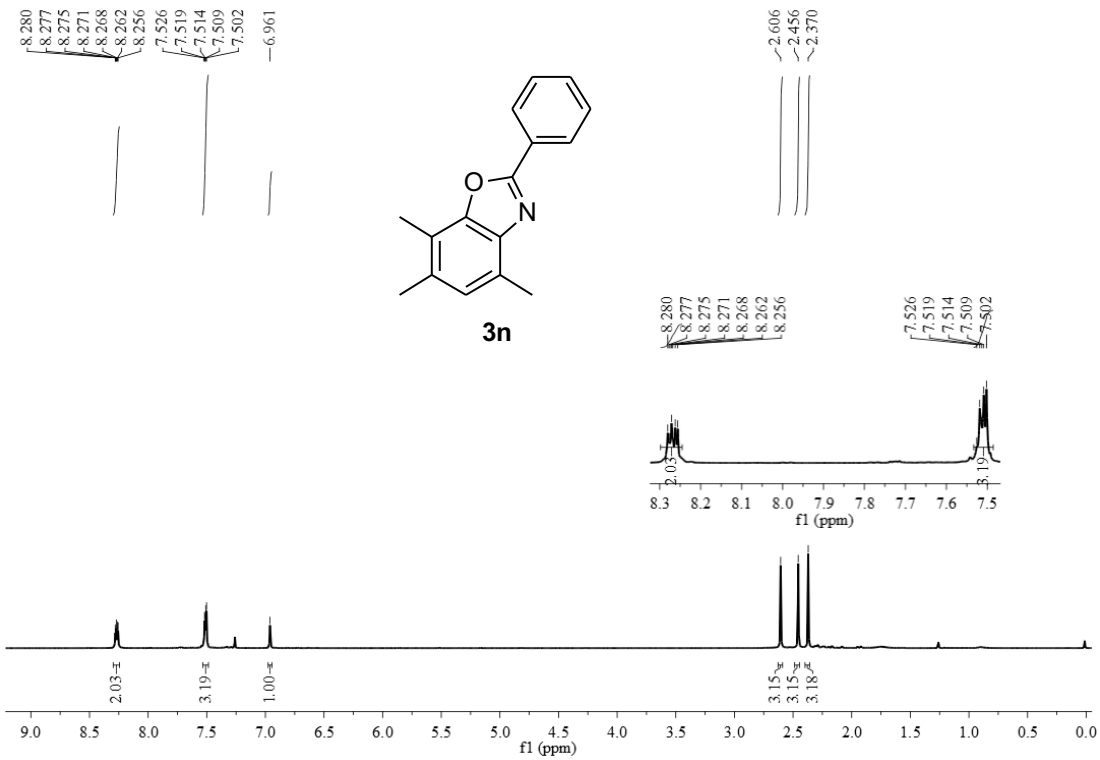

180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

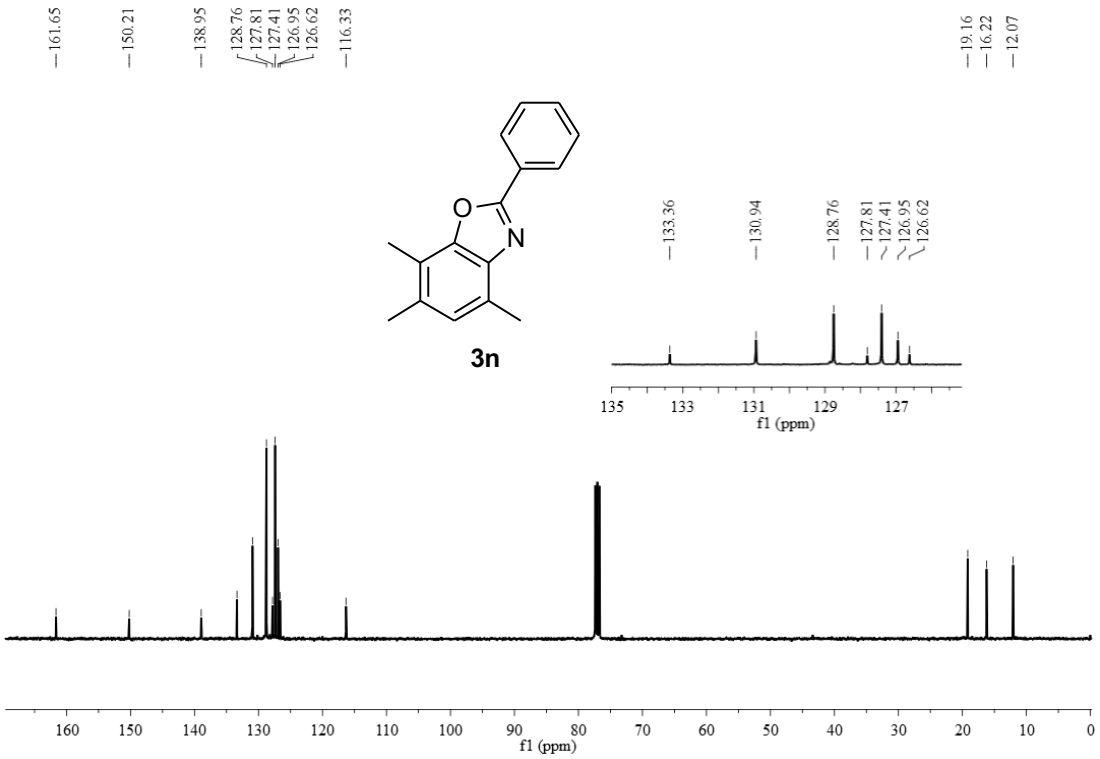

8.246
8.241
8.232
8.223
7.534
7.477
7.455
7.269
6.968
6.962
6.946
6.940
3.878
N
O
O
3l
2.01
3.13
1.07
0.82
1.00
3.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

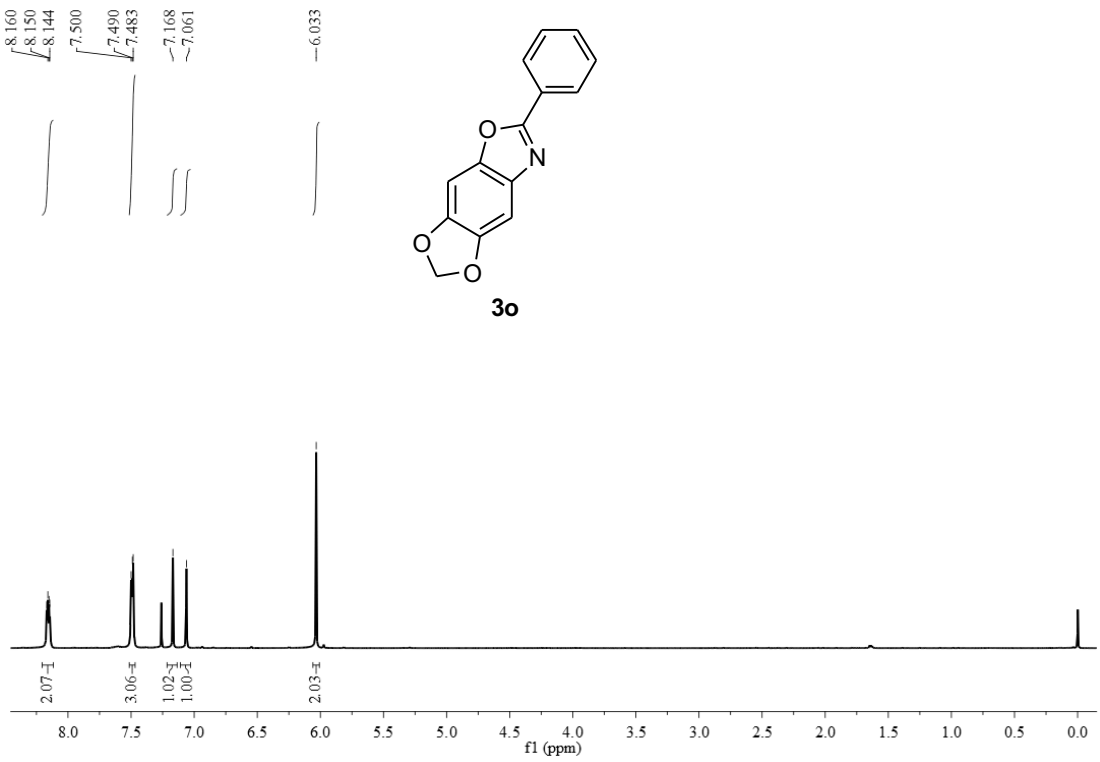

163.81
157.38
145.41
142.91
131.45
128.93
127.49
127.25
113.74
110.76
102.82
55.95
N
O
O
3l
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

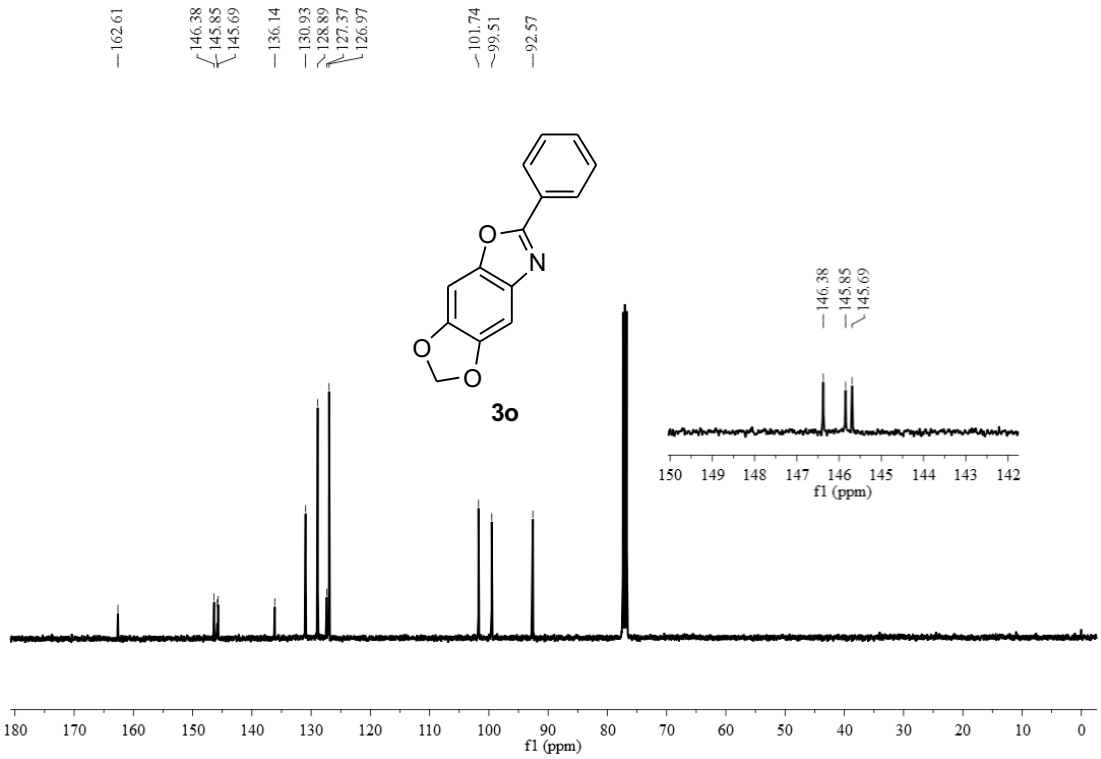

8.257
8.250
8.247
8.244
8.240
8.233
7.516
7.510
7.508
7.505
7.499
7.205
6.977
2.635
2.465
3m
2.00
3.05
8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5
f1 (ppm)
2.00
3.05
1.00
1.00
3.10
3.11
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

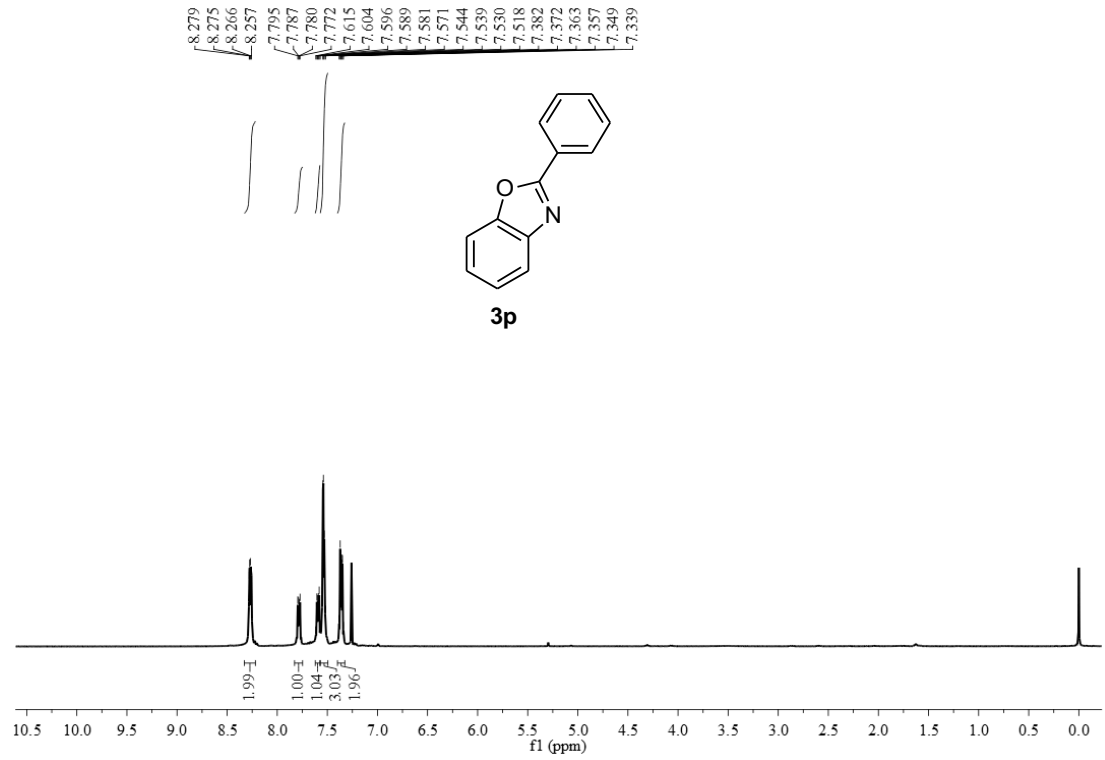

161.83
150.87
139.30
135.12
131.03
128.79
127.63
127.44
126.42
108.04
21.76
16.53
130.00
128.78
127.75
126.59
126.40
125.38
3m
132 130 128 126 124
f1 (ppm)
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.280
8.277
8.275
8.271
8.268
8.262
8.256
7.526
7.519
7.514
7.509
7.502
6.961
2.606
2.456
2.370
O
N
3n
2.03
3.19
f1 (ppm)
1.00
3.15
3.18

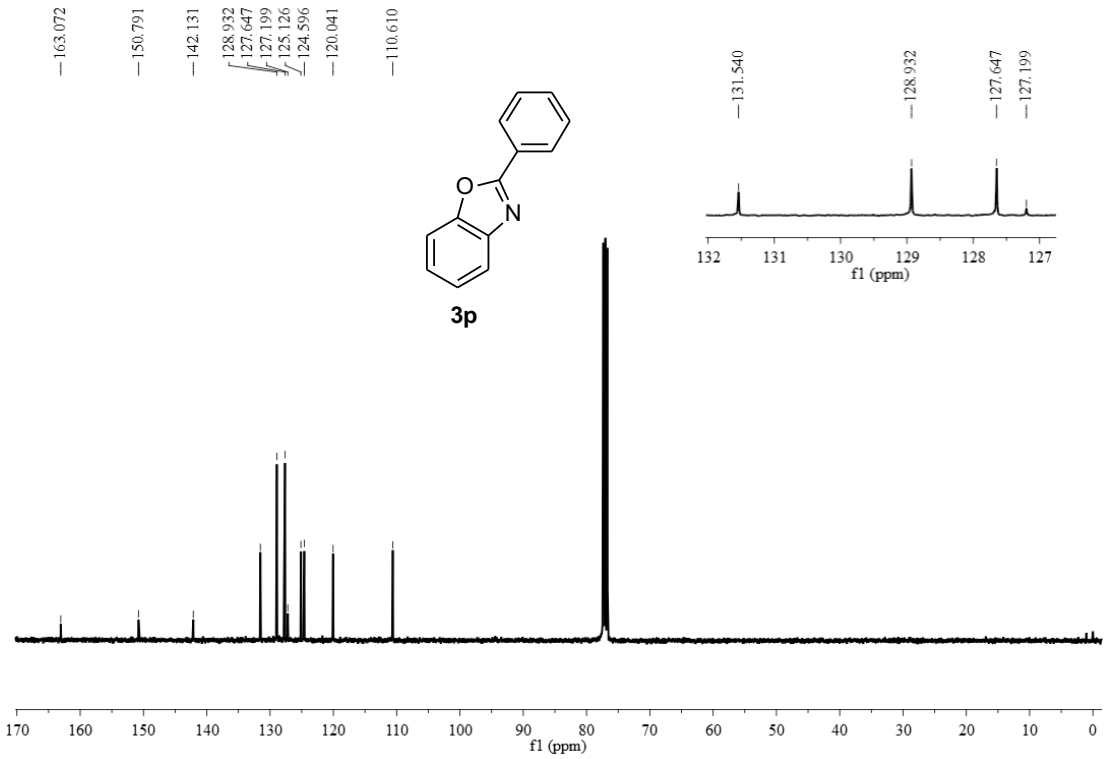

161.65
150.21
138.95
128.76
127.81
127.41
126.95
126.62
116.33
19.16
16.22
12.07
O
N
3n
133.36
130.94
128.76
127.81
127.41
126.95
126.62
f1 (ppm)


8.160
8.150
8.144
7.500
7.490
7.483
7.168
7.061
6.033
O
N
O
O
3o
2.07
3.06
1.02
1.00
2.03
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

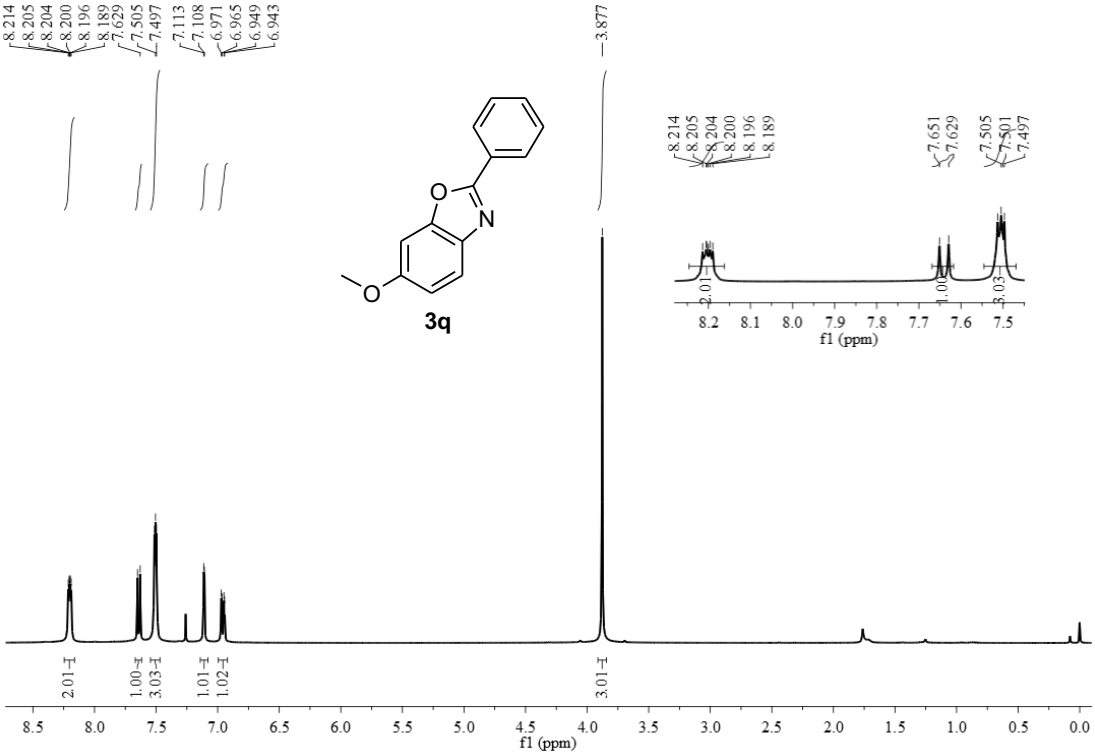

162.61
146.38
145.85
145.69
136.14
130.93
128.89
127.37
126.97
101.74
99.51
92.57
O
N
O
O
3o
146.38
145.85
145.69
150
149
148
147
146
145
144
143
142
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

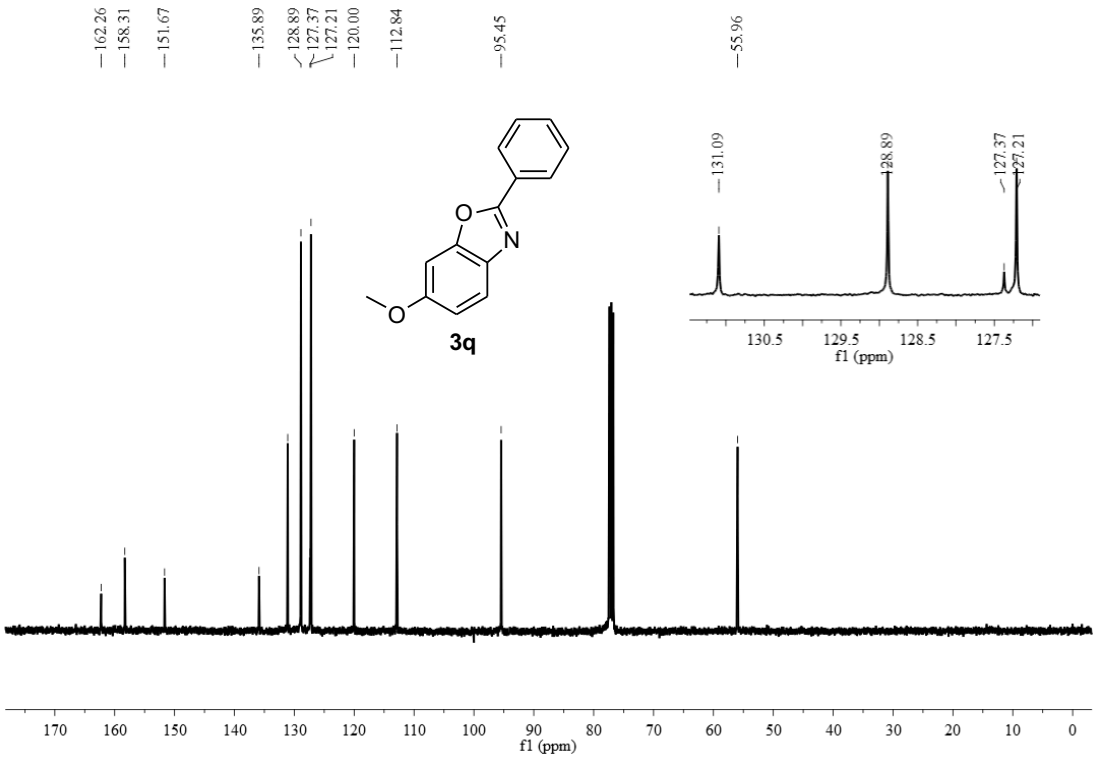

8.279
8.275
8.266
8.257
7.795
7.787
7.780
7.772
7.615
7.604
7.596
7.589
7.581
7.571
7.544
7.539
7.530
7.518
7.382
7.372
7.363
7.357
7.349
7.339
O
N
1.99
1.00
1.04
3.03
1.96
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

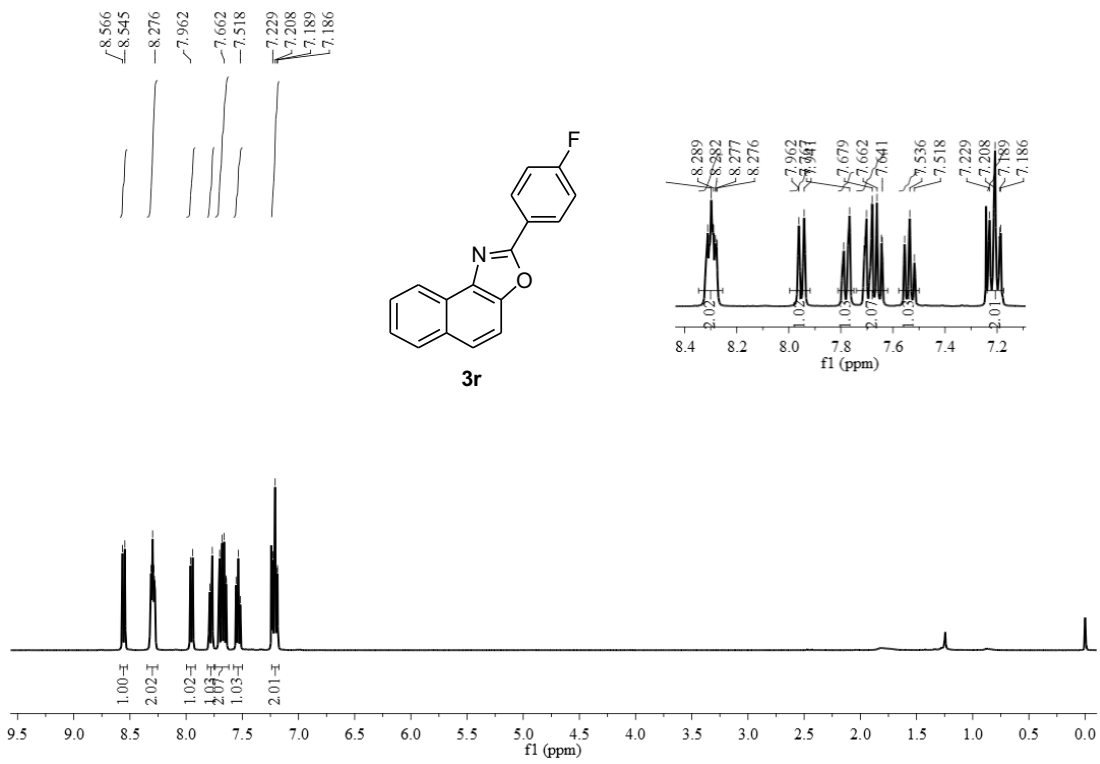
3p

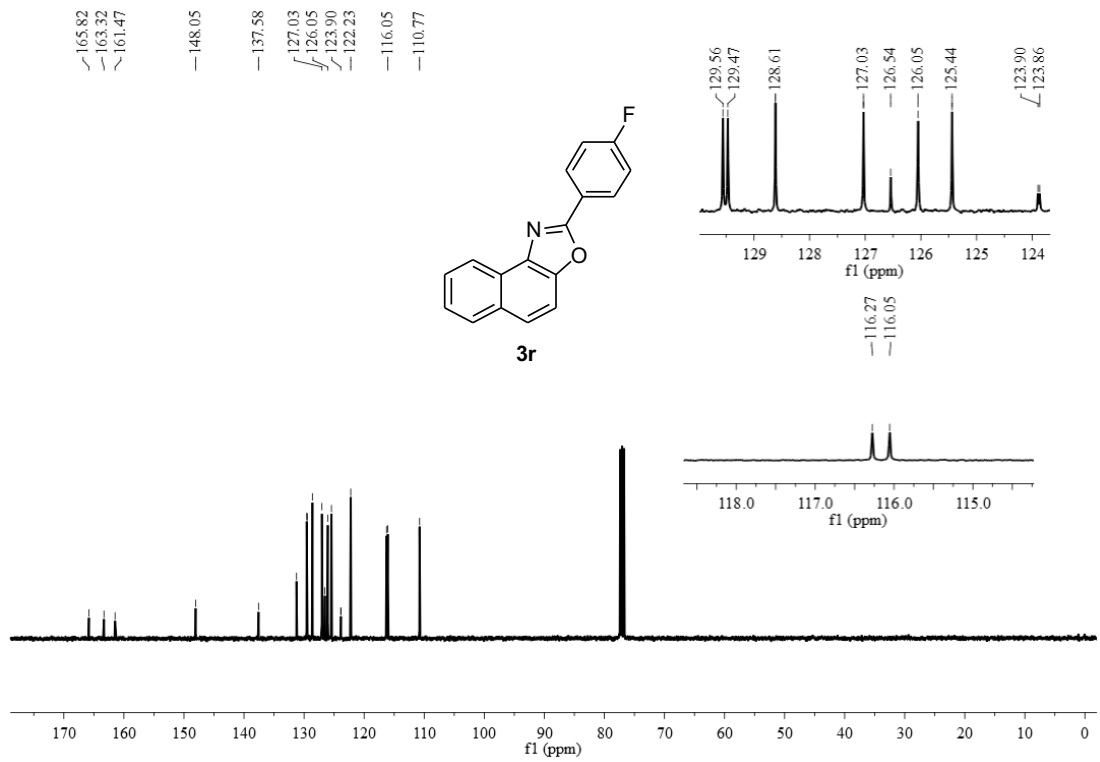

163.072
150.791
142.131
128.932
127.647
127.199
125.126
124.596
120.041
110.610
O
N
131.540
128.932
127.647
127.199
132 131 130 129 128 127
f1 (ppm)
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

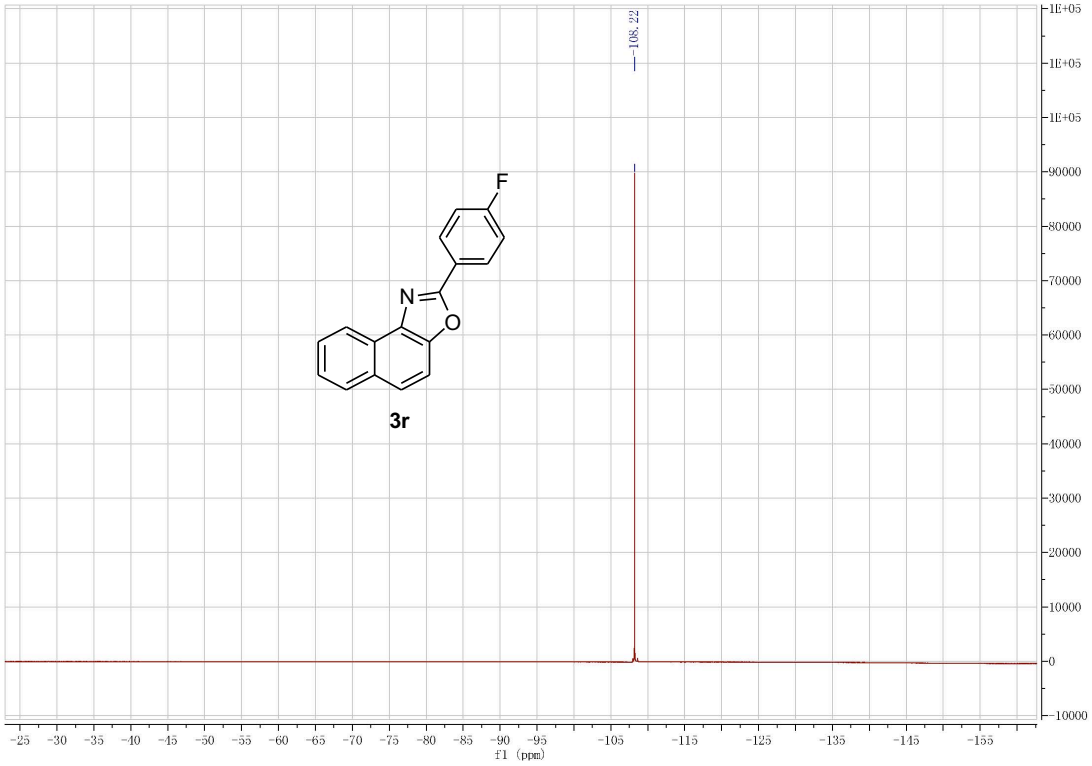
3p

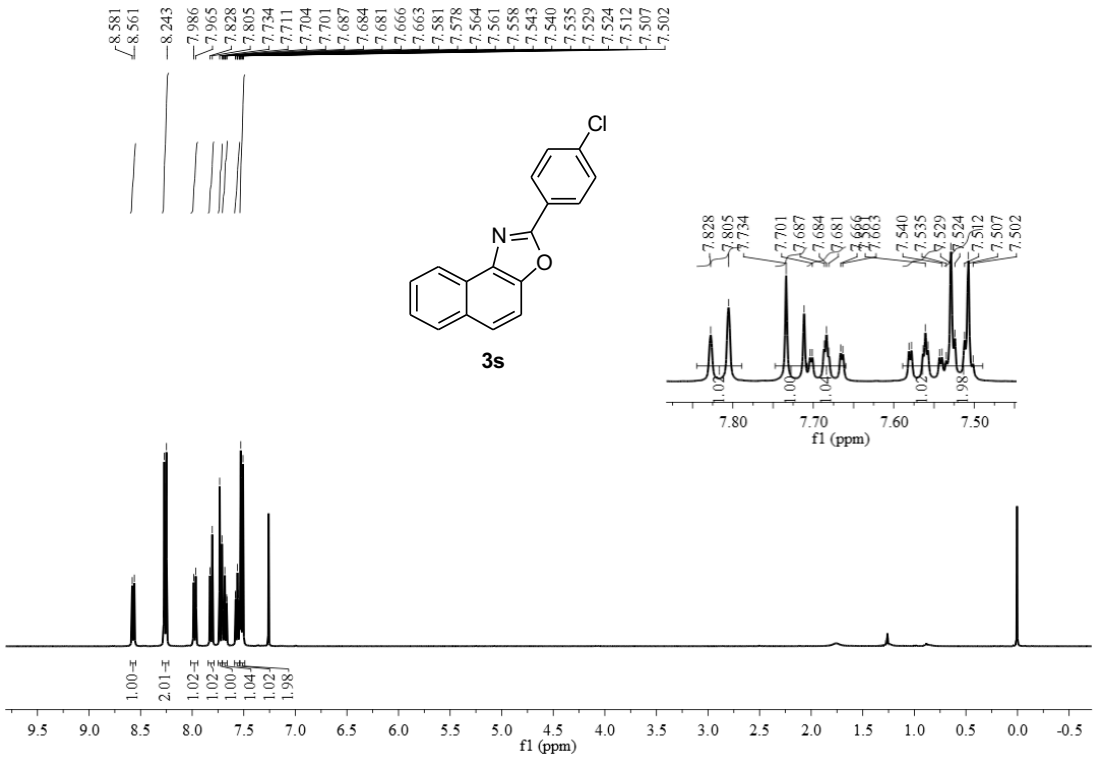

8.214
8.205
8.204
8.200
8.196
8.189
7.629
7.505
7.497
7.113
7.108
6.971
6.965
6.949
6.943
3.877
3q
2.01
1.00
3.03
1.01
1.02
3.01
f1 (ppm)

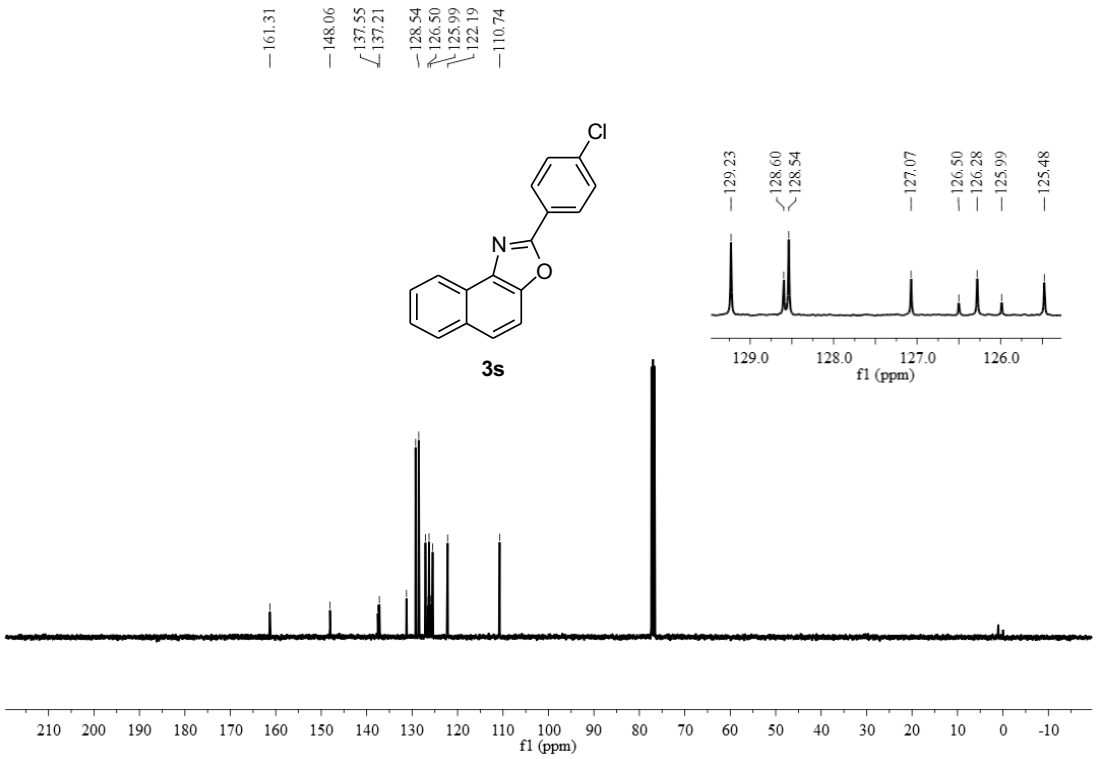

162.26
158.31
151.67
135.89
128.89
127.37
127.21
120.00
112.84
95.45
55.96
3q
131.09
128.89
127.37
127.21
f1 (ppm)

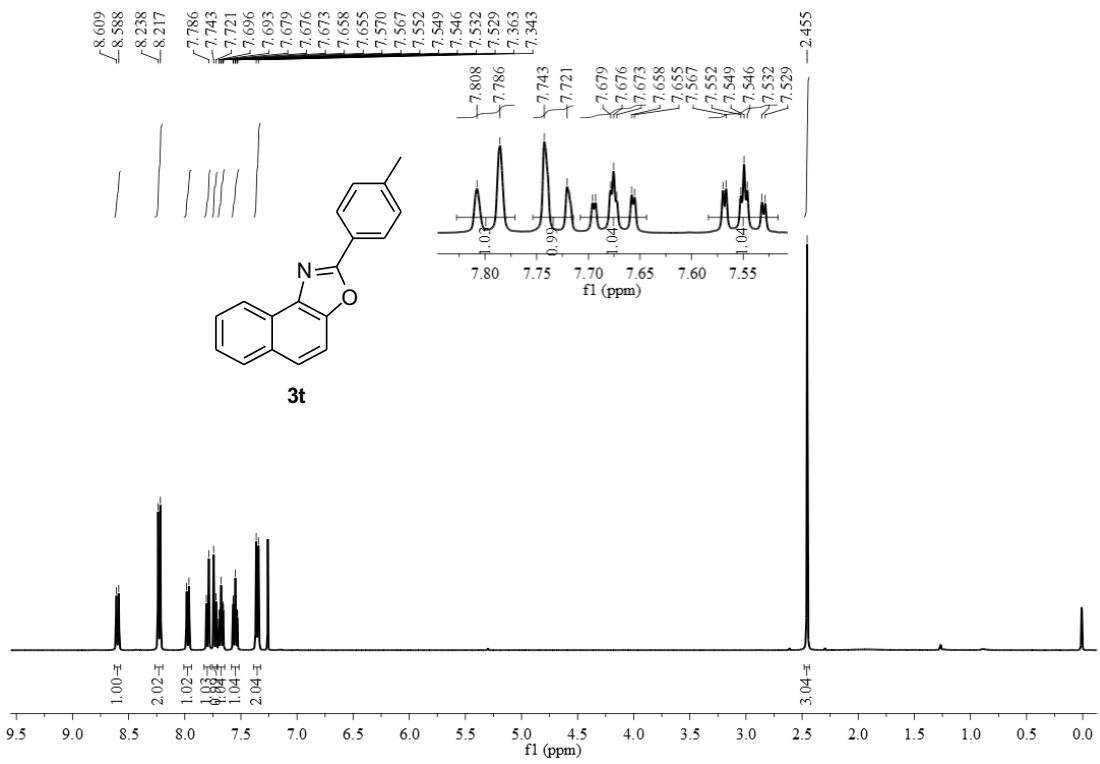

8.566
8.545
8.276
7.962
7.662
7.518
7.229
7.208
7.189
7.186
F
N
O
3r
8.289
8.282
8.277
8.276
7.962
7.947
7.941
7.679
7.662
7.641
7.536
7.518
7.229
7.208
7.189
7.186
2.02
1.02
1.03
2.07
1.03
2.01
8.4
8.2
8.0
7.8
7.6
7.4
7.2
f1 (ppm)
1.00
2.02
1.02
1.03
1.03
2.01
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

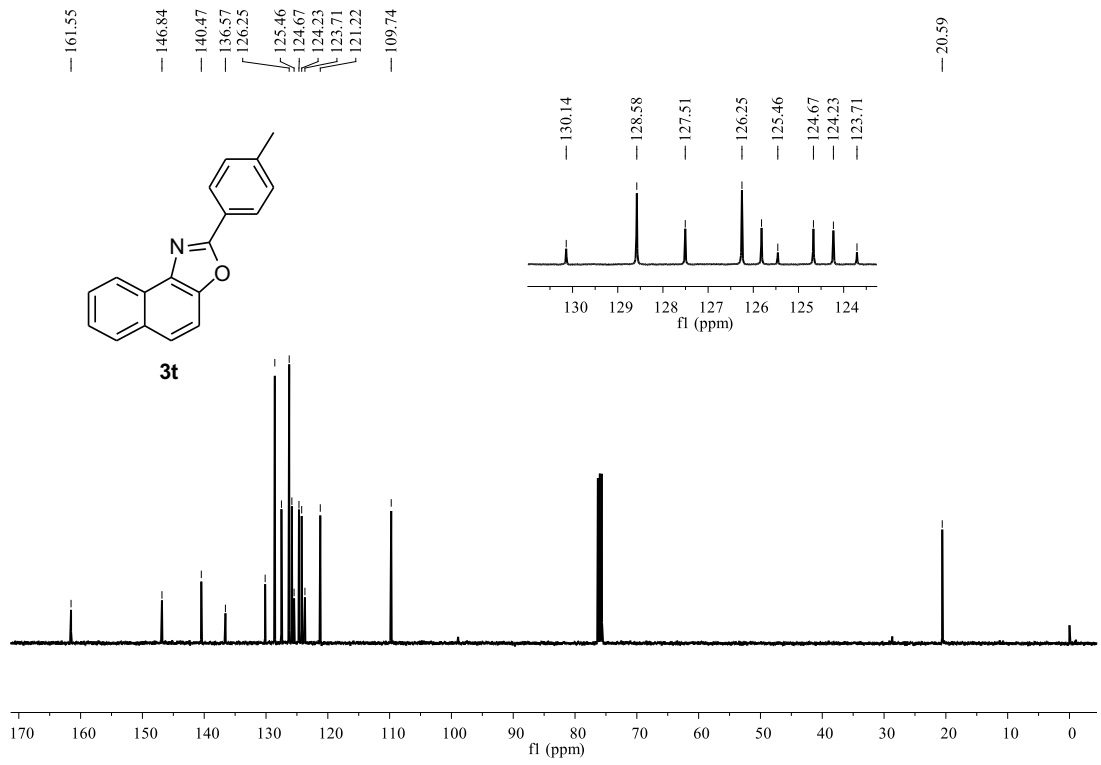

165.82
163.32
161.47
148.05
137.58
127.03
126.05
123.90
122.23
116.05
110.77
F
N
O
3r
129.56
129.47
128.61
127.03
126.54
126.05
125.44
123.90
123.86
129
128
127
126
125
124
f1 (ppm)
116.27
116.05
118.0
117.0
116.0
115.0
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

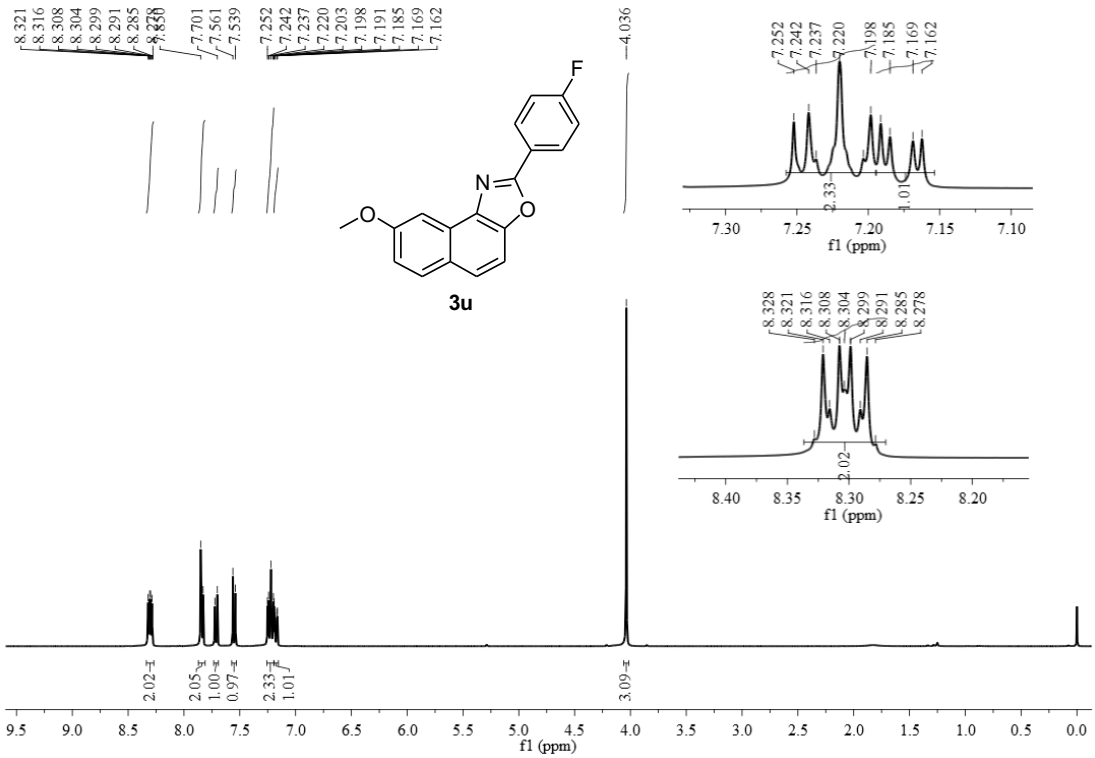

-108.22
F
N
O
3r
1E+05
1E+05
1E+05
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
-25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -105 -115 -125 -135 -145 -155
f1 (ppm)

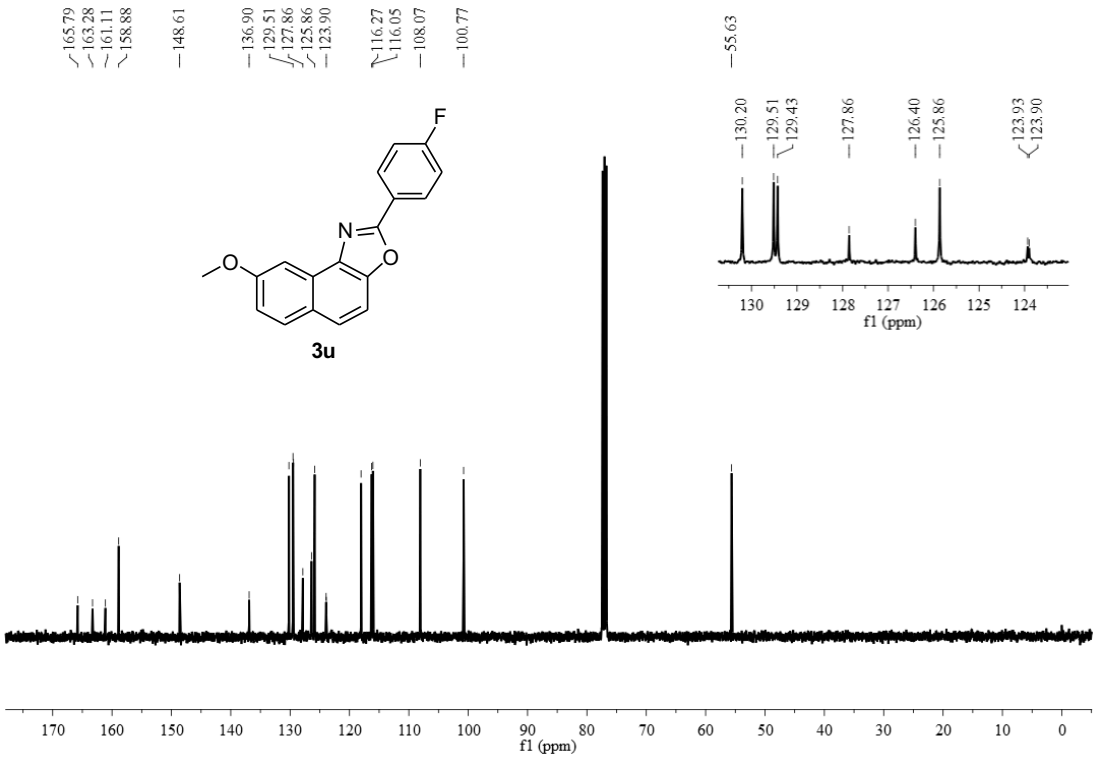

8.581
8.561
8.243
7.986
7.965
7.828
7.805
7.734
7.711
7.704
7.701
7.687
7.684
7.681
7.666
7.663
7.581
7.578
7.564
7.561
7.558
7.543
7.540
7.535
7.529
7.524
7.512
7.507
7.502
Cl
N
O
3s
7.828
7.805
7.734
7.701
7.687
7.684
7.681
7.666
7.663
7.581
7.540
7.535
7.529
7.524
7.512
7.507
7.502
1.02
1.00
1.04
1.02
1.98
7.80
7.70
7.60
7.50
f1 (ppm)
1.00
2.01
1.02
1.02
1.00
1.04
1.02
1.98
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
0.0
-0.5
f1 (ppm)

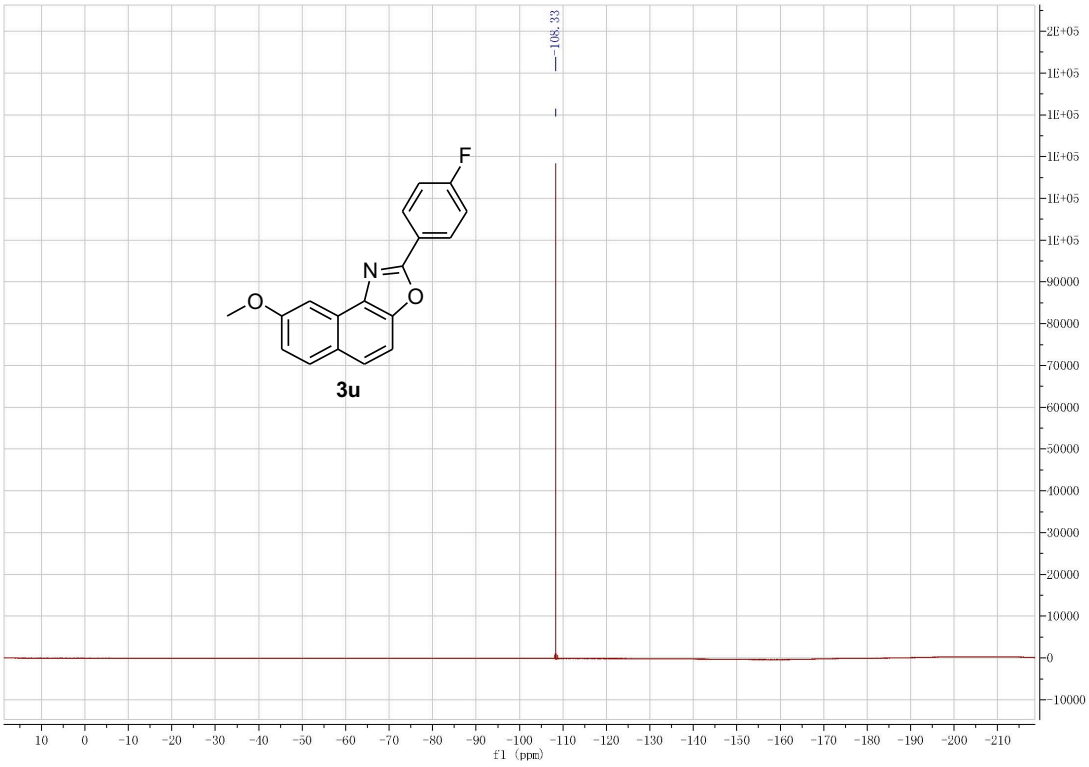

161.31
148.06
137.55
137.21
128.54
126.50
125.99
122.19
110.74
Cl
N
O
3s
129.23
128.60
128.54
127.07
126.50
126.28
125.99
125.48
129.0
128.0
127.0
126.0
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

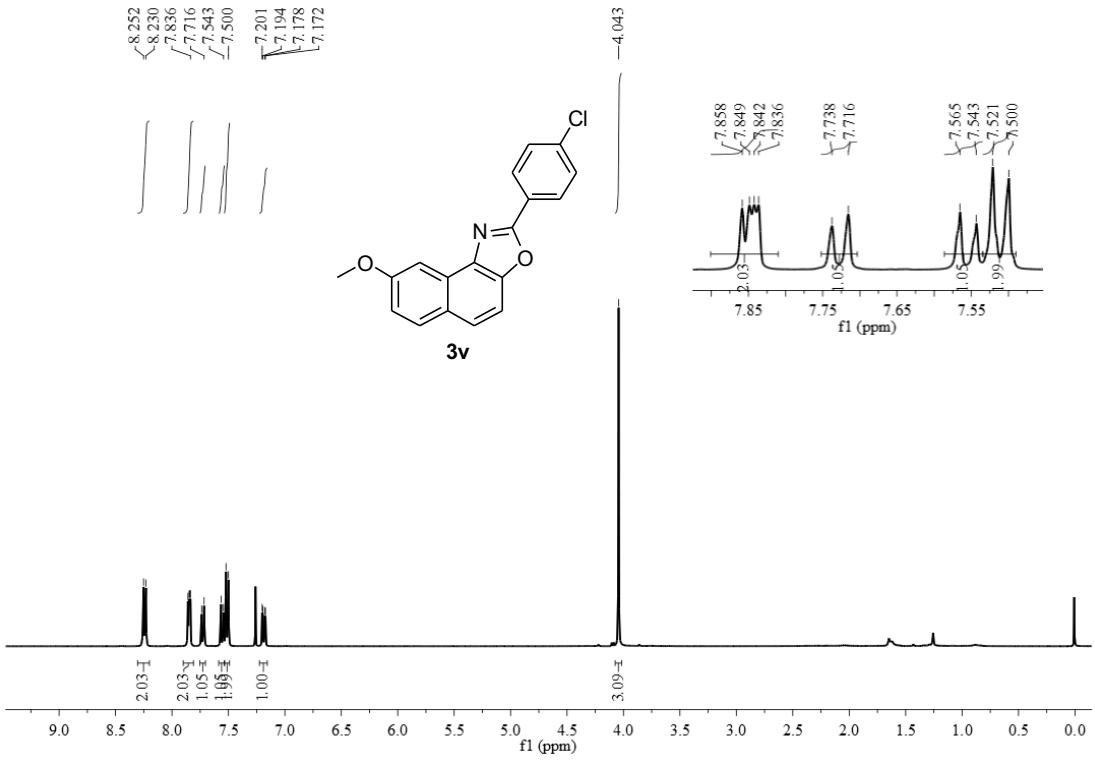

8.609
8.588
8.238
8.217
7.786
7.743
7.721
7.696
7.693
7.679
7.676
7.673
7.658
7.655
7.570
7.567
7.552
7.549
7.546
7.532
7.529
7.363
7.343
2.455
7.808
7.786
7.743
7.721
7.679
7.676
7.673
7.658
7.655
7.567
7.552
7.549
7.546
7.532
7.529
1.03
0.99
1.04
1.04
7.80 7.75 7.70 7.65 7.60 7.55
f1 (ppm)
N
O
3t
1.00
2.02
1.02
1.03
0.82
1.04
2.04
3.04
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 0.0
f1 (ppm)

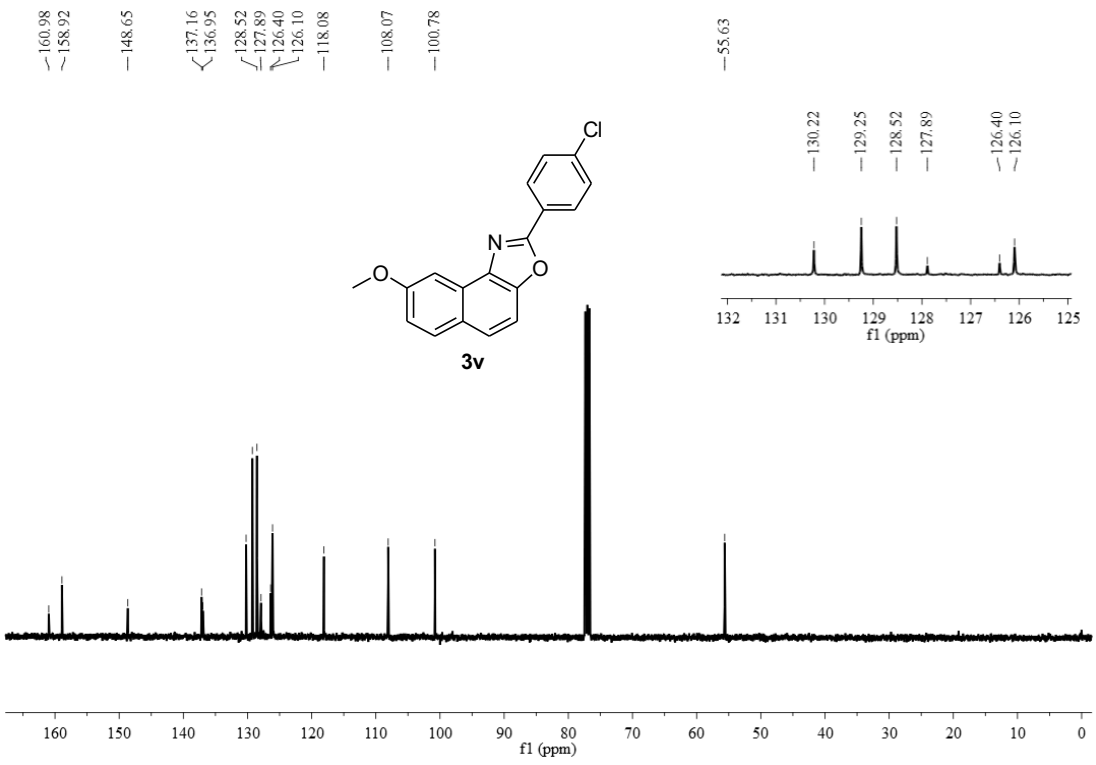

161.55
146.84
140.47
136.57
126.25
125.46
124.67
124.23
123.71
121.22
109.74
20.59
130.14
128.58
127.51
126.25
125.46
124.67
124.23
123.71
130 129 128 127 126 125 124
f1 (ppm)
N
O
3t
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

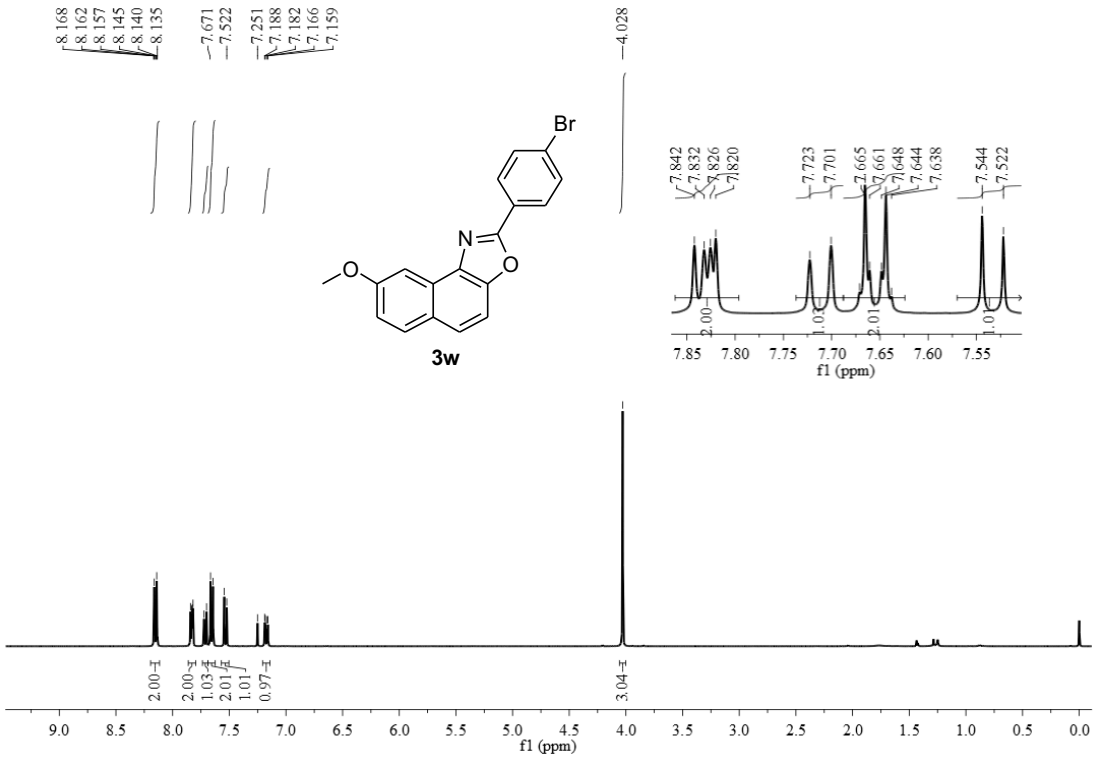

8.321
8.316
8.308
8.304
8.299
8.291
8.285
7.701
7.561
7.539
7.252
7.242
7.237
7.220
7.203
7.198
7.191
7.185
7.169
7.162
4.036
F
N
O
O
3u
2.02
2.05
1.00
0.97
2.33
1.01
3.09
f1 (ppm)
8.328
8.321
8.316
8.308
8.304
8.299
8.291
8.285
8.278
2.02
8.40
8.35
8.30
8.25
8.20
f1 (ppm)
7.252
7.242
7.237
7.220
7.198
7.185
7.169
7.162
2.33
1.01
7.30
7.25
7.20
7.15
7.10
f1 (ppm)

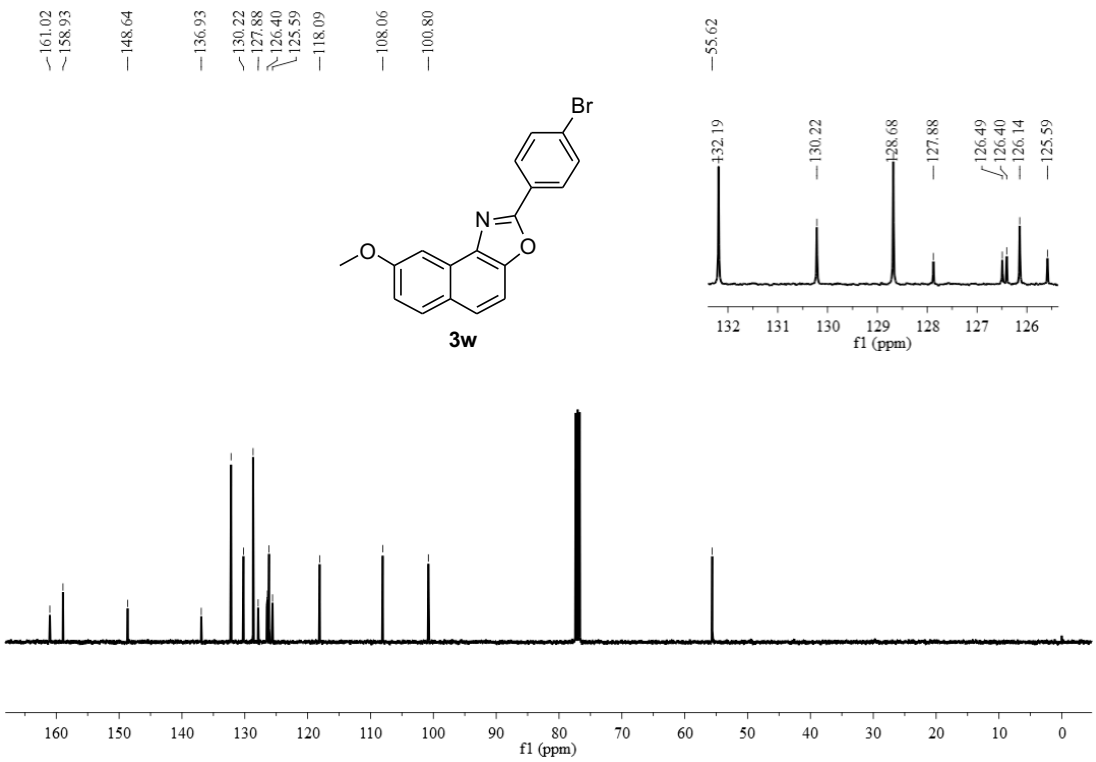

165.79
163.28
161.11
158.88
148.61
136.90
129.51
127.86
125.86
123.90
116.27
116.05
108.07
100.77
55.63
F
N
O
O
3u
130.20
129.51
129.43
127.86
126.40
125.86
123.93
123.90
130
129
128
127
126
125
124
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

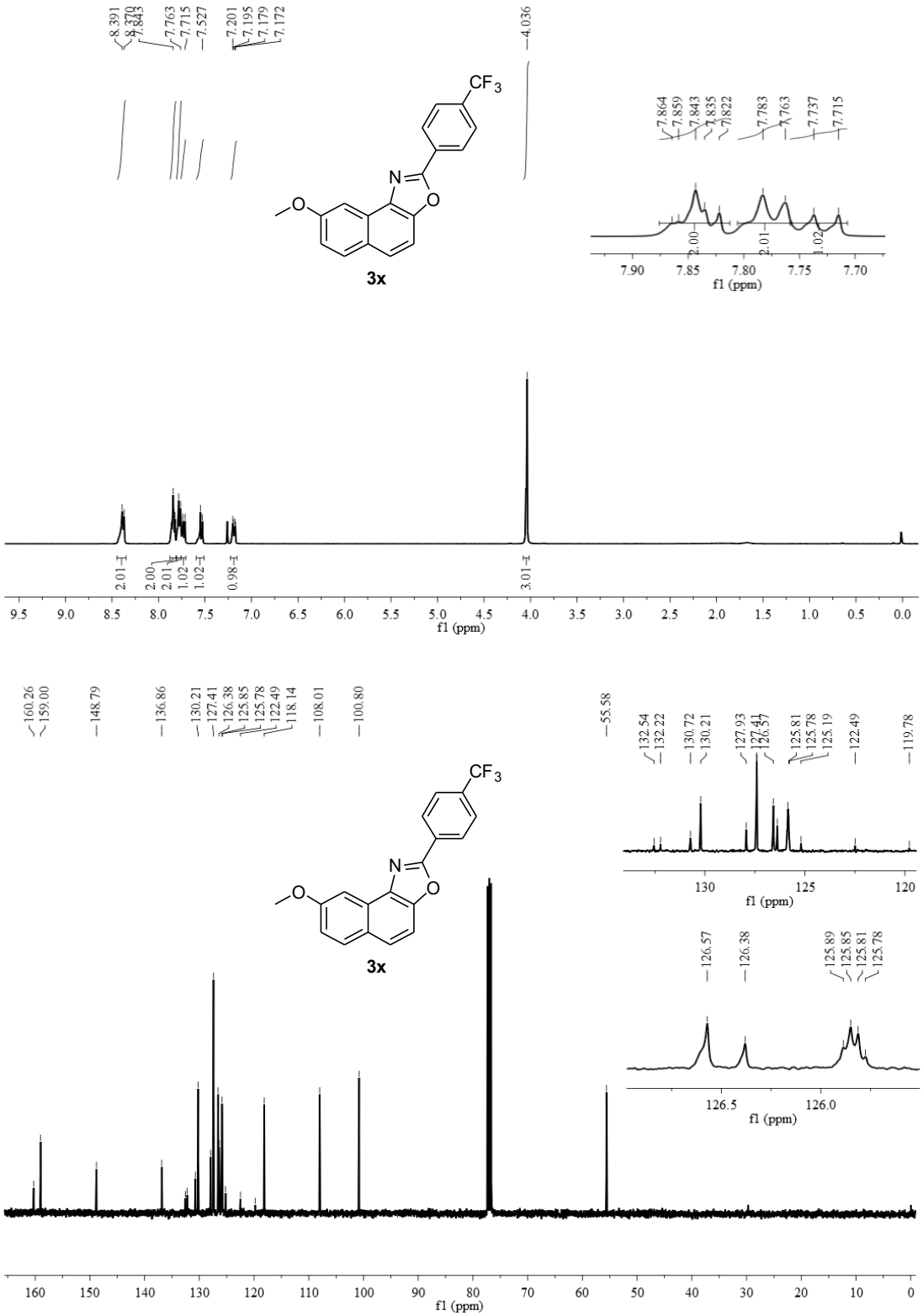

108.33
F
N
O
O
3u
2E+05
1E+05
1E+05
1E+05
1E+05
1E+05
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
−10000
10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)

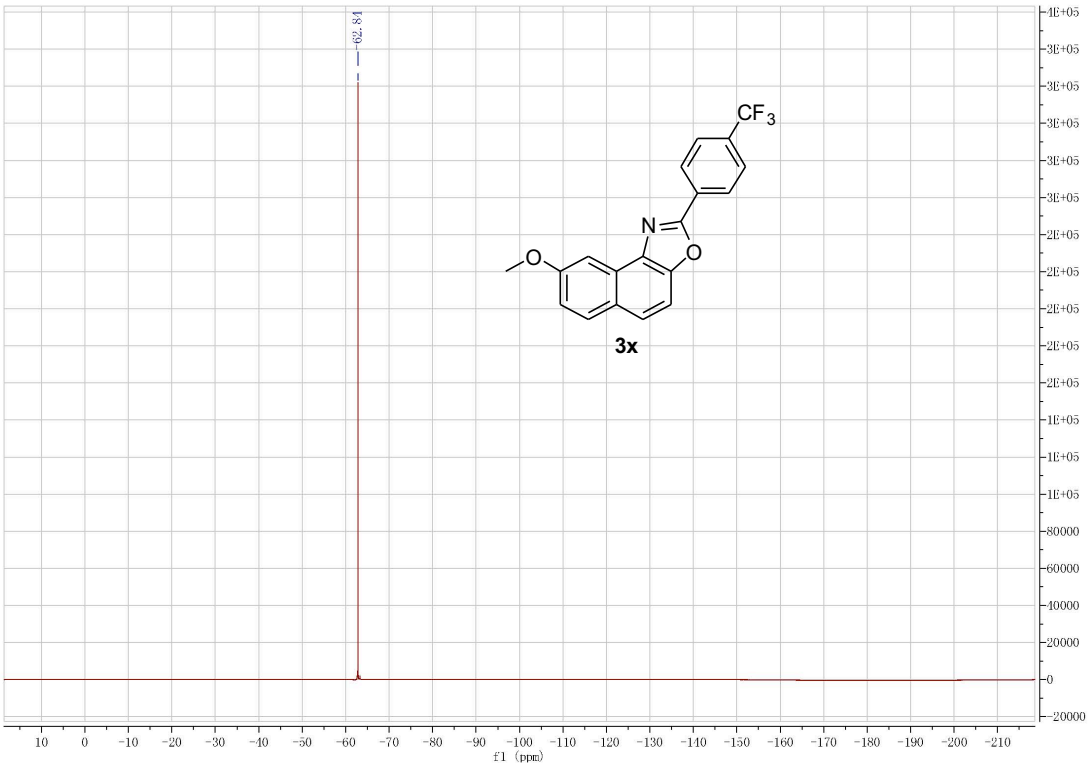

8.252
8.230
7.836
7.716
7.543
7.500
7.201
7.194
7.178
7.172
4.043
Cl
N
O
O
3v
7.858
7.849
7.842
7.836
7.738
7.716
7.565
7.543
7.521
7.500
2.03
1.05
1.03
1.99
7.85
7.75
7.65
7.55
f1 (ppm)
2.03
2.03
1.05
1.03
1.00
3.09
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

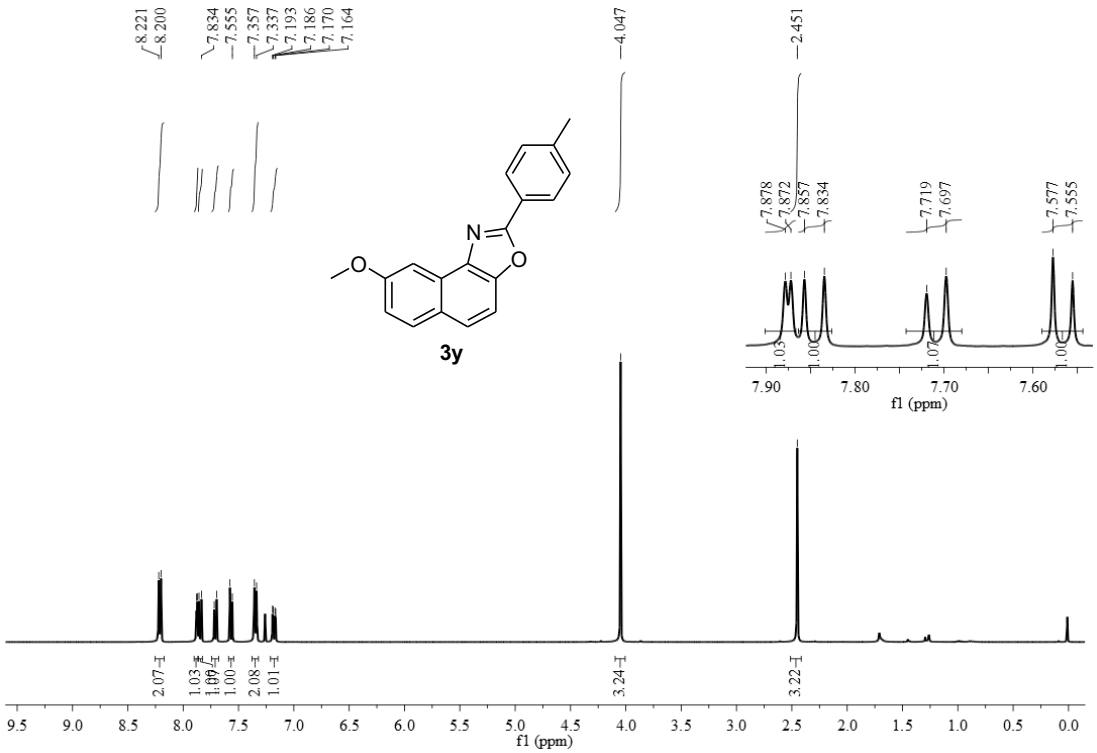

160.98
158.92
148.65
137.16
136.95
128.52
127.89
126.40
126.10
118.08
108.07
100.78
55.63
Cl
N
O
O
3v
130.22
129.25
128.52
127.89
126.40
126.10
132
131
130
129
128
127
126
125
f1 (ppm)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

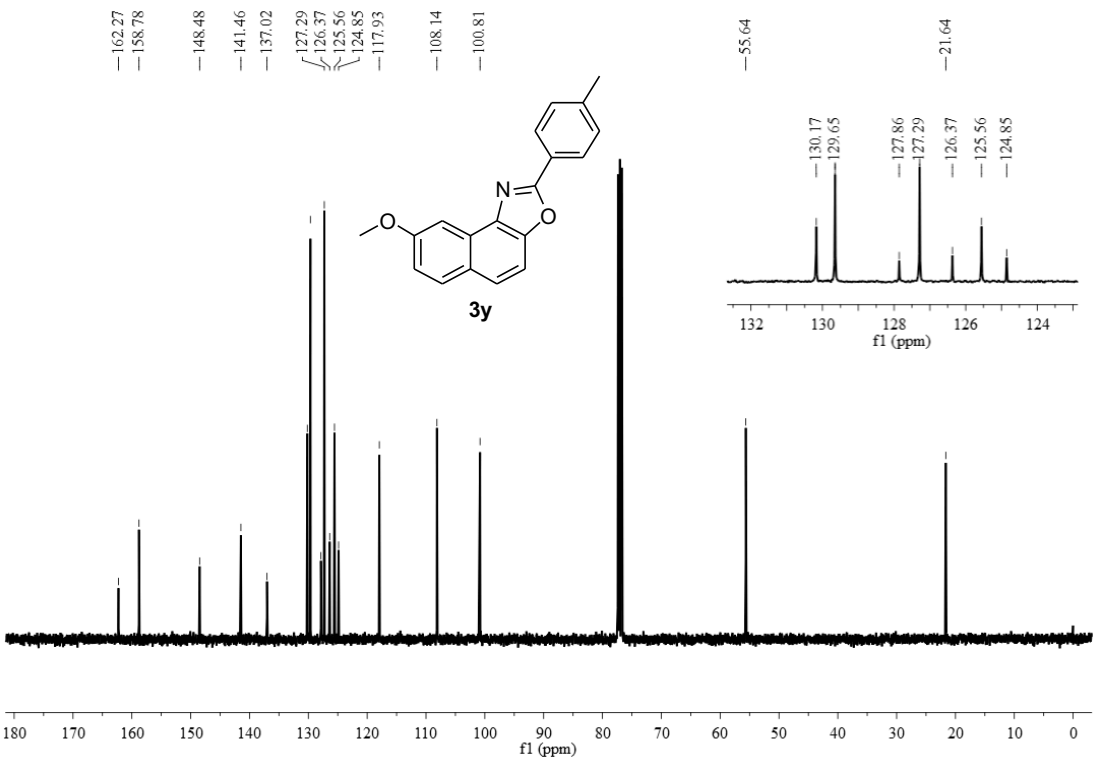

8.168
8.162
8.157
8.145
8.140
8.135
7.671
7.522
7.251
7.188
7.182
7.166
7.159
4.028
Br
N
O
O
3w
7.842
7.832
7.826
7.820
7.723
7.701
7.665
7.661
7.648
7.644
7.638
7.544
7.522
2.00
1.03
2.01
1.01
7.85 7.80 7.75 7.70 7.65 7.60 7.55
f1 (ppm)
2.00
2.00
1.03
2.01
1.01
0.97
3.04
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

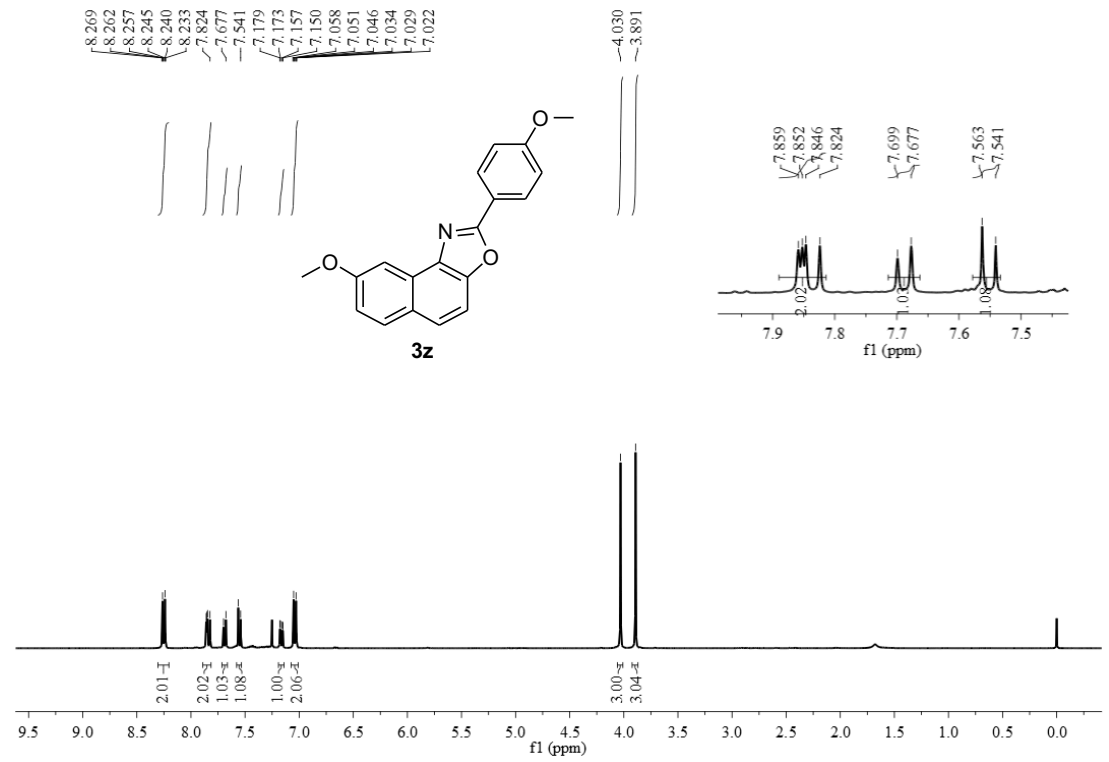

161.02
158.93
148.64
136.93
130.22
127.88
126.40
125.59
118.09
108.06
100.80
55.62
Br
N
O
O
3w
132.19
130.22
128.68
127.88
126.49
126.40
126.14
125.59
132 131 130 129 128 127 126
f1 (ppm)
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

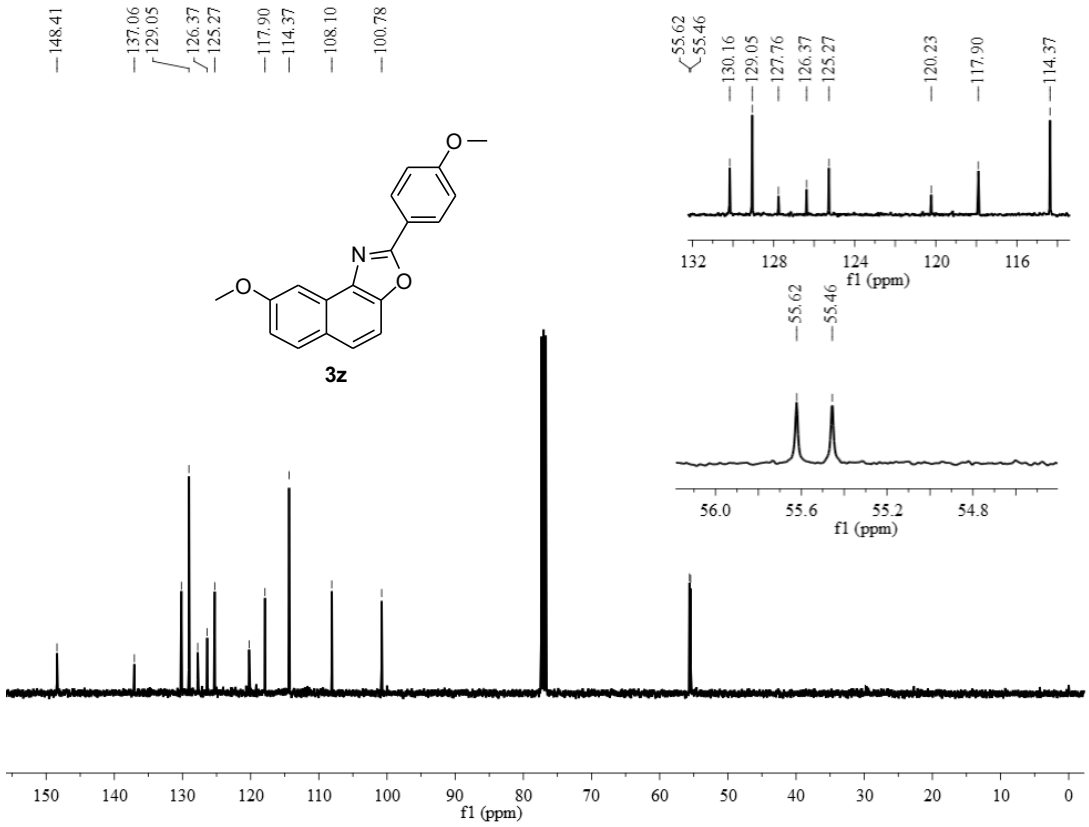

8.391
8.370
8.363
7.843
7.763
7.715
7.527
7.201
7.195
7.179
7.172
4.036
CF3
N
O
O
3x
7.864
7.859
7.843
7.835
7.822
7.783
7.763
7.737
7.715
2.00
2.01
1.02
7.90
7.85
7.80
7.75
7.70
f1 (ppm)
2.01
2.00
2.01
1.02
1.02
0.98
3.01
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
160.26
159.00
148.79
136.86
130.21
127.41
126.38
125.85
125.78
122.49
118.14
108.01
100.80
55.58
132.54
132.22
130.72
130.21
127.93
127.41
126.57
125.81
125.78
125.19
122.49
119.78
CF3
N
O
O
3x
130
125
120
f1 (ppm)
126.57
126.38
125.89
125.85
125.81
125.78
126.5
126.0
f1 (ppm)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

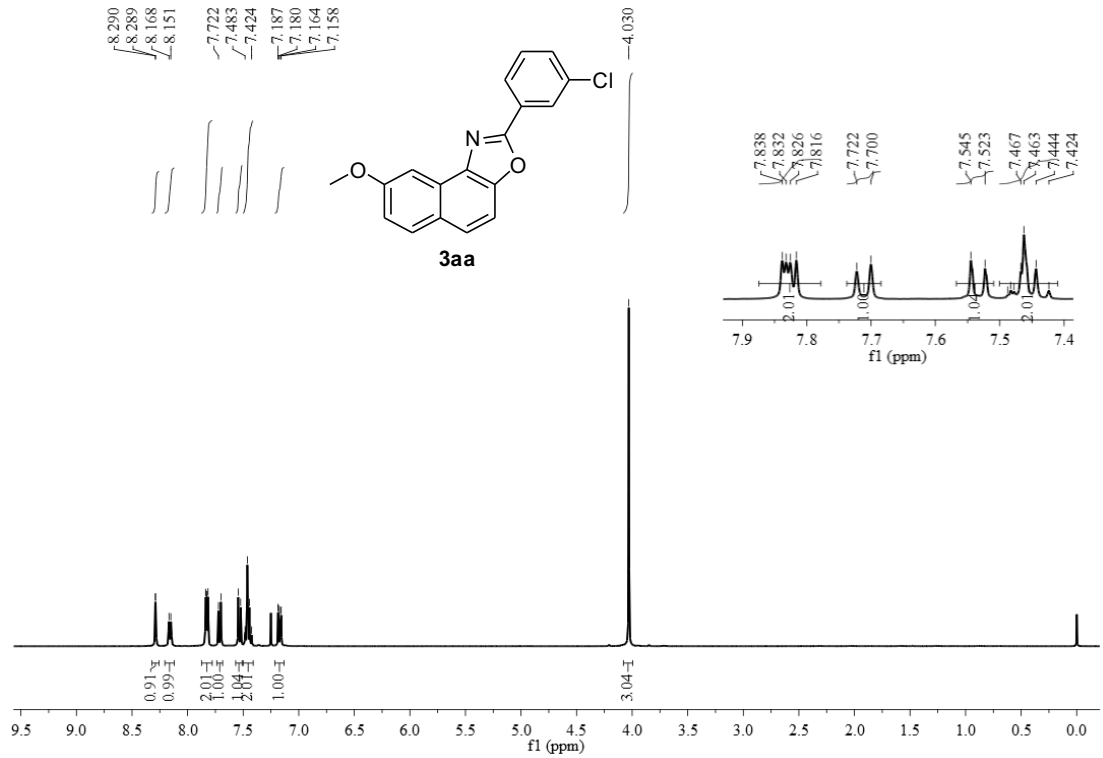

-62.84
CF3
N
O
O
3x
f1 (ppm)

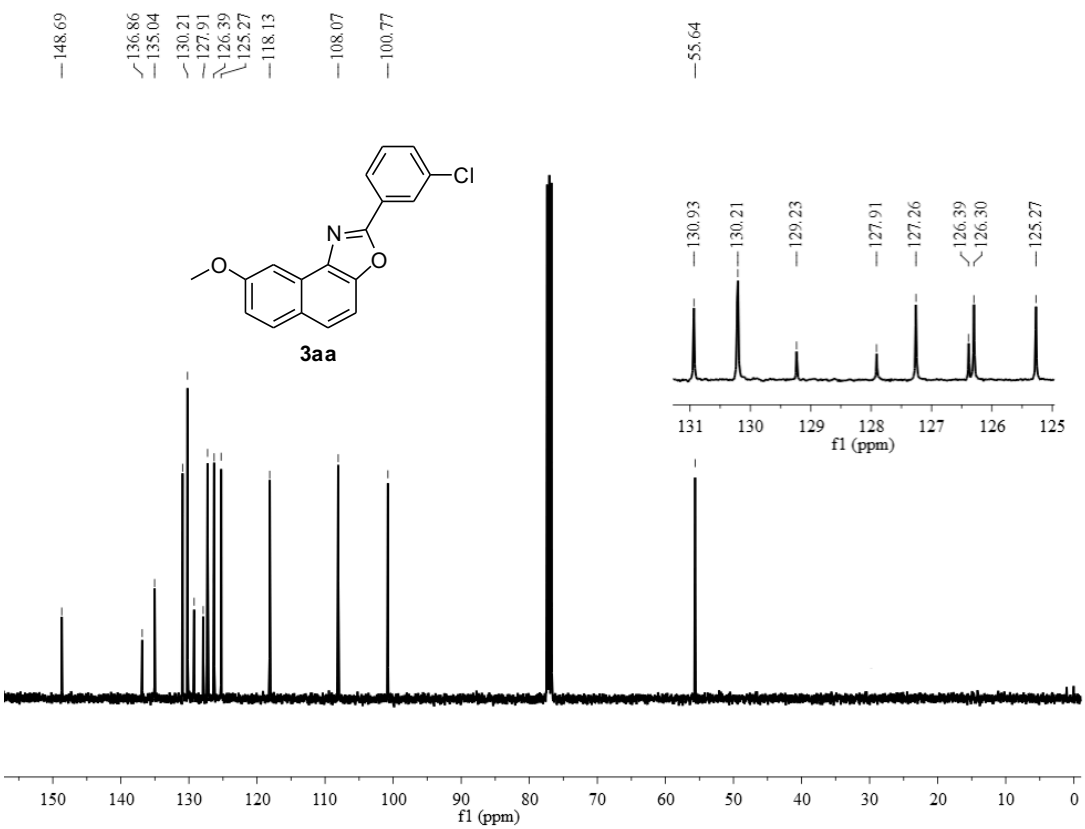

8.221
8.200
7.834
7.555
7.357
7.337
7.193
7.186
7.170
7.164
4.047
2.451
7.878
7.872
7.857
7.834
7.719
7.697
7.577
7.555
3y
2.07
1.03
1.00
1.00
2.08
1.01
3.24
3.22
f1 (ppm)

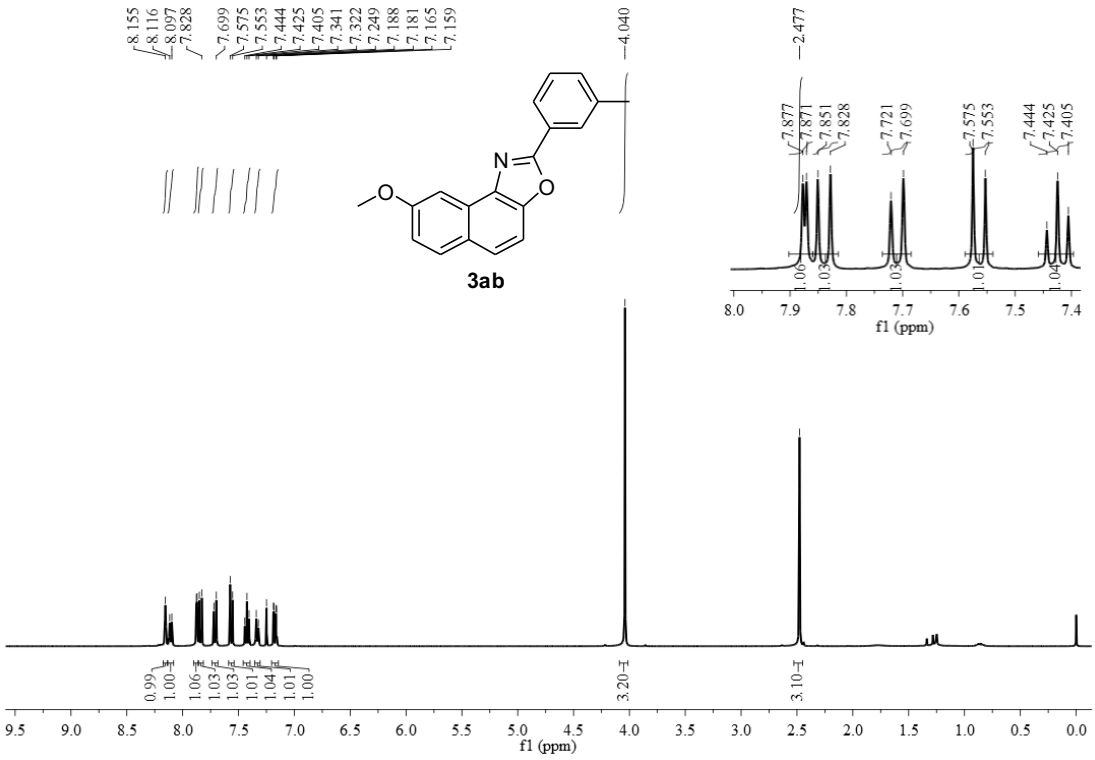

162.27
158.78
148.48
141.46
137.02
127.29
126.37
125.56
124.85
117.93
108.14
100.81
55.64
21.64
130.17
129.65
127.86
127.29
126.37
125.56
124.85
3y
f1 (ppm)

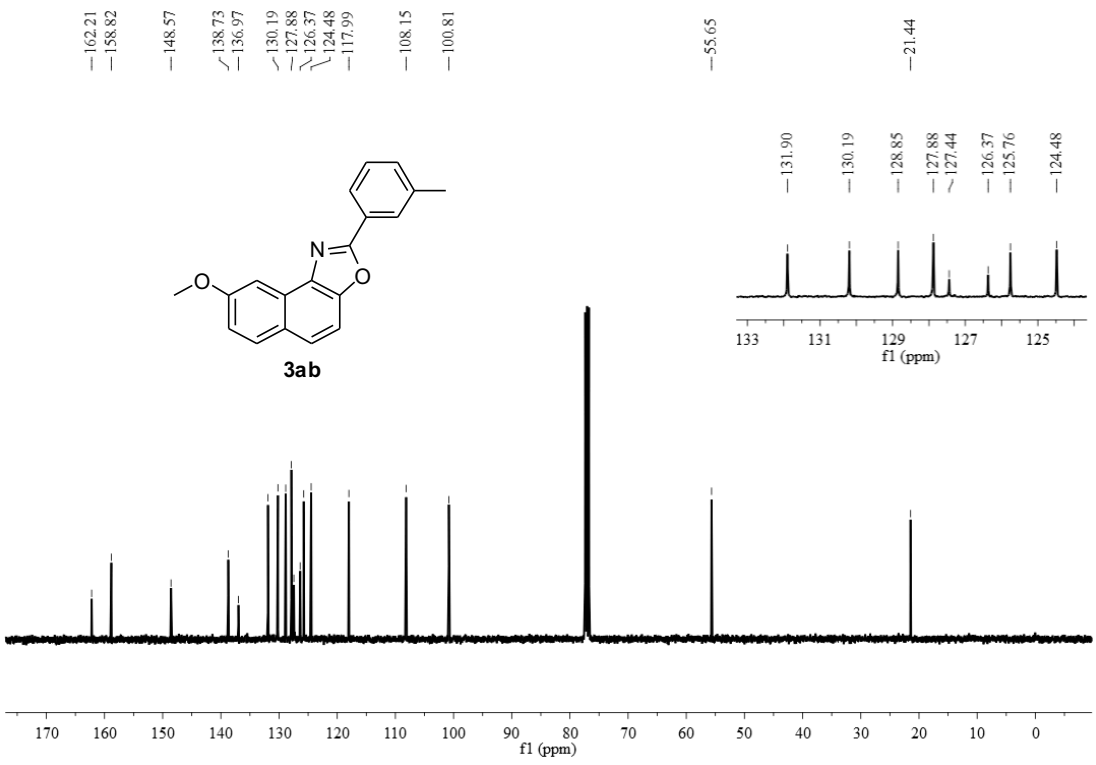

8.269
8.262
8.257
8.245
8.240
8.233
7.824
7.677
7.541
7.179
7.173
7.157
7.150
7.058
7.051
7.046
7.034
7.029
7.022
4.030
3.891
3z
7.859
7.852
7.846
7.824
7.699
7.677
7.563
7.541
2.02
1.03
1.08
7.9
7.8
7.7
7.6
7.5
f1 (ppm)
2.01
2.02
1.03
1.08
1.00
2.06
3.00
3.04
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

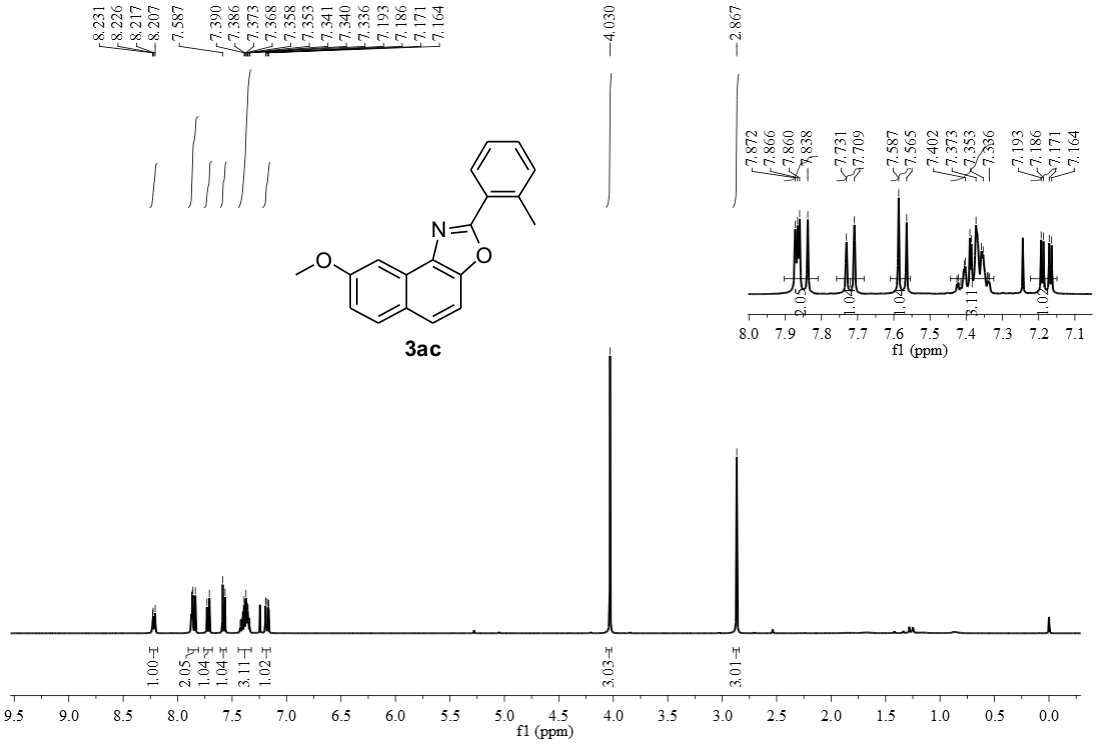

148.41
137.06
129.05
126.37
125.27
117.90
114.37
108.10
100.78
3z
55.62
55.46
130.16
129.05
127.76
126.37
125.27
120.23
117.90
114.37
132
128
124
120
116
f1 (ppm)
55.62
55.46
56.0
55.6
55.2
54.8
f1 (ppm)
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

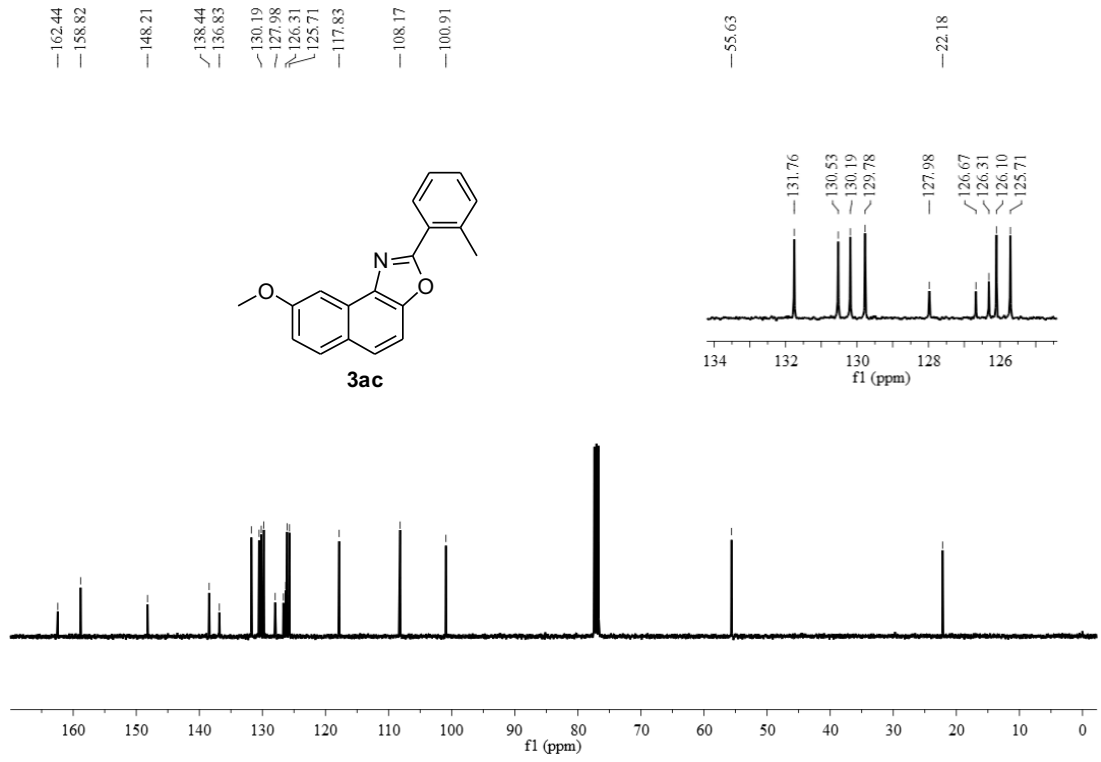

8.290
8.289
8.168
8.151
7.722
7.483
7.424
7.187
7.180
7.164
7.158
4.030
Cl
N
O
O
3aa
7.838
7.832
7.826
7.816
7.722
7.700
7.545
7.523
7.467
7.463
7.444
7.424
2.01
1.00
1.04
2.01
7.9
7.8
7.7
7.6
7.5
7.4
f1 (ppm)
0.91
0.99
2.01
1.00
1.04
2.01
1.00
3.04
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

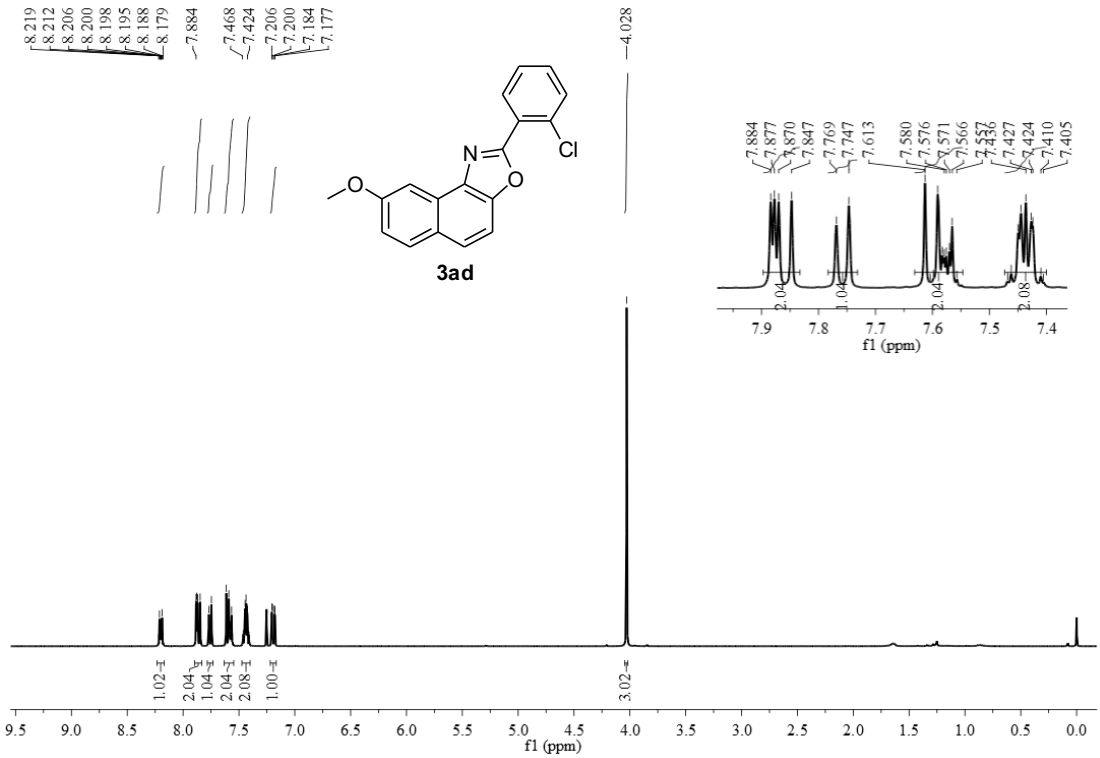

148.69
136.86
135.04
130.21
127.91
126.39
125.27
118.13
108.07
100.77
55.64
Cl
N
O
O
3aa
130.93
130.21
129.23
127.91
127.26
126.39
126.30
125.27
131
130
129
128
127
126
125
f1 (ppm)
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

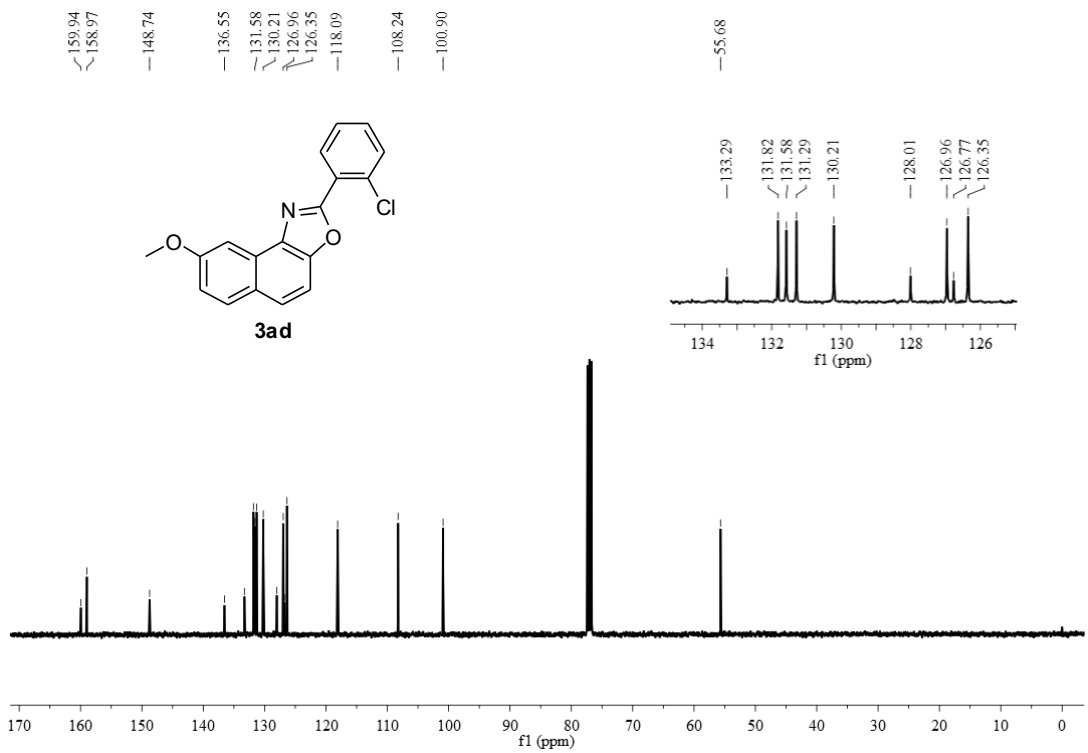

8.155
8.116
8.097
7.828
7.699
7.575
7.553
7.444
7.425
7.405
7.341
7.322
7.249
7.188
7.181
7.165
7.159
4.040
2.477
7.877
7.871
7.851
7.828
7.721
7.699
7.575
7.553
7.444
7.425
7.405
N
O
O
3ab
0.99
1.00
1.06
1.03
1.03
1.01
1.04
1.01
1.00
3.20
3.10
f1 (ppm)

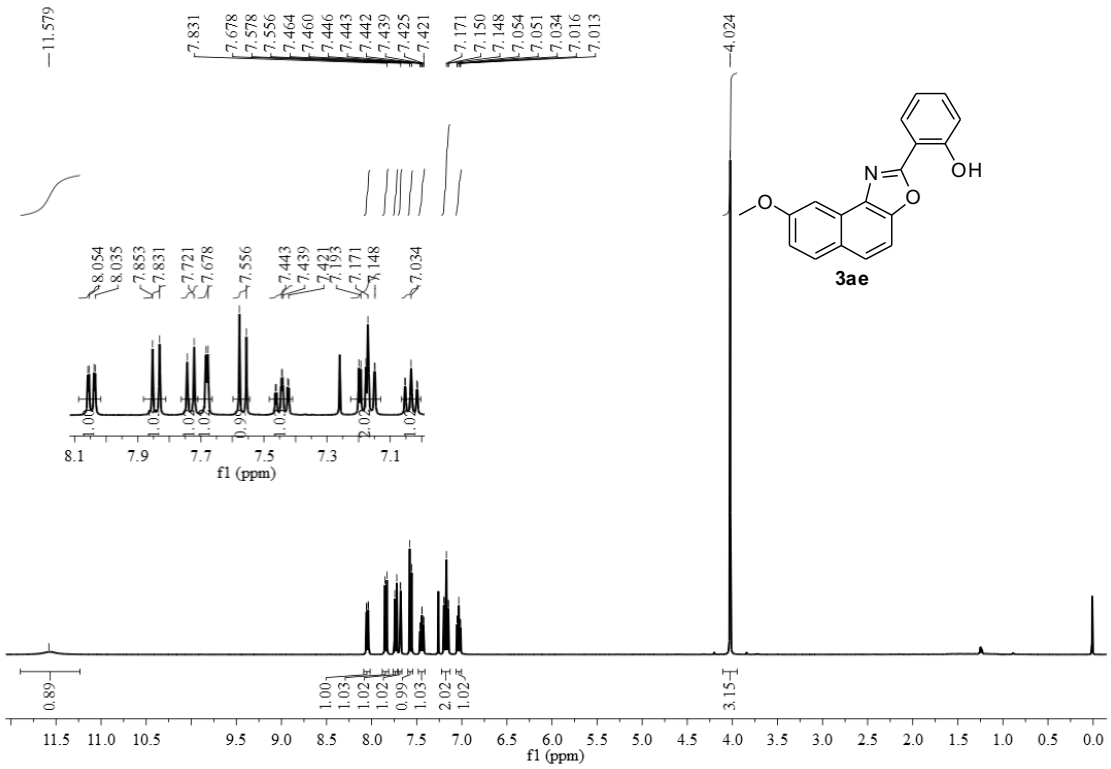

162.21
158.82
148.57
138.73
136.97
130.19
127.88
126.37
124.48
117.99
108.15
100.81
55.65
21.44
131.90
130.19
128.85
127.88
127.44
126.37
125.76
124.48
N
O
O
3ab
f1 (ppm)

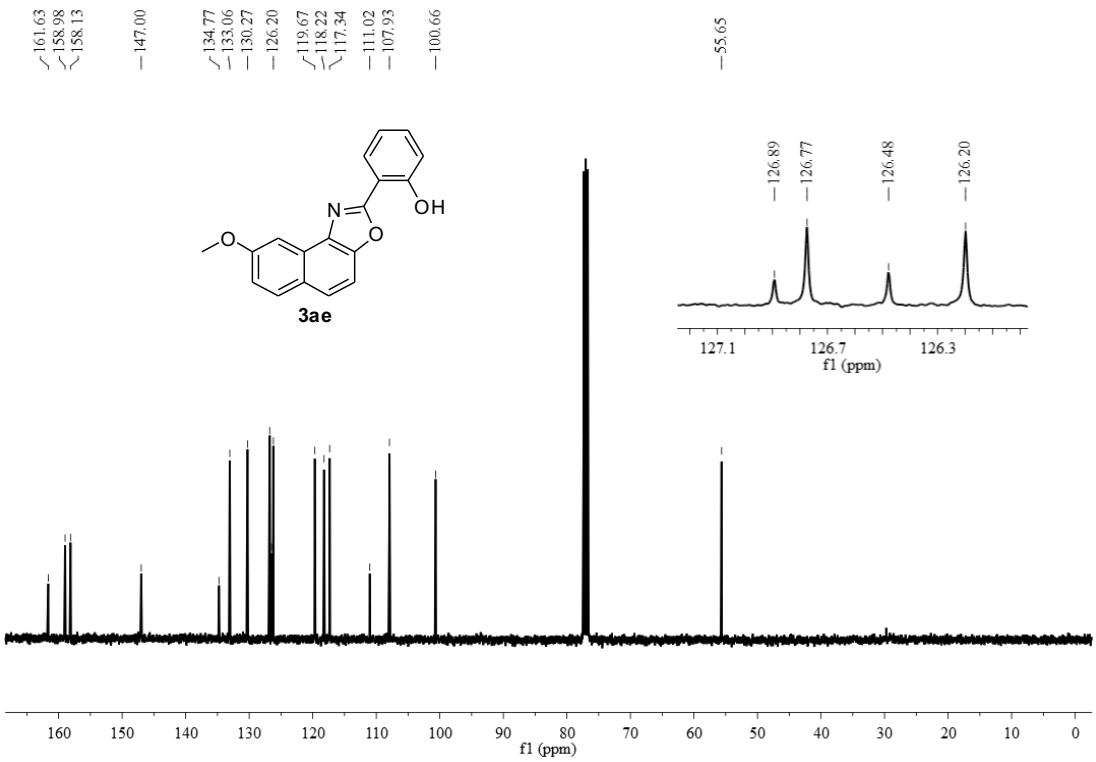

8.231
8.226
8.217
8.207
7.587
7.390
7.386
7.373
7.368
7.358
7.353
7.341
7.340
7.336
7.193
7.186
7.171
7.164
4.030
2.867
7.872
7.866
7.860
7.838
7.731
7.709
7.587
7.565
7.402
7.373
7.353
7.336
7.193
7.186
7.171
7.164
2.05
1.04
1.04
3.11
1.02
8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1
f1 (ppm)
N
O
O
3ac
1.00
2.05
1.04
1.04
3.11
1.02
3.03
3.01
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 0.0
f1 (ppm)

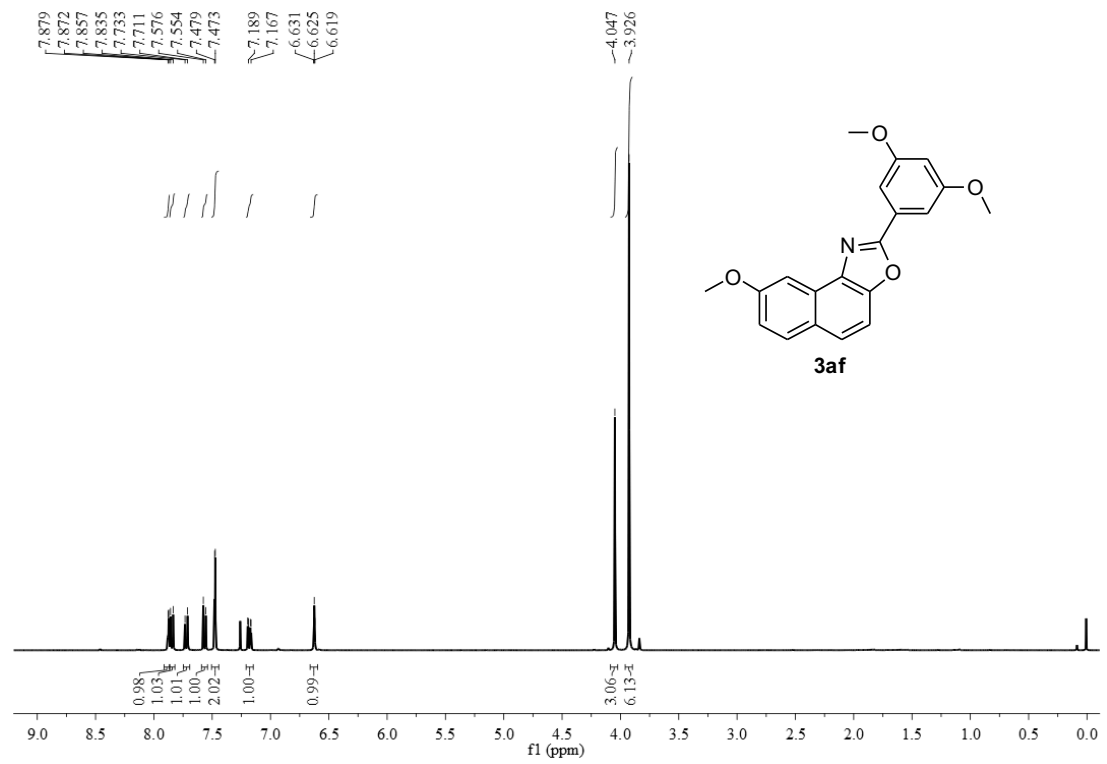

162.44
158.82
148.21
138.44
136.83
130.19
127.98
126.31
125.71
117.83
108.17
100.91
55.63
22.18
131.76
130.53
130.19
129.78
127.98
126.67
126.31
126.10
125.71
134 132 130 128 126
f1 (ppm)
N
O
O
3ac
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

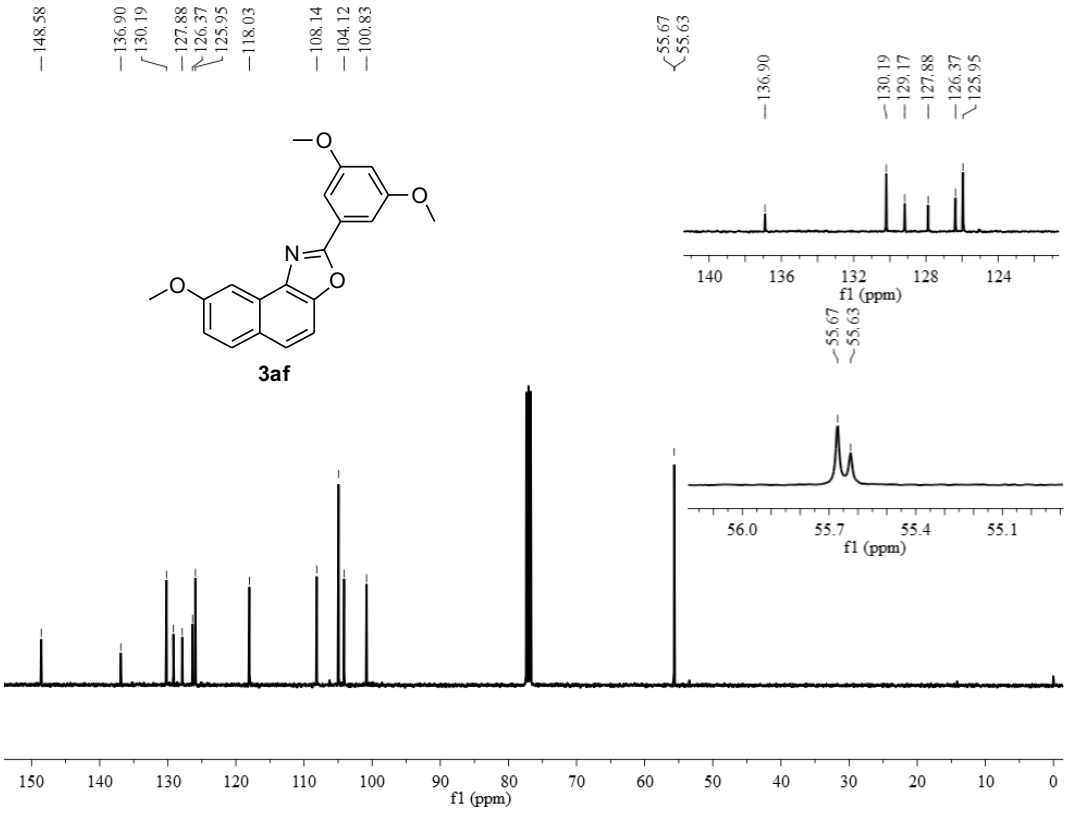

8.219
8.212
8.206
8.200
8.198
8.195
8.188
8.179
7.884
7.468
7.424
7.206
7.200
7.184
7.177
4.028
3ad
7.884
7.877
7.870
7.847
7.769
7.747
7.613
7.580
7.576
7.571
7.566
7.557
7.427
7.424
7.410
7.405
2.04
1.04
2.04
2.08
f1 (ppm)
1.02
2.04
1.04
2.04
2.08
1.00
3.02
f1 (ppm)

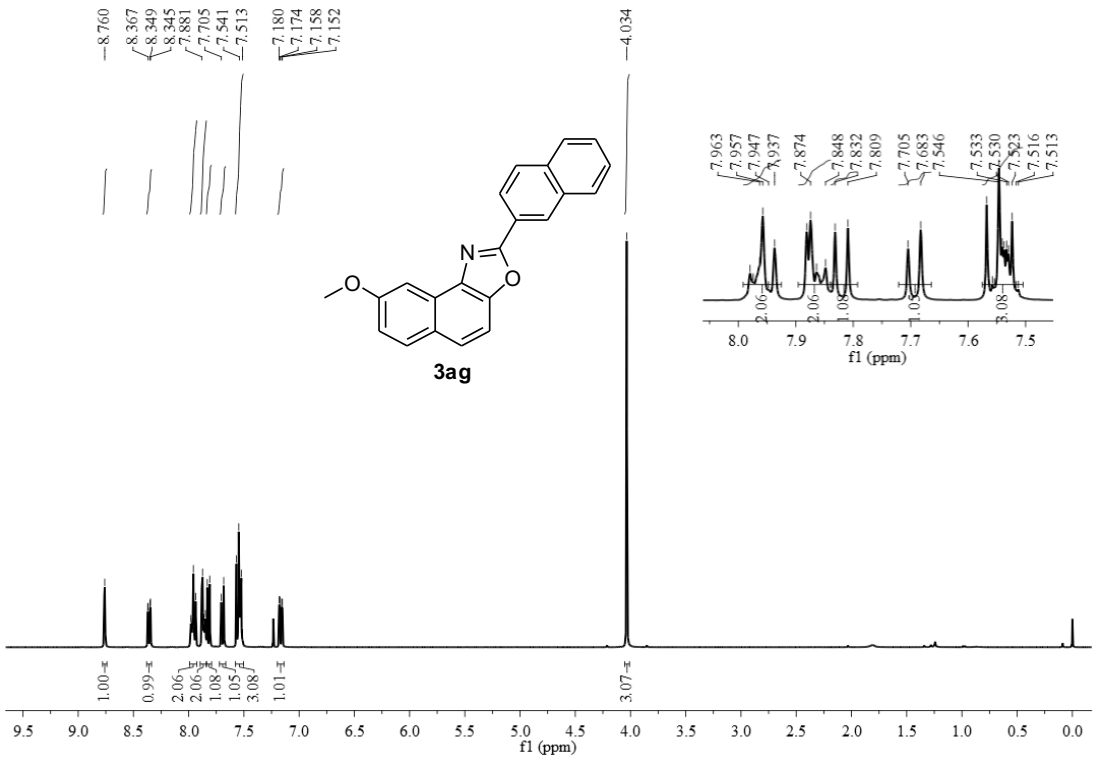

159.94
158.97
148.74
136.55
131.58
130.21
126.96
126.35
118.09
108.24
100.90
55.68
3ad
133.29
131.82
131.58
131.29
130.21
128.01
126.96
126.77
126.35
f1 (ppm)
f1 (ppm)

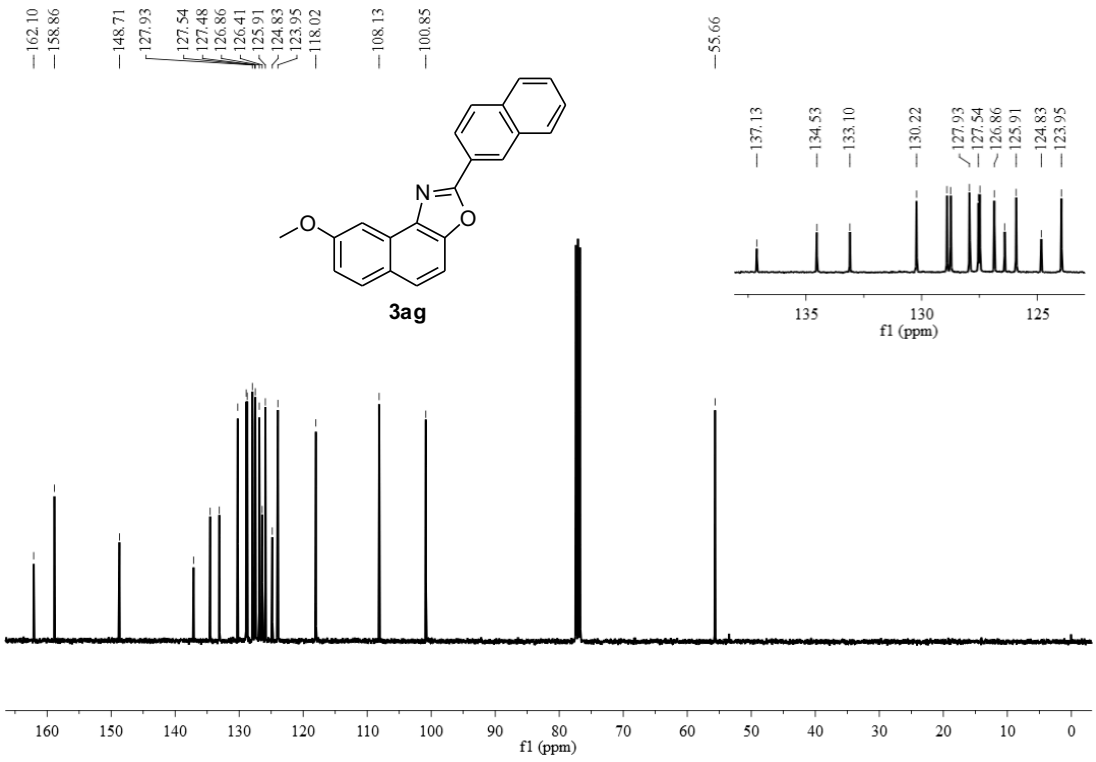

11.579
7.831
7.678
7.578
7.556
7.464
7.460
7.446
7.443
7.442
7.439
7.425
7.421
7.171
7.150
7.148
7.054
7.051
7.034
7.016
7.013
4.024
8.054
8.035
7.853
7.831
7.721
7.678
7.556
7.443
7.439
7.421
7.193
7.171
7.148
7.034
3ae
f1 (ppm)
0.89
1.00
1.03
1.02
1.02
0.99
1.03
2.02
1.02
3.15

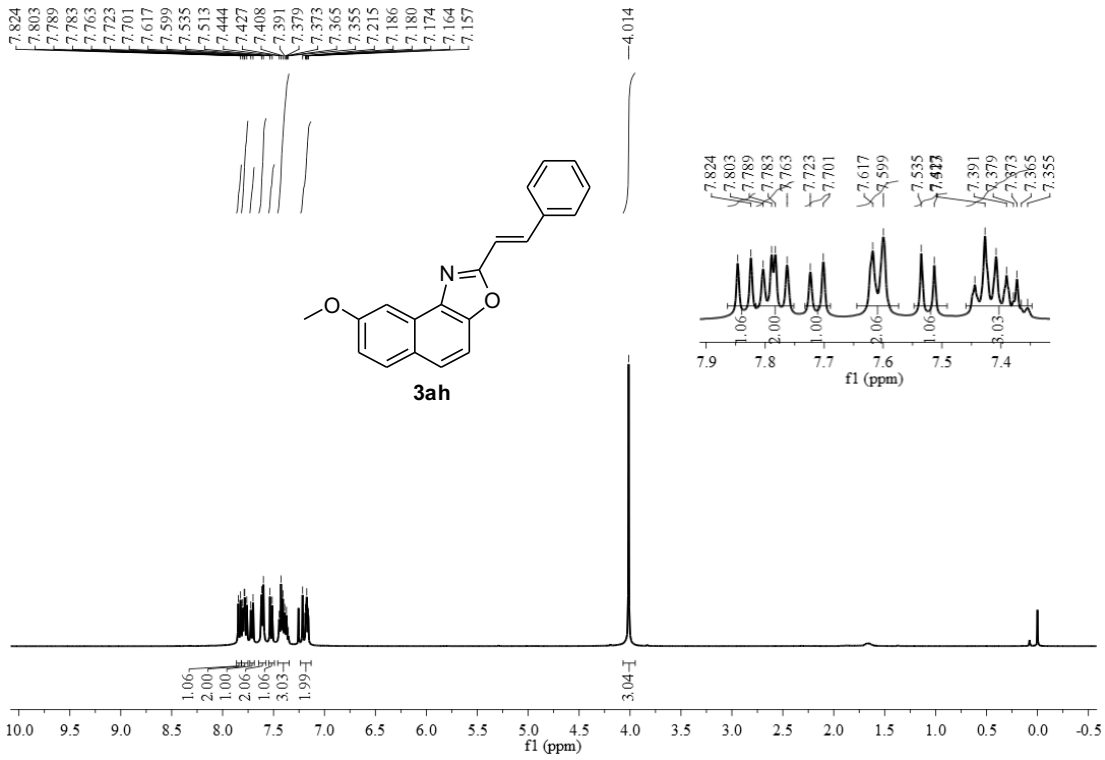

161.63
158.98
158.13
147.00
134.77
133.06
130.27
126.20
119.67
118.22
117.34
111.02
107.93
100.66
55.65
126.89
126.77
126.48
126.20
3ae
f1 (ppm)


7.879
7.872
7.857
7.835
7.733
7.711
7.576
7.554
7.479
7.473
7.189
7.167
6.631
6.625
6.619
4.047
3.926
0.98
1.03
1.01
1.00
2.02
1.00
0.99
3.06
6.13
f1 (ppm)
3af


148.58
136.90
130.19
127.88
126.37
125.95
118.03
108.14
104.12
100.83
55.67
55.63
136.90
130.19
129.17
127.88
126.37
125.95
f1 (ppm)
55.67
55.63
f1 (ppm)
f1 (ppm)
3af


8.760
8.367
8.349
8.345
7.881
7.705
7.541
7.513
7.180
7.174
7.158
7.152
4.034
7.963
7.957
7.947
7.937
7.874
7.848
7.832
7.809
7.705
7.683
7.546
7.533
7.530
7.523
7.516
7.513
1.00
0.99
2.06
2.06
1.08
1.05
3.08
1.01
3.07
f1 (ppm)
3ag


162.10
158.86
148.71
127.93
127.54
127.48
126.86
126.41
125.91
124.83
123.95
118.02
108.13
100.85
55.66
137.13
134.53
133.10
130.22
127.93
127.54
126.86
125.91
124.83
123.95
f1 (ppm)
3ag


7.824
7.803
7.789
7.783
7.763
7.723
7.701
7.617
7.599
7.535
7.513
7.444
7.427
7.408
7.391
7.379
7.373
7.365
7.355
7.215
7.186
7.180
7.174
7.164
7.157
4.014
3ah
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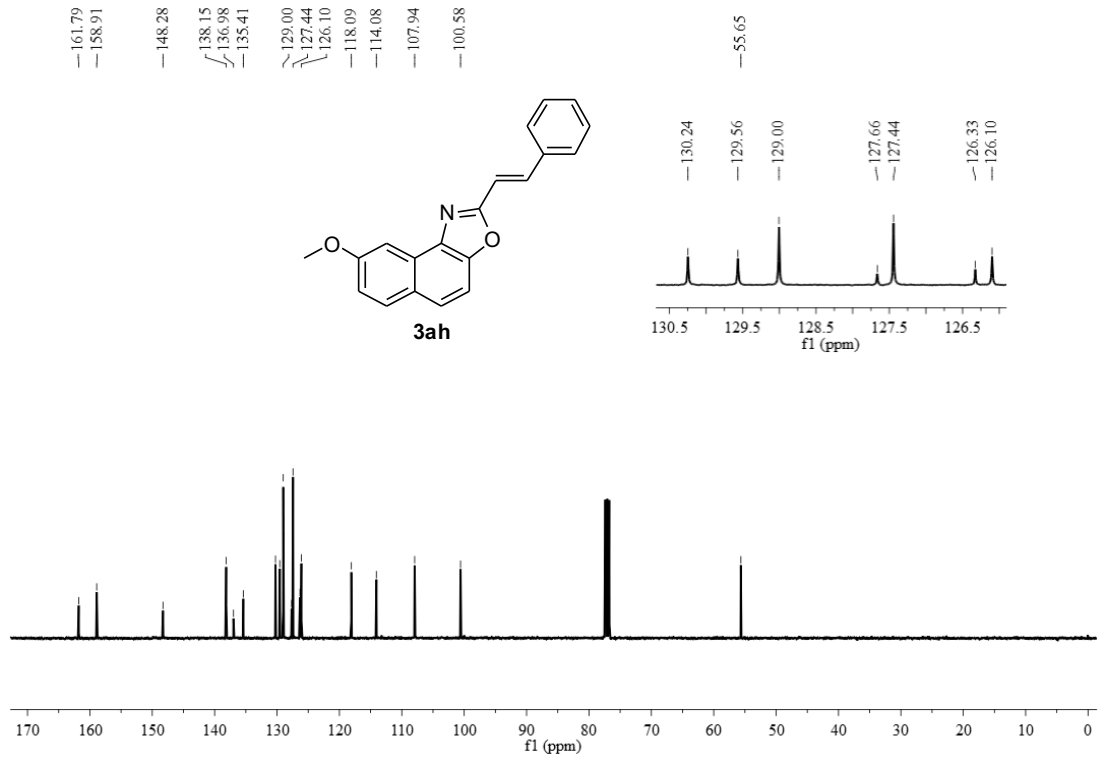
2.00
1.00
2.06
1.06
3.03
1.99
3.04
f1 (ppm)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158.91
148.28
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136.98
135.41
129.00
127.44
126.10
118.09
114.08
107.94
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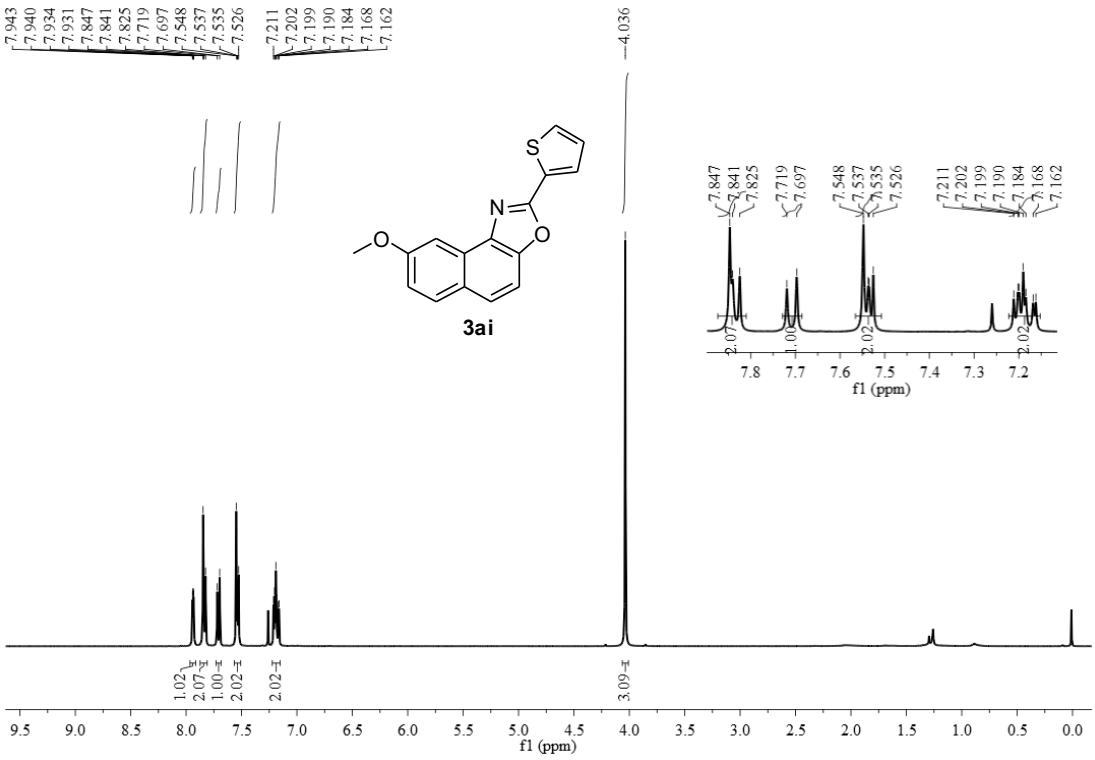
130.24
129.56
129.00
127.66
127.44
126.33
126.10
3ah
f1 (ppm)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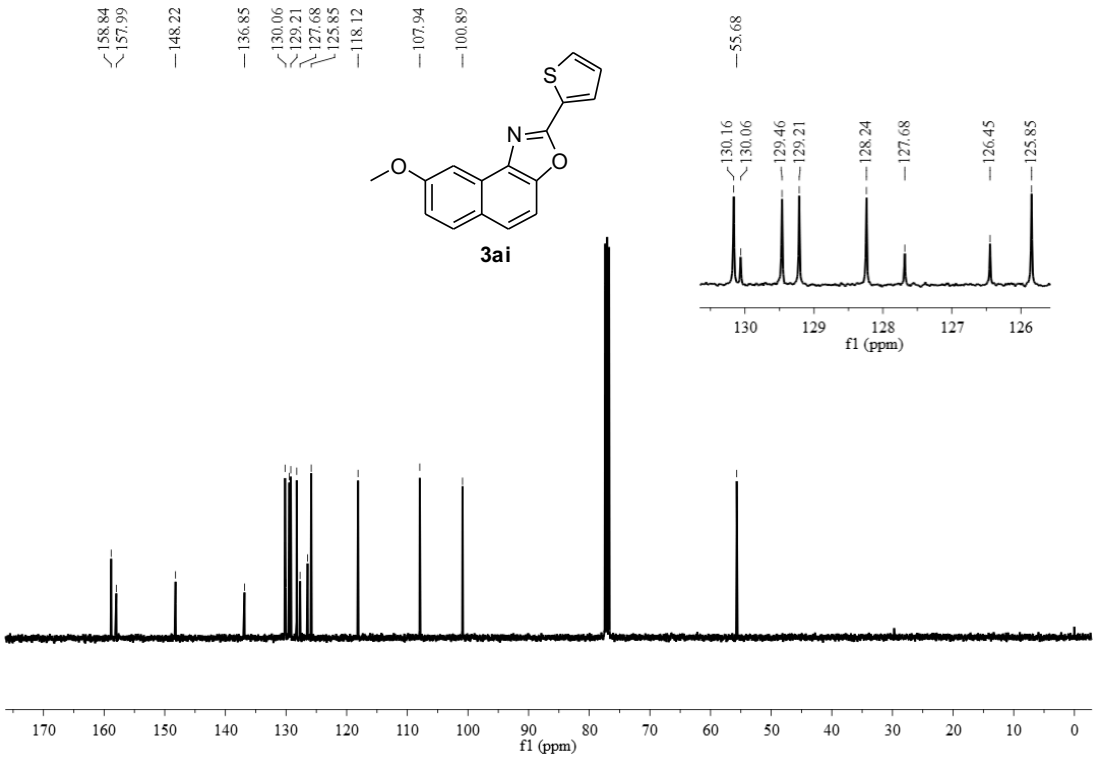
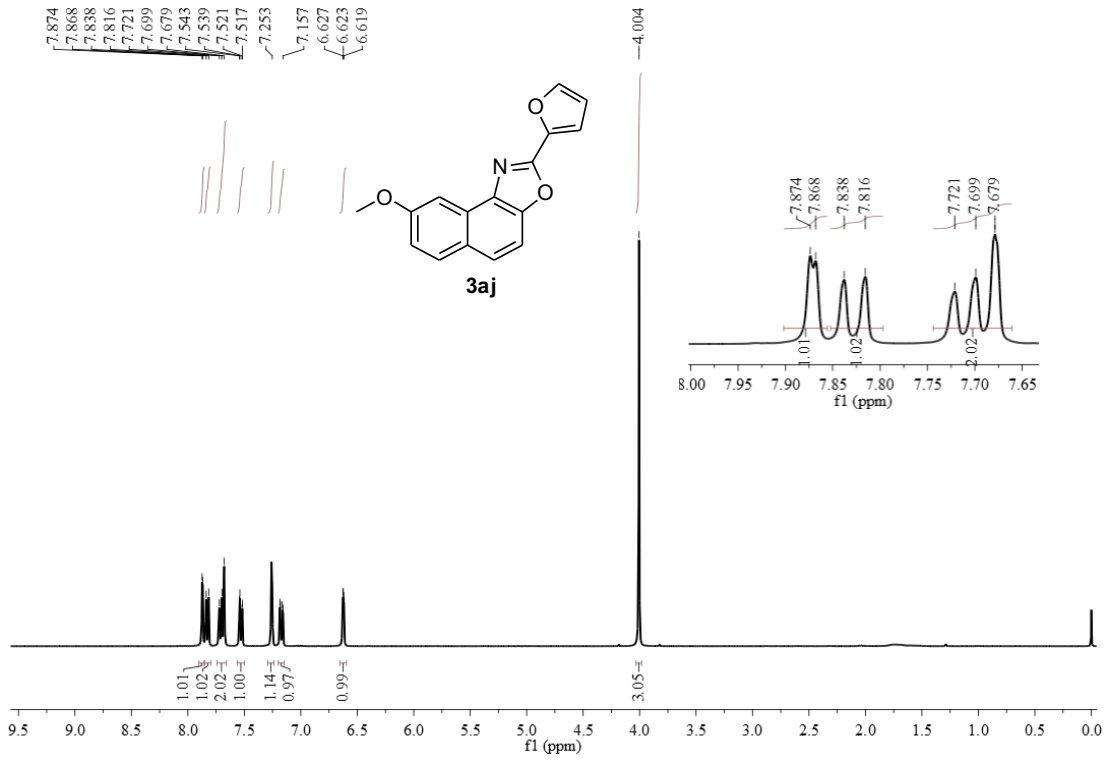
7.847
7.841
7.825
7.719
7.697
7.548
7.537
7.535
7.526
7.211
7.202
7.199
7.190
7.184
7.168
7.162
4.036
3ai
1.02
2.07
1.00
2.02
2.02
3.09
f1 (ppm)


158.84
157.99
148.22
136.85
130.06
129.21
127.68
125.85
118.12
107.94
100.89
55.68
3ai
f1 (ppm)


7.874
7.868
7.838
7.816
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7.699
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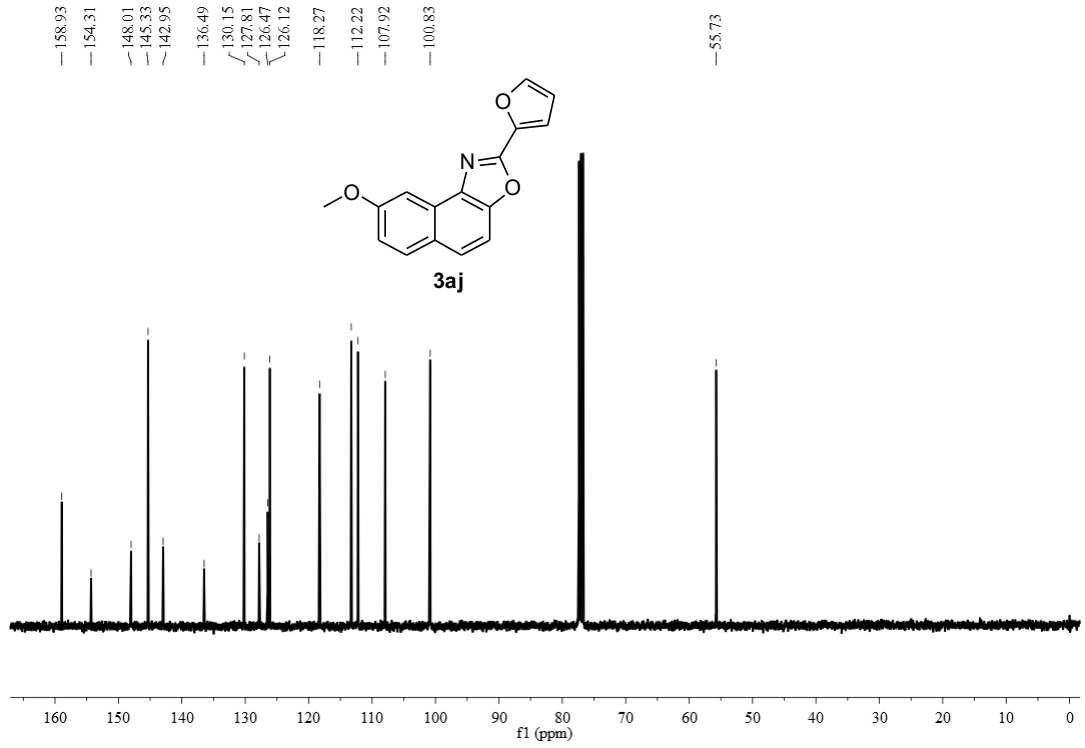
7.543
7.539
7.521
7.517
7.253
7.157
6.627
6.623
6.619
4.004
3aj
1.01
1.02
2.02
1.00
1.14
0.97
0.99
3.05
f1 (ppm)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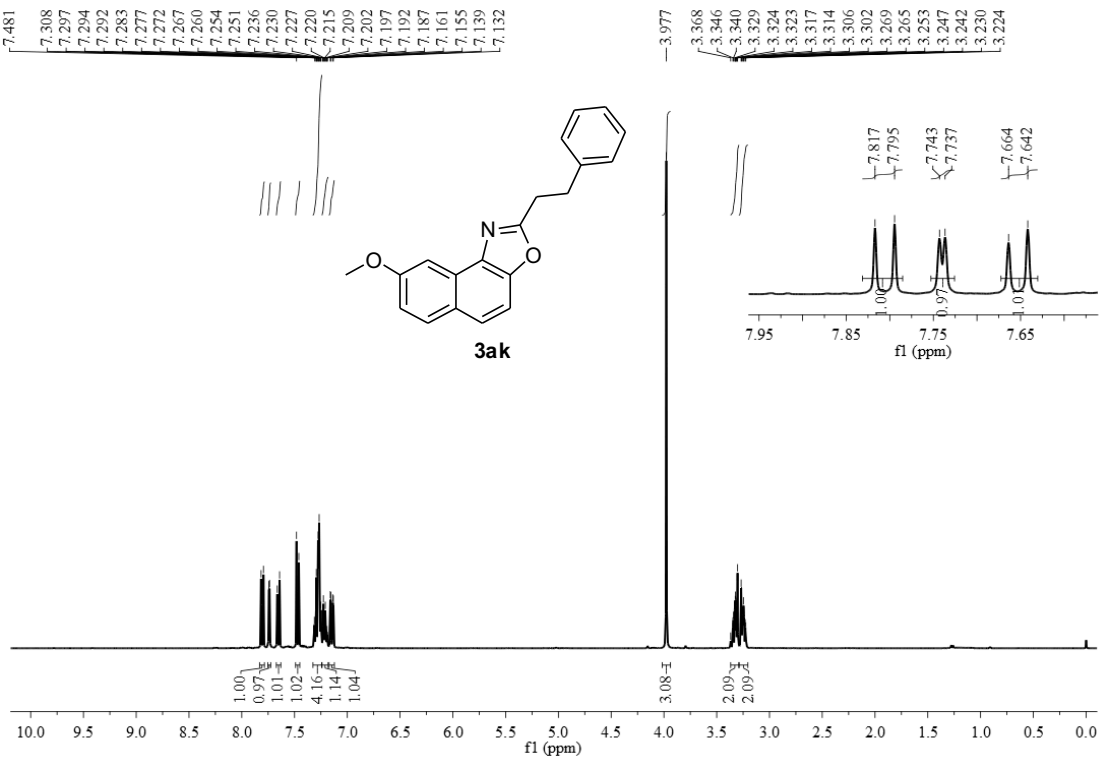
154.31
148.01
145.33
142.95
136.49
130.15
127.81
126.47
126.12
118.27
112.22
107.92
100.83
55.73
3aj
f1 (ppm)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7.294
7.292
7.283
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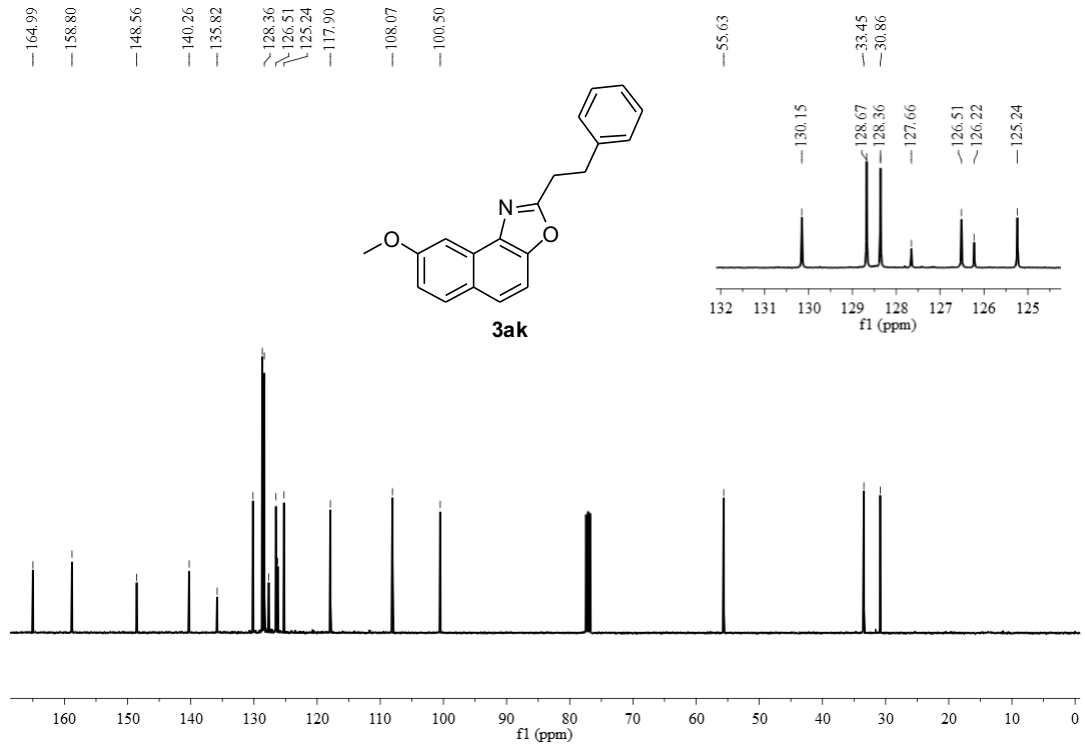
7.272
7.267
7.260
7.254
7.251
7.236
7.230
7.227
7.220
7.215
7.209
7.202
7.197
7.192
7.187
7.161
7.155
7.139
7.132
3.977
3.368
3.346
3.340
3.329
3.324
3.323
3.317
3.314
3.306
3.302
3.269
3.265
3.253
3.247
3.242
3.230
3.224
7.817
7.795
7.743
7.737
7.664
7.642
1.00
0.97
1.01
1.02
4.16
1.14
1.04
3.08
2.09
2.09
f1 (ppm)
3ak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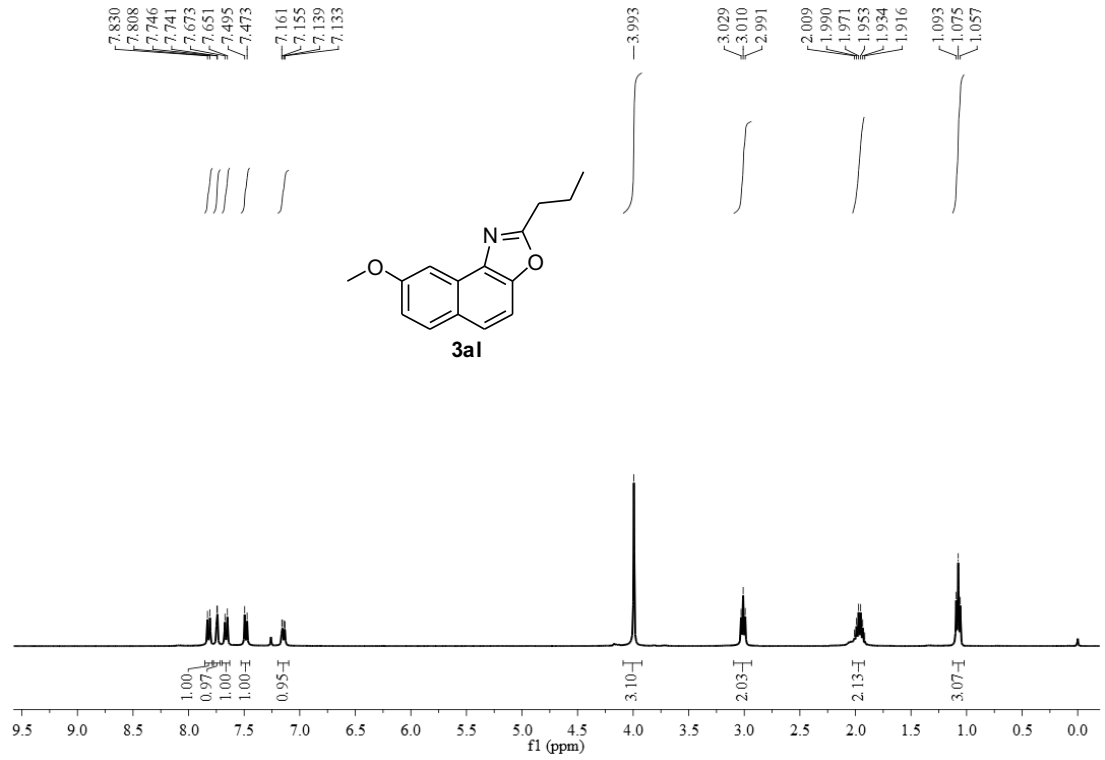
158.80
148.56
140.26
135.82
128.36
126.51
125.24
117.90
108.07
100.50
55.63
33.45
30.86
130.15
128.67
128.36
127.66
126.51
126.22
125.24
f1 (ppm)
3ak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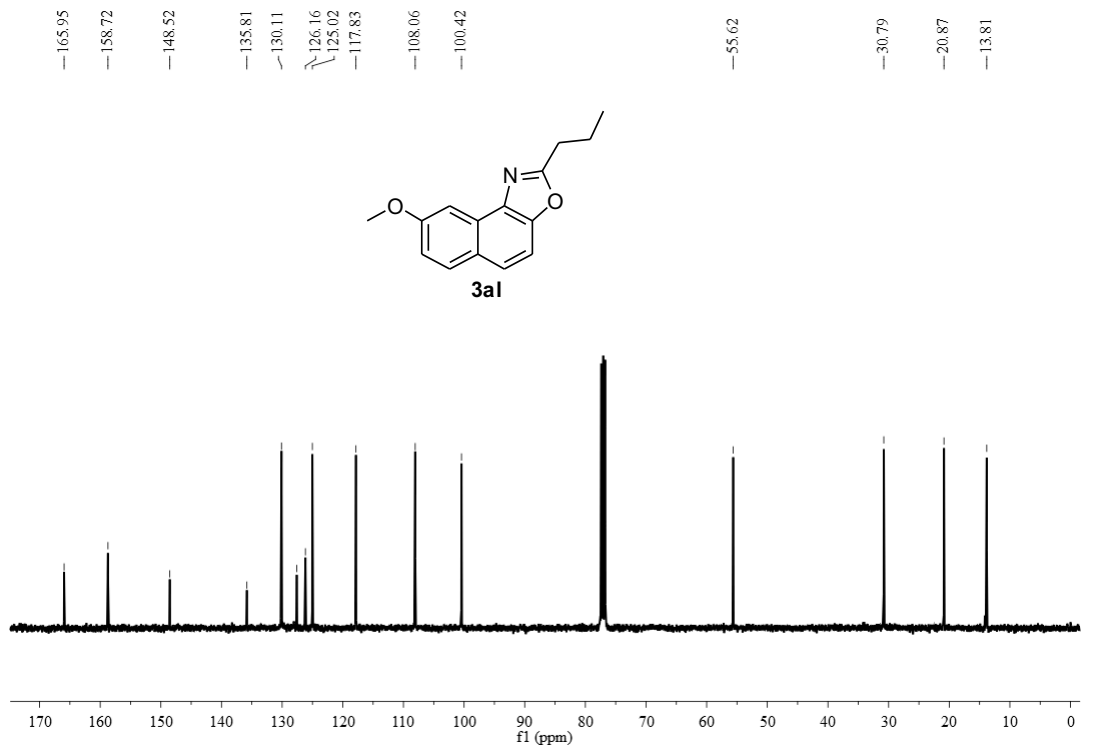
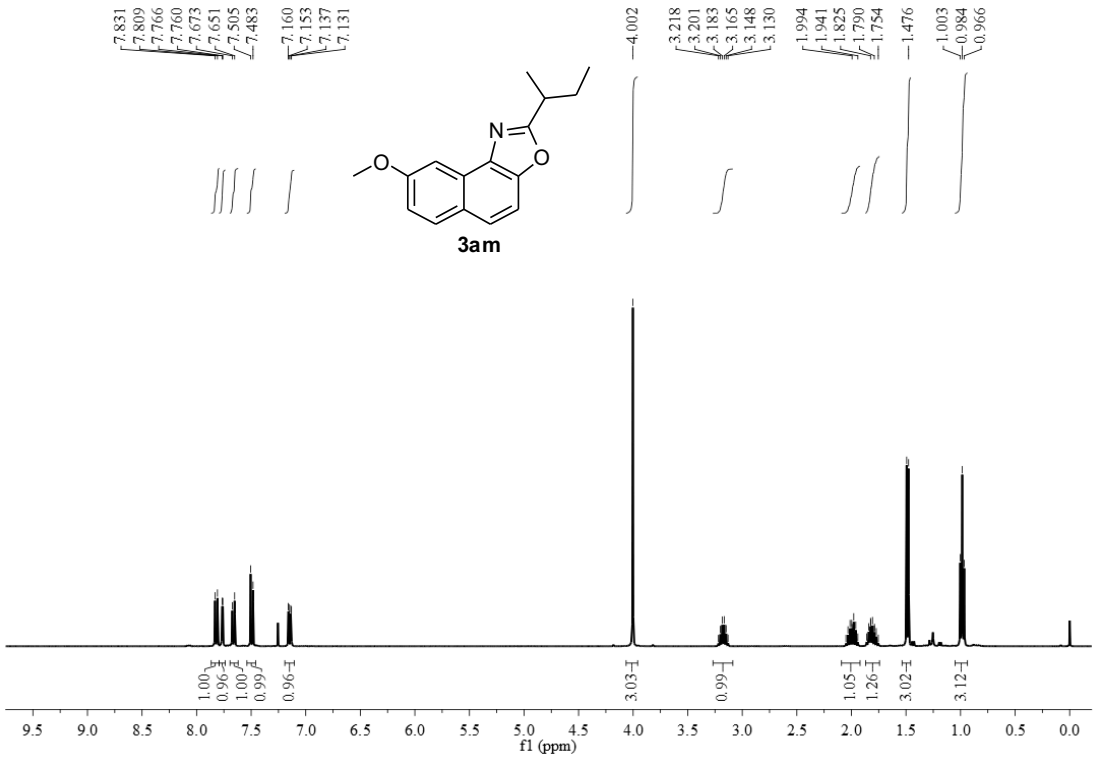
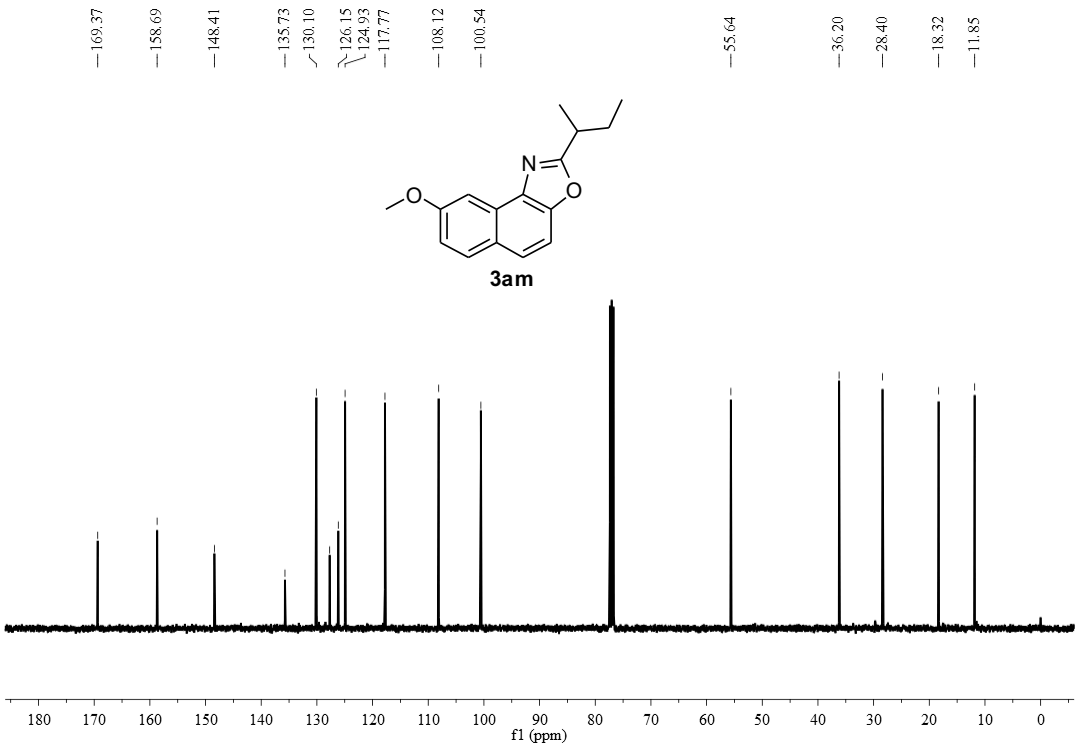
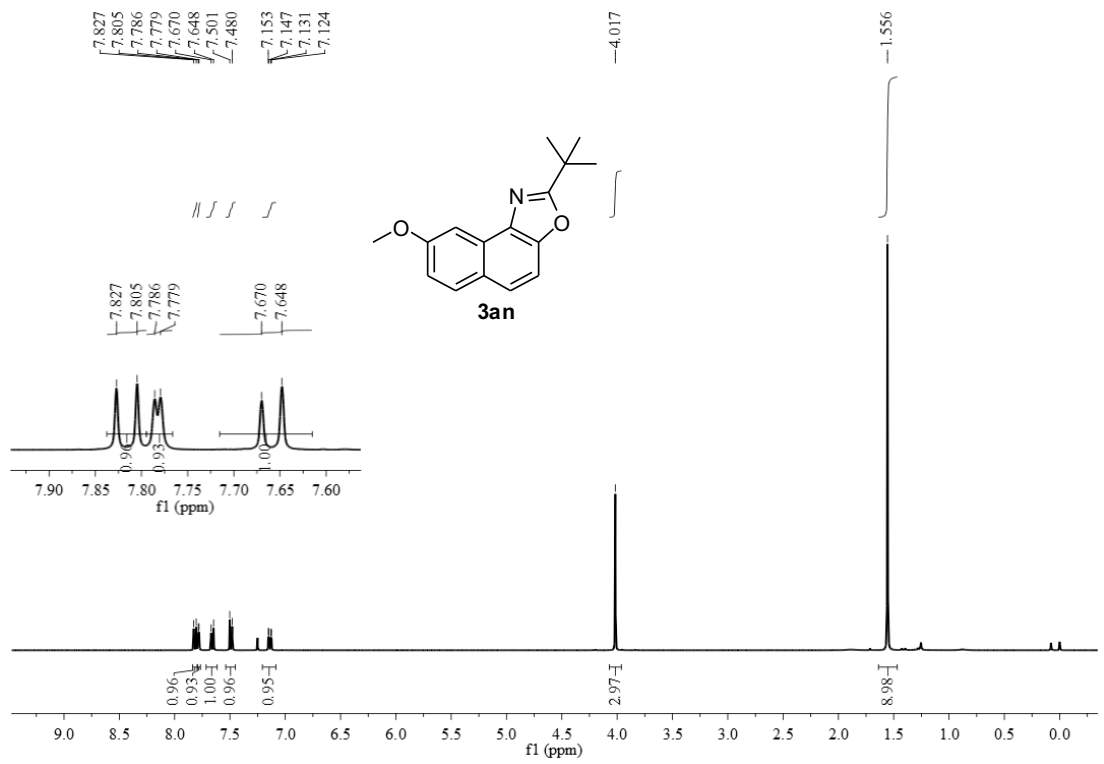
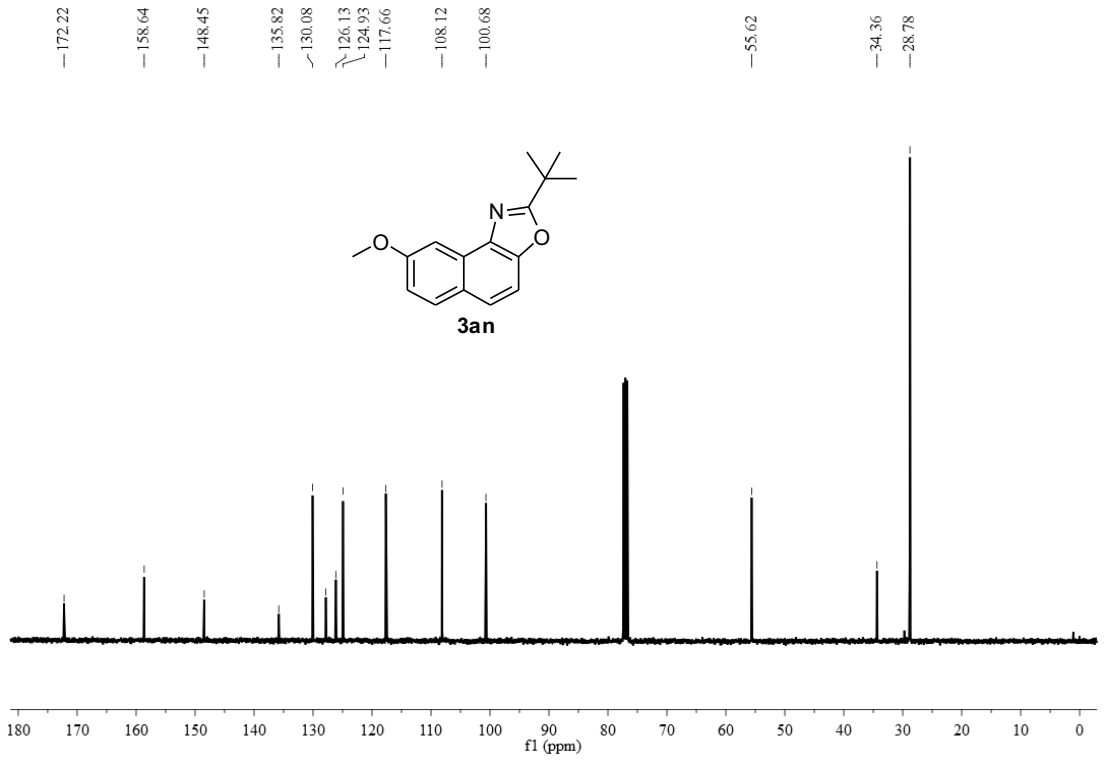
7.808
7.746
7.741
7.673
7.651
7.495
7.473
7.161
7.155
7.139
7.133
3.993
3.029
3.010
2.991
2.009
1.990
1.971
1.953
1.934
1.916
1.093
1.075
1.057
N
O
O
3al
1.00
0.97
1.00
1.00
0.95
3.10
2.03
2.13
3.07
f1 (ppm)


165.95
158.72
148.52
135.81
130.11
126.16
125.02
117.83
108.06
100.42
55.62
30.79
20.87
13.81
N
O
O
3al
f1 (ppm)


7.831
7.809
7.766
7.760
7.673
7.651
7.505
7.483
7.160
7.153
7.137
7.131
4.002
3.218
3.201
3.183
3.165
3.148
3.130
1.994
1.941
1.825
1.790
1.754
1.476
1.003
0.984
0.966
N
O
O
3am
1.00
0.96
1.00
0.99
0.96
3.03
0.99
1.05
1.26
3.02
3.12
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 0.0
f1 (ppm)


169.37
158.69
148.41
135.73
130.10
126.15
124.93
117.77
108.12
100.54
55.64
36.20
28.40
18.32
11.85
N
O
O
3am
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.827
7.805
7.786
7.779
7.670
7.648
7.501
7.480
7.153
7.147
7.131
7.124
4.017
1.556
3an
0.96
0.93
1.00
0.96
0.95
2.97
8.98
f1 (ppm)


172.22
158.64
148.45
135.82
130.08
126.13
124.93
117.66
108.12
100.68
55.62
34.36
28.78
3an
f1 (ppm)