# **Electronic Supplementary Information**

# General and practical synthesis of naphtho[2,1d]oxazoles from naphthols and amines

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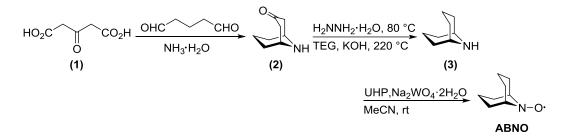
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# **1. General Information**

The reactions were carried out in Schlenk tubes of 25 mL under N<sub>2</sub> atmosphere. Reagents were used as received unless otherwise noted, and solvents were purified according to standard operation procedure. Column chromatography was performed using Silica Gel 60 (300–400 mesh). The reactions were monitored by GC and GC-MS, GC-MS results were recorded on GC-MS QP2010, and GC analysis was performed on GC 2010 plus. The <sup>1</sup>H, <sup>13</sup>C and <sup>19</sup>F NMR spectra were recorded on a Brucker ADVANCE III spectrometer at 400 MHz, 101 MHz, and 376 MHz, respectively, and chemical shifts were reported in parts per million (ppm). The HRMS measurements were recorded on MAT95XP high resolution mass spectrometer by the electron ionization (EI) method, and the mass analyzer type is TOF for EI. EPR spectra were recorded on Agilent Cary 100 UV-Vis Spectrophotometer. The absorption (UV) spectra were recorded on HITACHI F-7000 Fluorescence Spectrophotometer. The thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) curves were recorded on STA449F5 synchronous thermal analyzer. The single-crystal X-ray diffraction was conducted on the D8 Quest X-ray single crystal diffractometer. All solvents and reagents were purchased from Energy Chemical, Bide Pharmatech Ltd., Alfa Aesar, and Aladdin.

# 2. Preparation of the substrates

# 2.1 Synthesis of 9-Aza-bicyclo[3.3.1]nonane N-Oxyl (ABNO).<sup>1</sup>

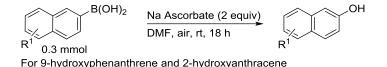


To a solution of acetonedicarboxylic acid (1) (2.1 g, 14.4 mmol) in  $H_2O$  (50 mL) was slowly added 23% ammonia-water (4.5 mL) at 0 °C. Then glutaraldehyde (1.44 g, 14.4 mmol) in water (52.5 mL) was added over 1 h. After the solution was stirred for 35 h at rt, the solvent ( $H_2O$ ) was removed under freezedrying condition. The resulting yellow solid (2) was used in the next reaction without further purification.

The mixture of (2) and  $H_2NNH_2 \cdot H_2O$  (2.2 mL, 43.1 mmol) was stirred at 80 °C for 2 h. To a solution of KOH (8.0 g, 144 mmol) in triethyleneglycol (21 mL) in a two-necked round-bottomed flask distillation apparatus, the solution of (2) and  $H_2NNH_2 \cdot H_2O$  was added dropwise. After the mixture was stirred at 220 °C for 30 min,  $H_2O$  (50 mL) was added dropwise over 2 h at 220 °C. During the reaction, the product, amine (3), was distillated with  $H_2O$  under azeotropic condition. The resulting aqueous solution was extracted with CHCl<sub>3</sub> and dried over  $K_2CO_3$ . Evaporation of the solvent afforded (3) as a colorless oil, which was used in the next reaction without further purification.

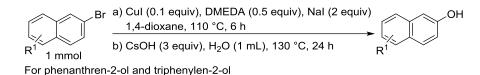
To a solution of the crude (3) in MeCN (14.4 mL) was added Na<sub>2</sub>WO<sub>4</sub>·H<sub>2</sub>O (0.95 g, 1.88 mmol) at ambient temperature and the mixture was stirred for 30 min. After the solution was cooled to 0 °C, urea hydrogen peroxide (2.7 g, 28.8 mmol) was added and the reaction mixture was stirred at 0 °C for 1 h and at ambient temperature for 4 h. H<sub>2</sub>O was added to the reaction mixture and the aqueous solution was extracted with CHCl<sub>3</sub>. The organic layer was dried over K<sub>2</sub>CO<sub>3</sub> and concentrated. The residue was purified by silica gel column chromatography to yield **ABNO** (0.56 g, 4 mmol) as a red solid.

#### 2.2 Synthesis of 9-hydroxyphenanthrene and 2-hydroxyanthracene.<sup>2</sup>



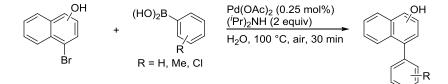
To a 25 mL round bottom flask in open air, arylboronic acid (0.3 mmol), sodium ascorbate (0.6 mmol, 0.119 g) and DMF (1.5 mL) were added. The suspension was vigorously stirred for 18 h, and it was diluted with water (10 mL) and extracted with ethyl acetate ( $3 \times 10$  mL). The combined organic layers were washed with brine (10 mL), dried over Na<sub>2</sub>SO<sub>4</sub>, and the solvent was removed under reduced pressure. Title compounds were purified by column chromatography on SiO<sub>2</sub> using a cyclohexane/ethyl acetate mixture as an eluent. As a result, 9-hydroxyphenanthrene was isolated in 46% yield, and 2-hydroxyanthracene in 79% yield.

#### 2.3 Synthesis of phenanthren-2-ol and triphenylen-2-ol.<sup>3</sup>



After standard cycles of evacuation and back-filling with dry and pure nitrogen, a Schlenk tube equipped with a magnetic stirring bar was charged with CuI (0.1 equiv), NaI (2 equiv) and the aryl bromides if a solid (1 mmol, 1 equiv). The tube was evacuated, back-filled with nitrogen. Then DMEDA (0.5 equiv) and degassed 1,4-dioxane (1.0 mL) were added under a stream of nitrogen by syringe at room temperature. The tube was sealed under a positive pressure of nitrogen, stirred and heated to 110 °C. After 6 h of reaction, add under a stream of nitrogen CsOH  $\cdot$ H<sub>2</sub>O (3 equiv), and 1 mL degassed water. The tube was sealed under a positive pressure of nitrogen, stirred and heated to 130 °C for 24 h. After cooling to room temperature, 10 mL of dichloromethane were added and 1 mL of HCl (37%). The mixture were stirred for 2 hours. The reaction mixture was filtered, and the filter cake being further washed with dichloromethane. The crude product was purified by flash column chromatography on silica gel to give the corresponding products. As a result, phenanthren-2-ol was isolated in 81% yield, and triphenylen-2-ol in 72% yield.

#### 2.4 Synthesis of para-arylnaphthols.<sup>4</sup>



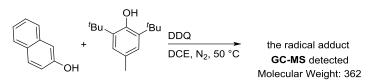
All Suzuki reactions were carried out under air. A mixture of aryl halide (0.5 mmol), arylboronic acid (0.75 mmol), base (1.0 mmol), Pd(OAc)<sub>2</sub> (0.25 mol%, 0.28 mg), H<sub>2</sub>O (1.0 mL) was stirred at 100 °C for the indicated time. The reaction mixture was added to brine (10 mL) and extracted with ethyl acetate (3 × 10 mL). The solvent was concentrated under vacuum and the product was isolated by short chromatography on a silica gel column to furnish the products in 78–85% yields.

# **3. Experimental Procedure**

By the treatment of 2-naphthol with 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) under the radical scavenger (RS) BHT, we only observed a radical adduct. Part of this adduct decomposed during isolation (for details, see the 3.1). Considering the relative instability of the radical adduct, we envisioned that the radical adduct might be further transformed by the attack of a nucleophile. Phenols would be selectively transformed into functional compounds in a new model with the suppression of other side reactions. In addition, RSs can strongly capture radical intermediates, and the reaction would be weakly

influenced by the electronic and steric effects of phenols, i.e., the generality and selectivity of phenol oxidation might be realized.

# 3.1 The BHT-captured experiment



In an oven dried 25 mL Schlenk tube charged with 2-naphthol (0.2 mmol), DDQ (0.2 mmol), BHT (0.4 mmol), after charging nitrogen for three times, DCE (1 mL) were added. The reaction mixture was reacted at 50 °C for 2 h. After completion, the reaction mixture was filtered and the filtrate was detected by GC-MS, and the result is show in Figure S1.

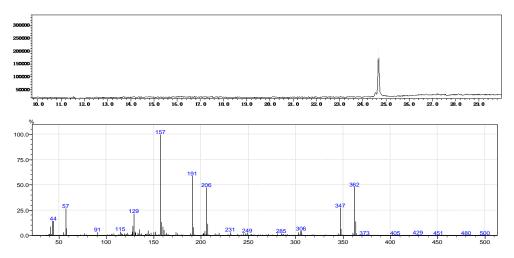
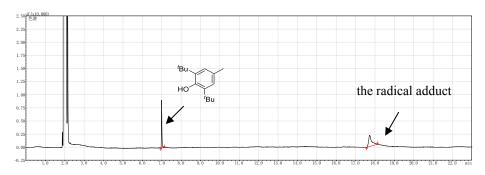
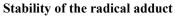


Figure S1. GC-MS chart of the radical adduct







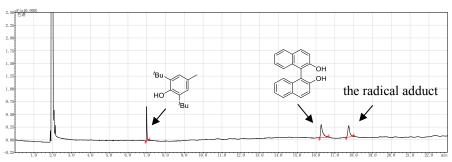


Figure S3. GC chart of the same mixture that standing for 24 h

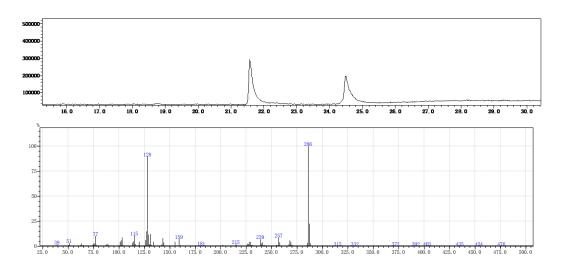
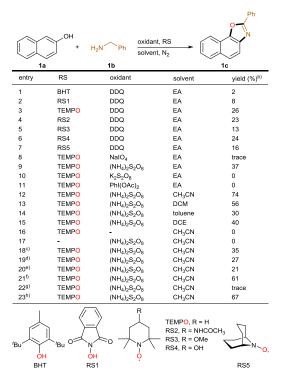


Figure S4. GC-MS chart of (1,1'-binaphthalene)-2,2'-diol

Figure S2 showed that the freshly separated mixture of BHT and the radical adduct was observed in GC chart. Figure S3 and Figure S4 showed that a new substance was observed in GC and GC-MS charts after the mixture was stood under the air for 24 h. And the peak times and molecular weight of this new substance in GC and GC-MS charts are the same as that of commercially available (1,1'binaphthalene)-2,2'-diol. The facts demonstrated that the structure of the radical adduct was formed by BHT and 2-naphthol at  $\alpha$  position, and it is instable even in (weakly oxidizing) atmospheric conditions, which made us envision that the radical adduct might be further transformed by the attack of a nucleophile.

# 3.2 Optimization of the reaction conditions

# Table S1 Optimization of the reaction conditions.<sup>a</sup>



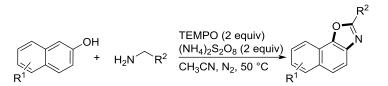
a) Reaction conditions: **1a** (0.2 mmol), **1b** (0.4 mmol), solvent (1 mL), oxidant (0.4 mmol), TEMPO (0.4 mmol), N<sub>2</sub> (1 atm), 25 mL glass tube, 50 °C, 8 h. b) GC yield using tridecane as an internal standard. c)

1 equiv TEMPO was added. d) 1 equiv  $(NH_4)_2S_2O_8$  was added. e) 1 equiv 1b was added. f) 70 °C. g) 30 °C. h) Under air.

As shown in Table S1, we initially tried to optimize the conditions by the treatment of 2-naphthol (1a) and benzylamine (1b) with DDQ and RS BHT in EA (1 mL) at 50 °C for 8 h (Table 1), but the desired product (1c) was given in only trace yield. This low reactivity is attributed to the over stability of the radical adduct. RSs containing N-O bonds that easily cleave were suitable for this reaction, and TEMPO was proved as the best RS (entries 2–7). Appropriate oxidant is essential for the 2-naphthol oxidation. Investigations on the other oxidants, such as NaIO<sub>4</sub>, (NH<sub>4</sub>)<sub>2</sub>S<sub>2</sub>O<sub>8</sub>, K<sub>2</sub>S<sub>2</sub>O<sub>8</sub> and PhI(OAc)<sub>2</sub> demonstrated that  $(NH_4)_2S_2O_8$  is superior to the others, and the desired product (1c) was produced in 37% yield (Table 1, entries 8–11). The solvent had great influence on the reaction yield (entries 12–15), and CH<sub>3</sub>CN was proven to be the most suitable candidate for this transformation. No product was detected in the absence of oxidant or TEMPO verifying their synergistic effect (entries 16 and 17). The stoichiometric quantities of the oxidant, TEMPO, and benzylamine (1b) were needed, very low yields of the desired product were observed using any of them with sub-stoichiometric amounts (entries 18–20). Further studies demonstrated that higher or lower temperature did not give better results for the reaction (entries 21 and 22). Notably, the reaction provided a slightly lower yield in air than in an inert atmosphere (entry 23). The use of easily available starting materials and mild metal-free conditions demonstrated the easy operation of this reaction to construct naphtho[2,1-d]oxazoles.

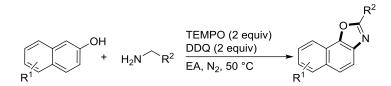
# 3.3 General experimental procedure for the synthesis of naphtho[2,1-d]oxazoles

# 3.3.1 General experimental procedure for the synthesis of naphtho[2,1-*d*]oxazoles 1c-16c, 26c-44c, 46c-49c, 55c



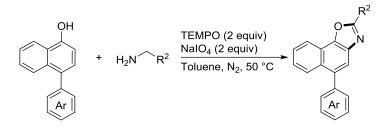
In an oven dried 25 mL Schlenk tube was charged with 2-naphthols (0.2 mmol),  $(NH_4)_2S_2O_8$  (0.4 mmol), TEMPO (0.4 mmol), after charging nitrogen for three times, the amines (0.4 mmol, 2.0 equiv), and CH<sub>3</sub>CN (1 mL) were added. The reaction mixture was reacted at 50 °C for 8 h. After completion of the reaction, the reaction mixture was filtered and the filtrate was concentrated under vacuum. The crude product was purified by flash column chromatography on silica gel to give the desired naphtho[2,1-*d*]oxazoles.

# 3.3.2 General experimental procedure for the synthesis of naphtho[2,1-*d*]oxazoles 17c, 18c, 20c-25c, 44c, 45c



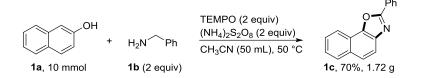
In an oven dried 25 mL Schlenk tube was charged with 2-naphthols (0.2 mmol), DDQ (0.4 mmol), TEMPO (0.4 mmol), after charging nitrogen for three times, the amines (0.4 mmol, 2.0 equiv), and EA (1 mL) were added (when ethylamine hydrochloride and methylamine hydrochloride were used as amine reagents, 1 equiv  $K_2CO_3$  was added). The reaction mixture was reacted at 50 °C for 8 h. After completion of the reaction, the reaction mixture was filtered and the filtrate was concentrated under vacuum. The crude product was purified by flash column chromatography on silica gel to give the desired naphtho[2,1-*d*]oxazoles.

# **3.3.3** General experimental procedure for the synthesis of naphtho[2,1-*d*]oxazoles 41c-43c using 1-naphthols and benzylamine



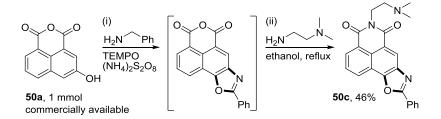
In an oven dried 25 mL Schlenk tube was charged with 1-naphthols (0.2 mmol), NaIO<sub>4</sub> (0.4 mmol), TEMPO (0.4 mmol), after charging nitrogen for three times, the benzylamine (**1b**, 0.4 mmol, 2.0 equiv), and Toluene (1 mL) were added. The reaction mixture was reacted at 50 °C for 8 h. After completion of the reaction, the reaction mixture was filtered and the filtrate was concentrated under vacuum. The crude product was purified by flash column chromatography on silica gel to give the desired naphtho[2,1-d]oxazoles.

# 3.3.4 Preparation of 2-phenyl-naphtho[2,1-d]oxazole (1c) at 10 mmol scale



**10 mmol scale:** In an oven dried 250 mL Schlenk tube was charged with 2-naphthol (**1a**, 10 mmol),  $(NH_4)_2S_2O_8$  (20 mmol), TEMPO (20 mmol), after charging nitrogen for three times, the amine (**1b**, 20 mmol, 2.0 equiv), and CH<sub>3</sub>CN (50 mL) were added. The reaction mixture was reacted at 50 °C for 8 h. After completion of the reaction, the reaction mixture was filtered and the filtrate was concentrated under vacuum. The crude product was purified by flash column chromatography on silica gel to give the desired 2-phenyl-naphtho[2,1-*d*]oxazole (**1c**) in 70% yield (1.72 g).

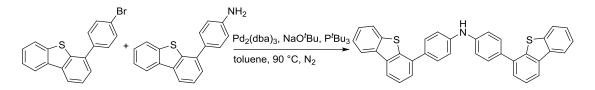
# 3.3.5 Experimental procedure for the synthesis of 5-(2-(dimethylamino)ethyl)-9-phenyl-4*H*-benzo[*de*]oxazolo[5,4-*g*]isoquinoline-4,6(5*H*)-dione (PBNI)



In an oven dried 25 mL Schlenk tube was charged with naphthol **50a** (1 mmol),  $(NH_4)_2S_2O_8$  (2 mmol), TEMPO (2 mmol), after charging nitrogen for three times, the amine (2 mmol, 2.0 equiv), and CH<sub>3</sub>CN (5 mL) were added. The reaction mixture was reacted at 50 °C for 8 h. After completion of the reaction, 15 mL of hydrochloric acid (25%) was added at room temperature. The precipitated solid was filtered and the aqueous layer was extracted with CH<sub>2</sub>Cl<sub>2</sub> (20 mL) and dried over Na<sub>2</sub>SO<sub>4</sub>. the afforded solid by evaporation of the solvent was further washed with petroleum ether, providing the crude product 9-phenyl-4*H*,6*H*-benzo[4,5]isochromeno[7,6-*d*]oxazole-4,6-dione, which was dissolved in 20 mL ethanol. After adding *N*,*N*-dimethylethylenediamine (0.163 mL, 0.0015 mol), the mixture were stirred and refluxed for 2-3 h, then the solution was evaporated in vacuum and the residue was purified on silica gel chromatography to give the desired PBNI (**50c**) in 46% yield.<sup>5</sup>

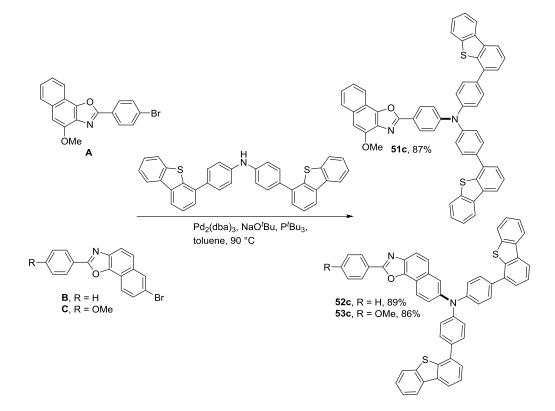
# **3.3.6** General experimental procedure for the synthesis of naphthoxazole-doped triarylamine materials 51c, 52c, 53c, 54c<sup>6</sup>

### 3.3.6.1 Synthesis of bis(4-(dibenzo[b,d]thiophen-4-yl)phenyl)amine



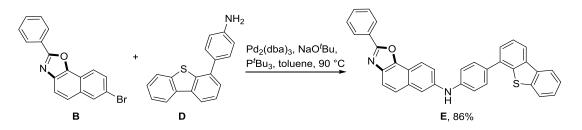
A mixture of 4-(4-bromophenyl)dibenzo[b,d]thiophene (1 mmol), 4-(dibenzo[b,d]thiophen-4yl)aniline (1.1 mmol), Pd<sub>2</sub>(dba)<sub>3</sub> (2 mol%),NaO'Bu (1.5 equiv), P'Bu<sub>3</sub> (4 mol%, 1.0 M in toluene), and anhydrous toluene (14 mL) was heated at 90 °C under N<sub>2</sub> atmosphere for 12 h. Then the mixture was cooled down to room temperature, filtered and the extracted with ethyl acetate. The organic layer was separated, dried over magnesium sulfate, filtered and evaporated. The crude product was purified by column chromatography to get bis(4-(dibenzo[b,d]thiophen-4-yl)phenyl)amine in 85% yield.

### 3.3.6.2 Synthesis of naphthoxazole-doped triarylamine materials 51c, 52c, 53c



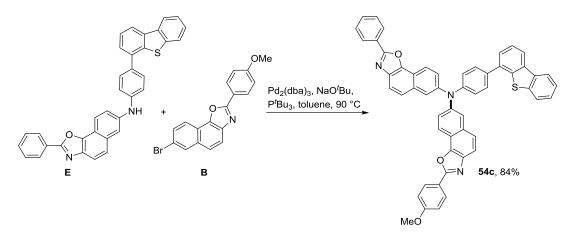
A mixture of Br-substituted naphthoxazole (**A**, **B**, or **C**, 0.2 mmol), bis(4-(dibenzo[b,d]thiophen-4yl)phenyl)amine (0.22 mmol), Pd<sub>2</sub>(dba)<sub>3</sub> (2 mol%), NaO'Bu (1.5 equiv), P'Bu<sub>3</sub> (4 mol%, 1.0 M in toluene), and anhydrous toluene (3 mL) was heated at 90 °C under N<sub>2</sub> atmosphere for 12 h. Then the mixture was cooled down to room temperature, filtered and the extracted with ethyl acetate. The organic layer was separated, dried over magnesium sulfate, filtered and evaporated. The crude product was purified by column chromatography to get naphthoxazole-doped triarylamine materials **51c**, **52c**, and **53c** in 87%, 89%, and 86% yields, respectively.

#### 3.3.6.3 Synthesis of secondary amine

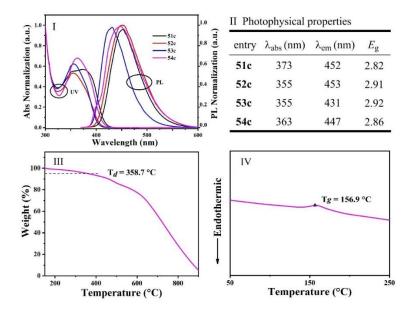


A mixture of 7-bromo-2-phenylnaphtho[2,1-*d*]oxazole (**B**, 1.0 mmol), 4-(dibenzo[*b*,*d*]thiophen-4yl)aniline (**D**, 1.1 mmol), Pd<sub>2</sub>(dba)<sub>3</sub> (2 mol%), NaO'Bu (1.5 equiv), P'Bu<sub>3</sub> (4 mol%, 1.0 M in toluene), and anhydrous toluene (14 mL) was heated at 90 °C under N<sub>2</sub> atmosphere for 12 h. Then the mixture was cooled down to room temperature, filtered and the extracted with ethyl acetate. The organic layer was separated, dried over magnesium sulfate, filtered and evaporated. The crude product was purified by column chromatography to get N-(4-(dibenzo[*b*,*d*]thiophen-4-yl)phenyl)-2-phenylnaphtho[2,1*d*]oxazol-7-amine (**E**) in 86% yield.

# 3.3.6.4 Synthesis of naphthoxazole-doped triarylamine material 54c



A mixture of 7-bromo-2-(4-methoxyphenyl)naphtho[2,1-*d*]oxazole (**B**, 1.0 mmol), *N*-(4-(dibenzo[*b*,*d*]thiophen-4-yl)phenyl)-2-phenylnaphtho[2,1-*d*]oxazol-7-amine (**E**, 1.1 mmol), Pd<sub>2</sub>(dba)<sub>3</sub> (2 mol%), NaO'Bu (1.5 equiv), P'Bu<sub>3</sub> (4 mol%, 1.0 M in toluene), and anhydrous toluene (14 mL) was heated at 90 °C under N<sub>2</sub> atmosphere for 12 h. Then the mixture was cooled down to room temperature, filtered and the extracted with ethyl acetate. The organic layer was separated, dried over magnesium sulfate, filtered and evaporated. The crude product was purified by column chromatography to get naphthoxazole-doped triarylamine material **54c** in 84% yield.



# 4. Photophysical Properties and Thermal of Naphthoxazole-doped Materials

Figure S5. Thermal and photophysical properties. I) Absorption (UV) and photoluminescence (PL) spectra of 51c, 52c, 53c, and 54c in dichloromethane (10<sup>-5</sup> mol/L). II) Photophysical properties of 51c, 52c, 53c, and 54c. III) Thermogravimetric analysis (TGA) of 54c. IV) Differential scanning calorimetry (DSC) curves of 54c.

The absorption (UV) and photoluminescence (PL) spectra of **51c**, **52c**, **53c**, and **54c** in dilute solutions (10<sup>-5</sup> mol/L dichloromethane) are depicted in Figure S5(I), and the corresponding data are summarized in Figure S5(II). The results indicated that these naphthoxazole-related compounds have similar UV absorption wavelengths ( $\lambda_{abs}$ , 355–373 nm), fluorescence emission wavelengths ( $\lambda_{em}$ , 431–453 nm), and band gap energies (E<sub>g</sub>, 2.82–2.92 eV). Furthermore, by taking **54c** as an example, the thermal properties were examined by thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) measurements (Figure S5(III) and (IV)). The results (T<sub>d</sub> = 358.7 °C, T<sub>g</sub> = 156.9 °C) disclosed that it was thermally and morphologically stable, which enabled it to function steadily as an organic electroluminescent material and may be applied as a hole transport layer material in OLED devices.

# 5. Investigations of the Reaction Mechanism

#### 5.1 Procedure for EPR Investigation of 2-naphthol.

In an oven dried 25 mL Schlenk tube equipped with a stir-bar, 2-naphthol (0.2 mmol) and  $(NH_4)_2S_2O_8$  (0.4 mmol) were charged. Then the reaction tube was vacuumed and purged with nitrogen for three times. CH<sub>3</sub>CN (1 mL) was added under nitrogen at room temperature. After the reaction mixture was reacted at 50 °C for 10 min, 20 µL of the mixture was taken out into a small tube and analyzed by EPR at 50 °C. As shown in Figure S6, the strong signal with *g*-factor as 2.0056 was observed in the overall catalytic process.

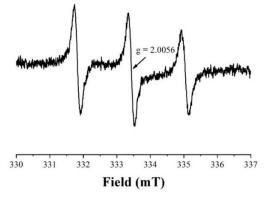


Figure S6. EPR spectra of 2-naphthol and (NH<sub>4</sub>)<sub>2</sub>S<sub>2</sub>O<sub>8</sub> mixture.

In an oven dried 25 mL Schlenk tube equipped with a stir-bar, 2-naphthol (0.2 mmol) and  $(NH_4)_2S_2O_8$  (0.4 mmol) were charged. Then the reaction tube was vacuumed and purged with nitrogen for three times. CH<sub>3</sub>CN (1 mL) was added under nitrogen at room temperature. After the reaction mixture was reacted at 50 °C for 10 min, *0.4 mmol TEMPO was added to the reaction mixture and mix*, 20 µL of the mixture was taken out into a small tube and analyzed by EPR at 50 °C. As shown in Figure S7, only the TEMPO signal was detected.

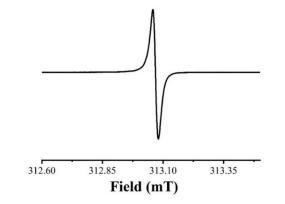
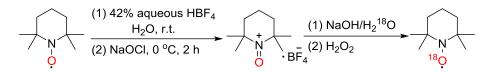


Figure S7. EPR spectra of 2-naphthol, (NH<sub>4</sub>)<sub>2</sub>S<sub>2</sub>O<sub>8</sub> and TEMPO mixture.

# 5.2 The <sup>18</sup>O-labeled experiment

# 5.2.1 Synthesis of TEMP<sup>18</sup>O.<sup>7</sup>



To a solution of TEMPO (4.68 g, 30 mmol) in  $H_2O$  (15 mL, 2M) was added dropwise 42% aqueous HBF<sub>4</sub> (14.9 mL, 30 mol) at room temperature. After the solution became to amber color, the aqueous NaOCl solution (16.0 mL, 30 mmol) was added dropwise at 0 °C. When it finished, the reaction mixture stirred for additional 1 h at 0 °C. Finally, the reaction mixture was filtered and the yellow crystalline precipitate was washed with ice-cold 5% aqueous NaHCO<sub>3</sub> (6.0 mL), water (6.0 mL), and ice-clod ether (60.0 mL). The bright yellow solid was dried at 50 °C in vacuo to gain the TEMPO<sup>+</sup>BF<sub>4</sub><sup>-</sup> (5.1 g, 70 %).

To the solution of TEMPO<sup>+</sup>BF<sub>4</sub><sup>-</sup> (0.9710 g, 4 mmol) in  $H_2^{18}O$  (1.7 mL) was added concentrated NaOH (12 N, 1.5 mL  $H_2^{18}O$ ) at 0 °C for 2 h and the color of solution was changed from orange to slightly yellow. Then, 30%  $H_2O_2$  (0.2 mL) was added to the reaction mixture. When the color of reaction mixture became slightly red, the reaction mixture was extracted with ether. The organic layer was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, filtered and concentrated under reduced pressure to gain the red crystalline solid (TEMP<sup>18</sup>O), which was dried at room temperature in vacuo. The ratio of TEMP<sup>18</sup>O/TEMP<sup>16</sup>O was **1:0.183** determined by the GC-MS analysis, and the result is show in Figure S8.

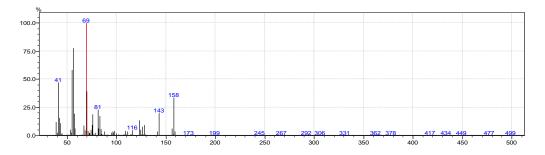
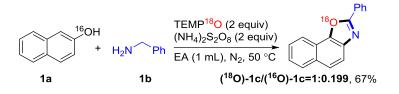


Figure S8. GC-MS Analysis of TEMP<sup>18</sup>O

[MS Spectrum] # of Peaks376 Raw Spectrum 5.875 -> 5.970 (scan: 576 -> 595) Base Peakm/z 69.05 (Inten: 1,598,702) Background 5.645 -> 5.905 (scan: 530 -> 582) m/z Absolute Intensity Relative Intensit								
39.00	189762	11.87	70.05	638531	39.94	116.05	72767	4.55
41.05	760496	47.57	71.05	68038	4.26	123.10	216473	13.54
42.05	248323	15.53	74.05	80779	5.05	124.10	85275	5.33
43.05	173759	10.87	75.05	154304	9.65	126.10	133266	8.34
53.05	84330	5.27	76.05	301865	18.88	128.05	154163	9.64
55.05	934849	58.48	81.05	375192	23.47	141.10	61502	3.85
56.05	1250688	78.23	82.05	99905	6.25	143.10	320465	20.05
57.05	310186	19.40	83.05	282223	17.65	<u>156.10</u>	98915	<u>6.19</u>
58.05	104719	6.55	84.05	94083	5.88	157.15	14671	0.92
67.00	138533	8.67	96.05	58154	3.64	<u>158.10</u>	540306	<u>33.80</u>
68.05	74726	4.67	98.05	64113	4.01	159.10	56464	3.53
69.05	1598702	100.00	109.05	54159	3.39	160.10	2622	0.16

5.2.2 The <sup>18</sup>O-labeled experiment of 2-naphthol (1a) and benzylamine (1b)



In an oven dried 25 mL Schlenk tube was charged with 2-naphthol (**1a**, 0.2 mmol),  $(NH_4)_2S_2O_8$  (0.4 mmol), TEMP<sup>18</sup>O (0.4 mmol), after charging nitrogen for three times, the amine **1b** (0.4 mmol), and CH<sub>3</sub>CN (1 mL) were added. The reaction mixture was reacted at 50 °C for 8 h. After completion, the reaction mixture was filtered and the filtrate was detected by GC-MS, and the results are shown in Figure S9 and Figure S10.

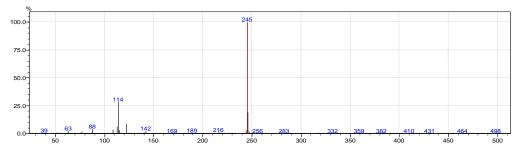


Figure S9. GC-MS analysis of 2-phenylnaphtho[2,1-d]oxazole under standard reaction conditions

[MS Spectrum] # of Peaks311								
Raw Sp	ectrum 17.	295 -> 17	.625 (scan: 1260	-> 1326)	Base Pea		nten: 1,478	,965)
Backgro	und 16.	890 -> 17	.450 (scan: 1179	-> 1291)				
m/z Ab	solute Inte	nsity Re	lative Intensity					
51.00	17076	1.15	108.55	53218	3.60	216.00	18293	1.24
62.00	15367	1.04	113.05	99108	6.70	244.15	47387	3.20
63.00	29731	2.01	114.05	455682	30.81	<u>245.05</u>	1478965	100.00
77.05	29344	1.98	115.05	45913	3.10	246.05	282045	19.07
87.00	14901	1.01	122.55	135659	9.17	247.05	28635	1.94
88.00	68192	4.61	142.05	35517	2.40	248.05	19940.13	

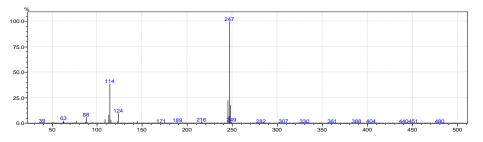


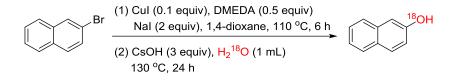
Figure S10. GC-MS analysis of TEMP<sup>18</sup>O-labeled 2-phenylnaphtho[2,1-*d*]oxazole

[MS Spectrum]								
# of Pea	ks304							
Raw Spe	ectrum 17.	090 -> 17.2	235 (scan: 1619	-> 1648)	Base Pea	km/z 247.10 (I	nten: 1,691	,150)
Backgro	und 17.	230 (scan:	1647)					
m/z Ab	solute Inte	nsity Rel	ative Intensity					
51.00	26961	1.59	108.55	70110	4.15	144.10	39254	2.32
62.00	23525	1.39	113.05	134848	7.97	216.10	23801	1.41
63.00	46502	2.75	114.05	637795	37.71	<u>245.10</u>	336535	<u> 19.90</u>
77.05	45137	2.67	115.05	64228	3.80	246.10	121846	7.20
87.05	21746	1.29	122.60	32784	1.94	<u>247.10</u>	1691150	<u>100.00</u>
88.05	99809	5.90	123.60	166638	9.85	248.10	310790	18.38
94.50	17815	1.05	140.10	17317	1.02	249.10	28539	1.69

Results showed that the oxidative cyclization of 2-naphthol and benzylamine could obtain the corresponding 2-phenylnaphtho[2,1-d]oxazole in 67% GC yield. The ratio of  $(^{18}O)$ -1c/ $(^{16}O)$ -1c was 1:0.199 determined by the GC-MS analysis, and almost all of oxygen of 2-phenylnaphtho[2,1-d]oxazole comes from TEMPO.

### 5.2.3 Experiment of <sup>18</sup>O-labeled 2-naphthol and benzylamine

# a) Synthesis of <sup>18</sup>O-labeled 2-naphthol.<sup>3</sup>



In an oven dried 25 mL Schlenk tube equipped with a magnetic stirring bar was charged with CuI (0.1 equiv), NaI (2 equiv) and the 2-bromonaphthalene (1 mmol, 1 equiv). The tube was evacuated, back-filled with nitrogen. If a liquid, aryl bromides was added under a stream of nitrogen by syringe at room temperature, followed by DMEDA (0.5 equiv) and degassed 1,4-dioxane (1.0 mL). The tube was sealed under a positive pressure of nitrogen, stirred and heated to 110 °C. After 6h of reaction, add under a stream of nitrogen CsOH·H<sub>2</sub>O (3 equiv), and 1 mL degassed H<sub>2</sub><sup>18</sup>O. The tube was sealed under a positive pressure of nitrogen, stirred and heated to 130 °C for 24h. After cooling to room temperature, 10 mL of dichloromethane were added and 1 mL of HCl (37%). Then, the mixture was stirred for 2 hours. The filtrate washed twice with water. Gathered aqueous phases were extracted with dichloromethane for five times. Organic layers were gathered, dried over Na<sub>2</sub>SO<sub>4</sub>, filtered and concentrated in vacuum to yield the crude product obtained was purified by silica gel chromatography with a mixture of heptanes/AcOEt and ethyl acetate. The ratio of TEMP<sup>18</sup>O/TEMP<sup>16</sup>O was 1:0.216 determined by the GC-MS analysis, and the result is show in Figure S11.

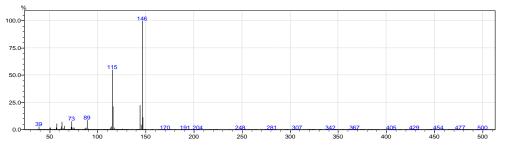


Figure S11. GC-MS analysis of <sup>18</sup>O-labeled 2-naphthol <sup>18</sup>O-1a

[MS Spectrum] # of Peaks184								
		35 -> 9.805 (sca	n· 728 -> ′	762) Bas	e Peakm/z 146	15 (Inten <sup>.</sup>	355 454)	
Backgrou		$15 \rightarrow 10.025$ (see		/		. 15 (Inten.	555,151)	
0		nsity Relative		000)				
39.05	12089	3.40	73.05	28979	8.15	115.10	203714	57.31
50.05	6581	1.85	74.00	7470	2.10	116.10	79939	22.49
51.05	8365	2.35	75.05	6944	1.95	117.10	6875	1.93
56.75	6768	1.90	86.05	4245	1.19	126.10	4132	1.16
57.70	21001	5.91	87.05	5973	1.68	<u>144.15</u>	76867	21.63
62.05	11635	3.27	88.10	8359	2.35	145.15	15831	4.45
63.05	27401	7.71	89.10	32695	9.20	<u>146.15</u>	355454	<u>100.00</u>
64.05	4660	1.31	90.10	3945	1.11	147.15	39198	11.03
65.05	13280	3.74	113.10	8215	2.31	148.10	1902	0.54
72.05	8647	2.43	114.15	10874	3.06			

b) Experiment of <sup>18</sup>O-labeled 2-naphthol <sup>18</sup>O-1a and amine 1b

In an oven dried 25 mL Schlenk tube was charged with <sup>18</sup>O-2-naphthol (<sup>18</sup>O-1a, 0.2 mmol),  $(NH_4)_2S_2O_8$  (0.4 mmol), TEMPO (0.4 mmol), after charging nitrogen for three times, the amine 1b (0.4 mmol), and CH<sub>3</sub>CN (1 mL) were added. The reaction mixture was reacted at 50 °C for 8 h. After completion, the reaction mixture was filtered and the filtrate was detected by GC-MS. As shown in Figure S9 and Figure S12, the molecular weight of 2-phenylnaphtho[2,1-*d*]oxazole under standard reaction conditions is same with that in <sup>18</sup>O-1a labeled experiment.

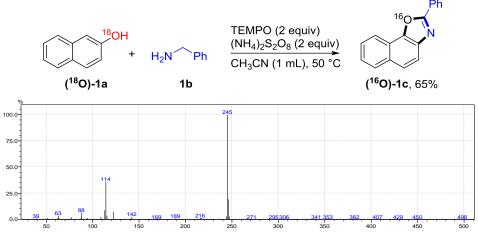


Figure S12. GC-MS analysis of 2-phenylnaphtho[2,1-d]oxazole

[MS Spectrum] # of Peaks310								
Raw Sp	ectrum 16	.960 -> 17.2	285 (scan: 1193	-> 1258)	Base Pea		nten: 105,0	036)
Backgro	und 16	.630 -> 17.0	085 (scan: 1127	-> 1218)				
m/z Ab	solute Inte	ensity Rel	ative Intensity					
39.05	1286	1.22	88.10	8743	8.32	142.10	3117	2.97
51.05	1905	1.81	94.55	1123	1.07	216.05	1818	1.73
62.05	2282	2.17	108.60	3272	3.12	217.10	1503	1.43
63.05	4115	3.92	113.10	11037	10.51	244.10	3728	3.55
64.05	1435	1.37	114.10	44019	41.91	<u>245.10</u>	105036	<u>100.00</u>
75.05	1181	1.12	115.10	4446	4.23	246.10	20000	19.04
77.05	2907	2.77	122.60	8607	8.19	<u>247.10</u>	3228	<b>3.07</b>
87.10	1993	1.90	140.10	1356	1.29	248.10	362	0.34

These results demonstrated that TEMPO is the source of the O atom of 2-phenylnaphtho[2,1-d]oxazole, but not the source of the O atom of 5,7-di-tert-butyl-2-phenylbenzo[d]oxazole.

# 5.2.4 The <sup>18</sup>O-labeled experiment of 4-phenyl-1-naphthol (41a) and benzylamine (1b)

In an oven dried 25 mL Schlenk tube was charged with <sup>16</sup>O-4-phenyl-2-naphthol (<sup>16</sup>O-41a, 0.2 mmol), NaIO<sub>4</sub> (0.4 mmol), TEMP<sup>18</sup>O (0.4 mmol), after charging nitrogen for three times, the benzylamine (1b, 0.4 mmol), and Toluene (1 mL) were added. The reaction mixture was reacted at 50 °C for 8 h. After completion, the reaction mixture was filtered and the filtrate was detected by GC-MS. As shown in Figure S13 and Figure S14, the molecular weight of 2,5-diphenylnaphtho[2,1-d]oxazole (41c) under standard reaction conditions is same with that in TEMP<sup>18</sup>O-involved experiment.



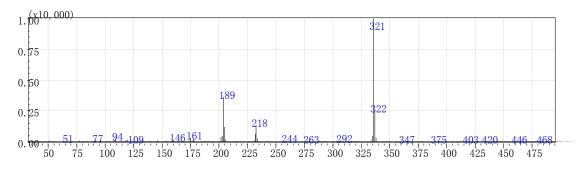


Figure S13. GC-MS analysis of 2,5-diphenylnaphtho[2,1-d]oxazole (41c) under standard reaction conditions

[MS Spectrum] # of Peaks 275 Raw Spectrum31.180 -> 32.725 (scan : 2237 -> 2546) Base Peak m/z 321.15 (Inten : 10,000) Background 32.545 (scan : 2510) m/z Absolute Intensity Relative Intensity

93.55	101	1.01	188.00	446	4.46	320.10	443	4 4 3
20100								
94.50	265	2.65	189.00	3625	36.25	<u>321.15</u>	10000	<u> 100.00</u>
105.05	144	1.44	190.00	1187	11.87	322.15	2545	25.45
145.60	135	1.35	191.00	127	1.27	323.10	336	3.36
160.60	285	2.85	217.00	621	6.21	324.15	31	0.31
163.05	273	2.73	218.00	1339	13.39			
187.00	380	3.80	219.00	228	2.28			

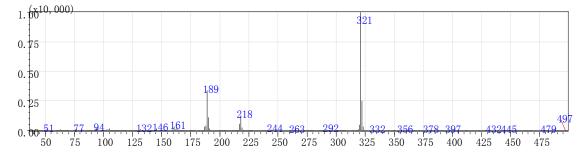


Figure S14. GC-MS analysis of 2,5-diphenylnaphtho[2,1-d]oxazole (41c) under TEMP<sup>18</sup>Oinvolved reaction conditions

[MS Spectrum] # of Peaks 239 Raw Spectrum31.650 -> 32.435 (scan : 2331 -> 2488) Base Peak m/z 321.15 (Inten : 10,000) Background 32.370 (scan : 2475) m/z Absolute Intensity Relative Intensity

93.55	137	1.37	188.00	427	4.27	320.10	441	4.41
94.50	185	1.85	189.00	3402	34.02	<u>321.15</u>	10000	100.00
105.05	131	1.31	190.00	1119	11.19	322.15	2551	25.51
145.60	136	1.36	191.00	119	1.19	<u>323.10</u>	335	3.35
160.60	286	2.86	217.00	574	5.74	324.15	28	0.28
163.05	246	2.46	218.00	1297	12.97			
187.00	336	3.36	219.00	218	2.18			

# 6. Characterization Data for the Products

6.1 X-ray crystallographic data of 7c.

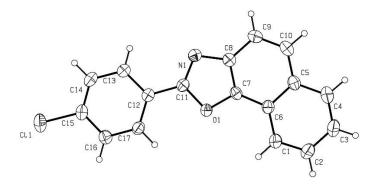


Figure S15. X-ray crystal structure of compound 7c (CCDC number: 2010209).

Table S7. Si	ummarv of X-rav	crystallographic	data for compound 7c.

le S7	e S7. Summary of X-ray crystallographic data for compound 7c.					
	formula	C <sub>17</sub> H <sub>10</sub> ClNO				
	Fw.	279.71				
	crystal system	triclinic				
	space group	P-1				
	a/Å	6.8033(7)				
	b/Å	7.2202(5)				
	$c/\text{\AA}$	13.3326(12)				
	a/deg	84.038(7)				
	$\beta/\deg$	89.246(8)				
	y/deg	82.696(7)				
	<i>V</i> /Å <sup>3</sup>	646.09(10)				
	Ζ	2				
	$D/g \text{ cm}^{-3}$	1.438				
	cryst size/mm	0.46  imes 0.4  imes 0.3				
	reflns collected	3930				
	ind reflns, Rint	2357, 0.0238				
	goodness-of-fit on $F^2$	1.033				
	$R1$ , $wR2$ $[I > 2\sigma(I)]$	0.0462, 0.1110				
	R1, wR2 (all data)	0.0663, 0.1264				
-						

6.2 X-ray crystallographic data of 41c.

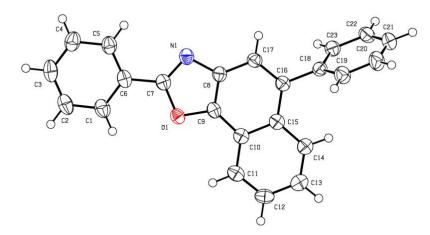


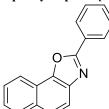
Figure S16. X-ray crystal structure of compound 41c (CCDC number: 2010211).

Table S8. Summar	v of X-rav	crystallogra	phic data fo	r compound 41c.

So. Summary of X ray crystanographic data for compound fite.				
formula	C <sub>23</sub> H <sub>15</sub> NO			
Fw.	321.36			
crystal system	monoclinic			
space group	$P2_1/n$			
a/Å	5.962(9)			
b/Å	15.52(3)			
$c/{ m \AA}$	17.60(3)			
$\alpha/\text{deg}$	90			
β/deg	99.36(6)			
y/deg	90			
$V/Å^3$	1607(5)			
Ζ	4			
$D/g \text{ cm}^{-3}$	1.328			
cryst size/mm	0.29 imes 0.09 imes 0.09			
reflns collected	13371			
ind reflns, Rint	2816, 0.1264			
goodness-of-fit on $F^2$	1.036			
$\tilde{R}1, wR2 [I > 2\sigma(I)]$	0.0568, 0.1464			
R1, wR2 (all data)	0.0690, 0.1595			
$\tilde{R}1, wR2 [I > 2\sigma(I)]$	0.0568, 0.1464			

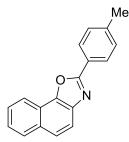
# 7. Characterization Data for the Products

2-phenylnaphtho[2,1-d]oxazole (1c)<sup>8</sup>



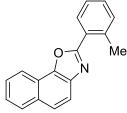
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a white solid in 70% yield (34.3 mg). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.40 – 8.24 (m, 3H), 7.96 (d, *J* = 8.2 Hz, 1H), 7.85 (d, *J* = 8.7 Hz, 1H), 7.78 (d, *J* = 8.7 Hz, 1H), 7.64 (t, *J* = 7.6 Hz, 1H), 7.51 – 7.55 (m, 4H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  162.4, 146.4, 138.6, 131.7, 131.1, 128.9, 128.7, 127.4, 127.3, 126.8, 125.6, 125.4, 120.4, 120.2, 118.6.

# 2-(p-tolyl)naphtho[2,1-d]oxazole (2c)<sup>9</sup>



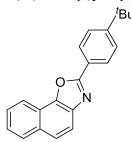
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a white solid in 71% yield (36.8 mg). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.29 (d, J = 8.2 Hz, 1H), 8.21 (d, J = 7.5 Hz, 2H), 7.96 (d, J = 8.2 Hz, 1H), 7.84 (d, J = 8.6 Hz, 1H), 7.77 (d, J = 8.7 Hz, 1H), 7.63 (t, J = 7.5 Hz, 1H), 7.52 (t, J = 7.5 Hz, 1H), 7.34 (d, J = 7.7 Hz, 2H), 2.44 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  162.7, 146.3, 141.6, 138.6, 131.6, 129.6, 128.7, 127.2, 126.7, 125.5, 125.3, 124.6, 120.3, 120.1, 118.5, 21.6.

2-(*o*-tolyl)naphtho[2,1-*d*]oxazole (3c)



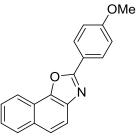
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a white solid in 68% yield (35.2 mg). mp 82.2–82.7 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.28 (t, *J* = 8.5 Hz, 2H), 7.96 (d, *J* = 8.2 Hz, 1H), 7.89 (d, *J* = 8.7 Hz, 1H), 7.78 (d, *J* = 8.7 Hz, 1H), 7.63 (t, *J* = 7.5 Hz, 1H), 7.52 (t, *J* = 7.6 Hz, 1H), 7.45 – 7.33 (m, 3H), 2.89 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  162.7, 145.9, 138.4, 138.3, 131.7, 131.5, 130.5, 129.6, 128.6, 126.7, 126.3, 126.0, 125.5, 125.1, 120.2, 120.2, 118.7, 22.3. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>18</sub>H<sub>13</sub>NO: 259.0997; found: 259.0996.

#### 2-(4-(*tert*-butyl)phenyl)naphtho[2,1-*d*]oxazole (4c)<sup>8</sup>



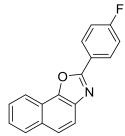
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a white solid in 82% yield (49.4 mg). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.32 (d, J = 8.2 Hz, 1H), 8.26 (d, J = 8.0 Hz, 2H), 7.97 (d, J = 8.2 Hz, 1H), 7.85 (d, J = 8.7 Hz, 1H), 7.79 (d, J = 8.7 Hz, 1H), 7.64 (t, J = 7.5 Hz, 1H), 7.58 (d, J = 8.0 Hz, 2H), 7.53 (t, J = 7.5 Hz, 1H), 1.39 (s, 9H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  162.7, 154.7, 146.3, 138.6, 131.6, 128.7, 127.1, 126.8, 125.9, 125.50, 125.3, 124.6, 120.4, 120.2, 118.6, 35.0, 31.2.

## 2-(4-methoxyphenyl)naphtho[2,1-d]oxazole (5c)<sup>9</sup>



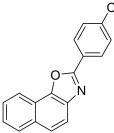
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a white solid in 80% yield (44.0 mg). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.27 (t, *J* = 7.3 Hz, 3H), 7.96 (d, *J* = 8.2 Hz, 1H), 7.82 (d, *J* = 8.7 Hz, 1H), 7.77 (d, *J* = 8.6 Hz, 1H), 7.62 (t, *J* = 7.5 Hz, 1H), 7.51 (t, *J* = 7.5 Hz, 1H), 7.04 (d, *J* = 7.8 Hz, 2H), 3.89 (s, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  162.6, 162.0, 146.2, 138.7, 131.5, 129.0, 128.7, 126.7, 125.4, 125.2, 120.3, 120.0, 120.0, 118.5, 114.4, 55.4.

2-(4-fluorophenyl)naphtho[2,1-d]oxazole (6c)



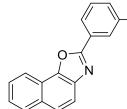
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a white solid in 76% yield (40.0 mg). mp 67.8–68.6 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.31 – 8.18 (m, 3H), 7.93 (d, J = 8.2 Hz, 1H), 7.81 – 7.74 (m, 2H), 7.61 (t, J = 7.6 Hz, 1H), 7.56 – 7.45 (m, 1H), 7.20 (t, J = 8.6 Hz, 2H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  165.7, 163.2, 161.4, 146.3, 138.5, 131.6, 129.4 (d, J = 8.8 Hz), 128.6, 126.8, 125.5 (d, J = 16.3 Hz), 123.6 (d, J = 3.2 Hz), 120.2, 120.0, 118.5, 116.1 (d, J = 22.2 Hz); <sup>19</sup>F NMR (377 MHz, CDCl<sub>3</sub>):  $\delta$  -108.00 (s). HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>17</sub>H<sub>10</sub>FNO: 263.0746; found: 263.0746.

2-(4-chlorophenyl)naphtho[2,1-d]oxazole (7c)<sup>9</sup>



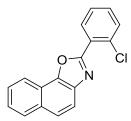
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a white solid in 64% yield (35.7 mg); mp 69.7–70.4 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.23 (d, *J* = 8.4 Hz, 1H), 8.20 (d, *J* = 7.8 Hz, 2H), 7.94 (d, *J* = 8.2 Hz, 1H), 7.80 (d, *J* = 8.7 Hz, 1H), 7.75 (d, *J* = 8.7 Hz, 1H), 7.62 (t, *J* = 7.5 Hz, 1H), 7.52 (d, *J* = 7.6 Hz, 1H), 7.48 (d, *J* = 8.3 Hz, 2H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  161.3, 146.4, 138.5, 137.3, 131.7, 129.2, 128.7, 128.4, 126.9, 125.8, 125.7, 125.6, 120.2, 120.1, 118.5.

#### 2-(3-chlorophenyl)naphtho[2,1-d]oxazole (8c)



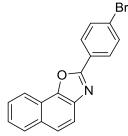
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a white solid in 67% yield (37.4 mg). mp 69.7–70.2 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.27 – 8.19 (m, 2H), 8.14 (d, J = 7.1 Hz, 1H), 7.92 (d, J = 8.2 Hz, 1H), 7.80 – 7.73 (m, 2H), 7.61 (t, J = 7.5 Hz, 1H), 7.51 (t, J = 7.5 Hz, 1H), 7.48 – 7.39 (m, 2H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  160.8, 146.4, 138.3, 135.0, 131.8, 131.0, 130.1, 128.9, 128.6, 127.1, 126.9, 125.8, 125.6, 125.2, 120.2, 120.1, 118.5. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>17</sub>H<sub>10</sub>CINO: 279.0451; found: 279.0450.

# 2-(2-chlorophenyl)naphtho[2,1-d]oxazole (9c)



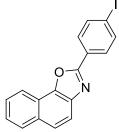
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a white solid in 63% yield (35.2 mg). mp 70.6–71.3 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): 8.29 (d, J = 8.2 Hz, 1H), 8.25 – 8.22 (m, 1H), 7.96 (d, J = 8.2 Hz, 1H), 7.90 (d, J = 8.7 Hz, 1H), 7.79 (d, J = 8.8 Hz, 1H), 7.63 (t, J = 7.6 Hz, 1H), 7.60 – 7.56 (m, 1H), 7.53 (t, J = 7.6 Hz, 1H), 7.47 – 7.36 (m, 2H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): 8 160.2, 146.4, 138.1, 133.1, 131.8, 131.5, 131.4, 128.6, 126.9, 126.8, 126.2, 125.8, 125.5, 120.3, 120.3, 118.8. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>17</sub>H<sub>10</sub>CINO: 279.0451; found: 279.0451.

### 2-(4-bromophenyl)naphtho[2,1-d]oxazole (10c)



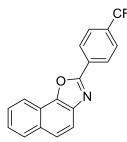
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a white solid in 65% yield (42.0 mg); mp 71.3–72.1 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.26 (d, *J* = 8.2 Hz, 1H), 8.15 (d, *J* = 8.0 Hz, 2H), 7.95 (d, *J* = 8.2 Hz, 1H), 7.79 (q, *J* = 8.7 Hz, 2H), 7.66 (d, *J* = 7.8 Hz, 2H), 7.62 (d, *J* = 7.7 Hz, 1H), 7.53 (t, *J* = 7.5 Hz, 1H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  161.5, 146.5, 138.5, 132.2, 131.8, 128.7, 128.6, 126.9, 126.3, 125.8, 125.6, 120.3, 120.1, 118.5. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>17</sub>H<sub>10</sub>BrNO: 322.9946; found: 322.9946.

# 2-(4-iodophenyl)naphtho[2,1-d]oxazole (11c)



The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a white solid in 60% yield (44.5 mg); mp 77.6–77.8 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.28 (d, *J* = 8.2 Hz, 1H), 8.03 (d, *J* = 7.8 Hz, 2H), 7.97 (d, *J* = 8.2 Hz, 1H), 7.89 (d, *J* = 8.0 Hz, 2H), 7.81 (q, *J* = 8.7 Hz, 2H), 7.64 (t, *J* = 7.5 Hz, 1H), 7.54 (t, *J* = 7.3 Hz, 1H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  161.7, 146.5, 138.5, 138.2, 131.8, 128.7, 128.6, 126.9, 126.9, 125.9, 125.7, 120.3, 120.2, 118.6, 97.9. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>17</sub>H<sub>10</sub>INO: 370.9807; found: 370.9804.

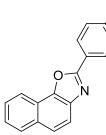
## 2-(4-(trifluoromethyl)phenyl)naphtho[2,1-d]oxazole (12c)



The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a white solid in 78% yield (48.8 mg); mp 124.8–125.1 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.31 (d, *J* = 8.1 Hz, 2H), 8.20 (d, *J* = 8.2 Hz, 1H), 7.90 (d, *J* = 8.2 Hz, 1H), 7.80 – 7.69 (m, 4H), 7.60 (t, *J* = 7.6 Hz, 1H), 7.50 (t, *J* = 7.5 Hz, 1H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  160.6, 146.6, 138.4, 132.4 (q, *J* = 32.8 Hz), 131.9, 130.4 (d, *J* = 0.9 Hz), 128.7, 127.3, 126.9, 125.9, 125.8 (q, *J* = 3.4 Hz), 123.8 (q, *J* = 270.7 Hz), 120.2, 120.1, 118.5. <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>):  $\delta$  -62.93. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>18</sub>H<sub>10</sub>F<sub>3</sub>NO: 313.0714; found: 313.0715.

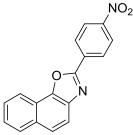
# 4-(naphtho[2,1-*d*]oxazol-2-yl)benzonitrile (13c)

CN



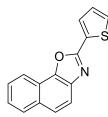
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a white solid in 51% yield (27.5 mg); mp 220–221 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.44 – 8.38 (m, 2H), 8.30 (d, *J* = 8.2 Hz, 1H), 7.99 (d, *J* = 8.2 Hz, 1H), 7.88 – 7.78 (m, 4H), 7.71 – 7.64 (m, 1H), 7.62 – 7.54 (m, 1H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  160.3, 146.9, 138.5, 132.7, 132.2, 131.2, 128.8, 127.6, 127.2, 126.3, 126.1, 120.3, 118.6, 118.2, 114.3. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>18</sub>H<sub>10</sub>N<sub>2</sub>O: 270.0793; found: 270.0792.

# 2-(4-nitrophenyl)naphtho[2,1-d]oxazole (14c)



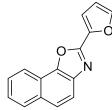
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a white solid in 60% yield (34.8 mg); mp 231.0–231.5 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.47 (d, *J* = 8.8 Hz, 2H), 8.38 (d, *J* = 8.8 Hz, 2H), 8.32 (d, *J* = 8.1 Hz, 1H), 8.00 (d, *J* = 8.2 Hz, 1H), 7.85 (q, *J* = 8.8 Hz, 2H), 7.68 (t, *J* = 7.4 Hz, 1H), 7.59 (t, *J* = 7.5 Hz, 1H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  160.0, 149.1, 147.1, 138.6, 132.9, 132.2, 128.8, 127.9, 127.2, 126.4, 126.2, 124.3, 120.3, 120.3, 118.7. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>17</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub>: 290.0691; found: 290.0692.

# 2-(thiophen-2-yl)naphtho[2,1-d]oxazole (15c)<sup>10</sup>



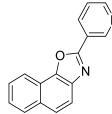
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a white solid in 47% yield (23.6 mg). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.24 (d, *J* = 8.2 Hz, 1H), 7.94 (d, *J* = 8.1 Hz, 2H), 7.78 (q, *J* = 8.7 Hz, 2H), 7.61 (t, *J* = 7.5 Hz, 1H), 7.54 – 7.49 (m, 2H), 7.19 (t, *J* = 4.0 Hz, 1H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  158.4, 146.0, 138.4, 131.6, 129.8, 129.6, 129.3, 128.6, 128.2, 126.8, 125.6, 125.5, 120.1, 120.1, 118.4.

2-(furan-2-yl)naphtho[2,1-d]oxazole (16c)<sup>11</sup>



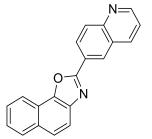
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a white solid in 41% yield (19.3 mg). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.27 (d, *J* = 8.2 Hz, 1H), 7.95 (d, *J* = 8.2 Hz, 1H), 7.80 (q, *J* = 8.7 Hz, 2H), 7.68 (s, 1H), 7.62 (t, *J* = 7.6 Hz, 1H), 7.52 (t, *J* = 7.5 Hz, 1H), 7.31 (d, *J* = 3.4 Hz, 1H), 6.66 - 6.59 (m, 1H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  154.8, 145.8, 145.8, 145.8, 138.2, 131.7, 128.6, 126.9, 125.7, 125.7, 120.2, 120.1, 118.5, 113.4, 112.2.

2-(pyridin-3-yl)naphtho[2,1-d]oxazole (17c)



The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a white solid in 31% yield (15.3 mg). mp 111.2–111.5 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  9.53 – 9.52 (m, 1H), 8.79 – 8.68 (m, 1H), 8.60 – 8.50 (m, 1H), 8.28 (d, *J* = 8.2 Hz, 1H), 7.96 (d, *J* = 8.2 Hz, 1H), 7.81 (q, *J* = 8.8 Hz, 2H), 7.65 (t, *J* = 7.5 Hz, 1H), 7.54 (t, *J* = 7.3 Hz, 1H), 7.47 (dd, *J* = 7.9, 4.9 Hz, 1H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  159.9, 151.6, 148.4, 146.6, 138.3, 134.3, 131.9, 128.7, 127.0, 126.0, 125.8, 123.7, 120.2, 120.2, 118.5. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>16</sub>H<sub>10</sub>N<sub>2</sub>O: 246.0793; found: 246.0795.

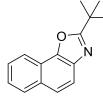
#### 2-(quinolin-6-yl)naphtho[2,1-d]oxazole (18c)



The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a white solid in 54% yield (32.0 mg). mp 160.5–161.1 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.99 – 8.97 (m, 1H), 8.79 (s, 1H), 8.61 (d, J = 8.8 Hz, 1H), 8.35 (d, J = 8.2 Hz, 1H), 8.30 (d, J = 8.1 Hz, 1H), 8.25 (d, J = 8.8 Hz, 1H), 8.35 (d, J = 8.2 Hz, 1H), 8.30 (d, J = 8.1 Hz, 1H), 8.25 (d, J = 8.8 Hz, 1H), 8.35 (d, J = 8.2 Hz, 1H), 8.30 (d, J = 8.1 Hz, 1H), 8.25 (d, J = 8.8 Hz, 1H), 8.35 (d, J = 8.2 Hz, 1H), 8.30 (d, J = 8.1 Hz, 1H), 8.25 (d, J = 8.8 Hz, 1H), 8.35 (d, J = 8.2 Hz, 1H), 8.30 (d, J = 8.1 Hz, 1H), 8.25 (d, J = 8.8 Hz, 1H), 8.35 (d, J = 8.2 Hz, 1H), 8.3

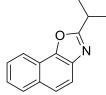
1H), 7.98 (d, J = 8.2 Hz, 1H), 7.87 (d, J = 8.7 Hz, 1H), 7.81 (d, J = 8.7 Hz, 1H), 7.67 (t, J = 7.5 Hz, 1H), 7.56 (t, J = 7.6 Hz, 1H), 7.48 (dd, J = 8.3, 4.2 Hz, 1H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  161.6, 151.7, 149.2, 146.6, 138.6, 136.7, 131.8, 130.3, 128.7, 128.0, 127.4, 127.1, 126.9, 125.8, 125.6, 125.3, 121.9, 120.2, 120.2, 118.5. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>20</sub>H<sub>12</sub>N<sub>2</sub>O: 296.0950; found: 296.0952.

2-(*tert*-butyl)naphtho[2,1-*d*]oxazole (19c)



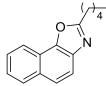
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a pale yellow oil in 66% yield (29.7 mg). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.22 (d, J = 8.2 Hz, 1H), 7.94 (d, J = 8.2 Hz, 1H), 7.80 (d, J = 8.7 Hz, 1H), 7.73 (d, J = 8.7 Hz, 1H), 7.60 (t, J = 7.6 Hz, 1H), 7.49 (t, J = 7.6 Hz, 1H), 1.58 (s, 9H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  172.7, 146.3, 137.4, 131.3, 128.5, 126.5, 125.2, 124.6, 120.3, 120.0, 118.5, 34.3, 28.7. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>15</sub>H<sub>15</sub>NO: 225.1154; found: 225.1155.

# 2-isopropylnaphtho[2,1-d]oxazole (20c)



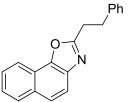
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a pale yellow oil in 64% yield (27.0 mg). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.20 (d, J = 8.2 Hz, 1H), 7.95 (d, J = 8.2 Hz, 1H), 7.76 (dd, J = 21.4, 8.7 Hz, 2H), 7.60 (t, J = 7.6 Hz, 1H), 7.50 (t, J = 7.6 Hz, 1H), 3.59 – 3.16 (m, 1H), 1.54 (d, J = 6.9 Hz, 6H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  170.4, 146.2, 137.4, 131.2, 128.5, 126.5, 125.1, 124.6, 120.2, 119.9, 118.4, 28.9, 20.5. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>14</sub>H<sub>13</sub>NO: 211.0997; found: 211.0994.

# 2-pentylnaphtho[2,1-d]oxazole (21c)



The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a pale yellow oil in 56% yield (26.8 mg). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.20 (d, J = 8.3 Hz, 1H), 7.96 (d, J = 8.2 Hz, 1H), 7.80 – 7.71 (m, 2H), 7.61 (t, J = 7.3 Hz, 1H), 7.51 (t, J = 7.1 Hz, 1H), 3.04 (t, J = 7.6 Hz, 2H), 2.05 – 1.87 (m, 2H), 1.55 – 1.34 (m, 4H), 0.93 (t, J = 7.0 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  166.6, 146.3, 137.6, 131.3, 128.5, 126.6, 125.2, 124.7, 120.2, 119.9, 118.4, 31.3, 28.7, 26.7, 22.3, 13.9. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>16</sub>H<sub>17</sub>NO: 239.1310; found: 239.1312.

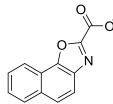
## 2-phenethylnaphtho[2,1-*d*]oxazole (22c)



The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a pale yellow oil in 42% yield (22.9 mg). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.17 (d, *J* = 8.2 Hz, 1H), 7.93 (d, *J* = 8.2 Hz,

1H), 7.74 (q, J = 8.7 Hz, 2H), 7.59 (t, J = 7.6 Hz, 1H), 7.49 (t, J = 7.6 Hz, 1H), 7.35 – 7.25 (m, 4H), 7.21 (dd, J = 7.9, 4.7 Hz, 1H), 3.37 – 3.23 (m, 4H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  165.4, 146.3, 140.1, 137.5, 131.3, 128.5, 128.2, 126.6, 126.4, 125.3, 124.8, 120.2, 119.9, 118.4, 33.0, 30.5. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>19</sub>H<sub>15</sub>NO: 273.1154; found: 273.1154.

Ethyl naphtho[2,1-*d*]oxazole-2-carboxylate (23c)



The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a white solid in 54% yield (26.0 mg). mp 101.2–101.7 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.25 (d, *J* = 8.1 Hz, 1H), 7.88 (d, *J* = 8.1 Hz, 1H), 7.75 (q, *J* = 8.8 Hz, 2H), 7.58 (t, *J* = 7.5 Hz, 1H), 7.52 (t, *J* = 7.4 Hz, 1H), 4.53 (q, *J* = 7.1 Hz, 2H), 1.47 (t, *J* = 7.1 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  156.2, 151.9, 147.3, 137.1, 132.8, 128.5, 127.2, 127.0, 126.7, 120.7, 120.1, 119.0, 62.9, 14.1. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>14</sub>H<sub>11</sub>NO<sub>3</sub>: 241.0739; found: 241.0737.

#### 2-methylnaphtho[2,1-d]oxazole (24c)<sup>12</sup>



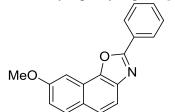
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (40/1) to afford a pale yellow oil in 33% yield (12.1 mg). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.16 (d, *J* = 8.2 Hz, 1H), 7.93 (d, *J* = 8.2 Hz, 1H), 7.79 – 7.67 (m, 2H), 7.61 – 7.56 (m, 4.0 Hz, 1H), 7.53 – 7.44 (m, 1H), 2.73 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  162.9, 146.5, 137.7, 131.3, 128.5, 126.6, 125.2, 124.7, 120.2, 119.8, 118.2, 14.5.

naphtho[2,1-d]oxazole (25c)<sup>13</sup>



The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (40/1) to afford a pale yellow oil in 31% yield (10.5 mg). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.28 – 8.24 (d, *J* = 10.5 Hz, 2H), 8.00 (d, *J* = 8.1 Hz, 1H), 7.87 (d, *J* = 8.7 Hz, 1H), 7.81 (d, *J* = 8.7 Hz, 1H), 7.66 (t, *J* = 7.5 Hz, 1H), 7.58 (t, *J* = 7.5 Hz, 1H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  151.2, 145.4, 135.9, 131.2, 128.0, 126.3, 125.3, 124.8, 119.8, 119.6, 118.2.

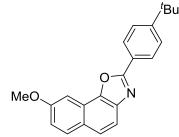
8-methoxy-2-phenylnaphtho[2,1-d]oxazole (26c)



The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a white solid in 83% yield (45.7 mg); mp 109.0-109.3 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.32 – 8.31 (m, 2H), 7.81 (d, *J* = 8.9 Hz, 1H), 7.67 (s, 2H), 7.53 – 7.52 (m, 3H), 7.48 (s, 1H), 7.14 (d, *J* = 8.9 Hz, 1H), 3.99 (s, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  162.3, 158.4, 145.9, 139.0, 131.1, 130.2, 128.8, 127.4, 127.2, 126.9,

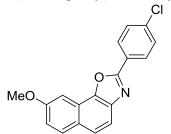
125.1, 121.2, 118.0, 115.9, 98.7, 55.5. HRMS (EI) m/z:  $[M]^+$  calcd. for  $C_{18}H_{13}NO_2$ : 275.0946; found: 275.0951.

# 2-(4-(*tert*-butyl)phenyl)-8-methoxynaphtho[2,1-d]oxazole (27c)



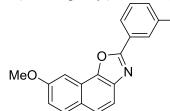
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a white solid in 66% yield (43.7 mg); mp 178.9–179.2 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.26 (d, *J* = 7.7 Hz, 2H), 7.84 (d, *J* = 8.9 Hz, 1H), 7.69 (s, 2H), 7.57 (d, *J* = 7.6 Hz, 2H), 7.53 (s, 1H), 7.16 (d, *J* = 8.9 Hz, 1H), 4.02 (s, 3H), 1.39 (s, 9H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  162.5, 158.4, 154.7, 145.9, 139.1, 130.3, 127.1, 126.9, 125.9, 125.0, 124.6, 121.2, 117.9, 115.9, 98.8, 55.5, 35.0, 31.1. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>22</sub>H<sub>21</sub>NO<sub>2</sub>: 331.1572; found: 331.1573.

#### 2-(4-chlorophenyl)-8-methoxynaphtho[2,1-d]oxazole (28c)



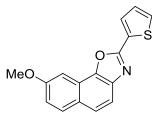
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a white solid in 68% yield (42.0 mg); mp 151.2–151.4 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.17 (d, *J* = 7.7 Hz, 2H), 7.77 (d, *J* = 8.9 Hz, 1H), 7.66 – 7.58 (m, 2H), 7.45 (d, *J* = 7.7 Hz, 2H), 7.39 (s, 1H), 7.12 (d, *J* = 8.9 Hz, 1H), 3.97 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  161.2, 158.4, 145.9, 138.8, 137.2, 130.2, 129.1, 128.4, 126.9, 125.8, 125.2, 121.1, 118.1, 115.7, 98.6, 55.4. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>18</sub>H<sub>12</sub>ClNO<sub>2</sub>: 309.0557; found: 309.0559.

#### 2-(3-chlorophenyl)-8-methoxynaphtho[2,1-d]oxazole (29c)



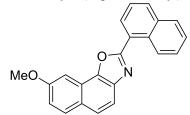
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a white solid in 57% yield (35.2 mg); mp 162.1–162.4 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.26 (s, 1H), 8.16 (d, *J* = 6.9 Hz, 1H), 7.81 (d, *J* = 8.9 Hz, 1H), 7.65 (q, *J* = 8.6 Hz, 2H), 7.50 – 7.39 (m, 3H), 7.14 (d, *J* = 8.9 Hz, 1H), 4.00 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  160.8, 158.5, 146.0, 138.8, 135.0, 131.0, 130.3, 130.2, 129.0, 127.2, 127.1, 125.3, 125.3, 121.2, 118.3, 115.8, 98.7, 55.5. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>18</sub>H<sub>12</sub>ClNO<sub>2</sub>: 309.0557; found: 309.0557.

## 8-methoxy-2-(thiophen-2-yl)naphtho[2,1-d]oxazole (30c)



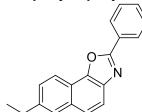
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a white solid in 50% yield (28.1 mg); mp 174.3–174.7 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  7.96 (s, 1H), 7.81 (d, *J* = 8.8 Hz, 1H), 7.65 (q, *J* = 8.5 Hz, 2H), 7.53 (s, 1H), 7.46 (s, 1H), 7.18 - 7.19 (m, 1H), 7.14 (d, *J* = 8.9 Hz, 1H), 3.99 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  158.5, 158.4, 145.5, 138.9, 130.3, 129.9, 129.6, 129.2, 128.2, 126.9, 125.2, 121.0, 118.1, 115.7, 98.6, 55.5. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>16</sub>H<sub>11</sub>NO<sub>2</sub>S: 281.0510; found: 281.0511.

8-methoxy-2-(naphthalen-1-yl)naphtho[2,1-d]oxazole (31c)



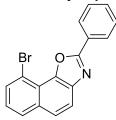
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a white solid in 45% yield (29.3 mg); mp 172.9–173.7 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  9.54 (d, *J* = 8.6 Hz, 1H), 8.52 (d, *J* = 7.2 Hz, 1H), 8.03 (d, *J* = 8.1 Hz, 1H), 7.94 (d, *J* = 8.2 Hz, 1H), 7.88 (d, *J* = 9.0 Hz, 1H), 7.80 (d, *J* = 8.6 Hz, 1H), 7.77 – 7.70 (m, 2H), 7.62 (dd, *J* = 18.2, 9.6 Hz, 3H), 7.19 (d, *J* = 8.9 Hz, 1H), 4.02 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  162.0, 158.5, 145.5, 139.2, 134.0, 131.9, 130.6, 130.3, 128.9, 128.6, 127.8, 127.1, 126.4, 126.3, 125.0, 124.9, 123.9, 121.2, 118.1, 116.2, 99.0, 55.5. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>22</sub>H<sub>15</sub>NO<sub>2</sub>: 325.1103; found: 325.1103.

#### 7-ethyl-2-phenylnaphtho[2,1-*d*]oxazole (32c)



The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (40/1) to afford a white solid in 62% yield (33.9 mg); mp 98.5–99.4 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.35 – 8.28 (m, 2H), 8.20 (d, J = 8.4 Hz, 1H), 7.81 (d, J = 8.7 Hz, 1H), 7.75 – 7.68 (m, 2H), 7.60 – 7.42 (m, 4H), 2.84 (q, J = 7.6 Hz, 2H), 1.36 (t, J = 7.6 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  162.0, 146.5, 141.7, 138.0, 132.1, 130.9, 128.8, 127.9, 127.5, 127.2, 126.5, 124.9, 120.1, 118.7, 118.5, 29.1, 15.5. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>19</sub>H<sub>15</sub>NO: 273.1154; found: 273.1152.

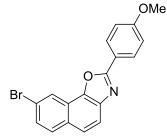
#### 9-bromo-2-phenylnaphtho[2,1-*d*]oxazole (33c)



The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (40/1) to afford a white solid

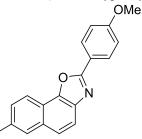
in 51% yield (32.9 mg); mp 147.1–148.0 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.38 – 8.30 (m, 2H), 7.90 – 7.84 (m, 3H), 7.77 (d, *J* = 8.7 Hz, 1H), 7.58 – 7.49 (m, 3H), 7.35 – 7.27 (m, 1H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  162.9, 145.2, 140.6, 133.4, 132.0, 131.3, 128.9, 128.2, 127.5, 127.1, 126.1, 125.7, 120.6, 119.7, 115.1. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>17</sub>H<sub>10</sub>BrNO: 322.9946; found: 322.9945.

8-bromo-2-(4-methoxyphenyl)naphtho[2,1-d]oxazole (34c)



The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a white solid in 72% yield (50.8 mg) ); mp 179.3–179.5 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.36 (s, 1H), 8.20 (d, J = 7.7 Hz, 2H), 7.77 (t, J = 7.3 Hz, 2H), 7.68 (d, J = 8.5 Hz, 1H), 7.53 (d, J = 8.6 Hz, 1H), 7.02 (d, J = 7.7 Hz, 2H), 3.88 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  163.0, 162.2, 145.0, 139.4, 130.2, 129.6, 129.1, 128.6, 125.0, 122.4, 121.1, 120.9, 119.5, 118.8, 114.3, 55.4. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>18</sub>H<sub>12</sub>BrNO<sub>2</sub>: 353.0051; found: 353.0051.

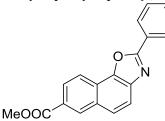
#### 7-bromo-2-(4-methoxyphenyl)naphtho[2,1-d]oxazole (35c)



Rr

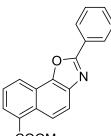
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a white solid in 67% yield (47.3 mg); mp 177.5–177.9 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.21 (d, *J* = 7.9 Hz, 2H), 8.09 (d, *J* = 8.4 Hz, 2H), 7.80 (d, *J* = 8.5 Hz, 1H), 7.65 (t, *J* = 11.1 Hz, 2H), 7.02 (d, *J* = 7.7 Hz, 2H), 3.88 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  162.9, 162.2, 146.0, 139.0, 132.4, 130.7, 130.0, 129.1, 124.3, 121.7, 119.6, 119.6, 119.2, 118.6, 114.4, 55.4. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>18</sub>H<sub>12</sub>BrNO<sub>2</sub>: 353.0051; found: 353.0052.

Methyl 2-phenylnaphtho[2,1-d]oxazole-7-carboxylate (36c)



The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a white solid in 68% yield (41.2 mg); mp 168.1–168.9 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.67 (s, 1H), 8.32 – 8.24 (m, 3H), 8.19 (d, *J* = 8.6 Hz, 1H), 7.88 – 7.82 (m, 2H), 7.54 (m, 3H), 3.98 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  166.9, 163.3, 146.0, 140.5, 131.6, 131.5, 130.6, 129.0, 127.4, 127.0, 126.7, 126.4, 122.2, 120.3, 119.5, 52.3. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>19</sub>H<sub>13</sub>NO<sub>3</sub>: 303.0895; found: 303.0896.

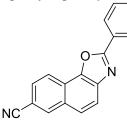
### Methyl 2-phenylnaphtho[2,1-d]oxazole-6-carboxylate (37c)



# ĊOOMe

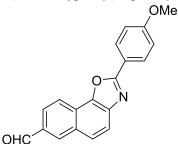
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a white solid in 67% yield (40.6 mg); mp 144.2–144.9 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.78 (d, *J* = 9.2 Hz, 1H), 8.34 (d, *J* = 8.1 Hz, 1H), 8.28 – 8.18 (m, 2H), 8.09 (d, *J* = 7.3 Hz, 1H), 7.88 (d, *J* = 9.2 Hz, 1H), 7.54 (t, *J* = 7.8 Hz, 1H), 7.51 – 7.43 (m, 3H), 3.97 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  167.7, 162.6, 146.3, 138.4, 131.2, 129.3, 129.0, 128.8, 128.0, 127.2, 127.0, 125.3, 124.7, 122.9, 120.8, 120.1, 52.2. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>19</sub>H<sub>13</sub>NO<sub>3</sub>: 303.0895; found: 303.0895.

#### 2-phenylnaphtho[2,1-d]oxazole-7-carbonitrile (38c)



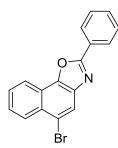
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a white solid in 51% yield (27.5 mg) ); mp 138.1–138.7 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.31 – 8.37 (m, 4H), 7.95 (d, *J* = 8.7 Hz, 1H), 7.83 (d, *J* = 8.6 Hz, 1H), 7.77 (d, *J* = 8.5 Hz, 1H), 7.58 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  163.9, 145.9, 141.2, 134.7, 131.9, 130.3, 129.1, 127.7, 127.6, 126.7, 125.8, 121.5, 121.5, 120.7, 119.0, 109.0. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>18</sub>H<sub>10</sub>N<sub>2</sub>O: 270.0793; found: 270.0791.

#### 2-(4-methoxyphenyl)naphtho[2,1-d]oxazole-7-carbaldehyde (39c)



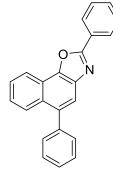
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a white solid in 42% yield (25.5 mg); mp 204.4–206.1 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  10.17 (s, 1H), 8.45 – 8.44 (m, 1H), 8.36 (d, *J* = 8.5 Hz, 1H), 8.32 – 8.22 (m, 2H), 8.10 (dd, *J* = 8.6, 1.4 Hz, 1H), 7.93 – 7.92 (m, 2H), 7.06 (d, *J* = 8.9 Hz, 2H), 3.91 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  191.8, 164.1, 162.5, 146.0, 141.6, 134.9, 133.5, 130.5, 129.4, 126.8, 124.2, 123.0, 121.2, 119.8, 119.5, 114.5, 55.5. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>19</sub>H<sub>13</sub>NO<sub>3</sub>: 303.0895; found: 303.0898.

#### 5-bromo-2-phenylnaphtho[2,1-d]oxazole (40c)



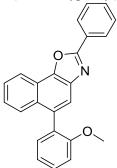
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a white solid in 71% yield (45.9 mg); mp 107.3–107.8 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.30 (d, *J* = 8.2 Hz, 1H), 8.28 – 8.23 (m, 2H), 8.21 (d, *J* = 8.3 Hz, 1H), 8.11 (s, 1H), 7.67 – 7.61 (m, 1H), 7.61 – 7.55 (m, 1H), 7.54 – 7.51 (m, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  162.8, 146.0, 138.6, 131.4, 129.5, 128.9, 128.3, 127.5, 127.3, 126.9, 126.8, 122.5, 120.8, 120.5, 118.6. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>17</sub>H<sub>10</sub>BrNO: 322.9946; found: 322.9945.

### 2, 5-diphenylnaphtho[2, 1-d]oxazole (41c)



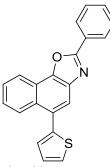
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a pale yellow solid in 67% yield (43.0 mg); mp 142.9–144.1 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.37 (s, 3H), 7.97 (d, J = 8.2 Hz, 1H), 7.81 (s, 1H), 7.65 (t, J = 6.8 Hz, 1H), 7.55 - 7.53 (m, 7H), 7.48 (t, J = 6.7 Hz, 2H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  162.6, 146.0, 140.5, 138.2, 138.0, 131.2, 130.3, 130.1, 128.9, 128.3, 127.4, 127.3, 126.7, 125.6, 120.4, 120.4, 119.3. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>23</sub>H<sub>15</sub>NO: 321.1154; found: 321.1151.

#### 5-(2-methoxyphenyl)-2-phenylnaphtho[2,1-d]oxazole (42c)



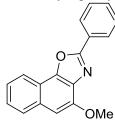
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a pale yellow solid in 68% yield (47.8 mg); mp 164–165 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.38 – 8.36 (m, 3H), 7.82 (s, 1H), 7.68 (d, *J* = 8.5 Hz, 1H), 7.64 (t, *J* = 7.6 Hz, 1H), 7.57 - 7.55 (m, 2H), 7.50 – 7.41 (m, 2H), 7.36 (d, *J* = 7.2 Hz, 1H), 7.13 (t, *J* = 7.4 Hz, 1H), 7.09 (d, *J* = 8.3 Hz, 1H), 3.72 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  162.4, 157.3, 146.1, 138.0, 134.7, 132.1, 131.0, 130.5, 129.2, 128.9, 127.5, 127.4, 127.3, 126.5, 125.3, 120.6, 120.2, 119.8, 111.0, 55.5. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>24</sub>H<sub>17</sub>NO<sub>2</sub>: 351.1259; found: 351.1259.

#### 2-phenyl-5-(thiophen-2-yl)naphtho[2, 1-d]oxazole (43c)



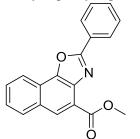
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a pale yellow solid in 65% yield (42.5 mg); mp 127.6–129 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.37 – 8.35 (m, 3H), 8.09 (d, J = 8.5 Hz, 1H), 7.85 (s, 1H), 7.65 (t, J = 7.5 Hz, 1H), 7.55 (s, 3H), 7.52 – 7.48 (m, 2H), 7.43 (s, 1H), 7.33 – 7.32 (m, 1H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  162.7, 146.2, 140.8, 138.0, 132.8, 131.2, 130.3, 129.7, 128.9, 127.3, 127.1, 126.8, 125.8, 125.4, 123.8, 120.5, 120.4, 119.4. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>21</sub>H<sub>13</sub>NOS: 327.0718; found: 327.0715.

#### 4-methoxy-2-phenylnaphtho[2,1-d]oxazole (44c)



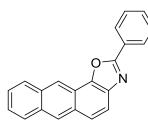
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a white solid in 88% yield (48.4 mg); mp 141.4–142.1 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.36 – 8.35 (m, 2H), 8.17 (s, 1H), 7.81 (s, 1H), 7.60 – 7.38 (m, 5H), 7.01 (d, *J* = 9.9 Hz, 1H), 4.12 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  162.1, 150.1, 147.6, 132.5, 131.4, 131.1, 128.8, 127.3, 127.2, 126.2, 124.3, 120.1, 116.3, 102.1, 55.9. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>18</sub>H<sub>13</sub>NO<sub>2</sub>: 275.0946; found: 275.0946.

# methyl 2-phenylnaphtho[2,1-d]oxazole-4-carboxylate (45c)



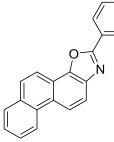
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a white solid in 29% yield (17.6 mg); mp 168.8–170.1 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.54 (s, 1H), 8.41 – 8.39 (m, 2H), 8.30 (d, *J* = 8.3 Hz, 1H), 8.05 (d, *J* = 8.2 Hz, 1H), 7.73 (t, *J* = 7.6 Hz, 1H), 7.59 (d, *J* = 7.4 Hz, 1H), 7.56 – 7.53 (m, 3H), 4.11 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  165.8, 163.3, 147.2, 136.8, 131.5, 130.3, 129.9, 129.4, 129.1, 128.8, 127.7, 127.0, 126.4, 122.1, 120.6, 120.3, 52.5. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>19</sub>H<sub>13</sub>NO<sub>3</sub>: 303.0895; found: 303.0895.

# 2-phenylanthra[2,1-*d*]oxazole (46c)



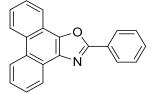
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a white solid in 73% yield (43.1 mg); mp 200.5–200.6 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.78 (s, 1H), 8.51 (s, 1H), 8.35 (d, *J* = 7.3 Hz, 2H), 8.09 (d, *J* = 8.2 Hz, 1H), 8.02 (d, *J* = 8.1 Hz, 1H), 7.91 (d, *J* = 9.0 Hz, 1H), 7.81 (d, *J* = 8.9 Hz, 1H), 7.60 – 7.46 (m, 6H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  162.2, 146.3, 137.9, 131.9, 131.3, 131.0, 130.2, 129.0, 128.5, 128.0, 127.7, 127.4, 127.2, 126.3, 126.2, 125.6, 119.5, 118.8, 118.4. HRMS (EI) m/z; [M]<sup>+</sup> calcd. for C<sub>21</sub>H<sub>13</sub>NO: 295.0997; found: 295.0997.

2-phenylphenanthro[2,1-d]oxazole (47c)



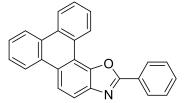
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a white solid in 70% yield (41.3 mg); mp 202.0–203.1 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.67 (d, *J* = 8.3 Hz, 1H), 8.62 (d, *J* = 8.8 Hz, 1H), 8.38 – 8.29 (m, 2H), 8.20 (d, *J* = 8.8 Hz, 1H), 7.97 (d, *J* = 8.8 Hz, 1H), 7.92 (d, *J* = 8.0 Hz, 1H), 7.89 (d, *J* = 9.1 Hz, 1H), 7.67 (t, *J* = 7.5 Hz, 1H), 7.60 (d, *J* = 7.5 Hz, 1H), 7.58 – 7.50 (m, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  162.9, 147.3, 139.4, 131.6, 131.3, 130.4, 129.0, 128.9, 128.2, 127.9, 127.4, 127.3, 127.2, 126.5, 122.9, 119.8, 118.7, 118.3, 118.1. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>21</sub>H<sub>13</sub>NO: 295.0997; found: 295.0995.

# 2-phenylphenanthro[9,10-d]oxazole (48c)<sup>14</sup>



The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a white solid in 47% yield (27.7 mg). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.74 (t, *J* = 8.5 Hz, 2H), 8.64 (d, *J* = 7.8 Hz, 1H), 8.40 - 8.36 (m, 2H), 8.34 (d, *J* = 7.7 Hz, 1H), 7.78 - 7.65 (m, 4H), 7.61 - 7.52 (m, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  162.2, 144.9, 135.5, 130.9, 129.3, 128.9, 127.6, 127.4, 127.3, 127.2, 126.4, 126.2, 126.1, 123.8, 123.4, 122.9, 121.1, 120.9.

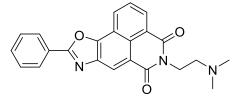
#### 8-phenyltriphenyleno[2,1-*d*]oxazole (49c)



The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a white solid in 31% yield (21.4 mg); mp 224.4–224.5 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  9.34 (d, *J* = 8.0 Hz, 1H),

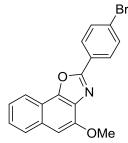
8.67 – 8.53 (m, 4H), 8.36 (d, J = 5.8 Hz, 2H), 7.94 (d, J = 8.7 Hz, 1H), 7.75 (t, J = 7.4 Hz, 1H), 7.68 (t, J = 7.6 Hz, 1H), 7.65 – 7.53 (m, 5H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  163.0, 148.1, 141.2, 131.5, 130.0, 129.6, 129.5, 129.0, 128.0, 127.6, 127.5, 127.4, 127.4, 127.2, 127.1, 123.7, 123.3, 123.0, 120.4, 118.8, 116.8. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>25</sub>H<sub>15</sub>NO: 345.1154; found: 345.1155.

5-(2-(dimethylamino)ethyl)-9-phenyl-4*H*-benzo[*de*]oxazolo[5,4-*g*]isoquinoline-4,6(5*H*)-dione (50c)<sup>5</sup>



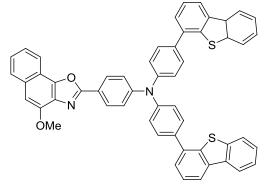
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a pale yellow solid in 46% yield (35.4 mg). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.93 (d, J = 1.8 Hz, 1H), 8.61 (d, J = 7.3 Hz, 1H), 8.57 (d, J = 8.3 Hz, 1H), 8.34 – 8.24 (m, 2H), 7.87 (t, J = 7.5 Hz, 1H), 7.57 (d, J = 6.6 Hz, 2H), 4.33 (t, J = 6.9 Hz, 2H), 2.67 (t, J = 7.0 Hz, 1H), 2.36 (s, 6H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  164.1, 164.0, 163.7, 149.9, 139.4, 132.1, 130.5, 129.1, 127.7, 127.6, 126.6, 126.2, 125.0, 123.4, 120.2, 118.3, 56.9, 45.7, 38.4.

#### 2-(4-bromophenyl)-4-methoxynaphtho[2,1-d]oxazole (A)



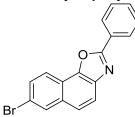
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a white solid in 72% yield (50.8 mg); mp 165.3–166.1 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.22 – 8.16 (m, 3H), 7.85 – 7.83 (m, 1H), 7.65 (d, *J* = 7.4 Hz, 2H), 7.49 – 7.48 (m, 2H), 7.04 (s, 1H), 4.12 (s, 4H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  161.2, 150.1, 147.7, 132.6, 132.1, 128.7, 127.4, 126.4, 126.1, 125.8, 124.5, 120.2, 116.3, 102.3, 56.0. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>18</sub>H<sub>10</sub>BrNO<sub>2</sub>: 353.0051; found: 353.0050.

# 4-(dibenzo[*b*,*d*]thiophen-4-yl)-*N*-(4-(5a,9a-dihydrodibenzo[*b*,*d*]thiophen-4-yl)phenyl)-*N*-(4-(4-methoxynaphtho[2,1-*d*]oxazol-2-yl)phenyl)aniline (51c)



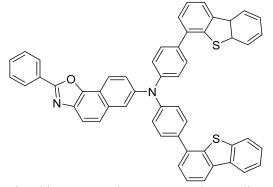
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a yellow solid in 87% yield (140.6 mg). mp 191.2–191.4 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.31 (d, *J* = 8.2 Hz, 2H), 8.20 – 8.16 (d, *J* = 5.9 Hz, 3H), 8.15 (d, *J* = 7.2 Hz, 2H), 7.85 (s, 3H), 7.76 (d, *J* = 7.7 Hz, 4H), 7.56 (q, *J* = 7.3 Hz, 4H), 7.48 (s, 6H), 7.41 – 7.35 (m, 6H), 7.06 (s, 1H), 4.14 (s, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  162.3, 150.2, 150.1, 147.4, 146.5, 139.5, 138.3, 136.3, 136.3, 136.2, 135.8, 132.3, 131.7, 129.4, 128.7, 127.4, 126.8, 126.0, 125.3, 125.1, 124.4, 124.3, 122.6, 121.7, 120.8, 120.3, 120.1, 116.4, 102.0, 55.9. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>54</sub>H<sub>36</sub>N<sub>2</sub>O<sub>2</sub>S<sub>2</sub>: 808.2218; found: 808.2215.

7-bromo-2-phenylnaphtho[2,1-d]oxazole (B)



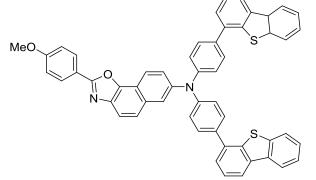
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a white solid in 61% yield (39.4 mg); mp 124.2–125.1 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.32 (s, 1H), 8.17 (d, *J* = 8.8 Hz, 1H), 8.14 (s, 1H), 7.87 (d, *J* = 8.7 Hz, 1H), 7.71 (t, *J* = 8.9 Hz, 1H), 7.55 (s, 1H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  162.7, 146.2, 138.9, 132.6, 131.3, 130.7, 130.1, 128.9, 127.3, 127.2, 124.4, 121.8, 119.8, 119.5, 118.7. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>17</sub>H<sub>10</sub>BrNO: 322.9946; found: 322.9945.

# *N*-(4-(dibenzo[*b*,*d*]thiophen-4-yl)phenyl)-*N*-(4-(5a,9a-dihydrodibenzo[*b*,*d*]thiophen-4-yl)phenyl)-2-phenylnaphtho[2,1-*d*]oxazol-7-amine (52c)



The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a yellow solid in 89% yield (138.5 mg). mp 186.5–186.9 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.35 (d, *J* = 6.5 Hz, 2H), 8.27 (d, *J* = 8.8 Hz, 1H), 8.22 – 8.15 (m, 2H), 8.13 (d, *J* = 6.7 Hz, 2H), 7.86 – 7.80 (m, 4H), 7.74 (d, *J* = 7.2 Hz, 4H), 7.63 (d, *J* = 8.7 Hz, 2H), 7.54 (d, *J* = 5.6 Hz, 7H), 7.48 – 7.45 (m, 4H), 7.38 (d, *J* = 7.3 Hz, 4H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  162.1, 147.1, 146.7, 145.0, 139.5, 138.3, 138.0, 136.4, 136.3, 135.8, 135.2, 133.0, 131.1, 129.3, 128.9, 127.4, 127.2, 126.8, 126.7, 125.6, 125.1, 124.7, 124.3, 124.2, 122.6, 122.5, 121.7, 121.6, 120.2, 119.2, 116.9. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>53</sub>H<sub>34</sub>N<sub>2</sub>OS<sub>2</sub>: 778.2113; found: 778.2111.

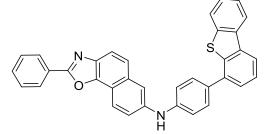
# *N*-(4-(dibenzo[*b*,*d*]thiophen-4-yl)phenyl)-*N*-(4-(5a,9a-dihydrodibenzo[*b*,*d*]thiophen-4-yl)phenyl)-2-(4-methoxyphenyl)naphtho[2,1-*d*]oxazol-7-amine (53c)



The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a yellow solid in 86% yield (139.0 mg). mp 261.3–261.8 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.31 (t, J = 9.4 Hz, 3H), 8.22 (t, J = 6.0 Hz, 2H), 8.17 (t, J = 9.6 Hz, 2H), 7.89 (d, J = 6.9 Hz, 2H), 7.84 (d, J = 9.4 Hz, 2H), 7.76 (d, J = 7.7 Hz, 4H), 7.66 (t, J = 8.3 Hz, 2H), 7.58 (q, J = 7.4 Hz, 4H), 7.53 – 7.46 (m, 4H), 7.41 (d, J = 7.7 Hz, 4H), 7.10 (d, J = 8.0 Hz, 2H), 3.94 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  162.3, 162.1, 147.2,

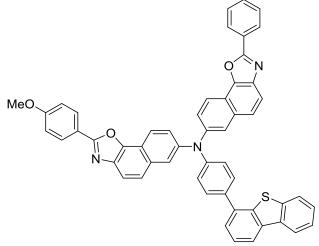
146.4, 144.8, 139.5, 138.3, 137.8, 136.5, 136.3, 135.8, 135.2, 132.8, 129.3, 129.1, 126.8, 126.7, 125.7, 125.1, 124.6, 124.4, 124.2, 122.6, 121.7, 121.5, 120.2, 119.8, 118.9, 116.9, 114.4, 55.5. HRMS (EI) m/z:  $[M]^+$  calcd. for  $C_{54}H_{36}N_2O_2S_2$ : 808.2218; found: 808.2214.

*N*-(4-(dibenzo[*b*,*d*]thiophen-4-yl)phenyl)-2-phenylnaphtho[2,1-*d*]oxazol-7-amine (E)



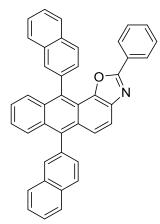
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (2/1) to afford a yellow solid in 81% yield (83.9 mg). mp 160.2–161.1 °C. HRMS (EI) m/z:  $[M]^+$  calcd. for  $C_{35}H_{22}N_2OS$ : 518.1453; found: 518.1455.

*N*-(4-(dibenzo[*b*,*d*]thiophen-4-yl)phenyl)-2-(4-methoxyphenyl)-*N*-(2-phenylnaphtho[2,1-*d*]oxazol-7-yl)naphtho[2,1-*d*]oxazol-7-amine (54c)



The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a yellow solid in 84% yield (132.9 mg). mp 194.5–194.9 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.33 (d, J = 6.2 Hz, 2H), 8.25 (t, J = 7.9 Hz, 4H), 8.17 (d, J = 5.3 Hz, 1H), 8.13 (d, J = 6.5 Hz, 1H), 7.84 (d, J = 6.3 Hz, 1H), 7.79 (t, J = 8.4 Hz, 2H), 7.76 – 7.71 (m, 4H), 7.63 – 7.50 (m, 9H), 7.47 – 7.45 (m, 2H), 7.35 (d, J = 7.5 Hz, 2H), 7.04 (d, J = 7.8 Hz, 2H), 3.88 (s, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  162.4, 162.1, 162.0, 147.2, 146.7, 146.4, 145.1, 144.8, 139.5, 138.2, 138.2, 138.0, 136.3, 136.3, 135.8, 135.2, 133.0, 132.7, 131.1, 129.3, 129.0, 128.9, 127.4, 127.2, 126.8, 126.6, 125.4, 125.3, 125.1, 124.6, 124.4, 124.4, 123.9, 122.5, 122.4, 122.2, 121.7, 121.6, 121.6, 120.2, 120.0, 119.2, 119.1, 116.9, 116.9, 114.4, 55.4. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>53</sub>H<sub>33</sub>N<sub>3</sub>O<sub>3</sub>S: 791.2243; found: 791.2245.

6,11-di(naphthalen-2-yl)-2-phenylanthra[2,1-d]oxazole (55c)



The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (1/1) to afford a yellow solid in 56% yield (61.3 mg). mp 107.9–108.4 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.10 (d, J = 16.0 Hz, 4H), 8.01 (s, 2H), 7.93 (s, 3H), 7.77 (d, J = 6.7 Hz, 1H), 7.69 (s, 4H), 7.61 (s, 4H), 7.42 – 7.36 (m, 2H), 7.24 (s, 1H), 7.18 (d, J = 5.5 Hz, 2H), 7.03 (s, 2H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  158.3, 142.6, 135.0, 134.6, 133.8, 132.7, 130.0, 129.6, 129.4, 129.1, 128.9, 127.2, 126.9, 126.5, 126.3, 125.9, 125.6, 125.3, 125.1, 124.8, 124.6, 124.5, 124.4, 124.3, 124.1, 123.7, 123.2, 123.0, 122.9, 122.8, 122.8, 122.7, 122.4, 121.8, 121.8, 115.1. HRMS (EI) m/z: [M]<sup>+</sup> calcd. for C<sub>41</sub>H<sub>25</sub>NO: 547.1936; found: 547.1938.

### 8. References

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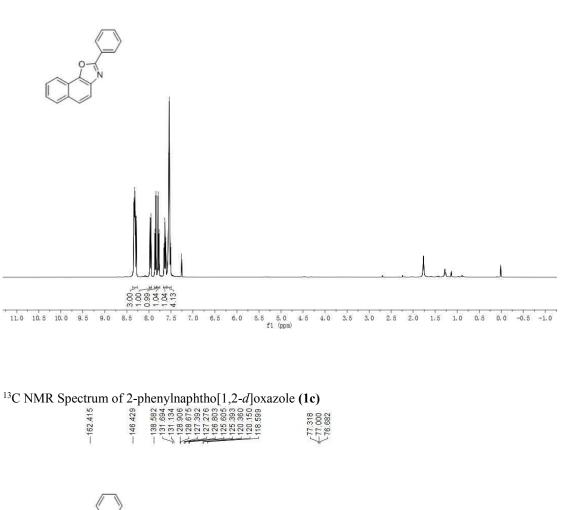
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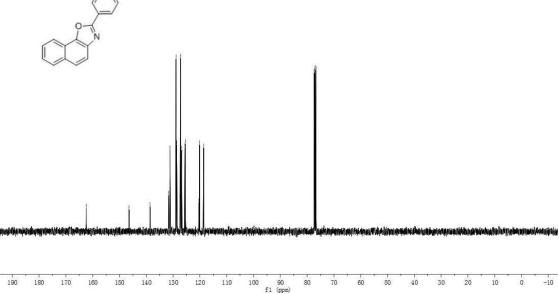
(13) Šagud, I., Šindler-Kulyk, M., Škorić, I. V., Ž. Marinić, Kelava, *Eur. J. Org. Chem.* **2018**, 3326 (2018).

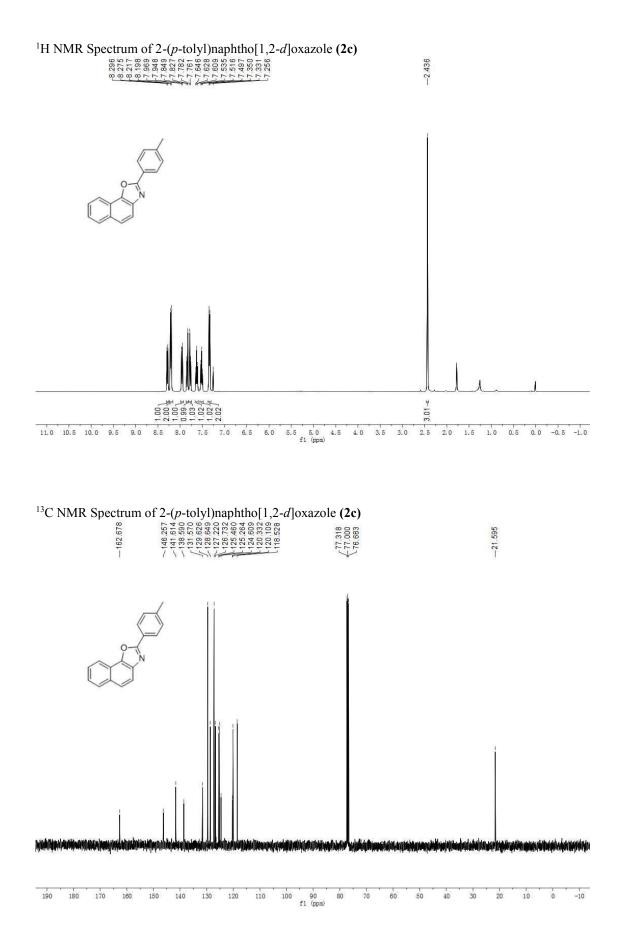
(14) Jang, J. H., et al. Org. Lett. 22, 1280 (2020).

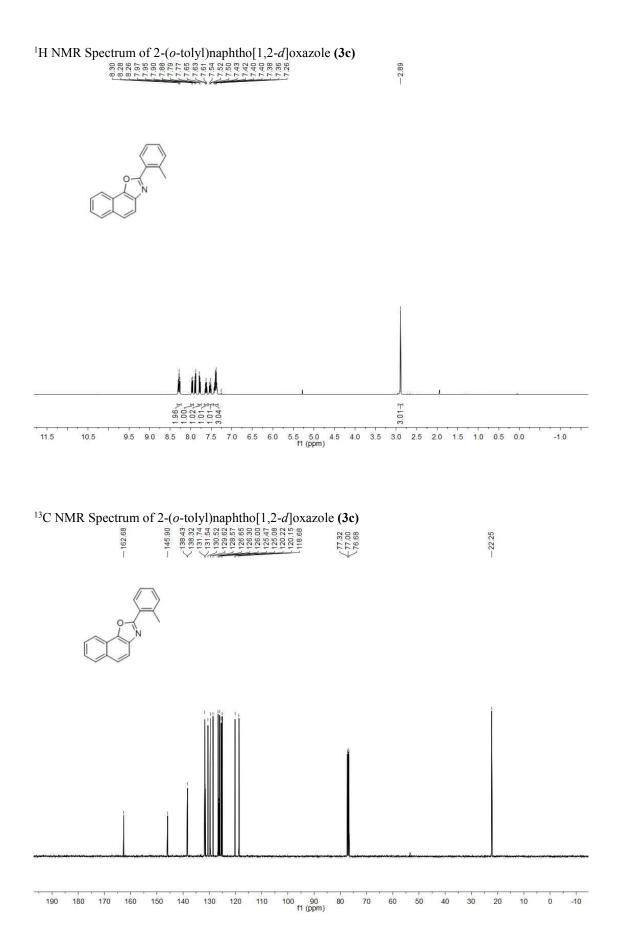
# 9. Copies of <sup>1</sup>H, <sup>13</sup>C and <sup>19</sup>F NMR Spectra of the Products

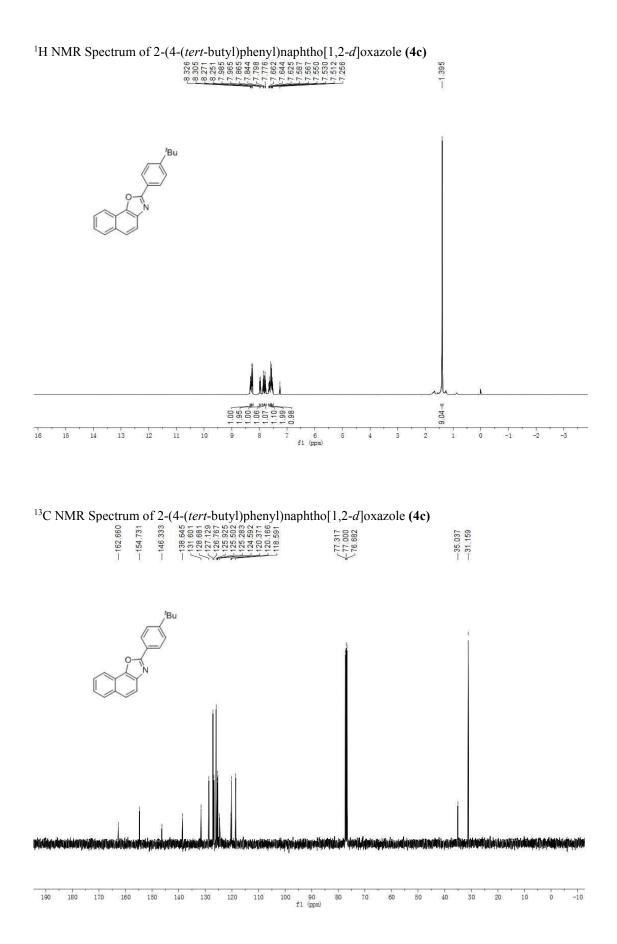
<sup>1</sup>H NMR Spectrum of 2-phenylnaphtho[1,2-*d*]oxazole (1c)

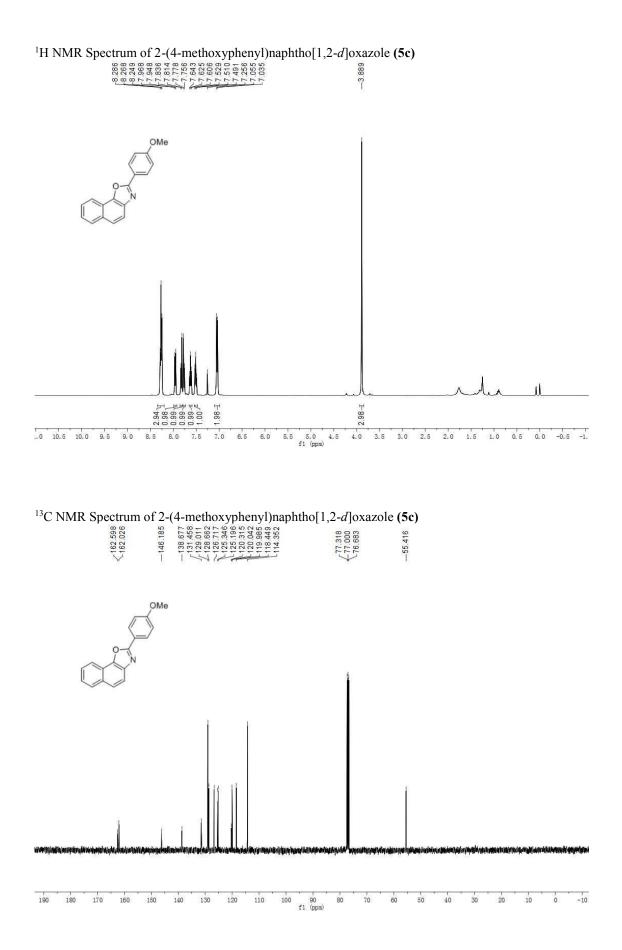




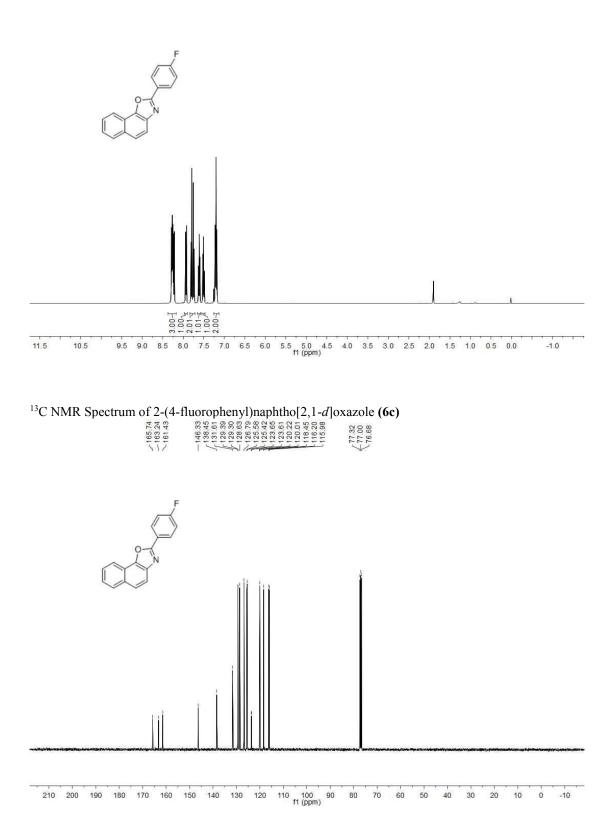




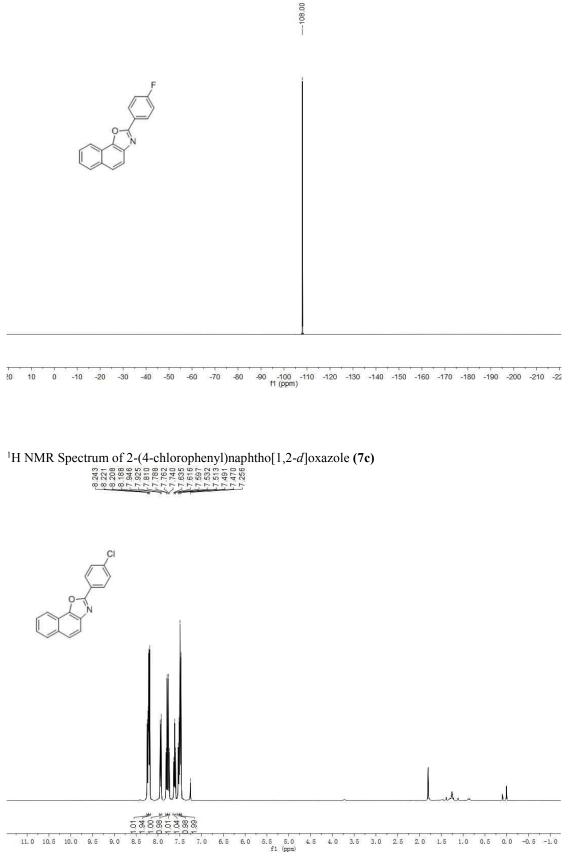


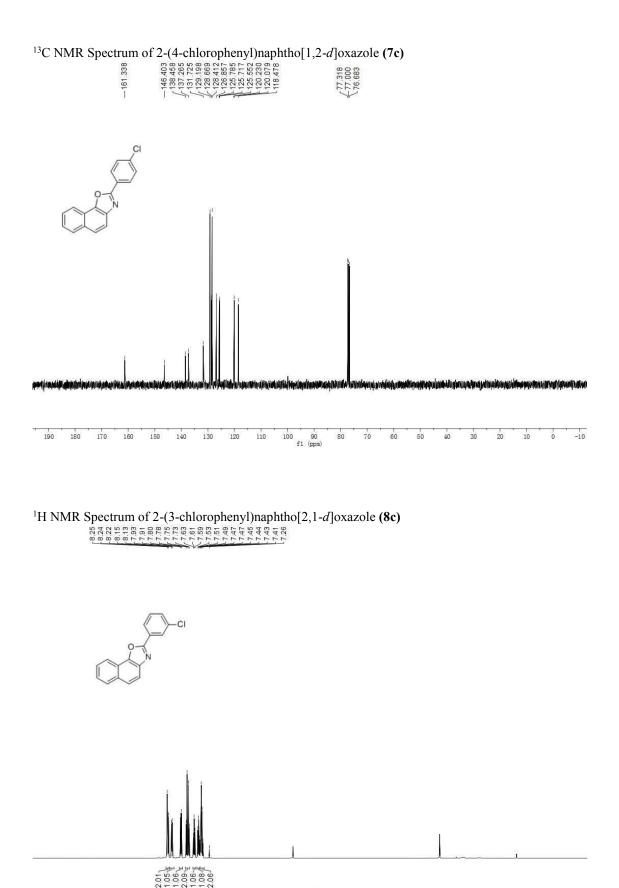


<sup>1</sup>H NMR Spectrum of 2-(4-fluorophenyl)naphtho[2,1-*d*]oxazole (6c)

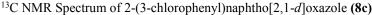


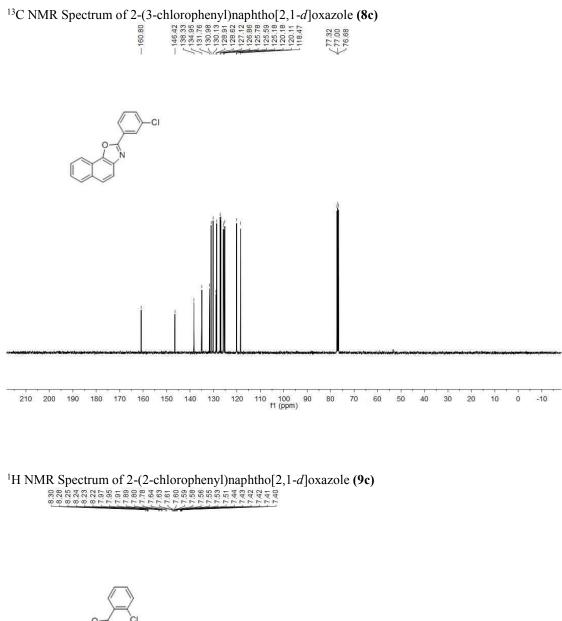
<sup>19</sup>F NMR Spectrum of 2-(4-fluorophenyl)naphtho[2,1-*d*]oxazole (6c)

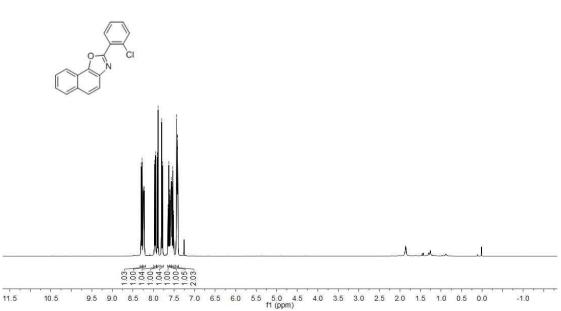


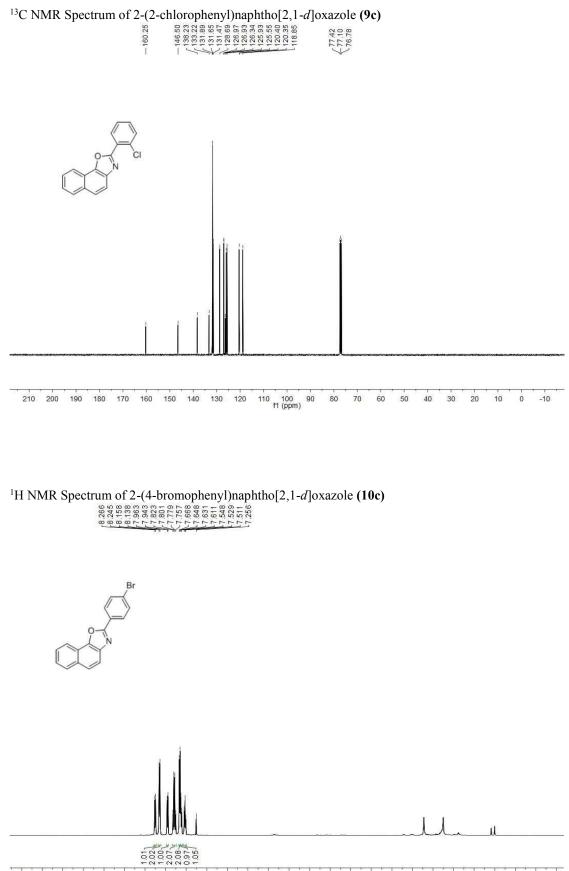


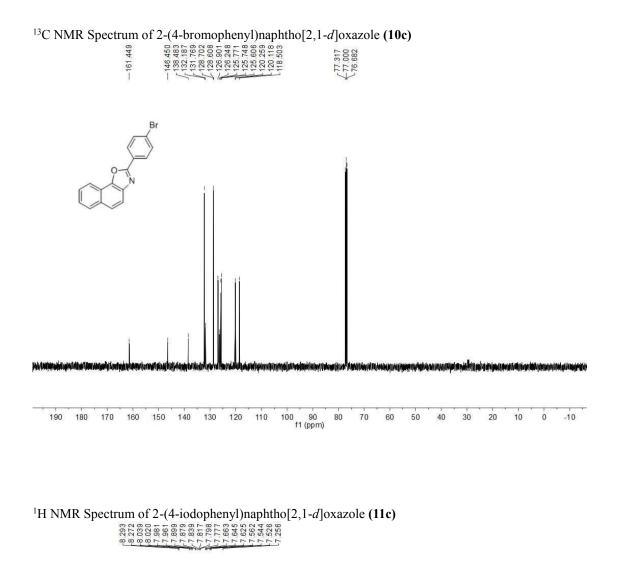


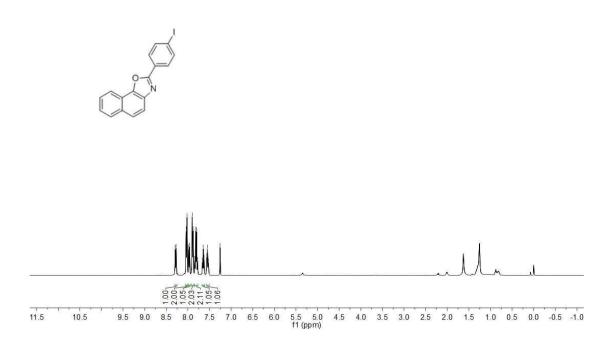


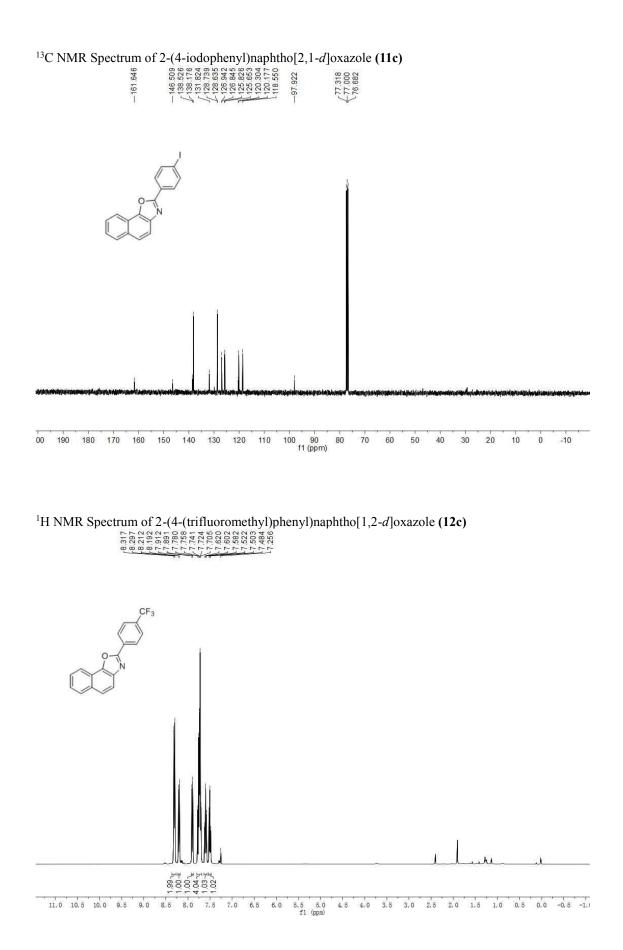


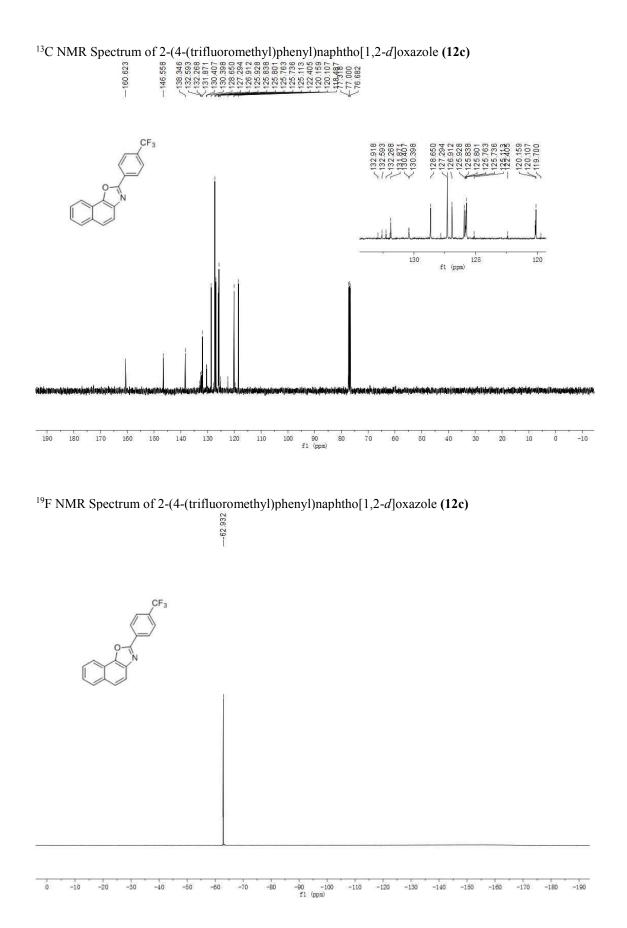




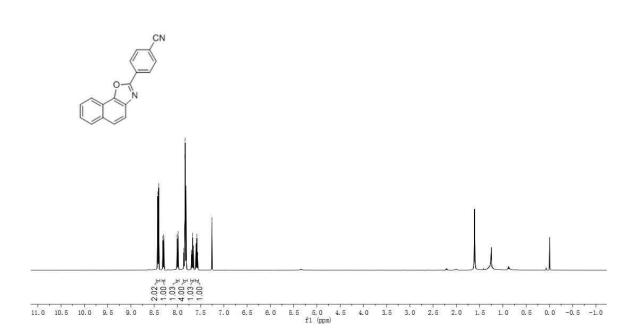






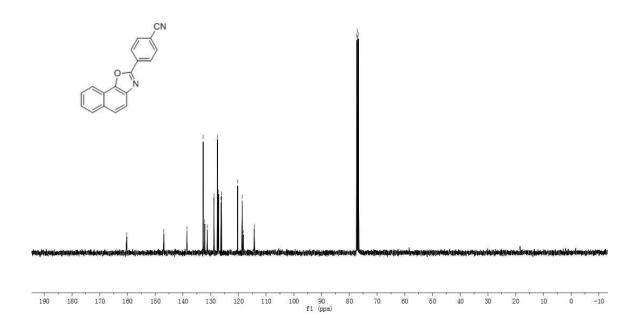


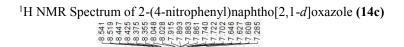
### <sup>1</sup>H NMR Spectrum of 4-(naphtho[2,1-*d*]oxazol-2-yl)benzonitrile (13c)

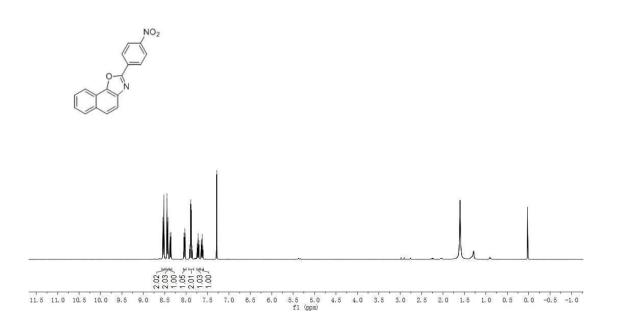


<sup>13</sup>C NMR Spectrum of 4-(naphtho[2,1-*d*]oxazol-2-yl)benzonitrile (13c)

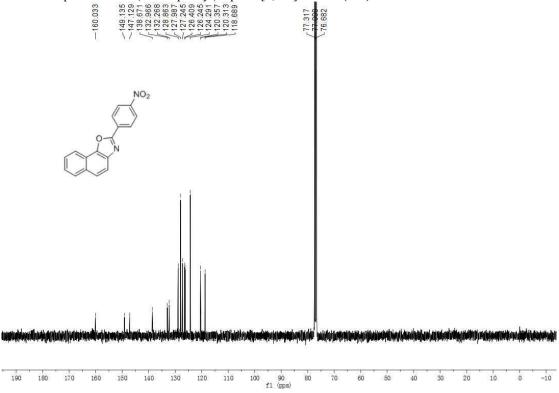
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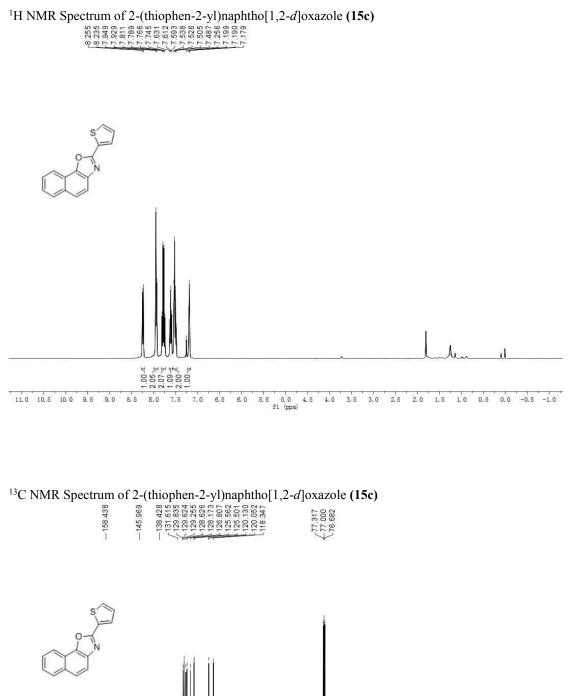


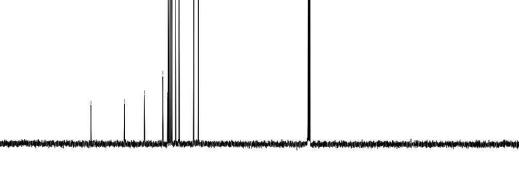


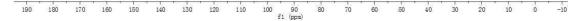


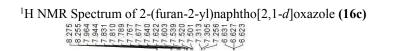
<sup>13</sup>C NMR Spectrum of 2-(4-nitrophenyl)naphtho[2,1-*d*]oxazole (14c)

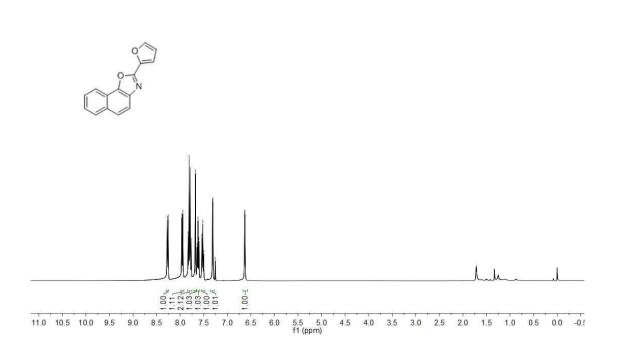






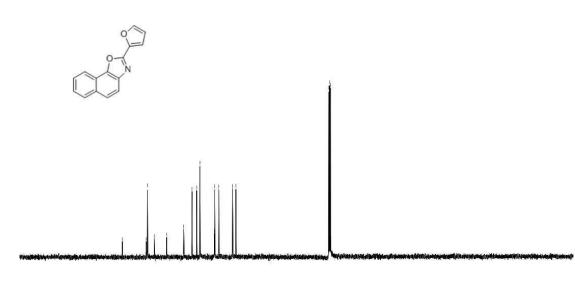




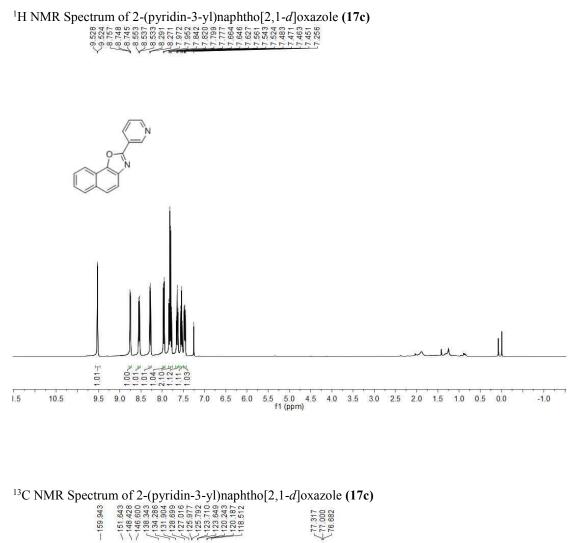


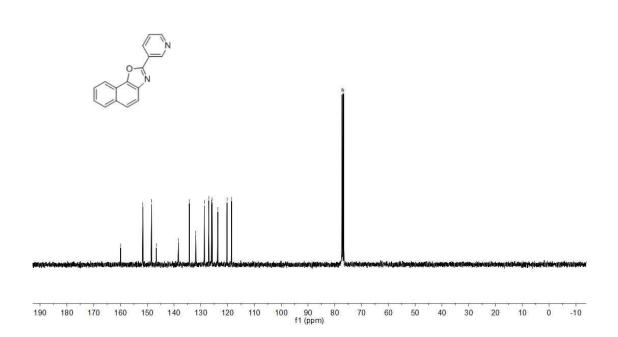
<sup>13</sup>C NMR Spectrum of 2-(furan-2-yl)naphtho[2,1-*d*]oxazole (16c)

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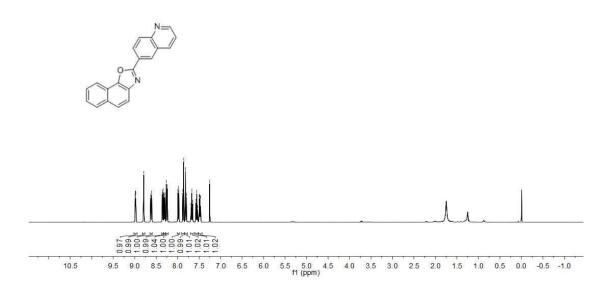


f1 (ppm) ò -10 



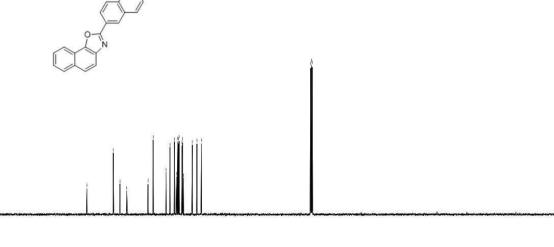


# <sup>1</sup>H NMR Spectrum of 2-(quinolin-6-yl)naphtho[2,1-*d*]oxazole (18c)

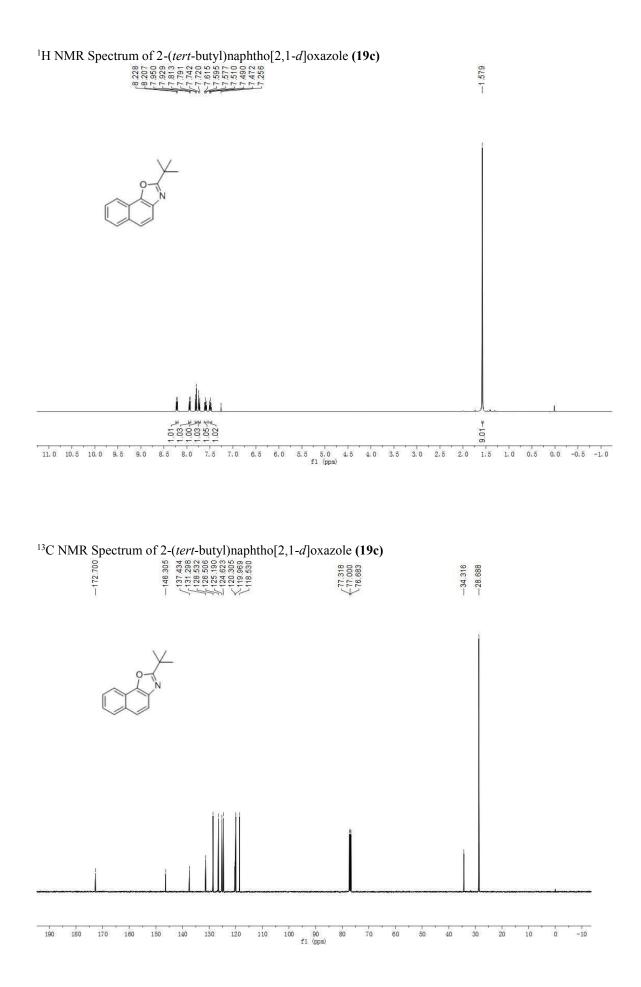


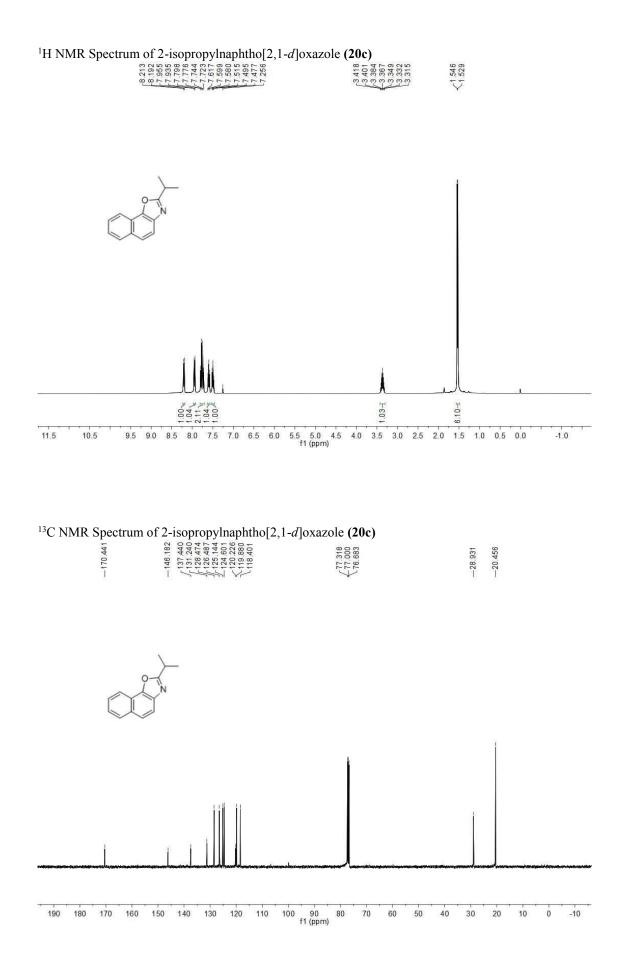
#### <sup>13</sup>C NMR Spectrum of 2-(quinolin-6-yl)naphtho[2,1-*d*]oxazole (18c)

-161.597	/161 679 /148 151 /148 5794 /138 5794 /138 552 /138 552 /138 567 /131 789 /131 789 /131 789 /131 789 /132 3867 /132 3867 /132 3867 /132 386 /132 3867 /132 3867 /132 38667 /132 3867 /132 387 /132 38	77.318 77.000 76.683	
	N		



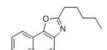
100 90 80 f1 (ppm) -10 

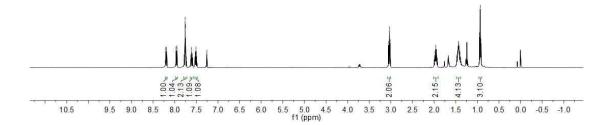


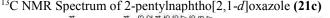


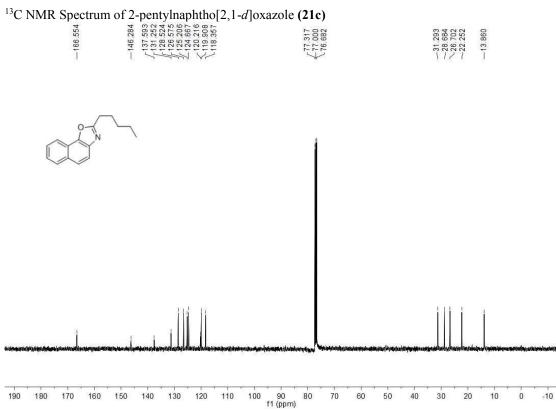
S55

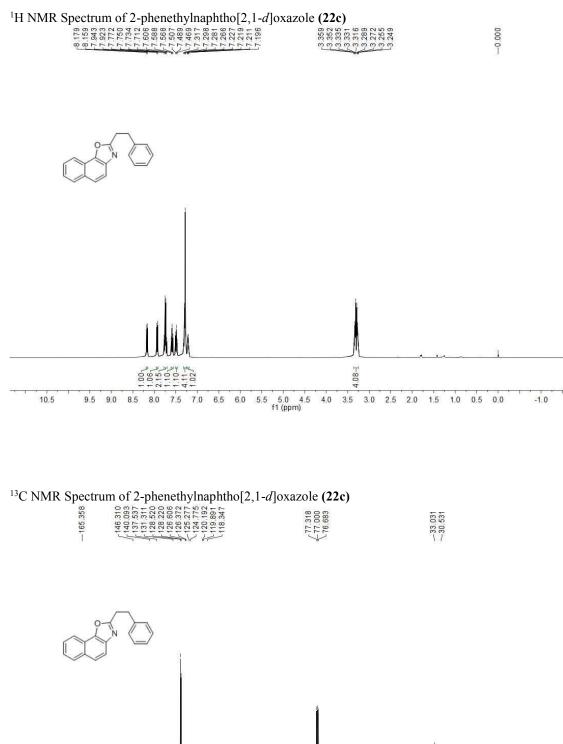
<sup>1</sup> H NMR Spectrum of 2-pentylnaphtho[2,1- <i>d</i> ]oxazole (21c)		
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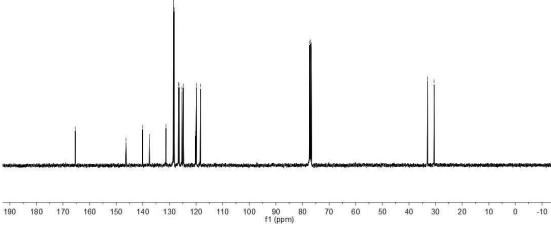


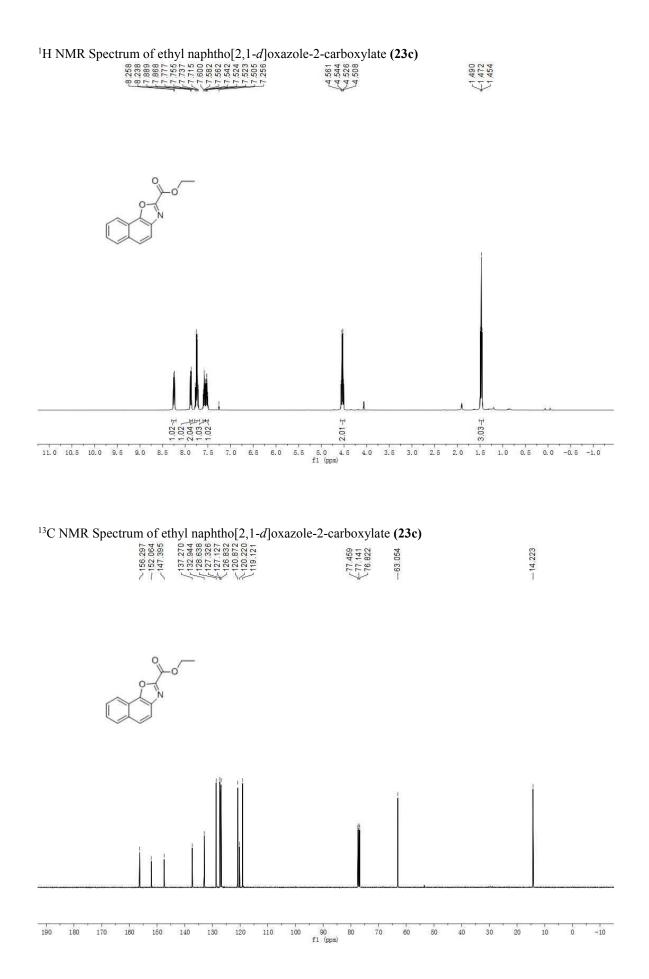


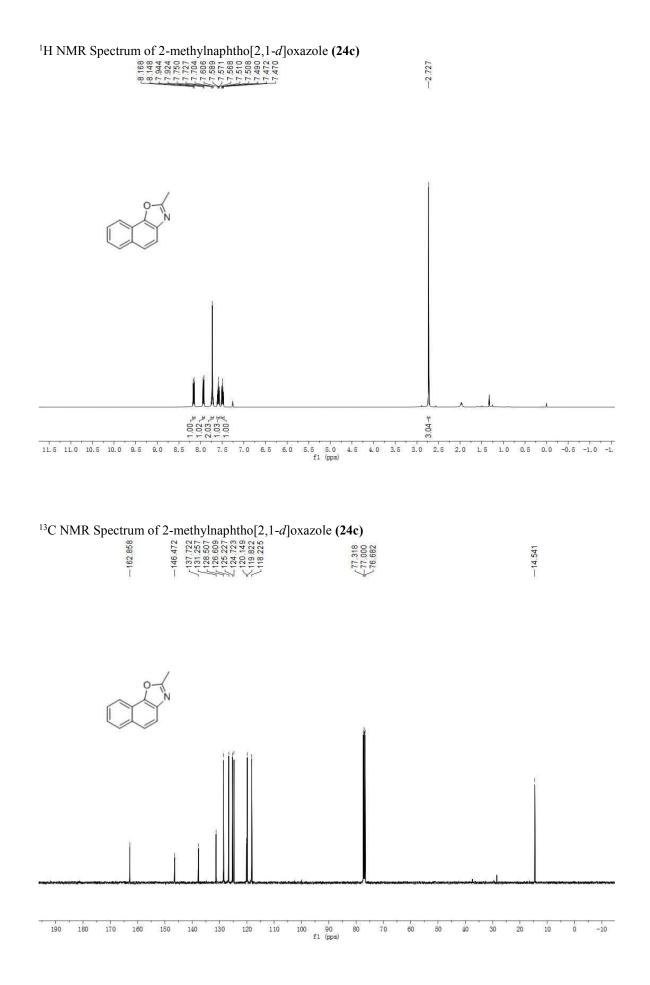




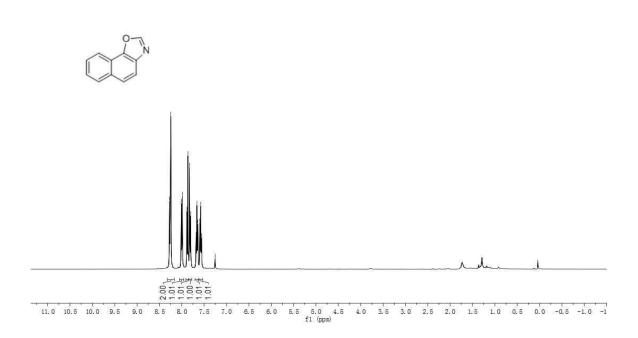






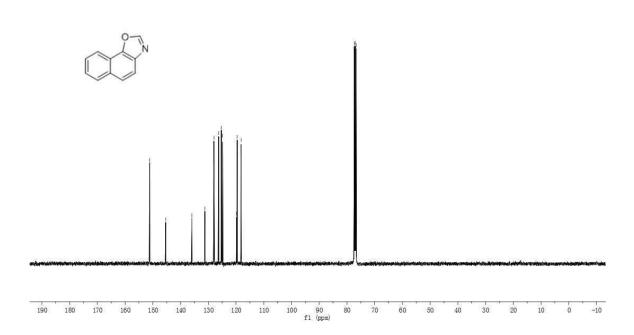


# <sup>1</sup>H NMR Spectrum of naphtho[2,1-*d*]oxazole (**25c**)

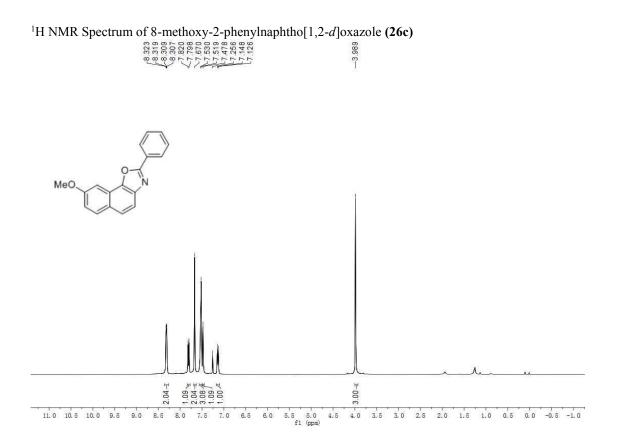


#### <sup>13</sup>C NMR Spectrum of naphtho[2,1-*d*]oxazole (25c)

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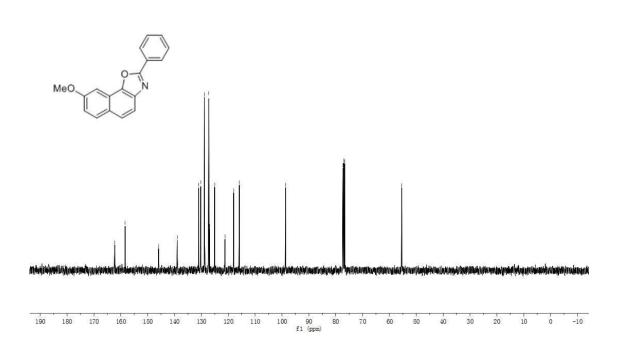


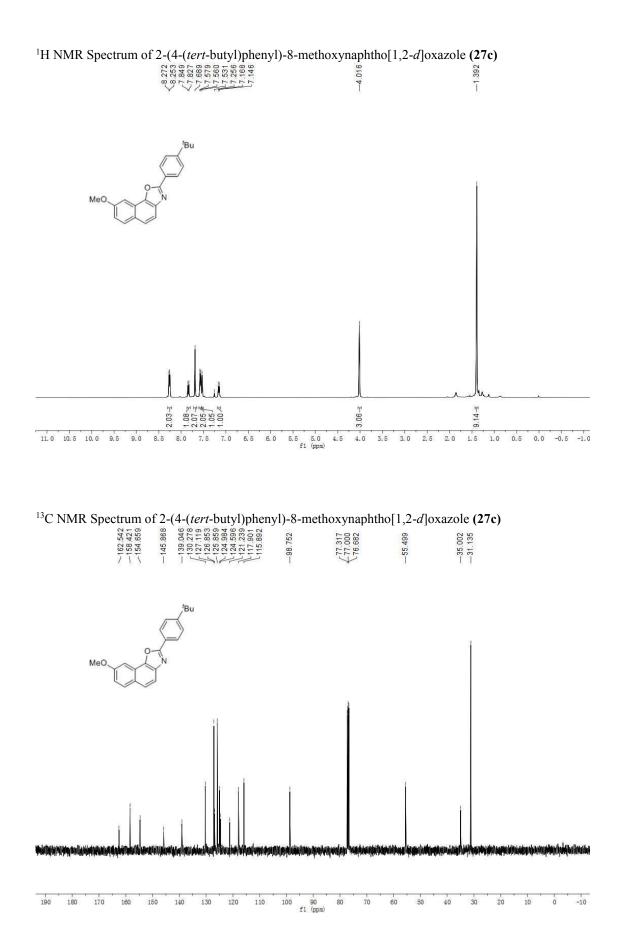
77.318 77.000 76.683

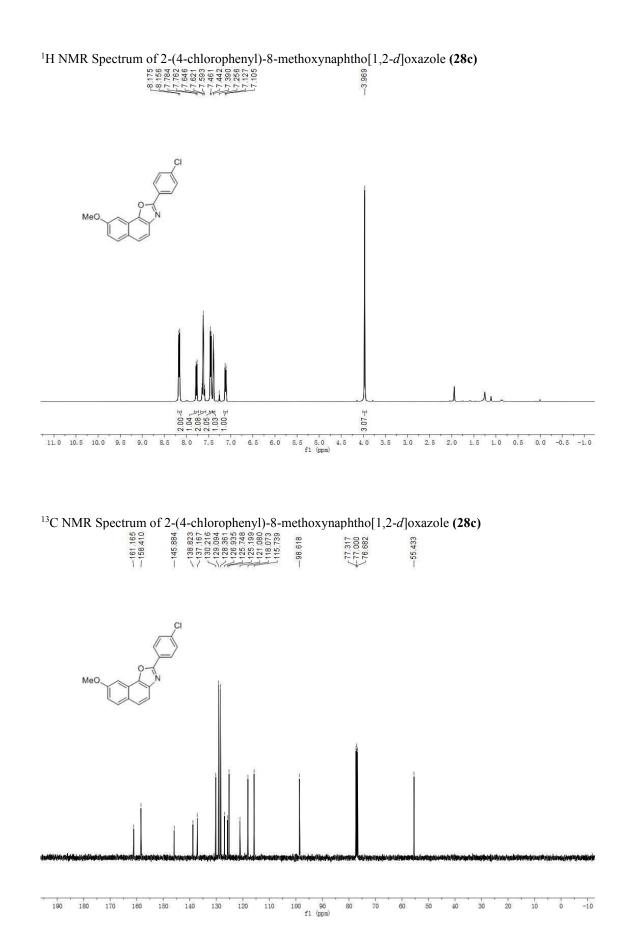


<sup>13</sup>C NMR Spectrum of 8-methoxy-2-phenylnaphtho[1,2-*d*]oxazole (26c)

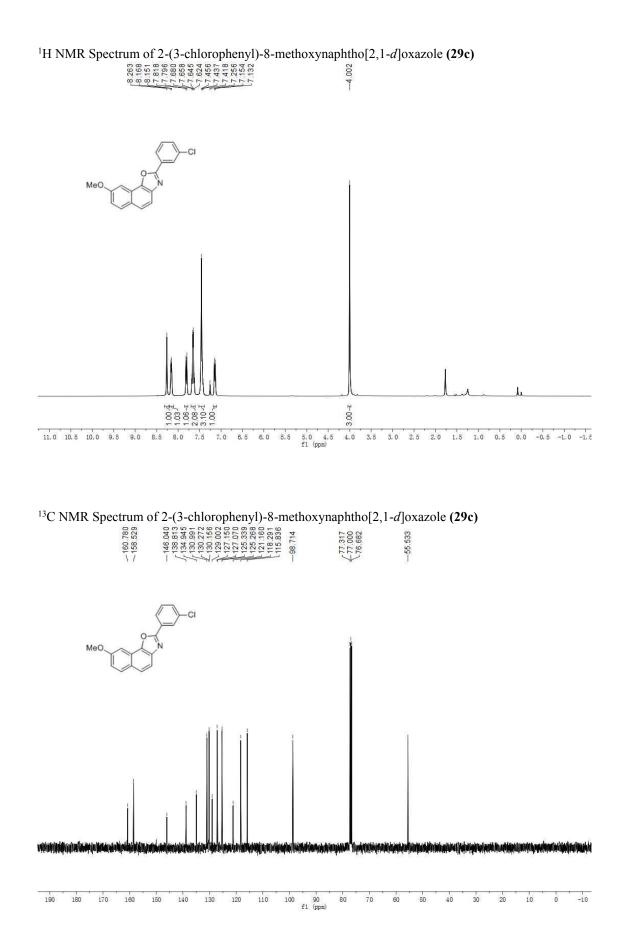
253	927	962 058 373 373 9058 9058 9055 9055 9055 9055 9055 9055	35	32	16
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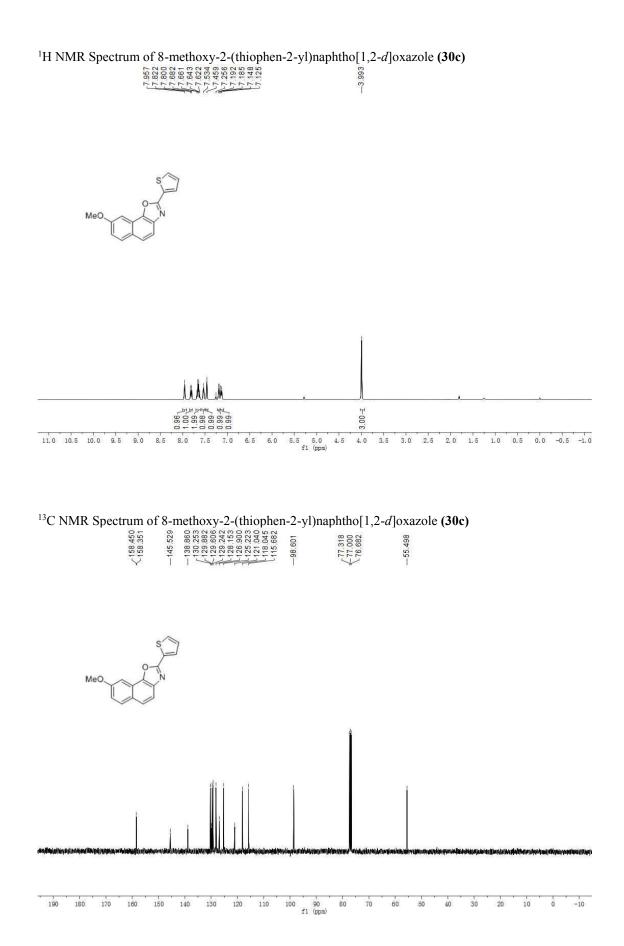


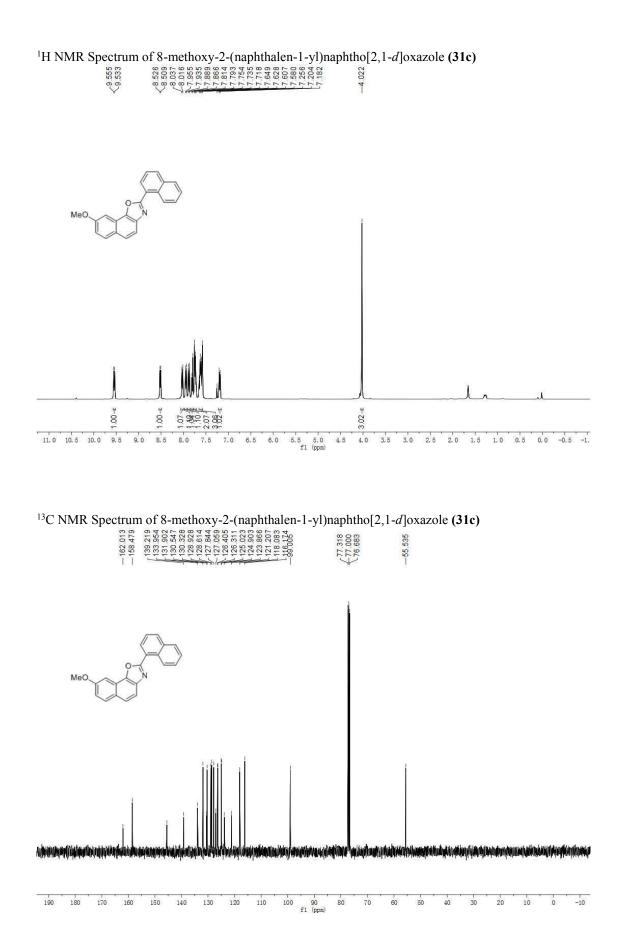


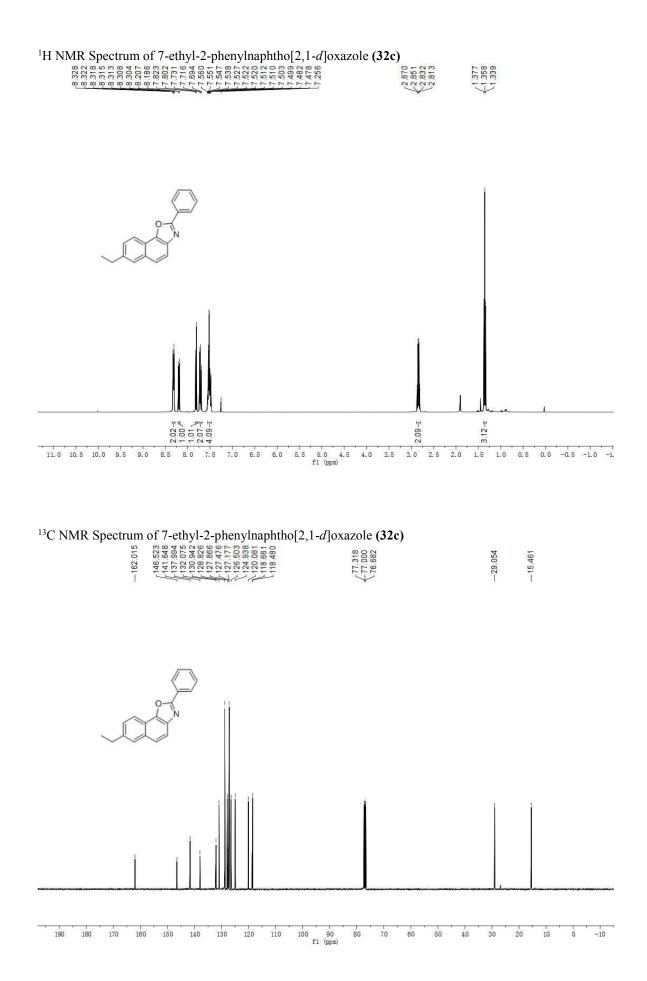


S63

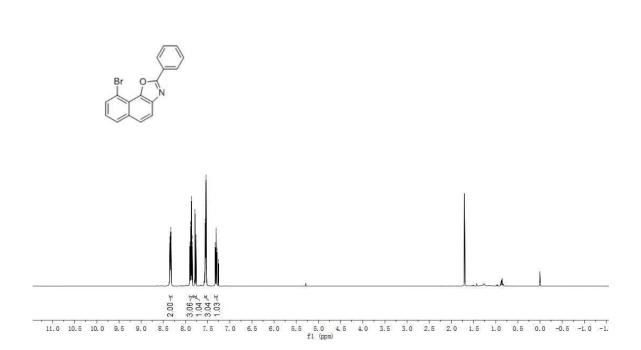






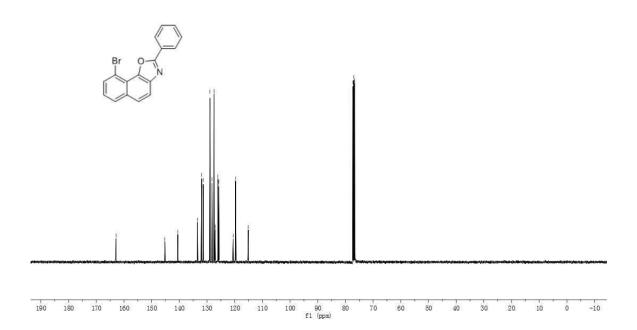


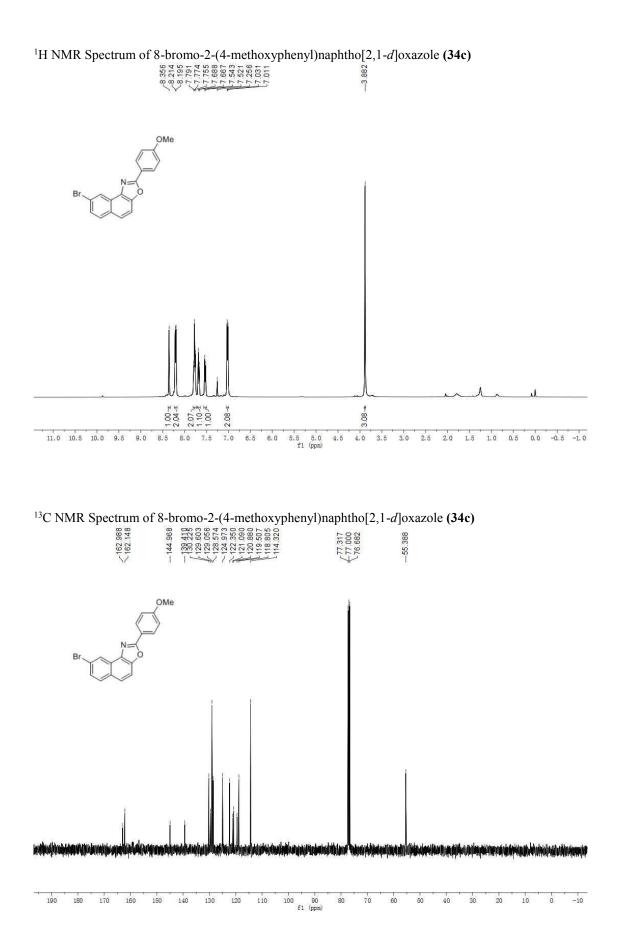
## <sup>1</sup>H NMR Spectrum of 9-bromo-2-phenylnaphtho[2,1-d]oxazole (33c)

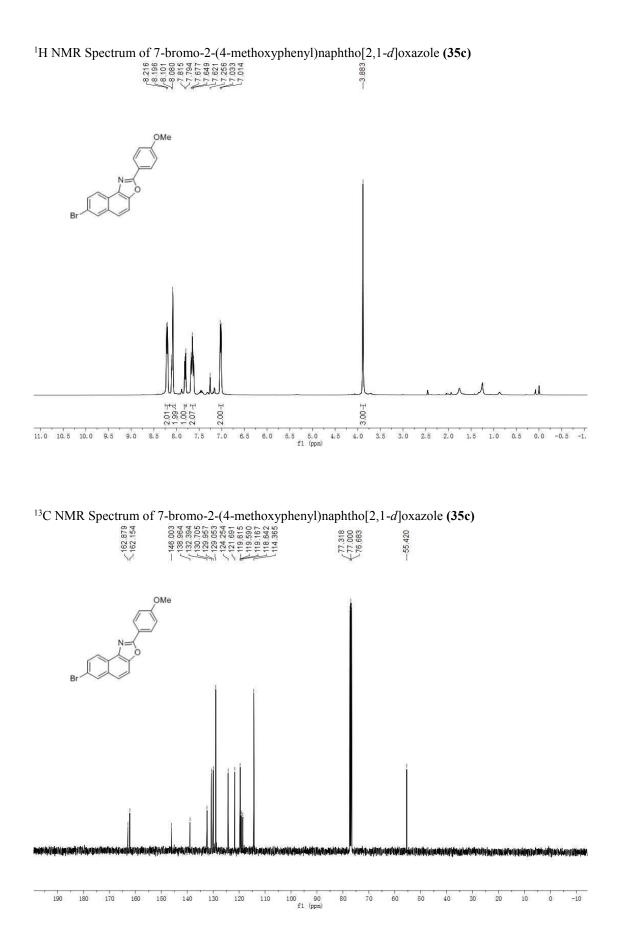


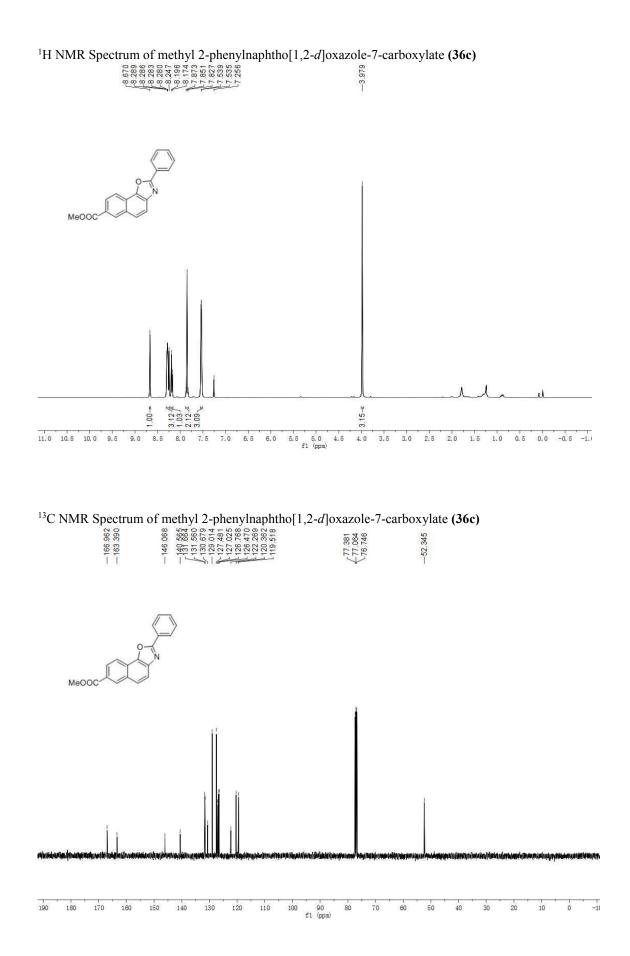
#### <sup>13</sup>C NMR Spectrum of 9-bromo-2-phenylnaphtho[2,1-*d*]oxazole (33c)

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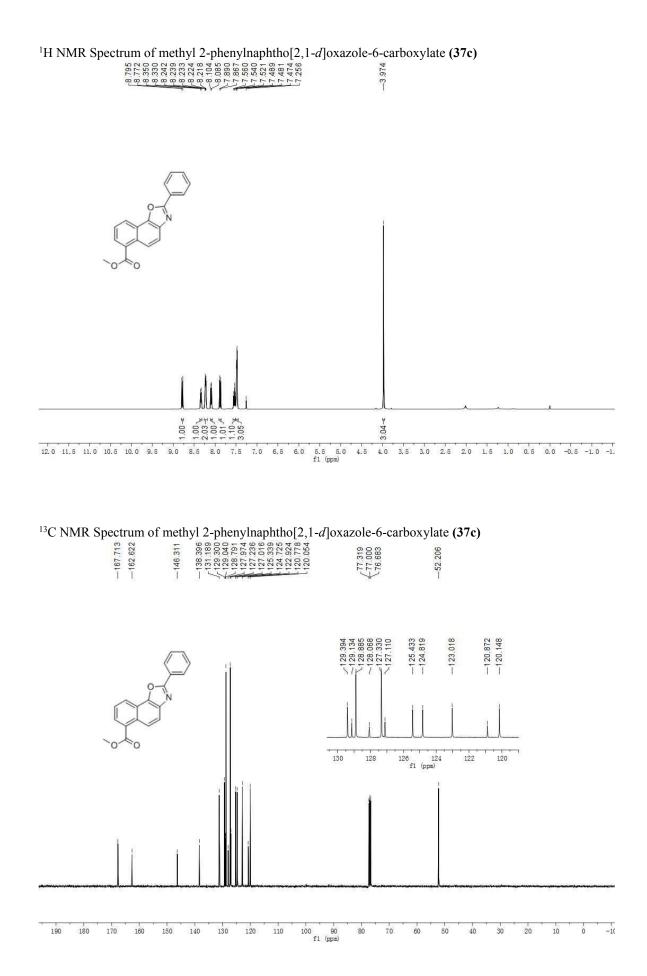


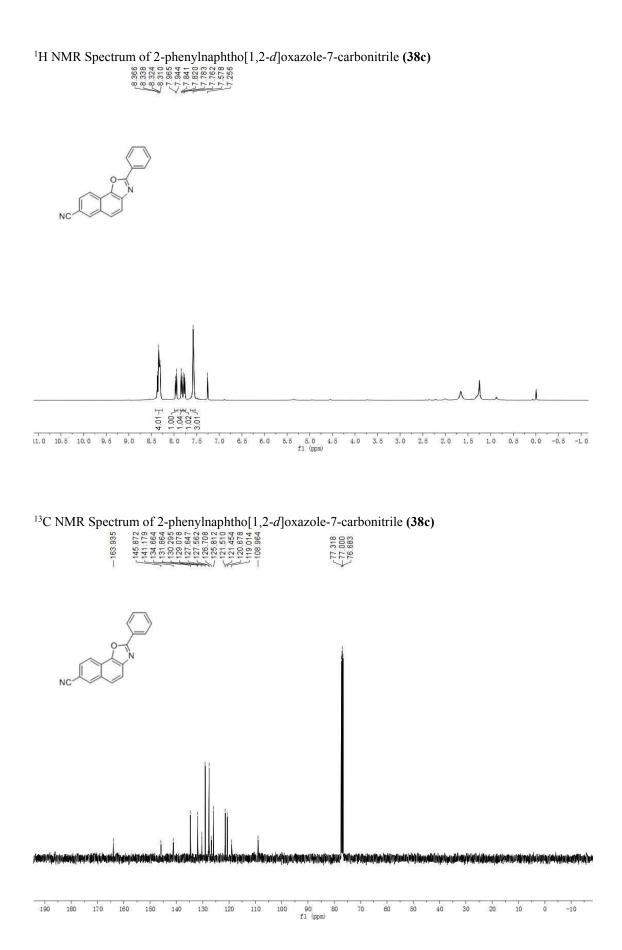




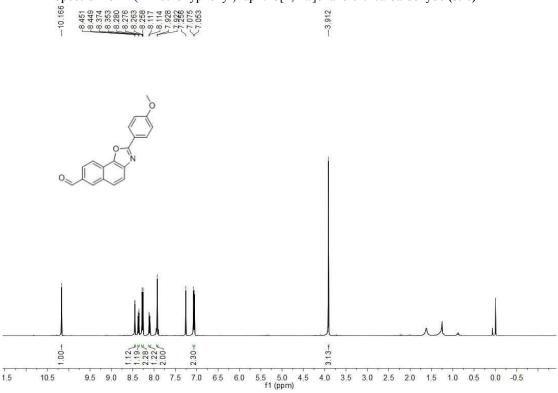


### S71

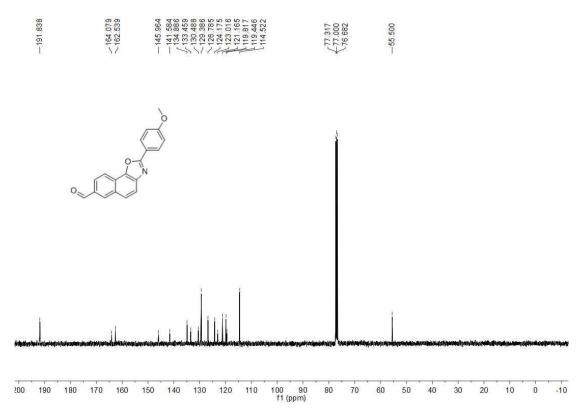


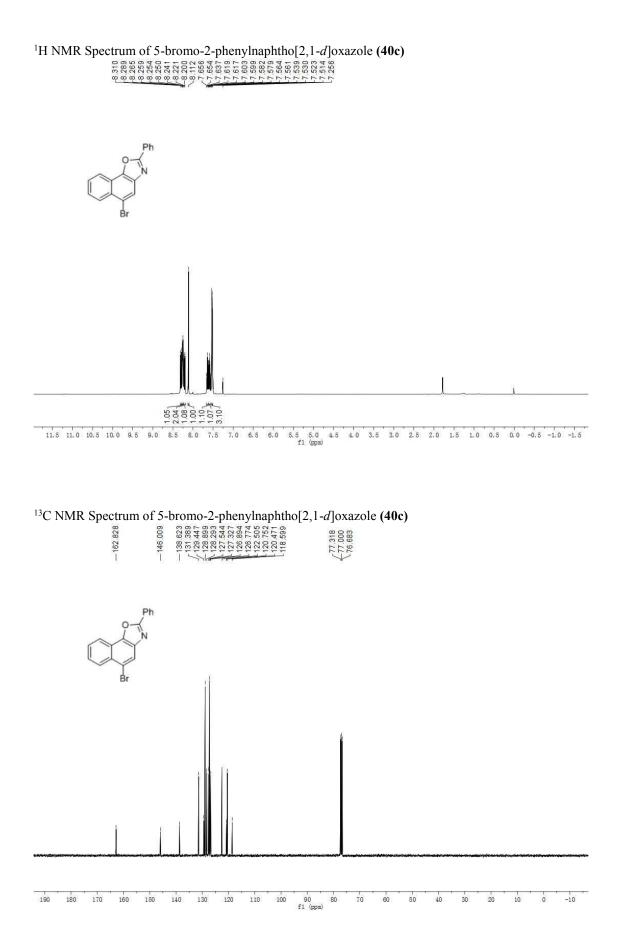


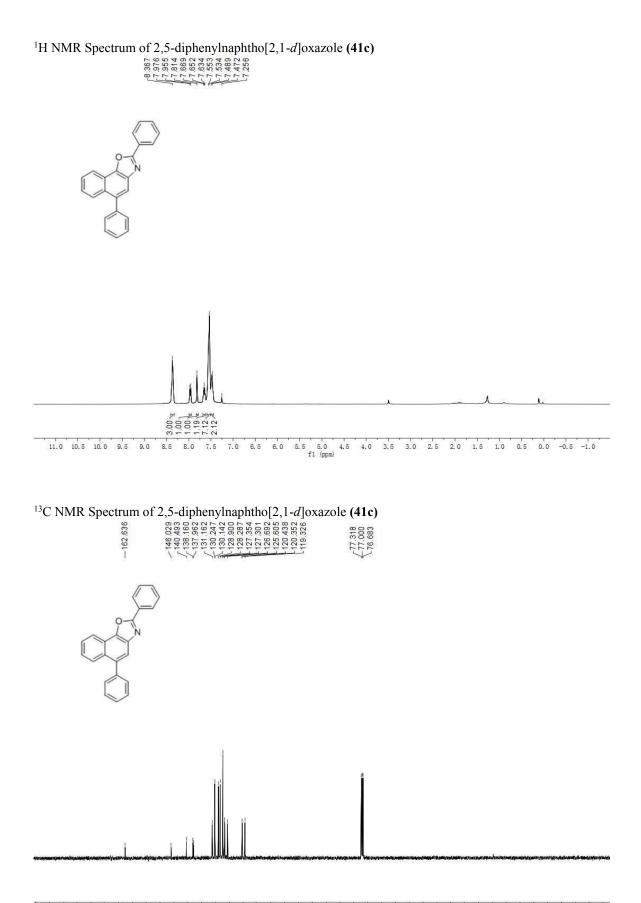
<sup>1</sup>H NMR Spectrum of 2-(4-methoxyphenyl)naphtho[2,1-*d*]oxazole-7-carbaldehyde (**39c**)



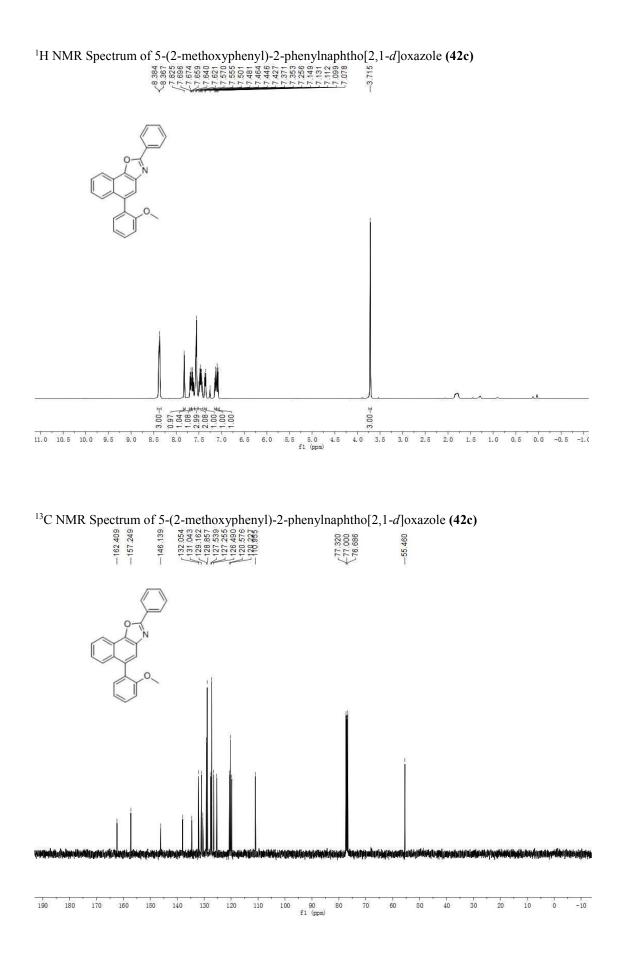
<sup>13</sup>C NMR Spectrum of 2-(4-methoxyphenyl)naphtho[2,1-*d*]oxazole-7-carbaldehyde (**39c**)

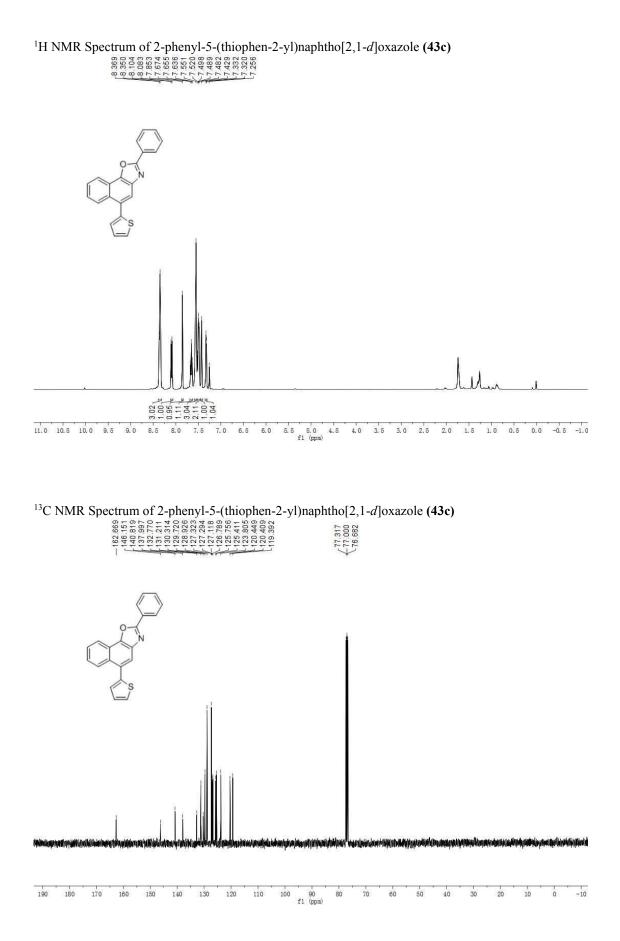


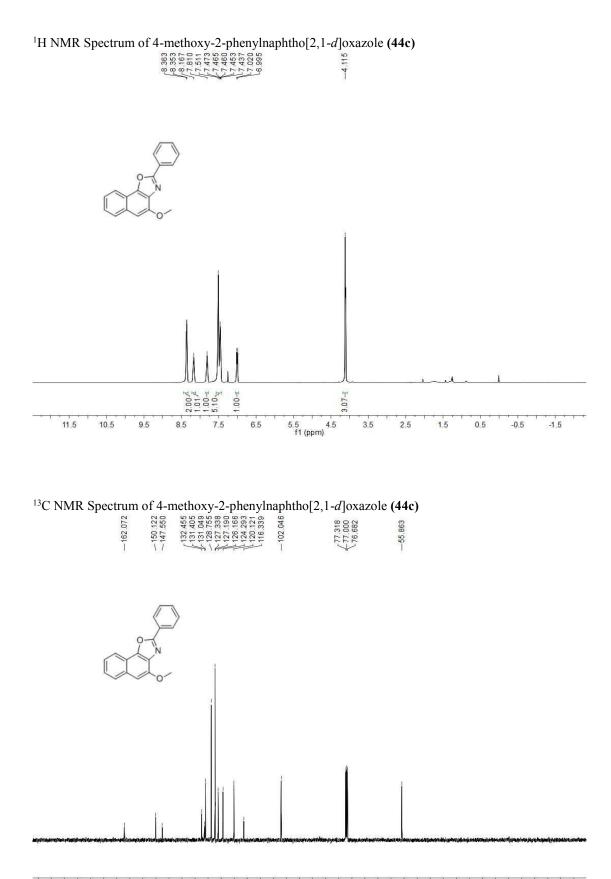


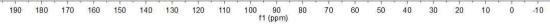


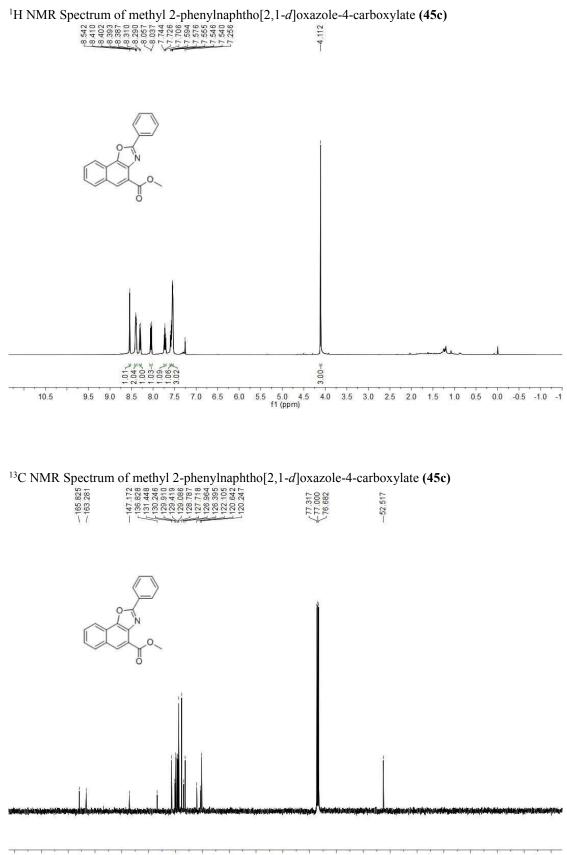
100 90 f1 (ppm) -10 



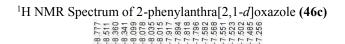


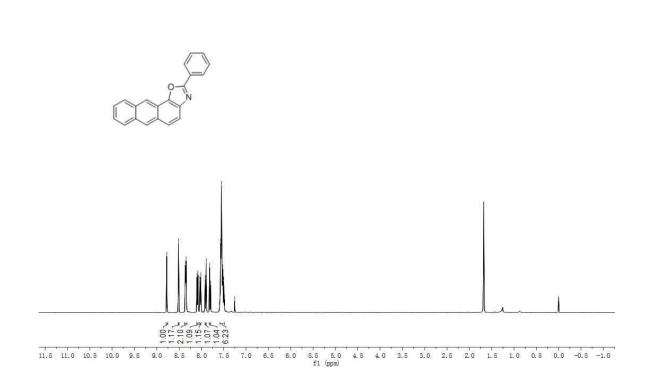


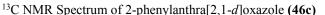


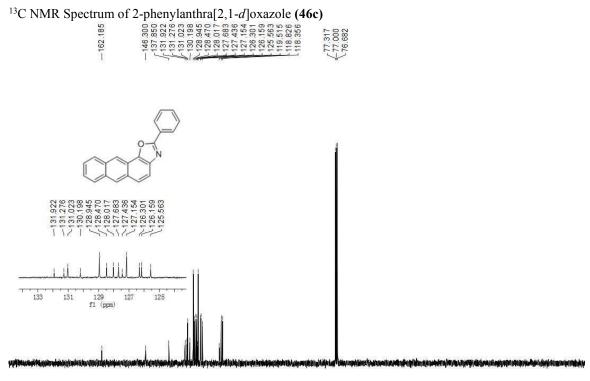


f1 (ppm) -10 ò

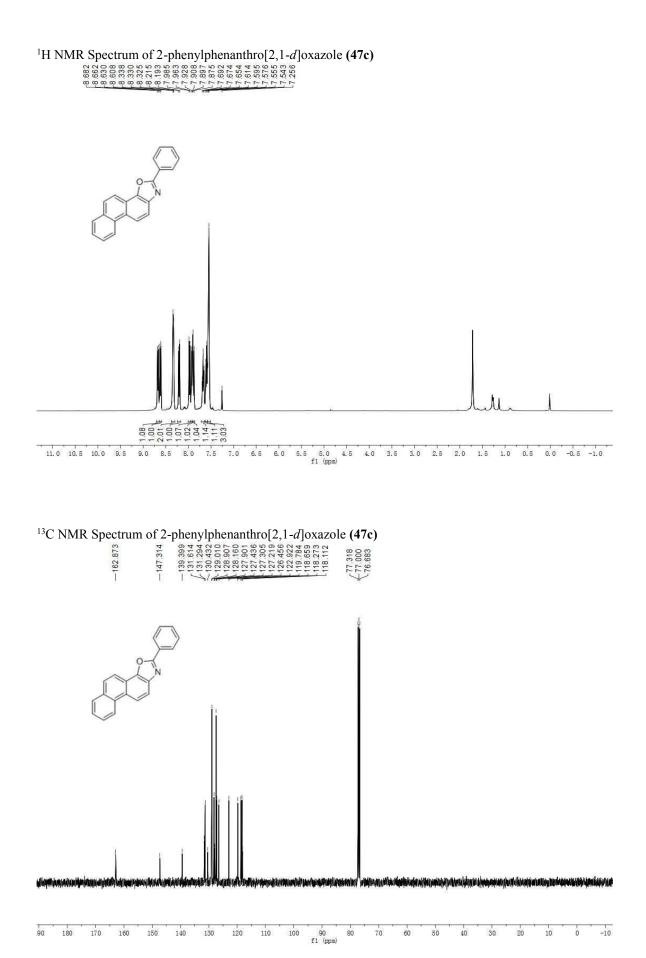


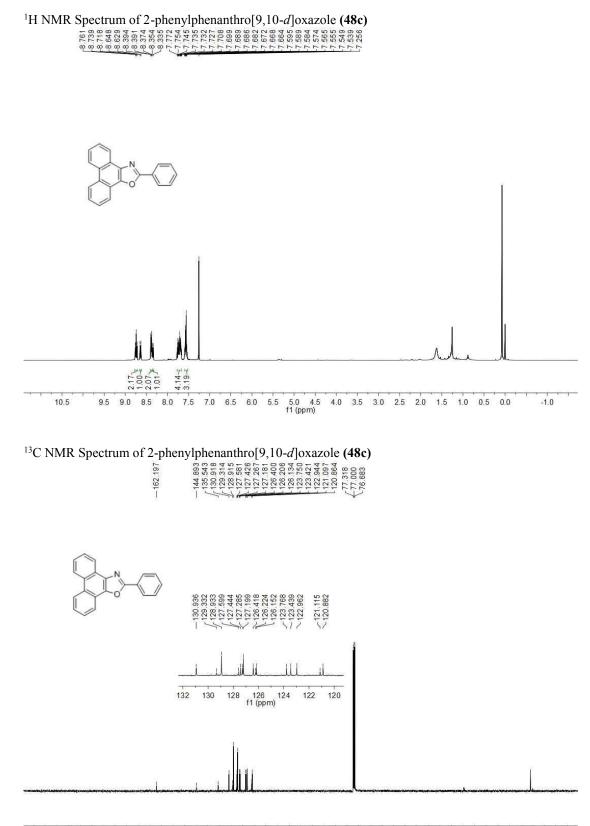




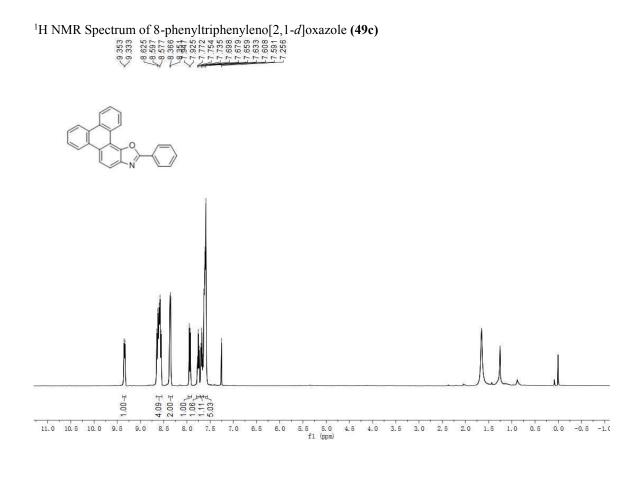


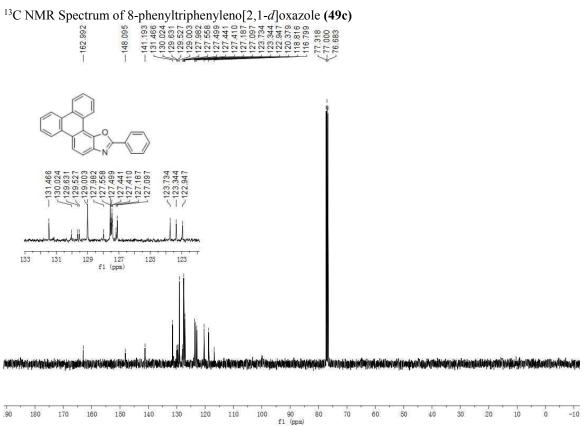
<sup>100 90</sup> f1 (ppm) ò -10 





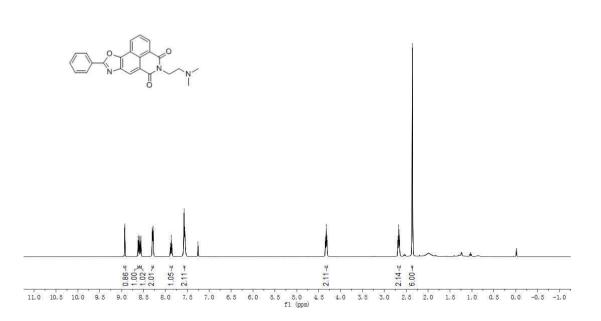
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 f1 (ppm)





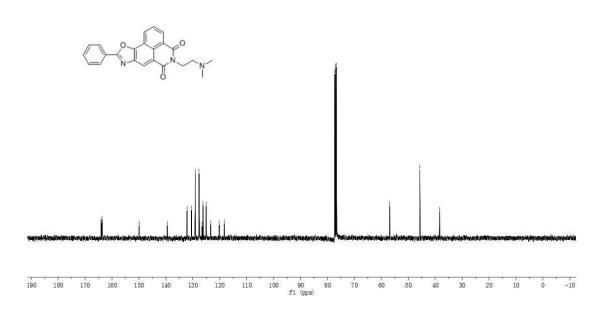
<sup>1</sup>H NMR Spectrum of 5-(2-(dimethylamino)ethyl)-9-phenyl-4*H*-benzo[*de*]oxazolo[5,4-*g*]isoquinoline-4,6(5*H*)-dione (50c)

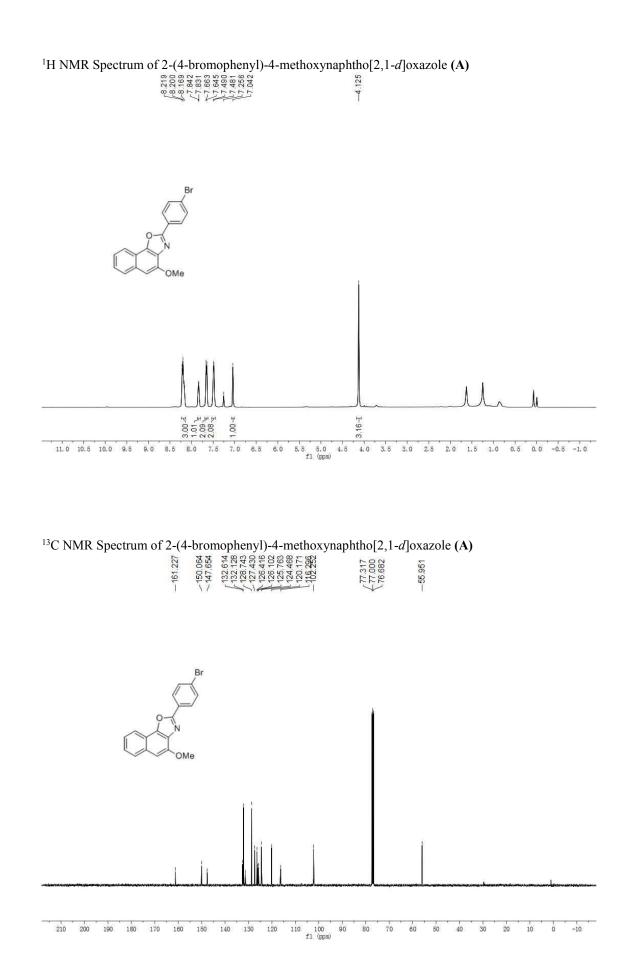
0 ~1 M D D D D D D D D M D D D M D D D M D D D D M D	40.00	004-
000000000000000000000000000000000000000	40-	00 1- 40 00
/ ກຸມານໜ້ອຍ ທ / ກ / ກຸມານ ພວກ ອ	ოოო	9000
a a a a a a a a a a a a a a a a a a a	444	2000
	Y	A P



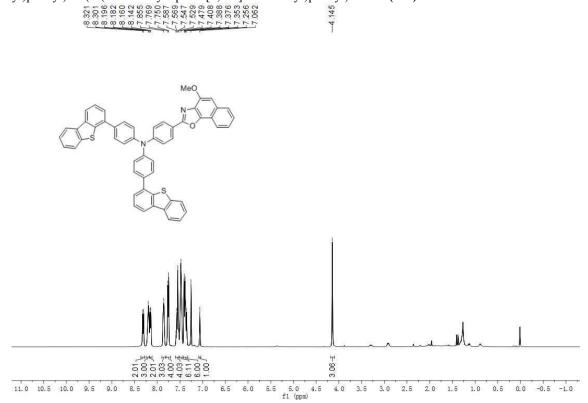
<sup>13</sup>C NMR Spectrum of 5-(2-(dimethylamino)ethyl)-9-phenyl-4*H*-benzo[*de*]oxazolo[5,4-*g*]isoquinoline-4,6(5*H*)-dione (**50c**)

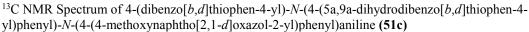
129 025 695	916	438 471 109 696 611 109 227 358 274 274	830083	26	17	381	
164 163	149	132 132 126 127 128 128 128 128 128 128 128 128 128 128	77.3 77.0 76.6	56.9	45.7	38.3	
$\checkmark$	1		$\downarrow$	1	T,	Щ.	

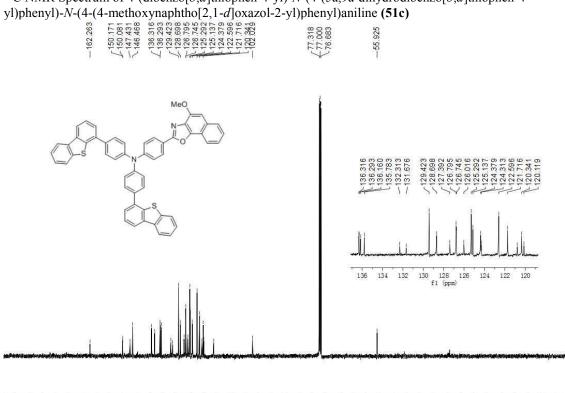




<sup>1</sup>H NMR Spectrum of 4-(dibenzo[*b*,*d*]thiophen-4-yl)-*N*-(4-(5a,9a-dihydrodibenzo[*b*,*d*]thiophen-4yl)phenyl)-*N*-(4-(4-methoxynaphtho[2,1-*d*]oxazol-2-yl)phenyl)aniline (51c)

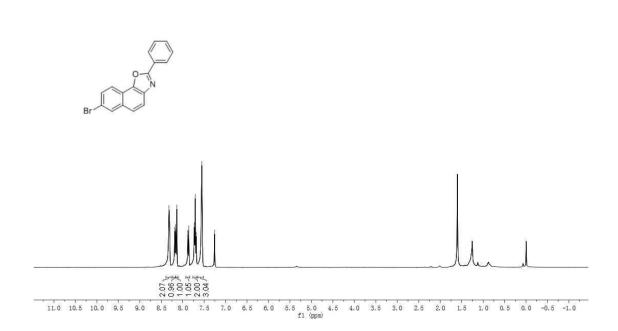






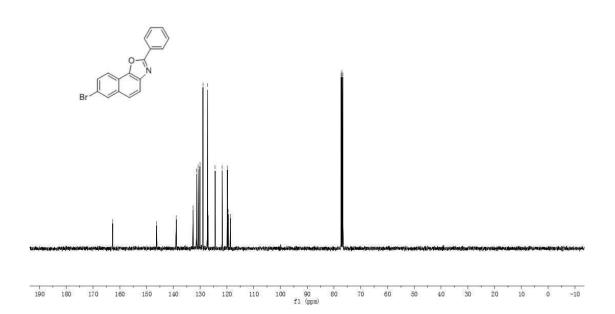
  f1 (ppm) -10

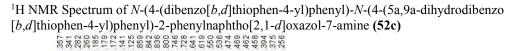
## <sup>1</sup>H NMR Spectrum of 7-bromo-2-phenylnaphtho[2,1-*d*]oxazole (**B**)

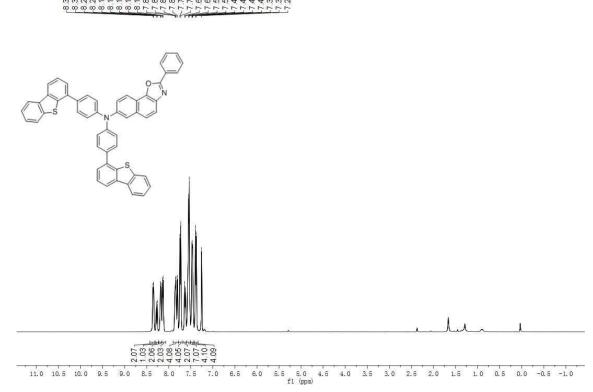


## <sup>13</sup>C NMR Spectrum of 7-bromo-2-phenylnaphtho[2,1-*d*]oxazole (**B**)

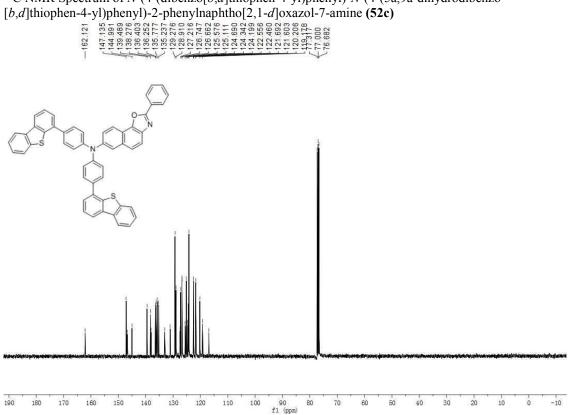
682	242 634 535 321 735 735 735 735 735 735 735 735 735 702 702	77.318 77.000 76.683
62.	321,331,331,331,331,331,331,331,331,332,3331,332,3331,332,3331,332,3331,332,3331,332,3331,332,3331,332,332	
ì		$\checkmark$

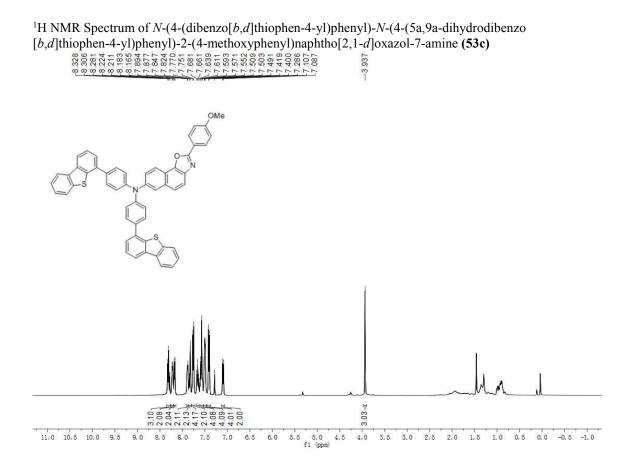


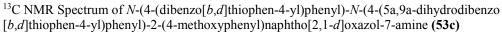


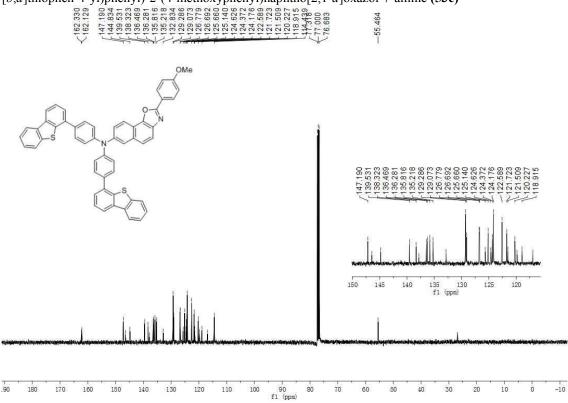


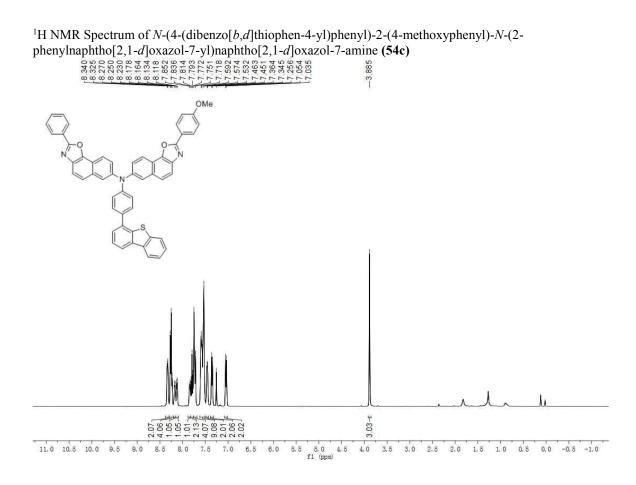
<sup>13</sup>C NMR Spectrum of N-(4-(dibenzo[b,d]thiophen-4-yl)phenyl)-N-(4-(5a,9a-dihydrodibenzo











<sup>13</sup>C NMR Spectrum of N-(4-(dibenzo[b,d]thiophen-4-yl)phenyl)-2-(4-methoxyphenyl)-N-(2-

