Electronic Supplementary Information

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

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Table of contents

1. General Information ............................................................................................................................................... S2
2. Preparation of the Substrates .................................................................................................................................. S2
3. Experimental Procedure ........................................................................................................................................ S3
4. Photophysical Properties and Thermal of Naphthoxazole-doped Materials .............................................. S9
5. Investigations of the Reaction Mechanism ........................................................................................................ S10
6. X-ray Crystallographic Data ................................................................................................................................ S16
7. Characterization Data for the Products ............................................................................................................. S17
8. References ............................................................................................................................................................ S35
9. Copies of $^1$H, $^{13}$C and $^{19}$F NMR Spectra of the Products .................................................................................... S36
1. General Information

The reactions were carried out in Schlenk tubes of 25 mL under N₂ 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 ¹H, ¹³C and ¹⁹F NMR spectra were recorded on a Bruker 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 JES-FA 200 electron spin resonance spectrometer. The absorption (UV) spectra were recorded on Agilent Cary 100 UV-Vis Spectrophotometer. The photoluminescence (PL) 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).¹

![Chemical structures](image)

To a solution of acetonedicarboxylic acid (1) (2.1 g, 14.4 mmol) in H₂O (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 (H₂O) was removed under freeze-drying condition. The resulting yellow solid (2) was used in the next reaction without further purification.

The mixture of (2) and H₂NNH₂·H₂O (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 triethylene glycol (21 mL) in a two-necked round-bottomed flask distillation apparatus, the solution of (2) and H₂NNH₂·H₂O was added dropwise. After the mixture was stirred at 220 °C for 30 min, H₂O (50 mL) was added dropwise over 2 h at 220 °C. During the reaction, the product, amine (3), was distilled with H₂O under azeotropic condition. The resulting aqueous solution was extracted with CHCl₃ and dried over K₂CO₃. 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 Na₂WO₄·H₂O (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. H₂O was added to the reaction mixture and the aqueous solution was extracted with CHCl₃. The organic layer was dried over K₂CO₃ 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.²
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 × 10 mL). The combined organic layers were washed with brine (10 mL), dried over Na₂SO₄, and the solvent was removed under reduced pressure. Title compounds were purified by column chromatography on SiO₂ 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.

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·H₂O (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.

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)₂ (0.25 mol%, 0.28 mg), H₂O (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

\[
\begin{align*}
\text{PhOH} + & \text{Bu}^\text{Bu} \text{DDQ} \rightarrow \text{PhOH} \text{Bu}^\text{Bu} \\
\text{DCE, N}_2, & \text{50 }\degree \text{C} \\
\text{GC-MS detected} \\
\text{Molecular Weight: } & 362
\end{align*}
\]

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](image)

Stability of the radical adduct

![Figure S2. GC chart of freshly separated mixture](image)

![Figure S3. GC chart of the same mixture that standing for 24 h](image)
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 α 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.

<table>
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<th>entry</th>
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<th>solvent, N₂</th>
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a) Reaction conditions: 1a (0.2 mmol), 1b (0.4 mmol), solvent (1 mL), oxidant (0.4 mmol), TEMPO (0.4 mmol), N₂ (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 (NH₄)₂S₂O₈ 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 NaIO₄, (NH₄)₂S₂O₈, K₂S₂O₈ and PhI(OAc)₂ demonstrated that (NH₄)₂S₂O₈ 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 CH₃CN 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

\[
\begin{align*}
\text{R}^1 \quad \text{OH} & \quad \text{+} \quad \text{H}_2\text{N} \quad \text{-} \quad \text{R}^2 \quad \text{TEMPO (2 equiv)} \quad \text{[NH}_4\text{]}_2\text{S}_2\text{O}_8 \quad \text{(2 equiv)} \\
\text{CH}_3\text{CN, N}_2, \quad \text{50} \quad \text{°C} & \quad \text{CH}_3\text{CN, N}_2, \quad \text{50} \quad \text{°C} \\
\end{align*}
\]

In an oven dried 25 mL Schlenk tube was charged with 2-naphthols (0.2 mmol), (NH₄)₂S₂O₈ (0.4 mmol), TEMPO (0.4 mmol), after charging nitrogen for three times, the amines (0.4 mmol, 2.0 equiv), and CH₃CN (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

\[
\begin{align*}
\text{R}^1 \quad \text{OH} & \quad \text{+} \quad \text{H}_2\text{N} \quad \text{-} \quad \text{R}^2 \quad \text{TEMPO (2 equiv)} \quad \text{DDQ (2 equiv)} \\
\text{EA, N}_2, \quad \text{50} \quad \text{°C} & \quad \text{EA, N}_2, \quad \text{50} \quad \text{°C} \\
\end{align*}
\]

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 K₂CO₃ 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), NaIO₄ (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 ºC 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), (NH₄)₂S₂O₈ (20 mmol), TEMPO (20 mmol), after charging nitrogen for three times, the amine (1b, 20 mmol, 2.0 equiv), and CH₃CN (50 mL) were added. The reaction mixture was reacted at 50 ºC 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-4H-benzo[de]oxazo[5,4-g]isoquinoline-4,6(5H)-dione (PBNI)

In an oven dried 25 mL Schlenk tube was charged with naphthol 50a (1 mmol), (NH₄)₂S₂O₈ (2 mmol), TEMPO (2 mmol), after charging nitrogen for three times, the amine (2 mmol, 2.0 equiv), and CH₃CN (5 mL) were added. The reaction mixture was reacted at 50 ºC 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 CH₂Cl₂ (20 mL) and dried over Na₂SO₄. the afforded solid by evaporation of the solvent was further washed with petroleum ether, providing the crude product 9-phenyl-4H,6H-benzo[4,5]isochromeno[7,6-d]oxazo[4,6-d]-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.

3.3.6 General experimental procedure for the synthesis of naphthoxazole-doped triarylamine materials 51c, 52c, 53c, 54c

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-4-yl)aniline (1.1 mmol), Pd\(_2\)(dba)\(_3\) (2 mol%), NaO\(\text{Bu}\) (1.5 equiv), P\(\text{Bu}_3\) (4 mol%, 1.0 M in toluene), and anhydrous toluene (14 mL) was heated at 90 °C under N\(_2\) 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-4-yl)phenyl)amine (0.22 mmol), Pd\(_2\)(dba)\(_3\) (2 mol%), NaO\(\text{Bu}\) (1.5 equiv), P\(\text{Bu}_3\) (4 mol%, 1.0 M in toluene), and anhydrous toluene (3 mL) was heated at 90 °C under N\(_2\) 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-\textit{d}]oxazole (B, 1.0 mmol), 4-(dibenzo[\textit{b,d}]thiophen-4-y)aniline (D, 1.1 mmol), Pd\textsubscript{2}(dba)\textsubscript{3} (2 mol%), NaO\textsubscript{t}Bu (1.5 equiv), P\textsubscript{t}Bu\textsubscript{3} (4 mol%, 1.0 M in toluene), and anhydrous toluene (14 mL) was heated at 90 °C under N\textsubscript{2} 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[\textit{b,d}]thiophen-4-y)phenyl)-2-phenylnaphtho[2,1-\textit{d}]oxazol-7-amine (E) in 86% yield.

### 3.3.6.4 Synthesis of naphthoxazole-doped triarylamine material 54c

![Chemical Structures](image)

A mixture of 7-bromo-2-(4-methoxyphenyl)naphtho[2,1-\textit{d}]oxazole (B, 1.0 mmol), \(N\)-(4-(dibenzo[\textit{b,d}]thiophen-4-y)phenyl)-2-phenylnaphtho[2,1-\textit{d}]oxazol-7-amine (E, 1.1 mmol), Pd\textsubscript{2}(dba)\textsubscript{3} (2 mol%), NaO\textsubscript{t}Bu (1.5 equiv), P\textsubscript{t}Bu\textsubscript{3} (4 mol%, 1.0 M in toluene), and anhydrous toluene (14 mL) was heated at 90 °C under N\textsubscript{2} 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

![Graphs](image)

<table>
<thead>
<tr>
<th>Entry</th>
<th>(\lambda_{\text{abs}}) (nm)</th>
<th>(\lambda_{\text{em}}) (nm)</th>
<th>(E_{\text{g}})</th>
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**Figure S5.** Thermal and photophysical properties. I) Absorption (UV) and photoluminescence (PL) spectra of 51c, 52c, 53c, and 54c in dichloromethane (10\textsuperscript{-5} 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 (10⁻⁵ 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 (λ<sub>abs</sub>, 355–373 nm), fluorescence emission wavelengths (λ<sub>em</sub>, 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 (NH₄)₂S₂O₈ (0.4 mmol) were charged. Then the reaction tube was vacuumed and purged with nitrogen for three times. CH₃CN (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 (NH₄)₂S₂O₈ mixture.](image)

In an oven dried 25 mL Schlenk tube equipped with a stir-bar, 2-naphthol (0.2 mmol) and (NH₄)₂S₂O₈ (0.4 mmol) were charged. Then the reaction tube was vacuumed and purged with nitrogen for three times. CH₃CN (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 mixed. 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, (NH₄)₂S₂O₈ and TEMPO mixture.](image)
5.2 The $^{18}$O-labeled experiment

5.2.1 Synthesis of TEMP$^{18}$O.\(^7\)

To a solution of TEMPO (4.68 g, 30 mmol) in H$_2$O (15 mL, 2M) was added dropwise 42% aqueous HBF$_4$ (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$_3$ (6.0 mL), water (6.0 mL), and ice-cold ether (60.0 mL). The bright yellow solid was dried at 50 °C in vacuo to gain the TEMPO$^+$$BF_4^-$ (5.1 g, 70 %).

To the solution of TEMPO$^+$$BF_4^-$ (0.9710 g, 4 mmol) in H$_2$O$^{18}$O (1.7 mL) was added concentrated NaOH (12 N, 1.5 mL H$_2$O$^{18}$O) at 0 °C for 2 h and the color of solution was changed from orange to slightly yellow. Then, 30% H$_2$O$_2$ (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$_2$SO$_4$, filtered and concentrated under reduced pressure to gain the red crystalline solid (TEMP$^{18}$O), which was dried at room temperature in vacuo. The ratio of TEMP$^{18}$O/TEMP$^{16}$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$^{18}$O](image)

<table>
<thead>
<tr>
<th>[MS Spectrum]</th>
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</tr>
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<td>Background 5.645 -&gt; 5.905 (scan: 530 -&gt; 582)</td>
</tr>
<tr>
<td>m/z</td>
</tr>
<tr>
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<td>69.05</td>
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</table>

5.2.2 The $^{18}$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$_4$)$_2$S$_2$O$_8$ (0.4 mmol), TEMP$^{18}$O (0.4 mmol), after charging nitrogen for three times, the amine 1b (0.4 mmol), and CH$_3$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]

<table>
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<th>Base Peak</th>
<th>Background</th>
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<td>16.890 -&gt; 17.450 (scan: 1179 -&gt; 1291)</td>
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<tr>
<td></td>
<td>m/z Absolute Intensity</td>
<td>Relative Intensity</td>
<td>m/z Absolute Intensity</td>
</tr>
<tr>
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<td>108.55</td>
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<tr>
<td>62.00</td>
<td>15367</td>
<td>1.04</td>
<td>113.05</td>
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<tr>
<td>63.00</td>
<td>29731</td>
<td>2.01</td>
<td>114.05</td>
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<tr>
<td>77.05</td>
<td>29344</td>
<td>1.98</td>
<td>115.05</td>
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<tr>
<td>87.00</td>
<td>68192</td>
<td>4.61</td>
<td>142.05</td>
</tr>
</tbody>
</table>

**Figure S10. GC-MS analysis of TEMP$^{18}$O-labeled 2-phenylnaphtho[2,1-d]oxazole**

[MS Spectrum]

<table>
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<tr>
<th># of Peaks</th>
<th>Raw Spectrum</th>
<th>Base Peak</th>
<th>Background</th>
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</thead>
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<tr>
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<td>17.090 -&gt; 17.235 (scan: 1619 -&gt; 1648)</td>
<td>247.10 (Inten: 1,691,150)</td>
<td>17.230 (scan: 1647)</td>
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<tr>
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<td>m/z Absolute Intensity</td>
<td>Relative Intensity</td>
<td>m/z Absolute Intensity</td>
</tr>
<tr>
<td>51.00</td>
<td>26961</td>
<td>1.59</td>
<td>108.55</td>
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<tr>
<td>62.00</td>
<td>23525</td>
<td>1.39</td>
<td>113.05</td>
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<td>63.00</td>
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<td>114.05</td>
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<td>77.05</td>
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<td>115.05</td>
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<td>87.05</td>
<td>21746</td>
<td>1.29</td>
<td>122.60</td>
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<td>88.05</td>
<td>99809</td>
<td>5.90</td>
<td>123.60</td>
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<tr>
<td>94.50</td>
<td>17815</td>
<td>1.05</td>
<td>140.10</td>
</tr>
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</table>
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 (18O)-1c/(16O)-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 18O-labeled 2-naphthol and benzylamine

a) Synthesis of 18O-labeled 2-naphthol

\[
\begin{align*}
18\text{O-}2\text{naphthol} & \rightarrow 18\text{O-2-phenylnaphtho[2,1-d]oxazole} \\
(1) \text{Cul (0.1 equiv), DMEDA (0.5 equiv)} & \rightarrow \text{Nal (2 equiv), 1,4-dioxane, 110 °C, 6 h} \\
(2) \text{CsOH (3 equiv), } H_2^{18}\text{O (1 mL)} & \rightarrow \text{100 °C, 24 h}
\end{align*}
\]

In an oven dried 25 mL Schlenk tube equipped with a magnetic stirring bar was charged with Cul (0.1 equiv), Nal (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·H2O (3 equiv), and 1 mL degassed H218O. 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 Na2SO4, 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 TEMP18O/TEMP16O was 1:0.216 determined by the GC-MS analysis, and the result is show in Figure S11.

![Figure S11. GC-MS analysis of 18O-labeled 2-naphthol 18O-1a](image)

[MS Spectrum]
\# of Peaks 184
Raw Spectrum 9.635 -> 9.805 (scan: 728 -> 762) Base Peak m/z 146.15 (Inten: 355,454)
Background 9.715 -> 10.025 (scan: 744 -> 806)
m/z Absolute Intensity Relative Intensity
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 1.68 144.15 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 9.20 146.15 355454 100.00
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 18O-labeled 2-naphthol 18O-1a and amine 1b
In an oven dried 25 mL Schlenk tube was charged with \(^{18}\text{O}\)-2-naphthol (\(^{18}\text{O}-1\text{a}, 0.2 \text{ mmol})\), (NH\(_2\))\(_2\)S\(_2\)O\(_8\) (0.4 mmol), TEMPO (0.4 mmol), after charging nitrogen for three times, the amine \(1\text{b} \) (0.4 mmol), and CH\(_3\)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-\text{d}]oxazole under standard reaction conditions is same with that in \(^{18}\text{O}-1\text{a} \) labeled experiment.

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

5.2.4 The \(^{18}\text{O}\)-labeled experiment of 4-phenyl-1-naphthol (41\text{a}) and benzylamine (1b)

In an oven dried 25 mL Schlenk tube was charged with \(^{16}\text{O}\)-4-phenyl-2-naphthol (\(^{16}\text{O}-4\text{1a}, 0.2 \text{ mmol})\), NaO\(_4\) (0.4 mmol), TEMP\(^{18}\text{O}\) (0.4 mmol), after charging nitrogen for three times, the benzylamine (\(1\text{b}, 0.4 \text{ mmol})\), 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-\text{d}]oxazole (41\text{c}) under standard reaction conditions is same with that in TEMP\(^{18}\text{O}\)-involved experiment.
Figure S13. GC-MS analysis of 2,5-diphenylnaphtho[2,1-d]oxazole (41c) under standard reaction conditions

[MS Spectrum]

<table>
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<tr>
<th># of Peaks</th>
<th>Raw Spectrum</th>
<th>Base Peak</th>
<th>m/z Absolute Intensity</th>
<th>Relative Intensity</th>
</tr>
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<tr>
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<tr>
<td></td>
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Figure S14. GC-MS analysis of 2,5-diphenylnaphtho[2,1-d]oxazole (41c) under TEMP\(^{18}\)O-involved reaction conditions

[MS Spectrum]

<table>
<thead>
<tr>
<th># of Peaks</th>
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<td>322.15 2545 25.45</td>
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S15
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. Summary of X-ray crystallographic data for compound 7c.

<table>
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<th>Value</th>
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</thead>
<tbody>
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</tr>
<tr>
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<td>279.71</td>
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<td>6.8033(7)</td>
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<tr>
<td>b/Å</td>
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<td>c/Å</td>
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<tr>
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<tr>
<td>β/deg</td>
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<tr>
<td>γ/deg</td>
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<tr>
<td>V/Å&lt;sup&gt;3&lt;/sup&gt;</td>
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<tr>
<td>Z</td>
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</tr>
<tr>
<td>D/g cm&lt;sup&gt;-3&lt;/sup&gt;</td>
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<tr>
<td>cryst size/mm</td>
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<tr>
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<tr>
<td>ind refins, Rint</td>
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<tr>
<td>goodness-of-fit on F&lt;sup&gt;2&lt;/sup&gt;</td>
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<td>R1, wR2 (all data)</td>
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6.2 X-ray crystallographic data of 41c.
Figure S16. X-ray crystal structure of compound 41c (CCDC number: 2010211).

Table S8. Summary of X-ray crystallographic data for compound 41c.

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</table>

7. Characterization Data for the Products

2-phenyl-naphtho[2,1-d]oxazole (1c)

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). ¹H NMR (400 MHz, CDCl₃): δ 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); ¹³C NMR (101 MHz, CDCl₃): δ 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)
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). \( ^1\)H NMR (400 MHz, CDCl\(_3\)): \( \delta \) 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); \( ^{13} \)C NMR (101 MHz, CDCl\(_3\)): \( \delta \) 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. \( ^1\)H NMR (400 MHz, CDCl\(_3\)): \( \delta \) 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); \( ^{13} \)C NMR (101 MHz, CDCl\(_3\)): \( \delta \) 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, 120.1, 118.7, 22.3. HRMS (EI) m/z: [M]+ calcd. for C\(_{18}\)H\(_{13}\)NO: 259.0997; found: 259.0996.

**2-(4-(tert-butyl)phenyl)naphtho[2,1-d]oxazole (4c)**

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). \( ^1\)H NMR (400 MHz, CDCl\(_3\)): \( \delta \) 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); \( ^{13} \)C NMR (101 MHz, CDCl\(_3\)): \( \delta \) 162.7, 154.7, 146.3, 138.6, 131.6, 128.7, 127.1, 126.8, 125.9, 125.5, 125.3, 125.0, 124.6, 120.1, 118.6, 35.0, 31.2.

**2-(4-methoxyphenyl)naphtho[2,1-d]oxazole (5c)**

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 92% yield (29.4 mg). \( ^1\)H NMR (400 MHz, CDCl\(_3\)): \( \delta \) 8.32 (d, \( J = 8.2 \) Hz, 1H), 7.77 (d, \( J = 8.2 \) Hz, 1H), 7.70 (t, \( J = 7.5 \) Hz, 1H), 7.54 (b, \( J = 8.7 \) Hz, 2H), 7.43 (s, 9H), 7.28 (t, \( J = 7.5 \) Hz, 1H), 1.39 (s, 9H); \( ^{13} \)C NMR (101 MHz, CDCl\(_3\)): \( \delta \) 162.7, 154.7, 146.3, 138.6, 131.6, 128.7, 127.1, 126.8, 125.9, 125.5, 125.0, 124.6, 120.1, 118.6, 35.0, 31.2.
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). $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 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).

$^{13}$C NMR (101 MHz, CDCl$_3$): $\delta$ 162.6, 162.0, 146.2, 138.7, 131.5, 129.0, 128.7, 126.7, 125.4, 125.2, 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. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 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); $^{13}$C NMR (101 MHz, CDCl$_3$): $\delta$ 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); $^{19}$F NMR (377 MHz, CDCl$_3$) $\delta$ -108.00 (s). HRMS (EI) m/z: [M$^+$] calcd. for C$_{17}$H$_{10}$FNO: 263.0746; found: 263.0746.

$^2$-(4-chlorophenyl)naphtho[2,1-$d$]oxazole (7e)

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. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 8.23 (d, $J$ = 8.4 Hz, 1H), 8.20 (d, $J$ = 7.8 Hz, 1H), 7.94 (d, $J$ = 8.2 Hz, 1H), 7.80 (d, $J$ = 8.7 Hz, 1H), 7.53 (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); $^{13}$C NMR (101 MHz, CDCl$_3$): $\delta$ 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 (8e)

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. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 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); $^{13}$C NMR (101 MHz, CDCl$_3$): $\delta$ 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$^+$] calcd. for C$_{17}$H$_{10}$ClNO: 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. \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) 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); \(^1^3\)C NMR (101 MHz, CDCl\(_3\)): \(\delta\) 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]\(^+\) calcd. for C\(_{17}\)H\(_{10}\)ClNO: 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. \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) 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). \(^1^3\)C NMR (101 MHz, CDCl\(_3\)): \(\delta\) 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]\(^+\) calcd. for C\(_{17}\)H\(_{10}\)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. \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) 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). \(^1^3\)C NMR (101 MHz, CDCl\(_3\)): \(\delta\) 161.7, 146.5, 138.5, 138.2, 131.8, 128.7, 128.6, 126.9, 126.3, 125.8, 125.6, 120.3, 120.2, 118.6, 97.9. HRMS (EI) m/z: [M]\(^+\) calcd. for C\(_{17}\)H\(_{10}\)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. $^1$H NMR (400 MHz, CDCl$_3$): δ 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); $^{13}$C NMR (101 MHz, CDCl$_3$): δ 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. $^{19}$F NMR (376 MHz, CDCl$_3$): δ -62.9. HRMS (EI) m/z: [M]$^+$ calcd. for C$_{18}$H$_{10}$F$_3$NO: 313.0714; found: 313.0715.

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

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. $^1$H NMR (400 MHz, CDCl$_3$): δ 8.44 – 8.38 (m, 2H), 8.30 (d, $J = 8.2$ Hz, 1H), 7.99 (d, $J = 8.2$ Hz, 1H), 7.80 – 7.78 (m, 4H), 7.71 – 7.64 (m, 1H), 7.62 – 7.54 (m, 1H); $^{13}$C NMR (101 MHz, CDCl$_3$): δ 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]$^+$ calcd. for C$_{18}$H$_{10}$N$_2$O: 270.0793; found: 270.0792.

2-(4-nitrophenyl)naptho[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. $^1$H NMR (400 MHz, CDCl$_3$): δ 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); $^{13}$C NMR (101 MHz, CDCl$_3$): δ 160.0, 149.1, 147.1, 138.6, 132.9, 132.2, 128.7, 127.9, 127.2, 126.4, 126.2, 124.3, 120.0, 120.3, 118.7. HRMS (EI) m/z: [M]$^+$ calcd. for C$_{17}$H$_{10}$N$_2$O$_3$: 290.0691; found: 290.0692.

2-(thiophen-2-yl)naptho[2,1-d]oxazole (15c)

S21
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). 

$^1$H NMR (400 MHz, CDCl$_3$): δ 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); $^{13}$C NMR (101 MHz, CDCl$_3$): δ 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, 118.4.

2-(furan-2-yl)naphtho[2,1-d]oxazole (16c)

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). 

$^1$H NMR (400 MHz, CDCl$_3$): δ 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); $^{13}$C NMR (101 MHz, CDCl$_3$): δ 154.8, 145.8, 145.3, 142.8, 138.2, 131.7, 128.6, 126.9, 125.7, 125.7, 120.2, 120.1, 118.5, 113.4, 112.2.

HRMS (EI) m/z: [M]$^+$ calcd. for C$_{16}$H$_{10}$N$_2$O: 246.0793; found: 246.0795.

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. 

$^1$H NMR (400 MHz, CDCl$_3$): δ 9.53 – 9.52 (m, 1H), 8.79 – 8.77 (m, 1H), 8.60 – 8.50 (m, 1H), 8.28 (d, $J$ = 8.2 Hz, 1H), 8.76 (d, $J$ = 8.2 Hz, 1H), 8.25 (d, $J$ = 8.2 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); $^{13}$C NMR (101 MHz, CDCl$_3$): δ 159.9, 151.6, 148.4, 146.6, 138.3, 134.3, 131.9, 128.7, 127.0, 126.0, 125.8, 123.7, 123.7, 120.2, 118.5. HRMS (EI) m/z: [M]$^+$ calcd. for C$_{16}$H$_{10}$N$_2$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. 

$^1$H NMR (400 MHz, CDCl$_3$): δ 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,
$^1$H NMR (400 MHz, CDCl$_3$): δ 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); $^{13}$C NMR (101 MHz, CDCl$_3$): δ 172.7, 146.3, 137.4, 131.3, 128.5, 126.5, 125.1, 124.6, 120.3, 120.2, 119.9, 118.4, 28.9, 20.5. HRMS (EI) m/z: [M]$^+$ calcd. for C$_{14}$H$_{13}$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). $^1$H NMR (400 MHz, CDCl$_3$): δ 8.20 (d, $J = 8.2$ 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); $^{13}$C NMR (101 MHz, CDCl$_3$): δ 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]$^+$ calcd. for C$_{16}$H$_{17}$NO: 239.1311; 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). $^1$H NMR (400 MHz, CDCl$_3$): δ 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); 13C NMR (101 MHz, CDCl3): δ 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]+ calcd. for C19H15NO: 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.

1H NMR (400 MHz, CDCl3): δ 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); 13C NMR (101 MHz, CDCl3): δ 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]+ calcd. for C14H11NO3: 241.0739; found: 241.0737.

**2-methylnaphtho[2,1-d]oxazole (24c)**

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). 1H NMR (400 MHz, CDCl3): δ 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); 13C NMR (101 MHz, CDCl3): δ 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)**

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). 1H NMR (400 MHz, CDCl3): δ 8.28 – 8.24 (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). 13C NMR (101 MHz, CDCl3): δ 162.9, 146.5, 137.7, 131.3, 128.5, 126.6, 125.2, 124.7, 120.2, 119.8, 118.2, 14.5.

**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. 1H NMR (400 MHz, CDCl3): δ 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). 13C NMR (101 MHz, CDCl3): δ 162.3, 158.4, 145.9, 139.0, 131.1, 130.2, 128.8, 127.4, 127.2, 126.9,
25.1, 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-buty)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. 1H NMR (400 MHz, CDCl3): δ 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); 13C NMR (101 MHz, CDCl3): δ 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]+ calcd. for C_{22}H_{21}NO_{2}: 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 (10/1) to afford a white solid in 66% yield (43.7 mg); mp 178.9–179.2 °C. 1H NMR (400 MHz, CDCl3): δ 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); 13C NMR (101 MHz, CDCl3): δ 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]+ calcd. for C_{22}H_{21}NO_{2}: 331.1572; found: 331.1573.

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. 1H NMR (400 MHz, CDCl3): δ 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); 13C NMR (101 MHz, CDCl3): δ 160.8, 158.5, 146.0, 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]+ calcd. for C_{18}H_{13}ClNO_{2}: 309.0557; found: 309.0559.

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. \(^1\)H NMR (400 MHz, CDCl\(_3\)): δ 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); \(^{13}\)C NMR (101 MHz, CDCl\(_3\)): δ 158.5, 158.4, 145.5, 138.9, 130.3, 129.9, 129.6, 129.2, 128.2, 126.9, 125.2, 121.0, 115.7, 98.6, 55.5. HRMS (EI) m/z: [M]\(^+\) calcd. for C\(_{16}\)H\(_{11}\)NO\(_2\)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. \(^1\)H NMR (400 MHz, CDCl\(_3\)): δ 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); \(^{13}\)C NMR (101 MHz, CDCl\(_3\)): δ 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]\(^+\) calcd. for C\(_{22}\)H\(_{15}\)NO: 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. \(^1\)H NMR (400 MHz, CDCl\(_3\)): δ 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); \(^{13}\)C NMR (101 MHz, CDCl\(_3\)): δ 162.0, 146.5, 141.7, 138.0, 132.1, 130.9, 128.8, 127.9, 127.5, 127.2, 126.5, 124.9, 124.0, 118.7, 118.5, 29.1, 15.5. HRMS (EI) m/z: [M]\(^+\) calcd. for C\(_{19}\)H\(_{15}\)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

S26
in 51% yield (32.9 mg); mp 147.1–148.0 °C. \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) 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); \(^1\)C NMR (101 MHz, CDCl\(_3\)): \(\delta\) 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]+ calcd. for C\(_{17}\)H\(_{10}\)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. \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) 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); \(^1\)C NMR (101 MHz, CDCl\(_3\)): \(\delta\) 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]+ calcd. for C\(_{18}\)H\(_{12}\)BrNO\(_2\): 353.0052; found: 353.0052.

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

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. \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) 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); \(^1\)C NMR (101 MHz, CDCl\(_3\)): \(\delta\) 162.9, 162.2, 146.0, 139.0, 132.4, 146.0, 130.7, 130.0, 129.1, 124.3, 121.7, 119.6, 119.2, 118.6, 114.5, 55.4. HRMS (EI) m/z: [M]+ calcd. for C\(_{18}\)H\(_{12}\)BrNO\(_2\): 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. \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) 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); \(^1\)C NMR (101 MHz, CDCl\(_3\)): \(\delta\) 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]+ calcd. for C\(_{19}\)H\(_{13}\)NO\(_3\): 303.0895; found: 303.0896.

Methyl 2-phenylnaphtho[2,1-d]oxazole-6-carboxylate (37c)
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. ¹H NMR (400 MHz, CDCl₃): δ 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);
¹³C NMR (101 MHz, CDCl₃) δ 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]+ calcd. for C₁₉H₁₃NO₃: 303.0895; found: 303.0895.

2-phenyl[naphtho[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. ¹H NMR (400 MHz, CDCl₃): δ 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); ¹³C NMR (101 MHz, CDCl₃) δ 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]+ calcd. for C₁₈H₁₀N₂O: 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. ¹H NMR (400 MHz, CDCl₃): δ 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); ¹³C NMR (101 MHz, CDCl₃) δ 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]+ calcd. for C₁₅H₁₃(NO): 303.0895; found: 303.0898.

5-bromo-2-phenyl[naphtho[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. \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) 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); \(^1^3\)C NMR (101 MHz, CDCl\(_3\)): \(\delta\) 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]\(^+\) calcd. for C\(_{17}\)H\(_{10}\)BrNO: 322.9946; found: 322.9945.

2, 5-diphenynaphtho[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. \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) 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); \(^1^3\)C NMR (101 MHz, CDCl\(_3\)): \(\delta\) 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, 119.3. HRMS (EI) m/z: [M]\(^+\) calcd. for C\(_{23}\)H\(_{15}\)NO: 321.1154; found: 321.1151.

5-(2-methoxyphenyl)-2-phenynaphtho[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. \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) 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); \(^1^3\)C NMR (101 MHz, CDCl\(_3\)): \(\delta\) 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]\(^+\) calcd. for C\(_{24}\)H\(_{17}\)NO\(_2\): 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. \( ^1H \) NMR (400 MHz, CDCl\(_3\)): \( \delta \) 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); \( ^{13}C \) NMR (101 MHz, CDCl\(_3\)): \( \delta \) 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]\(^+\) calcd. for C\(_{21}\)H\(_{13}\)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. \( ^1H \) NMR (400 MHz, CDCl\(_3\)): \( \delta \) 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); \( ^{13}C \) NMR (101 MHz, CDCl\(_3\)): \( \delta \) 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]\(^+\) calcd. for C\(_{18}\)H\(_{13}\)NO\(_2\): 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. \( ^1H \) NMR (400 MHz, CDCl\(_3\)): \( \delta \) 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); \( ^{13}C \) NMR (101 MHz, CDCl\(_3\)): \( \delta \) 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]\(^+\) calcd. for C\(_{19}\)H\(_{13}\)NO\(_3\): 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. \( ^1 \)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 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); \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \( \delta \) 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]+ calcd. for C\(_{21}\)H\(_{13}\)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. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 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, \( J = 7.8 \) 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); \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \( \delta \) 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]+ calcd. for C\(_{21}\)H\(_{13}\)NO: 295.0997; found: 295.0995.

2-phenylphenanthro[9,10-d]oxazole (48c)

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). \(^1\)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 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); \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \( \delta \) 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-phenyltriphenylene[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. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 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); 13C NMR (101 MHz, CDCl3): δ 163.0, 148.1, 141.2, 131.5, 130.0, 129.6, 129.5, 128.0, 127.6, 127.5, 127.4, 127.2, 127.1, 123.7, 123.3, 123.0, 120.4, 118.8, 116.8. HRMS (EI) m/z: [M]+ calcd. for C25H15NO: 345.1154; found: 345.1155.

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

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).

5-((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. 1H NMR (400 MHz, CDCl3): δ 8.22 – 8.16 (m, 3H), 7.85 – 7.73 (m, 1H), 7.65 (d, J = 7.4 Hz, 2H), 7.49 – 7.48 (m, 2H), 7.04 (s, 1H), 4.12 (s, 4H); 13C NMR (101 MHz, CDCl3): δ 164.1, 164.0, 163.7, 150.1, 147.4, 146.5, 139.5, 138.3, 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]+ calcd. for C18H10BrNO2: 353.0051; found: 353.0050.

4-(dibenzo[b,d]thiophen-4-yl)-N-(4-(5a,9a-dihydrdibenzo[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. 1H NMR (400 MHz, CDCl3): δ 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 (q, J = 7.3 Hz, 4H), 7.48 (s, 6H), 7.41 – 7.35 (m, 6H), 7.06 (s, 1H), 4.14 (s, 3H); 13C NMR (101 MHz, CDCl3): δ 162.3, 150.2, 150.1, 147.4, 146.5, 139.5, 138.3, 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]+ calcd. for C34H30N2O2S2: 808.2218; found: 808.2215.
7-bromo-2-phenynaphtho[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. $^1$H NMR (400 MHz, CDCl$_3$): δ 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); $^{13}$C NMR (101 MHz, CDCl$_3$): δ 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]$^+$ calcd. for C$_{17}$H$_{10}$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-phenynaphtho[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. $^1$H NMR (400 MHz, CDCl$_3$): δ 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); $^{13}$C NMR (101 MHz, CDCl$_3$): δ 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]$^+$ calcd. for C$_{53}$H$_{34}$N$_2$OS$_2$: 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. $^1$H NMR (400 MHz, CDCl$_3$): δ 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); $^{13}$C NMR (101 MHz, CDCl$_3$): δ 162.3, 162.1, 147.2,
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_{2}O_{3}S: 518.1453; found: 518.1455.

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N-(4-(dibenzo[b,d]thiophen-4-yl)phenyl)-2-phenylnaphtho[2,1-d]oxazol-7-amine (E)
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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. \(^{1}H\) NMR (400 MHz, CDCl\(_3\)): δ 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). \(^{13}C\) NMR (101 MHz, CDCl\(_3\)): δ 162.4, 162.1, 162.0, 147.2, 146.7, 146.4, 145.1, 144.8, 139.5, 138.2, 138.2, 138.0, 136.0, 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]+ calcd. for C_{35}H_{33}N_{3}O_{3}S: 791.2243; found: 791.2245.

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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)
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6,11-di(naphthalen-2-yl)-2-phenylantra[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. 1H NMR (400 MHz, CDCl3): δ 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); 13C NMR (101 MHz, CDCl3): δ 158.3, 142.6, 135.0, 134.6, 133.8, 132.7, 130.0, 129.4, 129.1, 128.9, 127.2, 126.9, 126.3, 125.9, 125.6, 125.3, 125.1, 124.8, 124.6, 124.5, 124.3, 124.1, 123.7, 123.2, 123.0, 122.9, 122.8, 122.7, 122.4, 121.8, 121.8, 115.1. HRMS (EI) m/z: [M]+ calcd. for C41H25NO: 547.1936; found: 547.1938.

8. References

9. Copies of $^1$H, $^{13}$C and $^{19}$F NMR Spectra of the Products

$^1$H NMR Spectrum of 2-phenylnaphtho[1,2-d]oxazole (1c)

$^{13}$C NMR Spectrum of 2-phenylnaphtho[1,2-d]oxazole (1c)
$^1$H NMR Spectrum of 2-(p-tolyl)naphtho[1,2-d]oxazole (2c)

$^{13}$C NMR Spectrum of 2-(p-tolyl)naphtho[1,2-d]oxazole (2c)
$^1$H NMR Spectrum of 2-(4-(tert-butyl)phenyl)naphtho[1,2-$d$]oxazole (4c)

$^{13}$C NMR Spectrum of 2-(4-(tert-butyl)phenyl)naphtho[1,2-$d$]oxazole (4c)
$^1$H NMR Spectrum of 2-(4-methoxyphenyl)naphtho[1,2-$d$]oxazole (5c)

$^{13}$C NMR Spectrum of 2-(4-methoxyphenyl)naphtho[1,2-$d$]oxazole (5c)
$^1$H NMR Spectrum of 2-(4-fluorophenyl)naphtho[2,1-$d$]oxazole (6c)

$^{13}$C NMR Spectrum of 2-(4-fluorophenyl)naphtho[2,1-$d$]oxazole (6c)
$^{19}$F NMR Spectrum of 2-(4-fluorophenyl)naphtho[2,1-$d$]oxazole (6c)

$^1$H NMR Spectrum of 2-(4-chlorophenyl)naphtho[1,2-$d$]oxazole (7c)
$^{13}$C NMR Spectrum of 2-(4-chlorophenyl)naphtho[1,2-$d$]oxazole (7c)

$^1$H NMR Spectrum of 2-(3-chlorophenyl)naphtho[2,1-$d$]oxazole (8c)
$^{13}$C NMR Spectrum of 2-(3-chlorophenyl)naphtho[2,1-$d$]oxazole (8c)

$^1$H NMR Spectrum of 2-(2-chlorophenyl)naphtho[2,1-$d$]oxazole (9c)
$^{13}$C NMR Spectrum of 2-(2-chlorophenyl)naphtho[2,1-$d$]oxazole (9c)

$^1$H NMR Spectrum of 2-(4-bromophenyl)naphtho[2,1-$d$]oxazole (10c)
$^{13}$C NMR Spectrum of 2-(4-bromophenyl)naphtho[2,1-$d$]oxazole (10c)

$^1$H NMR Spectrum of 2-(4-iodophenyl)naphtho[2,1-$d$]oxazole (11c)
$^{13}$C NMR Spectrum of 2-(4-iodophenyl)naphtho[2,1-d]oxazole (11c)

$^1$H NMR Spectrum of 2-(4-(trifluoromethyl)phenyl)naphtho[1,2-d]oxazole (12c)
$^{13}$C NMR Spectrum of 2-(4-(trifluoromethyl)phenyl)naphtho[1,2-$d$]oxazole (12c)

$^{19}$F NMR Spectrum of 2-(4-(trifluoromethyl)phenyl)naphtho[1,2-$d$]oxazole (12c)
$^1$H NMR Spectrum of 4-(naphtho[2,1-$d$/]oxazol-2-yl)benzonitrile (13c)

$^{13}$C NMR Spectrum of 4-(naphtho[2,1-$d$/]oxazol-2-yl)benzonitrile (13c)
$^1$H NMR Spectrum of 2-(4-nitophenyl)naphtho[2,1-$d$]oxazole (14c)

$^{13}$C NMR Spectrum of 2-(4-nitophenyl)naphtho[2,1-$d$]oxazole (14c)
$^1$H NMR Spectrum of 2-(thiophen-2-yl)naphtho[1,2-$d$]oxazole (15c)

$^{13}$C NMR Spectrum of 2-(thiophen-2-yl)naphtho[1,2-$d$]oxazole (15c)
$^1$H NMR Spectrum of 2-(furan-2-yl)naphtho[2,1-$d$]oxazole (16c)

$^{13}$C NMR Spectrum of 2-(furan-2-yl)naphtho[2,1-$d$]oxazole (16c)
$^1$H NMR Spectrum of 2-(pyridin-3-yl)naphtho[2,1-$d$]oxazole (17c)

$^{13}$C NMR Spectrum of 2-(pyridin-3-yl)naphtho[2,1-$d$]oxazole (17c)
$^1$H NMR Spectrum of 2-(quinolin-6-yl)naphtho[2,1-$d$]oxazole (18c)

$^{13}$C NMR Spectrum of 2-(quinolin-6-yl)naphtho[2,1-$d$]oxazole (18c)
$^1$H NMR Spectrum of 2-(tert-butyl)naphtho[2,1-$d$]oxazole (19c)

$^{13}$C NMR Spectrum of 2-(tert-butyl)naphtho[2,1-$d$]oxazole (19c)
$^1$H NMR Spectrum of 2-isopropynaphtho[2,1-$d$]oxazole (20c)

$^{13}$C NMR Spectrum of 2-isopropynaphtho[2,1-$d$]oxazole (20c)
$^1$H NMR Spectrum of 2-pentylnaphtho[2,1-d]oxazole (21c)

$^{13}$C NMR Spectrum of 2-pentylnaphtho[2,1-d]oxazole (21c)
$^1$H NMR Spectrum of 2-phenethynaphtho[2,1-$d$]oxazole (22c)

$^{13}$C NMR Spectrum of 2-phenethynaphtho[2,1-$d$]oxazole (22c)
$^1$H NMR Spectrum of ethyl naphtho[2,1-$d$]oxazole-2-carboxylate (23c)

$^{13}$C NMR Spectrum of ethyl naphtho[2,1-$d$]oxazole-2-carboxylate (23c)
$^1$H NMR Spectrum of naphtho[2,1-d]oxazole (25c)

$^{13}$C NMR Spectrum of naphtho[2,1-d]oxazole (25c)
$^1$H NMR Spectrum of 8-methoxy-2-phenynaphtho[1,2-$d$]oxazole (26c)

$^{13}$C NMR Spectrum of 8-methoxy-2-phenynaphtho[1,2-$d$]oxazole (26c)
$^1$H NMR Spectrum of 2-(4-((tert-butyl)phenyl)-8-methoxynaphtho[1,2-$d$]oxazole (27c)

$^{13}$C NMR Spectrum of 2-(4-((tert-butyl)phenyl)-8-methoxynaphtho[1,2-$d$]oxazole (27c)
$^1$H NMR Spectrum of 2-(4-chlorophenyl)-8-methoxynaphtho[1,2-$d$]oxazole (28c)

$^{13}$C NMR Spectrum of 2-(4-chlorophenyl)-8-methoxynaphtho[1,2-$d$]oxazole (28c)
$^1$H NMR Spectrum of 2-(3-chlorophenyl)-8-methoxynaphtho[2,1-$d$]oxazole (29c)

$^{13}$C NMR Spectrum of 2-(3-chlorophenyl)-8-methoxynaphtho[2,1-$d$]oxazole (29c)
$^1$H NMR Spectrum of 8-methoxy-2-(thiophen-2-yl)naphtho[1,2-$d$]oxazole (30c)

$^{13}$C NMR Spectrum of 8-methoxy-2-(thiophen-2-yl)naphtho[1,2-$d$]oxazole (30c)
$^1$H NMR Spectrum of 8-methoxy-2-(naphthalen-1-yl)naphtho[2,1-$d$]oxazole (31c)

$^{13}$C NMR Spectrum of 8-methoxy-2-(naphthalen-1-yl)naphtho[2,1-$d$]oxazole (31c)
\(^1\)H NMR Spectrum of 7-ethyl-2-phenylnaphtho[2,1-d]oxazole (32c)

\[^1^C\) NMR Spectrum of 7-ethyl-2-phenylnaphtho[2,1-d]oxazole (32c)
$^1$H NMR Spectrum of 9-bromo-2-phenylnaphtho[2,1-$d$]oxazole (33c)

$^{13}$C NMR Spectrum of 9-bromo-2-phenylnaphtho[2,1-$d$]oxazole (33c)
$^1$H NMR Spectrum of 8-bromo-2-(4-methoxyphenyl)naphtho[2,1-$d$]oxazole (34c)

$^{13}$C NMR Spectrum of 8-bromo-2-(4-methoxyphenyl)naphtho[2,1-$d$]oxazole (34c)
$^1$H NMR Spectrum of 7-bromo-2-(4-methoxyphenyl)naphtho[2,1-\textit{d}]oxazole (35c)

$^{13}$C NMR Spectrum of 7-bromo-2-(4-methoxyphenyl)naphtho[2,1-\textit{d}]oxazole (35c)
$^1$H NMR Spectrum of methyl 2-phenyl)naphtho[2,1-$d$]oxazole-6-carboxylate (37c)

$^{13}$C NMR Spectrum of methyl 2-phenyl)naphtho[2,1-$d$]oxazole-6-carboxylate (37c)
$^1$H NMR Spectrum of 2-phenylnaphtho[1,2-d]oxazole-7-carbonitrile (38c)

$^{13}$C NMR Spectrum of 2-phenylnaphtho[1,2-d]oxazole-7-carbonitrile (38c)
$^1$H NMR Spectrum of 2-(4-methoxyphenyl)naphtho[2,1-d]oxazole-7-carbaldehyde (39c)

$^{13}$C NMR Spectrum of 2-(4-methoxyphenyl)naphtho[2,1-d]oxazole-7-carbaldehyde (39c)
$^1$H NMR Spectrum of 5-bromo-2-phenylnaptho[2,1-$d$]oxazole (40c)

$^{13}$C NMR Spectrum of 5-bromo-2-phenylnaptho[2,1-$d$]oxazole (40c)
$^1$H NMR Spectrum of 2,5-diphenylnaptho[2,1-$d$]oxazole (41c)

$^{13}$C NMR Spectrum of 2,5-diphenylnaptho[2,1-$d$]oxazole (41c)

S76
\( ^1H \) NMR Spectrum of 5-(2-methoxyphenyl)-2-phenylnaphtho[2,1-\(d\)]oxazole (42c)

\( ^13C \) NMR Spectrum of 5-(2-methoxyphenyl)-2-phenylnaphtho[2,1-\(d\)]oxazole (42c)
$^1$H NMR Spectrum of 2-phenyl-5-(thiophen-2-yl)naphtho[2,1-\textit{d}]oxazole (43c)

$^{13}$C NMR Spectrum of 2-phenyl-5-(thiophen-2-yl)naphtho[2,1-\textit{d}]oxazole (43c)
$^1$H NMR Spectrum of 4-methoxy-2-phenylnaphtho[2,1-$d$]oxazole (44c)

$^{13}$C NMR Spectrum of 4-methoxy-2-phenylnaphtho[2,1-$d$]oxazole (44c)
\(^1\)H NMR Spectrum of methyl 2-phenylnaphtho[2,1-d]oxazole-4-carboxylate (45c)

\(^{13}\)C NMR Spectrum of methyl 2-phenylnaphtho[2,1-d]oxazole-4-carboxylate (45c)
$^1$H NMR Spectrum of 2-phenylanthra[2,1-d]oxazole (46c)

$^{13}$C NMR Spectrum of 2-phenylanthra[2,1-d]oxazole (46c)
$^1$H NMR Spectrum of 2-phenylphenanthro[2,1-$d$]oxazole (47c)

$^{13}$C NMR Spectrum of 2-phenylphenanthro[2,1-$d$]oxazole (47c)
$^1$H NMR Spectrum of 2-phenylphenanthro[9,10-d]oxazole (48c)

$^{13}$C NMR Spectrum of 2-phenylphenanthro[9,10-d]oxazole (48c)
$^1$H NMR Spectrum of 8-phenyltriphenyleno[2,1-$d$/]oxazole (49c)

$^{13}$C NMR Spectrum of 8-phenyltriphenyleno[2,1-$d$/]oxazole (49c)
$^1$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)

$^{13}$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)
$^1$H NMR Spectrum of 2-(4-bromophenyl)-4-methoxynaphtho[2,1-$d$]oxazole (A)

$^{13}$C NMR Spectrum of 2-(4-bromophenyl)-4-methoxynaphtho[2,1-$d$]oxazole (A)
$^1$H NMR Spectrum of 4-(dibenzo[\textit{b,d}]thiophen-4-yl)-N-(4-(5a,9a-dihydrodibenzo[\textit{b,d}]thiophen-4-yl)phenyl)-N-(4-(4-methoxynaphtho[2,1-\textit{d}]oxazol-2-yl)phenyl)aniline (51c)

$^{13}$C NMR Spectrum of 4-(dibenzo[\textit{b,d}]thiophen-4-yl)-N-(4-(5a,9a-dihydrodibenzo[\textit{b,d}]thiophen-4-yl)phenyl)-N-(4-(4-methoxynaphtho[2,1-\textit{d}]oxazol-2-yl)phenyl)aniline (51c)
$^1$H NMR Spectrum of 7-bromo-2-phenyl naptho[2,1-d]oxazole (B)

$^{13}$C NMR Spectrum of 7-bromo-2-phenyl naptho[2,1-d]oxazole (B)
$^1$H NMR Spectrum of $N$-(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)

$^{13}$C NMR Spectrum of $N$-(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)
\(^1\)H NMR Spectrum of \(N\)-(4-(dibenz[\text{b,d}]thiophen-4-yl)phenyl)-\(N\)-(4-(5a,9a-dihydrodibenz[\text{b,d}]thiophen-4-yl)phenyl)-2-(4-methoxyphenyl)naphtho[2,1-\text{d}]oxazol-7-amine (53c)

\(^13\)C NMR Spectrum of \(N\)-(4-(dibenz[\text{b,d}]thiophen-4-yl)phenyl)-\(N\)-(4-(5a,9a-dihydrodibenz[\text{b,d}]thiophen-4-yl)phenyl)-2-(4-methoxyphenyl)naphtho[2,1-\text{d}]oxazol-7-amine (53c)
$^1$H NMR Spectrum of \( N-(4-(dibenzo[\text{b},\text{d}]\text{thiophen}-4-\text{yl})\text{phenyl})-2-(4\text{-methoxyphenyl})-N-(2\text{-phenylnaphtho}[2,1-\text{d}]\text{oxazol}-7-\text{yl})\text{naphtho}[2,1-\text{d}]\text{oxazol}-7\text{-amine (54c)} \)

$^{13}$C NMR Spectrum of \( N-(4-(dibenzo[\text{b},\text{d}]\text{thiophen}-4-\text{yl})\text{phenyl})-2-(4\text{-methoxyphenyl})-N-(2\text{-phenylnaphtho}[2,1-\text{d}]\text{oxazol}-7-\text{yl})\text{naphtho}[2,1-\text{d}]\text{oxazol}-7\text{-amine (54c)} \)
$^1$H NMR Spectrum of 6,11-di(naphthalen-2-yl)-2-phenylanthra[2,1-$d$]oxazole (55c)

$^{13}$C NMR Spectrum of 6,11-di(naphthalen-2-yl)-2-phenylanthra[2,1-$d$]oxazole (55c)