Supporting Information

Facile Protocols towards C2-Arylated Benzoazoles using Fe(III)-Catalyzed C(sp²-H) Functionalization and Metal-free Domino Approach

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1. General Methods

All starting materials were purchased from commercial suppliers (Sigma-Aldrich, Alfa-Aesar, SD fine chemicals, Merck, HI Media) and were used without further purification unless otherwise indicated. All reactions were carried out under an argon atmosphere in oven-dried glassware with magnetic stirring. The reactions were performed in pressure tube purchased from Sigma-Aldrich glassware. Solvents used in extraction and purification were distilled prior to use. Thin-layer chromatography (TLC) was performed on TLC plates purchase from Merck. Compounds were visualized with UV light ($\lambda = 254$ nm) and/or by immersion in KMnO$_4$ staining solution followed by heating. Products were purified by column chromatography on silica gel, 100 - 200 mesh. $^1$H ($^{13}$C) NMR spectra were recorded at 300 (75) MHz, 400 (100) MHz, 500 (125) MHz, 600 (150) MHz on a Brucker spectrometer using CDCl$_3$ as a solvent. The $^1$H and $^{13}$C chemical shifts were referenced to residual solvent signals at $\delta$ H/C 7.26 /77.28 (CDCl$_3$) relative to TMS as internal standards. Coupling constants J [Hz] were directly taken from the spectra and are not averaged. Splitting patterns are designated as s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet) and br (broad).

2. Further optimization of the reaction conditions for the catalytic C-H functionalization of benzoxazoles 1a with boronic acids 2a

Table 1. Further optimization of the reaction conditions towards Fe(III) catalytic C-H functionalization of 1a with 2a.$^{a,b,c}$

<table>
<thead>
<tr>
<th>S.N</th>
<th>Catalyst / Ligand</th>
<th>Reagents and Conditions</th>
<th>% Yield 3a$^b$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-</td>
<td>DCIB (1.3 equiv.), Cs$_2$CO$_3$ (1.5 equiv.), DMF, 100 °C, 16 h</td>
<td>0$^c$</td>
</tr>
<tr>
<td>2</td>
<td>FeCl$_3$ (5 mol%), DMEDA (20 mol%)</td>
<td>DCIB (1.3 equiv.), Cs$_2$CO$_3$ (1.5 equiv.), DMF, 100 °C, 16 h</td>
<td>49</td>
</tr>
<tr>
<td>3</td>
<td>FeCl$_3$ (5 mol%), 1,2-cyclohexane diamine (20 mol%)</td>
<td>DCIB (1.3 equiv.), Cs$_2$CO$_3$ (1.5 equiv.), DMF, 100 °C, 16 h</td>
<td>33</td>
</tr>
<tr>
<td>4</td>
<td>FeCl$_3$ (5 mol%), 2,2'-bipyridine (10 mol%)</td>
<td>DCIB (1.3 equiv.), Cs$_2$CO$_3$ (1.5 equiv.), DMF, 100 °C, 16 h</td>
<td>61</td>
</tr>
</tbody>
</table>
3. Screening of the conditions for the domino reaction between 1-nitroso-2-naphthol 4a and acetophenone 5a

Table 2. Screening of the conditions for the domino reaction between 4a and 5a.a,b

<table>
<thead>
<tr>
<th>Entry</th>
<th>Reagents</th>
<th>Solvent</th>
<th>T(°C)/t (h)</th>
<th>3a, Yield%</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>KBr (1.1 equiv.), TBHP (1.2 equiv.), Cs₂CO₃ (2.5 equiv.)</td>
<td>CH₃CN</td>
<td>80 °C/6 h</td>
<td>NR</td>
</tr>
<tr>
<td>2</td>
<td>KI (1.1 equiv.), TBHP (1.2 equiv.), Cs₂CO₃ (2.5 equiv.)</td>
<td>CH₃CN</td>
<td>80 °C/6 h</td>
<td>NR</td>
</tr>
<tr>
<td>3</td>
<td>TBAB (1.1 equiv.), Cs₂CO₃ (2.5 equiv.)</td>
<td>CH₃CN</td>
<td>80 °C/6 h</td>
<td>trace</td>
</tr>
<tr>
<td>4</td>
<td>NBS (1.1 equiv.), Cs₂CO₃ (2.5 equiv.)</td>
<td>CH₃CN</td>
<td>80 °C/6 h</td>
<td>18%</td>
</tr>
<tr>
<td>5</td>
<td>I₂ (0.5 equiv.), Cs₂CO₃ (2.5 equiv.)</td>
<td>CH₃CN</td>
<td>80 °C/6 h</td>
<td>NR</td>
</tr>
</tbody>
</table>

aAll reactions were performed using 1.0 mmol 1a and 1.0 mmol 2a in 2 mL solvent under nitrogen atmosphere. bIsolated yields. cStarting material 1a was recovered. dReaction was performed under air.
<table>
<thead>
<tr>
<th>Reaction</th>
<th>Conditions</th>
<th>Yield</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>I$_2$ (0.5 equiv.), Cs$_2$CO$_3$ (2.5 equiv.) DMF 80 °C/6 h</td>
<td>NR</td>
</tr>
<tr>
<td>7</td>
<td>CBr$_4$ (1 equiv.), Cs$_2$CO$_3$ (2.5 equiv.) CH$_3$CN 80 °C/6 h</td>
<td>52%</td>
</tr>
<tr>
<td>8</td>
<td>CBr$_4$ (0.5 equiv.), NaO'Bu (2.0 equiv.) THF 100 °C/6 h</td>
<td>NR</td>
</tr>
<tr>
<td>9</td>
<td>CBr$_4$ (0.5 equiv.), NaOAc (2.0 equiv.) CH$_3$CN 100 °C/6 h</td>
<td>NR</td>
</tr>
<tr>
<td>10</td>
<td>CBr$_4$ (0.5 equiv.), Na$_2$CO$_3$ (3 equiv.) CH$_3$CN 100 °C/6 h</td>
<td>trace</td>
</tr>
<tr>
<td>11</td>
<td>CBr$_4$ (0.5 equiv.), piperidine (2.5 equiv.) CH$_3$CN 100 °C/6 h</td>
<td>NR</td>
</tr>
<tr>
<td>12</td>
<td>CBr$_4$ (0.5 equiv.), DBU (2.5 equiv.) CH$_3$CN 80 °C/6 h</td>
<td>NR</td>
</tr>
<tr>
<td>13</td>
<td>CBr$_4$ (0.5 equiv.), Cs$_2$CO$_3$ (2.5 equiv.) DMF 100 °C/6 h</td>
<td>trace</td>
</tr>
<tr>
<td>14</td>
<td>CBr$_4$ (0.5 equiv.), Cs$_2$CO$_3$ (2.5 equiv.) DMSO 100 °C/6 h</td>
<td>trace</td>
</tr>
<tr>
<td>15</td>
<td>CBr$_4$ (0.5 equiv.), Cs$_2$CO$_3$ (2.5 equiv.) THF 60 °C/8 h</td>
<td>NR</td>
</tr>
<tr>
<td>16</td>
<td>CBr$_4$ (0.5 equiv.), Cs$_2$CO$_3$ (2.5 equiv.) DCE 60 °C/8 h</td>
<td>NR</td>
</tr>
<tr>
<td>17</td>
<td>CBr$_4$ (0.5 equiv.), Cs$_2$CO$_3$ (2.5 equiv.) 1,4-dioxane 100 °C/6 h</td>
<td>NR</td>
</tr>
<tr>
<td>18</td>
<td>CBr$_4$ (0.5 equiv.), Cs$_2$CO$_3$ (2.5 equiv.) DMA 100 °C/6 h</td>
<td>trace</td>
</tr>
<tr>
<td>19</td>
<td>CBr$_4$ (0.5 equiv.), Cs$_2$CO$_3$ (2.5 equiv.) H$_2$O 80 °C/6 h</td>
<td>NR</td>
</tr>
<tr>
<td>20</td>
<td>CBr$_4$ (0.5 equiv.), Cs$_2$CO$_3$ (2.5 equiv.) CH$_3$CN 50 °C/6 h</td>
<td>37%</td>
</tr>
<tr>
<td>21</td>
<td>CBr$_4$ (0.5 equiv.), Cs$_2$CO$_3$ (2.5 equiv.) CH$_3$CN 80 °C/3 h</td>
<td>42%</td>
</tr>
</tbody>
</table>

*All reactions were performed using 1.0 mmol 4a and 1.0 mmol 5a in 10 mL solvent under nitrogen atmosphere. Isolated yields.*

4. General experimental procedure for the synthesis of products (3a-v) using Fe(III)-catalyzed reactions (Method A)

A 10 mL pressure tube was charged with a mixture of oxazoles or thiazoles 1a-f (1.0 mmol), boronic acids 2a-o (1.0 mmol), FeCl$_3$ (0.05 mmol), 1,10-Phenanthroline (0.1 mmol), DCIB (1.3 mmol), Cs$_2$CO$_3$ (1.5 mmol) and DMF (2 mL). The pressure tube was then sealed and heated at 100 °C for 16 h. After completion of the reaction (progress was monitored by TLC; SiO$_2$, Hexane/EtOAc = 9:1), the mixture was diluted with hot ethyl acetate (20 mL) and water (40 mL) and extracted with ethyl acetate (3 × 10 mL). The combined organic layer was washed with brine (2 × 10 mL) and dried over anhydrous Na$_2$SO$_4$. Solvent was removed under reduced pressure and the remaining residue was purified by column chromatography.
over silica gel using hexane / ethyl acetate = 9:1 as an eluent to obtain the desired products 3a-v in high yields.

5. General experimental procedure for the synthesis of products (3a-f, 3h-3i, 3k, 3m, 3w, 3x) using CBr₄-catalyzed reactions (Method B)

In an oven dried 100 mL round bottomed flask 1-nitrosonaphthalene-2-ol 4a or 2-nitrosophenol 4b (1.0 mmol), acetophenones 5a-k (1.0 mmol), CBr₄ (0.5 mmol, 165 mg), Cs₂CO₃ (2.1 mmol, 682 mg) and 10 mL CH₃CN were added successively and the reaction mixture was heated for 6h at 80 °C under nitrogen atmosphere. After completion of the reaction (progress was monitored by TLC; SiO₂, Hexane/EtOAc = 9:1), the reaction mixture was allowed to cool at room temperature and then solvent was removed under vacuum. The crude product was purified by using column chromatography over silica gel using hexane / ethyl acetate = 9:1 as an eluent to obtain the desired products (3a-f, 3h-3i, 3k, 3m, 3w, 3x) in high yields.

6. Experimental procedures and analytical data of synthesized compounds (3a-x).

Synthesis of 2-phenynaptho [1,2-d]oxazole (3a); known compound¹ using (Method A)

According to the general procedure, reactions between naphthoxazole 1a (1.0 mmol, 169 mg), phenylboronic acid 2a (1.0 mmol, 122 mg) were performed using FeCl₃ (0.05 mmol, 8.1 mg), 1,10-Phenanthroline (0.1 mmol, 18 mg), DCIB (1.3 mmol, 165 mg), Cs₂CO₃ (1.5 mmol 487 mg) and DMF (2 mL) to obtain the desired 2-phenynaptho [1,2-d]oxazole 3a in 85% (208 mg) yield as pale yellow solid.

Synthesis of 2-phenynaptho [1,2-d]oxazole (3a); known compound¹ using (Method B)

According to the general procedure, reactions between 1-nitrosonaphthalene-2-ol 4a (1.0 mmol, 173 mg), acetophenone 5a (1.0 mmol, 120 mg) were performed using CBr₄ (0.5 mmol, 165 mg), Cs₂CO₃ (2.1 mmol, 682 mg) and 10 mL CH₃CN to obtain the desired 2-phenynaptho [1,2-d]oxazole 3a in 69% (169 mg) yield as pale yellow solid.
Figure 1. $^1$H (400 MHz) NMR spectra of 3a in CDCl$_3$
**Figure 2.** $^1$H (100 MHz) NMR spectra of 3a in CDCl$_3$

$^1$H NMR (400 MHz, CDCl$_3$): $\delta = 7.45 - 7.49$ (m, 5H; 8-H, 9-H, 10-H, 11-H and 12-H), 7.69 (dd, $^3$J (1-H, 2-H) = 7.0 Hz, $^3$J (2-H, 3-H) = 8.0 Hz, $^3$J (3-H, 4-H) = 8.1 Hz, $^3$J (2-H, 3-H) = 8.1 Hz, 2H; 2-H, 3-H), 7.89 (d, $^3$J (3-H, 4-H) = 7.0 Hz, 1H; 4-H), 8.23 – 8.29 (m, 2H; 5-H and 6-H), 8.52 (d, $^3$J (1-H, 2-H) = 8.0 Hz, 1H; 1-H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta = 109.8$ (C-6), 115.5 (C-14), 121.2 (C-1), 123.4 (C-15), 124.3 (C-2), 124.9 (C-3), 125.9 (C-4), 126.2 (C-8 and C-12), 127.5 (C-10), 127.8 (C-9 and C-11), 130.0 (C-5), 130.1 (C-19), 136.5 (C-16), 147.0 (C-17), 161.2 ppm (C-18); HRMS (EI, [M + H]$^+$) calculated for C$_{17}$H$_{12}$NO (246.0918); found (246.0914).
Synthesis of 2-(4-methoxyphenyl)naphtho[1,2-d]oxazole (3b); known compound\(^1\) using (Method A)

According to the general procedure, reactions between naphthoxazole 1a (1.0 mmol, 169 mg), 4-Methoxyphenylboronic acid 2b (1.0 mmol, 152 mg) were performed using FeCl\(_3\) (0.05 mmol, 8.1 mg), 1,10-Phenanthroline (0.1 mmol, 18 mg), DCIB (1.3 mmol, 165 mg), Cs\(_2\)CO\(_3\) (1.5 mmol 487 mg) and DMF (2 mL) to obtain the desired 2-(4-methoxyphenyl)naphtho[1,2-d]oxazole 3b in 88% (242 mg) yield as pale yellow solid.

Synthesis of 2-(4-methoxyphenyl)naphtho[1,2-d]oxazole (3b); known compound\(^1\) using (Method B)

According to the general procedure, reactions between 1-nitrosonaphthalene-2-ol 4a (1.0 mmol, 173 mg), 4’-methoxyacetophenone 5b (1.0 mmol, 150 mg) were performed using CBr\(_4\) (0.5 mmol, 165 mg), Cs\(_2\)CO\(_3\) (2.1 mmol, 682 mg) and 10 mL CH\(_3\)CN to obtain the desired 2-(4-methoxyphenyl)naphtho[1,2-d]oxazole 3b in 76% (209 mg) yield as pale yellow solid.

\(^1\)H NMR (300 MHz, CDCl\(_3\)): \(\delta = 3.89\) (s, 3H), 7.03 - 7.06 (m, 2H; 9-H, 11-H), 7.54 (ddd, \(^3\)J (2-H, 4-H) = 0.9Hz, \(^3\)J (1-H, 2-H) = 7.0 Hz, \(^3\)J (2-H, 3-H) = 7.9 Hz, 1H; 2-H), 7.64 - 7.68 (m, 1H; 3-H), 7.71 (d, \(^3\)J (5-H, 6-H) = 8.8 Hz, 1H; 5-H), 7.78 (d, \(^3\)J (5-H, 6-H) = 8.8 Hz, 1H; 6-H), 7.96 (d, \(^3\)J (3-H, 4-H) = 8.2 Hz, 1H; 4-H), 8.25 - 8.28 (m, 2H; 8-H, 12-H), 8.58 ppm (d, \(^3\)J (1-H, 2-H) = 8.2 Hz, 1H; 1-H).
Synthesis of 2-(2-methoxyphenyl)naphtho[1,2-d]oxazole (3c); known compound\(^1\) using (Method A)

![Chemical Structure](image)

According to the general procedure, reactions between naphthoxazole 1a (1.0 mmol, 169 mg), 2-Methoxyphenylboronic acid 2c (1.0 mmol, 152 mg) were performed using FeCl\(_3\) (0.05 mmol, 8.1 mg), 1,10-Phenanthroline (0.1 mmol, 18 mg), DCIB (1.3 mmol, 165 mg), Cs\(_2\)CO\(_3\) (1.5 mmol 487 mg) and DMF (2 mL) to obtain the desired 2-(2-methoxyphenyl)naphtho[1,2-d]oxazole 3c in 84% (231 mg) yield as pale yellow solid.

Synthesis of 2-(2-methoxyphenyl)naphtho[1,2-d]oxazole (3c); known compound\(^1\) using (Method-B)

According to the general procedure, reactions between 1-nitrosonaphthalene-2-ol 4a (1.0 mmol, 173 mg), 2'-methoxyacetophenone 5c (1.0 mmol,150 mg) were performed using CBr\(_4\) (0.5 mmol, 165 mg), Cs\(_2\)CO\(_3\) (2.1 mmol, 682 mg) and 10 mL CH\(_3\)CN to obtain the desired 2-(2-methoxyphenyl)naphtho[1,2-d]oxazole 3c in 71% (195 mg) yield as pale yellow solid.

\(^1\)HNMR (300 MHz, CDCl\(_3\)) \(\delta = 4.05\) (s, 3H), 7.08 - 7.16 (m, 2H; 9-H,11-H), 7.47 - 7.57 (m, 2H; 2-H, 3-H), 7.67 (ddd, 4\(J\) (8-H, 10-H) = 0.9 Hz, 3\(J\) (9-H, 10-H) = 7.2 Hz, 2\(J\) (10-H, 11-H) = 7.8 Hz, 1H; 10-H), 7.76 (d, 3\(J\) (8-H, 9-H) = 8.9 Hz, 1H; 8-H), 7.81 (dd, 3\(J\) (5-H, 6-H) = 8.9 Hz, 2H; 5-H, 6-H), 8.22 (d, 3\(J\) (3-H, 4-H) = 7.8 Hz, 1H; 3-H), 8.63 ppm (d, 3\(J\) (1-H, 2-H) = 8.2 Hz, 1H; 1-H)
Synthesis of 2-(p-tolyl)naphtho[1,2-d]oxazole (3d); known compound\textsuperscript{1} using (Method A)

According to the general procedure, reactions between naphthoxazole 1\textsuperscript{a} (1.0 mmol, 169 mg), 4-Methylphenylboronic acid 2\textsuperscript{d} (1.0 mmol, 136 mg) were performed using FeCl\textsubscript{3} (0.05 mmol, 8.1 mg), 1,10-Phenanthroline (0.1 mmol, 18 mg), DCIB (1.3 mmol, 165 mg), Cs\textsubscript{2}CO\textsubscript{3} (1.5 mmol 487 mg) and DMF (2 mL) to obtain the desired 2-(p-tolyl)naphtho[1,2-d]oxazole 3\textsuperscript{d} in 86\% (223 mg) yield as yellow crystalline solid.

Synthesis of 2-(p-tolyl)naphtho[1,2-d]oxazole (3d); known compound\textsuperscript{1} using (Method B)

According to the general procedure, reactions between 1-nitrosonaphthalene-2-ol 4\textsuperscript{a} (1.0 mmol, 173 mg), 4'-methylacetophenone 5\textsuperscript{d} (1.0 mmol, 134 mg) were performed using CBr\textsubscript{4} (0.5 mmol, 165 mg), Cs\textsubscript{2}CO\textsubscript{3} (2.1 mmol, 682 mg) and 10 mL CH\textsubscript{3}CN to obtain the desired 2-(p-tolyl)naphtho[1,2-d]oxazole 3\textsuperscript{d} in 78\% (202 mg) yield as yellow crystalline solid.
Figure 3. $^1$H (400 MHz) NMR spectra of $3d$ in CDCl$_3$

Figure 4. $^{13}$C (100 MHz) NMR spectra of $3d$ in CDCl$_3$
**1H NMR** (400 MHz, CDCl₃): δ = 2.38 (s, 3H; 20-H), 7.27 (d, 3J (8-H, 9-H) = 7.2 Hz, 2H; 9-H and 11-H), 7.47 (ddd, 3J (2-H, 3-H) = 7.0 Hz, 3J (3-H, 4-H) = 8.2 Hz, 4J (1-H, 3-H) = 0.82 Hz, 1H; 3-H), 7.59 (ddd, 3J (1-H, 2-H) = 8.2 Hz, 3J (2-H, 3-H) = 7.0 Hz, 4J (2-H, 4-H) = 0.81 Hz, 1H; 2-H), 7.68 (dd, 3J (11-H, 12-H) = 7.1 Hz, 2H; 8-H, 12-H), 7.89 (d, 3J (3-H, 4-H) = 8.2 Hz, 1H; 4-H), 8.15 (d, 3J (5-H, 6-H) = 8.9 Hz, 2H; 5-H, 6-H), 8.51 (d, 3J (1-H, 2-H) = 8.2 Hz, 1H; 1-H); **13C NMR** (100 MHz, CDCl₃): δ = 20.51 (C-20), 109.7 (C-6), 121.2 (C-1), 123.7 (C-14), 124.1 (C-2), 124.6 (C-3), 125.5 (C-10), 125.8 (C-4), 126.2 (C-9, C-11), 127.5 (C-5), 128.5 (C-8, C-12), 130.2 (C-18), 136.6 (C-15), 140.4 (C-19), 146.8 (C-16), 161.5 ppm (C-17); **HRMS** (EI, [M + H]+) calculated for C₁₈H₁₄NO (260.1075); found (260.1070).

**Synthesis of 2-(4-chlorophenyl)naphtho[1,2-d]oxazole (3e); known compound¹ using (Method A)**

![Image of structure 3e](image)

According to the general procedure, reactions between naphthoxazole 1a (1.0 mmol, 169 mg), 4-chlorophenylboronic acid 2e (1.0 mmol, 156 mg) were performed using FeCl₃ (0.05 mmol, 8.1 mg), 1,10-Phenanthroline (0.1 mmol, 18 mg), DCIB (1.3 mmol, 165 mg), Cs₂CO₃ (1.5 mmol 487 mg) and DMF (2 mL) to obtain the desired 2-(4-chlorophenyl)naphtho[1,2-d]oxazole 3e in 79% (220 mg) yield as pale yellow solid.

**Synthesis of 2-(4-chlorophenyl)naphtho[1,2-d]oxazole (3e); known compound¹ using (Method B)**

According to the general procedure, reactions between 1-nitrosonaphthalene-2-ol 4a (1.0 mmol, 173 mg), 4'-chloroacetophenone 5e (1.0 mmol, 154 mg) were performed using CBr₄ (0.5 mmol, 165 mg), Cs₂CO₃ (2.1 mmol, 682 mg) and 10 mL CH₃CN to obtain the desired 2-(4-chlorophenyl)naphtho[1,2-d]oxazole 3e in 73% (204 mg) yield as pale yellow solid.
Figure 5. $^1$H (600 MHz) NMR spectra of 3e in CDCl$_3$

Figure 6. $^{13}$C (150 MHz) NMR spectra of 3e in CDCl$_3$
\[^{1}\text{H NMR} (600 \text{ MHz, CDCl}_3)\]: \(\delta = 7.52 \text{ (d, }^{3}J (8-\text{H, 9-}\text{H}) = 7.0 \text{ Hz, 2H; 9-}\text{H, 11-H), 7.56 \text{ (ddd, }^{3}J (2-\text{H, 3-}\text{H}) = 7.0 \text{ Hz, }^{3}J (3-\text{H, 4-}\text{H}) = 8.2 \text{ Hz, }^{4}J (1-\text{H, 3-}\text{H}) = 0.8 \text{ Hz, 1H; 3-}\text{H), 7.68 \text{ (ddd, }^{3}J (1-\text{H, 2-}\text{H}) = 8.2 \text{ Hz, }^{3}J (2-\text{H, 3-}\text{H}) = 7.0 \text{ Hz, }^{4}J (2-\text{H, 4-}\text{H}) = 0.81 \text{ Hz, 1H; 2-}\text{H), 7.73 \text{ (d, }^{3}J (11-\text{H, 12-}\text{H}) = 7.0 \text{ Hz, 1H; 12-}\text{H), 7.82 \text{ (d, }^{3}J (8-\text{H, 9-}\text{H}) = 7.0 \text{ Hz, 1H; 8-}\text{H), 7.98 \text{ (dd, }^{3}J (3-\text{H, 4-}\text{H}) = 8.2 \text{ Hz, }^{4}J (2-\text{H, 4-}\text{H}) = 0.8 \text{ Hz, 1H; 4-}\text{H), 8.27 \text{ (d, }^{3}J (5-\text{H, 6-}\text{H}) = 8.9 \text{ Hz, 2H; 5-}\text{H, 6-}\text{H), 8.57 \text{ (dd, }^{3}J (1-\text{H, 2-}\text{H}) = 8.2 \text{ Hz, }^{4}J (1-\text{H, 3-}\text{H}) = 0.8 \text{ Hz, 1H; 1-}\text{H); }^{13}\text{C NMR} (150 \text{ MHz, CDCl}_3): \delta = 110 \text{ (C-6), 122.1 \text{ (C-14), 125.4 \text{ (C-15), 126.2 \text{ (C-1), 127 \text{ (C-5), 128.55 \text{ (C-2, C-3, C-4), 128.59 \text{ (C-18), 129.2 \text{ (C-8, C-9, C-11, C-12), 131.2 \text{ (C-10, 137.10 \text{ (C-19), 148.0 \text{ (C-16), 161.3 ppm (C-17); HRMS (EI, [M + H]^+) calculated for C}_{17}\text{H}_{11}\text{ClNO (280.0529); found (280.0521).}}}

\text{Synthesis of 2-(3-chlorophenyl)naphtho[1,2-d]oxazole (3f); unknown compound using (Method A)}}

\text{According to the general procedure, reactions between naphthoxazole 1a (1.0 mmol, 169 mg), 3-chlorophenylboronic acid 2f (1.0 mmol, 156 mg) were performed using FeCl}_3 \text{ (0.05 mmol, 8.1 mg), 1,10-Phenanthroline (0.1 mmol, 18 mg), DCIB (1.3 mmol, 165 mg), Cs}_2\text{CO}_3 \text{ (1.5 mmol 487 mg) and DMF (2 mL) to obtain the desired 2-(3-chlorophenyl)naphtho[1,2-d]oxazoles 3f in 71\% (198 mg) yield as pale yellow solid.}}

\text{Synthesis of 2-(3-chlorophenyl)naphtho[1,2-d]oxazole (3f); unknown compound using (Method B)}}

\text{According to the general procedure, reactions between 1-nitrosonaphthalene-2-ol 4a (1.0 mmol, 173 mg), 3'-chloroacetophenone 5f (1.0 mmol, 154 mg) were performed using CBr}_4 \text{ (0.5 mmol, 165 mg), Cs}_2\text{CO}_3 \text{ (2.1 mmol, 682 mg) and 10 mL CH}_3\text{CN to obtain the desired 2-(3-chlorophenyl)naphtho[1,2-d]oxazoles 3f in 66\% (184 mg) yield as pale yellow solid.}
**Figure 7.** $^1$H (400 MHz) NMR spectra of 3f in CDCl$_3$

**Figure 8.** $^{13}$C (100 MHz) NMR spectra of 3f in CDCl$_3$
$^1$H NMR (400 MHz, CDCl$_3$): $\delta$ = 7.41 (d, $^3$J (10-H, 11-H) = 7.2 Hz, 7.41 (t, $^3$J (10-H, 11-H) = 7.1 Hz, $^3$J (11-H, 12-H) = 7.0 Hz, 2H; 10-H, 11-H), 7.49 (ddd, $^3$J (3-H, 4-H) = 7.0 Hz, $^3$J (2-H, 3-H) = 8.2 Hz, $^4$J (1-H, 3-H) = 0.8 Hz, 1H; 3-H), 7.61 (ddd, $^3$J (1-H, 2-H) = 8.2 Hz, $^3$J (2-H, 3-H) = 7.0 Hz, $^4$J (2-H, 4-H) = 0.81 Hz, 1H; 2-H), 7.70 (dd, $^3$J (5-H, 6-H) = 7.0 Hz, 2H; 5-H, 6-H), 7.90 (d, $^3$J (11-H, 12-H) = 7.0 Hz, 1H; 12-H), 8.01 (dd, $^3$J (3-H, 4-H) = 8.2 Hz, $^4$J (2-H, 4-H) = 0.8 Hz, 1H; 4-H), 8.25 (s, 1H; 8-H), 8.50 (dd, $^3$J (1-H, 2-H) = 8.2 Hz, $^4$J (1-H, 3-H) = 0.8 Hz, 1H; 1-H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ = 110 (C-6), 122.3 (C-14), 125.3 (C-15), 125.6 (C-1), 126 (C-5), 127.1 (C-2, C-3 and C-4), 128.59 (C-18), 130 (C-8, C-9, C-11 and C-12), 131.2 (C-10), 137.10 (C-19), 148.3 (C-16), 160.9 ppm (C-17); HRMS (EI, [M + H]$^+$) calculated for C$_{17}$H$_{11}$ClNO (280.0529); found (280.0521).

**Synthesis of 2-(3,4-dichlorophenyl)naphtho[1,2-d]oxazole (3g); known compound** using (Method A)

According to the general procedure, reactions between naphthoxazole 1a (1.0 mmol, 169 mg), 3,4-dichlorophenylboronic acid 2g (1.0 mmol, 191 mg) were performed using FeCl$_3$ (0.05 mmol, 8.1 mg), 1,10-Phenanthroline (0.1 mmol, 18 mg), DCIB (1.3 mmol, 165 mg), Cs$_2$CO$_3$ (1.5 mmol 487 mg) and DMF (2 mL) to obtain the desired 2-(3,4-dichlorophenyl)naphtho[1,2-d]oxazole 3g in 73% (228 mg) yield as pale yellow solid.

$^1$H NMR (300 MHz, CDCl$_3$): $\delta$ = 7.57 (ddd, $^4$J (7-H, 9-H) = 1.3 Hz, $^3$J (7-H, 8-H) = 7.0 Hz, $^3$J (6-H, 7-H) = 8.3 Hz, 1H; 7-H), 7.62 (d, $^3$J (5'-H, 6'-H) = 8.5 Hz, 1H; 5'-H), 7.69 (ddd, $^4$J (6-H, 8-H) = 1.2 Hz, $^3$J (7-H, 8-H) = 6.9 Hz, $^3$J (8-H, 9-H) = 8.2 Hz, 1H; 8-H), 7.72 (d, $^3$J (4-H, 5-H) = 8.9 Hz, 1H; 4-H), 7.84 (brd, $^3$J (4-H, 5-H) = 8.9 Hz, 1H; 5-H), 7.98 (brd, $^3$J (6-H, 7-H) = 8.3 Hz, 1H; 6-H), 8.15 (dd, $^4$J (2'-H, 6'-H) = 2.1 Hz, $^3$J (5'-H, 6'-H) = 8.5 Hz, 1H; 6'-H), 8.42 (d, $^4$J (2'-H, 6'-H) = 2.0 Hz, 1H; 2'H), 8.56 ppm (brd, $^3$J (8-H, 9-H) = 8.2 Hz, 1H; 9-H).
Synthesis of 2-(4-fluorophenyl)naphtho[1,2-d]oxazole (3h); known compound\textsuperscript{1} using (Method A)

According to the general procedure, reactions between naphthoazole 1a (1.0 mmol, 169 mg), 4-fluorophenylboronic acid 2h (1.0 mmol, 140 mg) were performed using FeCl\textsubscript{3} (0.05 mmol, 8.1 mg), 1,10-Phenanthroline (0.1 mmol, 18 mg), DCIB (1.3 mmol, 165 mg), Cs\textsubscript{2}CO\textsubscript{3} (1.5 mmol 487 mg) and DMF (2 mL) to obtain the desired 2-(4-fluorophenyl)naphtho[1,2-d]oxazole 3h in 65% (171 mg) yield as yellow crystalline solid.

Synthesis of 2-(4-fluorophenyl)naphtho[1,2-d]oxazole (3h); known compound\textsuperscript{1} using (Method B)

According to the general procedure, reactions between 1-nitrosonaphthalene-2-ol 4a (1.0 mmol, 173 mg), 4'-fluoroacetophenone 5g (1.0 mmol, 138 mg) were performed using CBr\textsubscript{4} (0.5 mmol, 165 mg), Cs\textsubscript{2}CO\textsubscript{3} (2.1 mmol, 682 mg) and 10 mL CH\textsubscript{3}CN to obtain the desired 2-(4-fluorophenyl)naphtho[1,2-d]oxazole 3h in 59% (155 mg) yield as yellow crystalline solid.
**Figure 9.** $^1$H (600 MHz) NMR spectra of 3h in CDCl$_3$

**Figure 10.** $^{13}$C (150 MHz) NMR spectra of 3h in CDCl$_3$
\[ \textbf{H NMR} (600 MHz, CDCl}_3\): \(\delta = 7.24 \text{ (d, } {^3}J \text{ (8-H, 9-H) = 7.2 Hz, 2H; 12-H, 8-H), 7.56 \text{ (ddd, } {^3}J \text{ (2-H, 3-H) = 7.0 Hz, } {^3}J \text{ (3-H, 4-H) = 8.2 Hz, } {^4}J \text{ (1-H, 3-H) = 0.8 Hz, 1H; 3-H), 7.68 \text{ (ddd, } {^3}J \text{ (1-H, 2-H) = 8.2 Hz, } {^3}J \text{ (2-H, 3-H) = 7.0 Hz, } {^4}J \text{ (2-H, 4-H) = 0.8 Hz, 1H; 2-H), 7.73 \text{ (d, } {^3}J \text{ (11-H, 12-H) = 7.0 Hz, 1H; 11-H), 7.81 \text{ (d, } {^3}J \text{ (8-H, 9-H) = 7.2 Hz, 1H; 9-H), 7.98 \text{ (dd, } {^3}J \text{ (1-H, 2-H) = 8.2 Hz, } {^4}J \text{ (2-H, 4-H) = 0.8 Hz, 1H; 4-H), 8.31 - 8.35 \text{ (m, 2H; 5-H, 6-H), 8.57 \text{ (dd, } {^3}J \text{ (1-H, 2-H) = 8.2 Hz, } {^4}J \text{ (1-H, 3-H) = 0.8 Hz, 1H; 1-H); \text{ C NMR} (150 MHz, CDCl}_3\): \(\delta = 110 \text{ (C-6), 116.2 \text{ (C-9), 116.0 \text{ (C-11), 122.0 \text{ (C-14), 125.3 \text{ (C-1), 126.5 \text{ (C-15), 131.1 \text{ (C-18), 126 \text{ (C-3), 126.9 \text{ (C-2), 128.5 \text{ (C-4), 129.4 \text{ (C-12), 129.5 \text{ (C-8), 148 \text{ (C-19), 161.41 \text{ (C-16), 163.71 \text{ (C-10), 165.3 ppm (C-17); HRMS (EI, [M + H]}) calculated for C}_{17}H_{11}FNO (264.0824); found (264.0814).}

\textbf{Synthesis of methyl 4-(naphtho[1,2-d]oxazol-2-yl)benzoate (3i); known compound\textsuperscript{1} using (Method A)}

\[
\begin{align*}
\text{3i}
\end{align*}
\]

According to the general procedure, reactions between naphthoxazole 1a (1.0 mmol, 169 mg), 4-Methoxycarbonylphenylboronic acid 2i (1.0 mmol, 180 mg) were performed using FeCl\(_3\) (0.05 mmol, 8.1 mg), 1,10-Phenanthroline (0.1 mmol, 18 mg), DCIB (1.3 mmol, 165 mg), Cs\(_2\)CO\(_3\) (1.5 mmol 487 mg) and DMF (2 mL) to obtain the desired methyl 4-(naphtho[1,2-d]oxazol-2-yl)benzoate 3i in 76\% (230 mg) yield as pale yellow solid.

\textbf{Synthesis of methyl 4-(naphtho[1,2-d]oxazol-2-yl)benzoate (3i); known compound\textsuperscript{1} using (Method B)}

According to the general procedure, reactions between 1-nitrosonaphthalene-2-ol 4a (1.0 mmol,173 mg), methyl 4-acetylbenzoate 5h (1.0 mmol, 178 mg) were performed using CBr\(_4\) (0.5 mmol, 165 mg), Cs\(_2\)CO\(_3\) (2.1 mmol, 682 mg) and 10 mL CH\(_3\)CN to obtain the desired methyl 4-(naphtho[1,2-d]oxazol-2-yl)benzoate 3i in 65\% (197 mg) yield as pale yellow solid.
\[ {^1} \text{HNMR} \ (300 \text{ MHz, CDCl}_3) \delta = 3.97 \ (s, 3\text{H}), 7.57 \ (dd, ^3J (2\text{-H, 3\text{-H}}) = 7.0 \text{ Hz, 2H; 2\text{-H, 3\text{-H}}}) \]
\[ 7.68 \ (dd, ^3J (8\text{-H, 9\text{-H}}) = 7.3 \text{ Hz, 3\text{H}}} \]
\[ 7.74 \ (dd, ^3J (8\text{-H, 9\text{-H}}) = 7.0 \text{ Hz, 3\text{H}}} \]
\[ 7.82 (\text{d-like}, ^3J (2\text{-H, 3\text{-H}}) = 8.5 \text{ Hz, 2H; 3\text{-H and 5\text{-H}}}) \]
\[ 7.99 \ (\text{brd,} \ ^3J (4\text{-H, 5\text{-H}}) = 9.1 \text{ Hz, 1H; 5\text{-H}}) \]
\[ 8.41 \ (\text{d-like}, ^3J (2\text{-H, 3\text{-H}}) = 8.5 \text{ Hz, 2H; 2\text{-H and 6\text{-H}}}) \]
\[ 8.57 \ (\text{brd}, ^3J (8\text{-H, 9\text{-H}}) = 8.3 \text{ Hz, 1H, 9\text{-H}}) \]

Synthesis of 4-(naphtho[1,2-d]oxazol-2-y1)benzonitrile (3j); known compound\(^1\) using (Method-A)

According to the general procedure, reactions between naphthoazole 1a (1.0 mmol, 169 mg), 4-cyanophenylboronic acid 2j (1.0 mmol, 147 mg) were performed using FeCl\(_3\) (0.05 mmol, 8.1 mg), 1,10-Phenanthroline (0.1 mmol, 18 mg), DCIB (1.3 mmol, 165 mg), Cs\(_2\)CO\(_3\) (1.5 mmol 487 mg) and DMF (2 mL) to obtain the desired 4-(naphtho[1,2-d]oxazol-2-yl)benzonitrile 3j in 64% (173 mg) yield as pale yellow solid.

\[ {^1} \text{HNMR} \ (300 \text{ MHz, CDCl}_3) \delta = 7.59 \ (\text{ddd,} ^4J (7\text{-H, 9\text{-H}}) = 1.2 \text{ Hz,} ^3J (7\text{-H, 8\text{-H}}) = 6.9 \text{ Hz,} ^3J (6\text{-H, 7\text{-H}}) = 8.2 \text{ Hz, 1H; 7\text{-H}}) \]
\[ 7.71 \ (\text{ddd,} ^4J (6\text{-H, 8\text{-H}}) = 1.2 \text{ Hz,} ^3J (7\text{-H, 8\text{-H}}) = 7.0 \text{ Hz,} ^3J (8\text{-H, 9\text{-H}}) = 8.2 \text{ Hz, 1H; 8\text{-H}}) \]
\[ 7.82 \ (\text{d-like,} ^3J (2\text{-H, 3\text{-H}}) = 8.5 \text{ Hz, 2H; 3\text{-H and 5\text{-H}}}) \]
\[ 7.99 \ (\text{brd,} ^3J (4\text{-H, 5\text{-H}}) = 9.1 \text{ Hz, 1H; 5\text{-H}}) \]
\[ 8.41 \ (\text{d-like,} ^3J (2\text{-H, 3\text{-H}}) = 8.5 \text{ Hz, 2H; 2\text{-H and 6\text{-H}}}) \]
\[ 8.57 \ (\text{brd,} ^3J (8\text{-H, 9\text{-H}}) = 8.3 \text{ Hz, 1H, 9\text{-H}}) \]
Synthesis of 2-(4-nitrophenyl)naphtho[1,2-d]oxazole (3k); unknown compound using (Method A)

According to the general procedure, reactions between naphthooxazole 1a (1.0 mmol, 169 mg), 4-nitrophenylboronic acid 2k (1.0 mmol, 167 mg) were performed using FeCl₃ (0.05 mmol, 8.1 mg), 1,10-Phenanthroline (0.1 mmol, 18 mg), DCIB (1.3 mmol, 165 mg), Cs₂CO₃ (1.5 mmol 487 mg) and DMF (2 mL) to obtain the desired 2-(4-nitrophenyl)naphtho[1,2-d]oxazole 3k in 55% (159 mg) yield as yellow crystalline solid.

Synthesis of 2-(4-nitrophenyl)naphtho[1,2-d]oxazole (3k); unknown compound using (Method B)

According to the general procedure, reactions between 1-nitrosonaphthalene-2-ol 4a (1.0 mmol, 173 mg), 4'-nitroacetophenone 5i (1.0 mmol, 165 mg) were performed using CBr₄ (0.5 mmol, 165 mg), Cs₂CO₃ (2.1 mmol, 682 mg) and 10 mL CH₃CN to obtain the desired 2-(4-nitrophenyl)naphtho[1,2-d]oxazole 3k in 55% (159 mg) yield as yellow crystalline solid.
Figure 11. $^1$H (400 MHz) NMR spectra of 3k in CDCl$_3$

$^1$H NMR (400 MHz, CDCl$_3$): $\delta$ = 7.07 (ddd, $^3$J (2-H, 3-H) = 7.0 Hz, $^3$J (3-H, 4-H) = 8.2 Hz, $^4$J (1-H, 3-H) = 0.83 Hz, $^3$J (1-H, 2-H) = 8.2 Hz, $^3$J (2-H, 3-H) = 7.0 Hz, $^4$J (2-H, 4-H) = 0.82 Hz, 2H; 2-H, 3-H), 7.19 (d, $^3$J (3-H, 4-H) = 8.2 Hz, 1H; 4-H), 7.40 – 7.84 (m, 4H; 8-H, 9-H, 11-H and 12-H), 7.91 (d, $^3$J (5-H, 6-H) = 8.9 Hz, 1H; 5-H), 8.32 (d, $^3$J (5-H, 6-H) = 8.9 Hz, 1H; 6-H), 8.44 ppm (d, $^3$J (1-H, 2-H) = 8.1Hz, 1H; 1-H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ = 110 (C-6), 122.1 (C-14), 125.4 (C-15), 126.2 (C-1), 127 (C-5), 128.55 (C-2, C-3 and C-4), 128.59 (C-18), 129.2 (C-8, C-9, C-11 and C-12), 131.2 (C-10), 137.10 (C-19), 148.0 (C-16), 161.3 ppm (C-17); HRMS (EI, [M + H]$^+$) calculated for C$_{17}$H$_{11}$N$_2$O$_3$ (291.0769); found (291.0760).
Synthesis of 2-(napthalen-2-yl)naphtho[1,2-d]oxazole (3l); known compound\(^1\) using (Method A)

According to the general procedure, reactions between naphthoxazole 1a (1.0 mmol, 169 mg), 2-naphthylboronic acid 2l (1.0 mmol, 172 mg) were performed using FeCl\(_3\) (0.05 mmol, 8.1 mg), 1,10-Phenanthroline (0.1 mmol, 18 mg), DCIB (1.3 mmol, 165 mg), Cs\(_2\)CO\(_3\) (1.5 mmol 487 mg) and DMF (2 mL) to obtain the desired 2-(napthalen-2-yl)naphtho[1,2-d]oxazole 3l in 62% (183 mg) yield as pale yellow solid.

\(^1\)HNMR (500 MHz, CDCl\(_3\)) \(\delta \) = 7.54 - 7.59 (m, 3H; 6'-H, 7'-H and 7-H), 7.70 (ddd, \(^4\)J (6-H, 8-H) = 1.3 Hz, \(^3\)J (7-H, 8-H) = 6.9 Hz, \(^5\)J (8-H, 9-H) = 8.1 Hz, 1H; 8-H), 7.78 (d, \(^5\)J (4-H, 5-H) = 8.9 Hz, 1H; 4-H), 7.84 (d, \(^5\)J (4-H, 5-H) = 8.9 Hz, 1H; 5-H), 7.87 - 7.91 (m, 1H; 5'-H), 7.97 (d, \(^3\)J (6-H, 7-H) = 8.2 Hz, 1H; 6-H), 7.98 (d, \(^5\)J (3'-H, 4'-H) = 8.7 Hz, 1H; 4'-H), 7.99 - 8.02 (m, 1H; 8'-H), 8.40 (dd, \(^4\)J (1'-H, 3'-H) = 1.7 Hz, \(^3\)J (3'-H, 4'-H) = 8.5 Hz, 1H; 3'-H), 8.65 (brd, \(^3\)J (8-H, 9-H) = 8.1 Hz, 1H; 9-H), 8.84 ppm (brs, 1H; 1'-H).

Synthesis of 2-phenylbenzo[d]oxazole (3m); known compound\(^2\) using (Method A)

According to the general procedure, reactions between benzoazole 1b (1.0 mmol, 119 mg), phenylboronic acid 2a (1.0 mmol, 122 mg) were performed using FeCl\(_3\) (0.05 mmol, 8.1 mg), 1,10-Phenanthroline (0.1 mmol, 18 mg), DCIB (1.3 mmol, 165 mg), Cs\(_2\)CO\(_3\) (1.5 mmol 487 mg) and DMF (2 mL) to obtain the desired 2-phenylbenzo[d]oxazole 3m in 89% (173 mg) yield as pale yellow solid.
Synthesis of 2-phenylbenzo[d]oxazole (3m); known compound\(^2\) using (Method B)

According to the general procedure, reactions between 2-nitrosophenol 4b (1.0 mmol, 123 mg), acetophenone 5a (1.0 mmol, 120 mg) were performed using CBr\(_4\) (0.5 mmol, 165 mg), Cs\(_2\)CO\(_3\) (2.1 mmol, 682 mg) and 10 mL CH\(_3\)CN to obtain the desired 2-phenylbenzo[d]oxazole 3m in 57% (111 mg) yield as pale yellow solid.

\[\text{Figure 12.} \quad \text{\(^1\)H (400 MHz) NMR spectra of 3m in CDCl}_3\]
\[ \delta = 7.38 \text{ (dd, } J(6-H, 7-H) = 8.5 \text{ Hz, } J(5-H, 7-H) = 1.7 \text{ Hz, } J(4-H, 5-H) = 8.5 \text{ Hz, } J(4-H, 6-H) = 1.7 \text{ Hz, } J(4'-H, 5'-H) = 6.9 \text{ Hz, } J(4'-H, 5'-H) = 8.1 \text{ Hz, } J(5'-H, 6'-H) = 8.1 \text{ Hz, } J(5'-H, 6'-H) = 6.9 \text{ Hz, } J(6'-H, 7'-H) = 8.1 \text{ Hz, } J(6'-H, 7'-H) = 1.2 \text{ Hz, } J(5'-H, 6'-H) = 8.9 \text{ Hz, } J(5'-H, 6'-H) = 8.9 \text{ Hz, } J(4-H, 6-H) = 1.2 \text{ Hz, } J(5-H, 6-H) = 8.9 \text{ Hz, } J(4-H, 6-H) = 1.2 \text{ Hz, } J(5-H, 7-H) = 8.9 \text{ Hz, } J(5-H, 6-H) = 8.9 \text{ Hz, } J(6'-H, 7'-H) = 8.9 \text{ Hz, } J(6'-H, 7'-H) = 2H; J(3'-H and 7'-H); } \]

\[ \delta = 110 \text{ (C-4), } 120.1 \text{ (C-7), } 124 \text{ (C-5), } 125 \text{ (C-6), } 127 \text{ (C-5'), } 127.8 \text{ (C-3' and C-7'), } 128 \text{ (C-4' and C-6'), } 131 \text{ (C-2'), } 142 \text{ (C-7a), } 150 \text{ (C-3a), } 163 \text{ ppm (C-2); } \]

**HRMS** (EI, [M + H]^+) calculated for C_{13}H_{10}NO (196.0762); found (196.0757).
Synthesis of 2-(4-methoxyphenyl)benzo[d]oxazole (3n); known compound\textsuperscript{2} using (Method A)

According to the general procedure, reactions between benzoxazole 1b (1.0 mmol, 119 mg), 4-methoxyphenylboronic acid 2b (1.0 mmol, 152 mg) were performed using FeCl\textsubscript{3} (0.05 mmol, 8.1 mg), 1,10-Phenanthroline (0.1 mmol, 18 mg), DCIB (1.3 mmol, 165 mg), Cs\textsubscript{2}CO\textsubscript{3} (1.5 mmol 487 mg) and DMF (2 mL) to obtain the desired 2-(4-methoxyphenyl)benzo[d]oxazole 3n in 87\% (196 mg) yield as pale yellow solid.

\textbf{Figure 14.} \textsuperscript{1}H (400 MHz) NMR spectra of 3n in CDCl\textsubscript{3}
**Figure 15.** $^{13}$C (100 MHz) NMR spectra of 3n in CDCl$_3$

$^1$HNMR (400 MHz, CDCl$_3$) $\delta$ = 3.92 (s, 3H; 8′-H), 7.05 (dd, $^3$J (6-H, 7-H) = 8.5 Hz, $^4$J (5-H, 7-H) = 1.7 Hz, $^3$J (4-H, 5-H) = 8.5 Hz, $^4$J (4-H, 6-H) = 1.7 Hz, 2H; 4-H, 7-H), 7.35 (dd, $^3$J (3′-H, 4′-H) = 6.9 Hz, $^3$J (6′-H, 7′-H) = 8.1 Hz, 2H; 4′-H and 6′-H), 7.58 (ddd, $^3$J (4-H, 5-H) = 8.9 Hz, $^3$J (5-H, 6-H) = 8.9 Hz, $^4$J (7-H, 5-H) = 1.2 Hz, 1H; 5-H), 7.75 (ddd, $^3$J (6-H, 7-H) = 8.9 Hz, $^3$J (5-H, 6-H) = 8.9 Hz, $^4$J (4-H, 6-H) = 1.2 Hz, 1H; 6-H), 8.22 (dd, $^3$J (3′-H, 4′-H) = 8.9 Hz, $^3$J (6′-H, 7′-H) = 8.9 Hz, 2H; 3′-H, 7′-H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ = 55 (C-8′), 110 (C-4), 114.1 (C-7), 119 (C-5), 119.7 (C-6), 124 (C-5′), 124.6 (C-3′ and C-7′), 129 (C-4′ and C-6′), 142 (C-2′), 150 (C-7a), 162 (C-3a), 163 ppm (C-2); HRMS (EI, [M + H]$^+$) calculated for C$_{14}$H$_{12}$NO$_2$ (226.0868); found (226.0859).
Synthesis of 2-(2-bromo-4-methylphenyl)benzo[d]oxazole (3o); unknown compound using (Method A)

According to the general procedure, reactions between benzoxazole 1b (1.0 mmol, 119 mg), 2-bromo-4-methylphenylboronic acid 2m (1.0 mmol, 215 mg) were performed using FeCl₃ (0.05 mmol, 8.1 mg), 1,10-Phenanthroline (0.1 mmol, 18 mg), DCIB (1.3 mmol, 165 mg), Cs₂CO₃ (1.5 mmol 487 mg) and DMF (2 mL) to obtain the desired 2-(2-bromo-4-methylphenyl)benzo[d]oxazole 3o in 83% (238 mg) yield as pale yellow solid.

Figure 16. ¹H (400 MHz) NMR spectra of 3o in CDCl₃
**Figure 17.** $^{13}$C (100 MHz) NMR spectra of 3o in CDCl$_3$

$^1$HNMR (400 MHz, CDCl$_3$) δ = 2.43 (s, 3H; 8′-H), 7.26 (d, $^3$J (6′-H, 7′-H) = 8.5 Hz, 1H; 6′-H), 7.38 (dd, $^3$J (4-H, 5-H) = 6.9 Hz, $^4$J (4-H, 6-H) = 1.2 Hz, $^3$J (6-H, 7-H) = 6.9 Hz, $^4$J (5-H, 7-H) = 1.2 Hz, 2H; 4-H and 7-H), 7.60 (s, 1H; 4′-H), 7.84 (d, $^3$J (6′-H, 7′-H) = 8.5 Hz, 1H; 6′-H), 7.98 (dd, $^3$J (4-H, 5-H) = 8.9 Hz, $^3$J (5-H, 6-H) = 8.9 Hz, $^3$J (5-H, 6-H) = 8.9 Hz, $^3$J (6-H, 7-H) = 8.9 Hz, 2H; 5-H and 6-H); $^{13}$C NMR (100 MHz, CDCl$_3$): δ = 21 (C-8′), 110 (C-4), 120 (C-7), 121 (C-3′), 124 (C-6), 125 (C-5), 125.4 (C-6′), 128 (C-4′), 131 (C-7), 135 (C-2′), 141 (C-5′), 142.4 (C-7′), 150 (C-3′), 161 (C-2) ; HRMS (EI, [M + H]$^+$) calculated for C$_{14}$H$_{11}$BrNO (288.0023); found (288.0019).
Synthesis of 2-(2-bromophenyl)benzo[d]oxazole (3p); unknown compound using (Method A)

According to the general procedure, reactions between benzoxazole 1b (1.0 mmol, 119 mg), 2-bromophenylboronic acid 2n (1.0 mmol, 201 mg) were performed using FeCl₃ (0.05 mmol, 8.1 mg), 1,10-Phenanthroline (0.1 mmol, 18 mg), DCIB (1.3 mmol, 165 mg), Cs₂CO₃ (1.5 mmol 487 mg) and DMF (2 mL) to obtain the desired 2-(2-bromophenyl)benzo[d]oxazole 3p in 66% (180 mg) yield as pale yellow solid.

![Figure 18. ¹H (400 MHz) NMR spectra of 3p in CDCl₃](image)
$^1$HNMR (400 MHz, CDCl$_3$) $\delta = 7.33$ - 7.40 (m, 3H; 4-H, 7-H and 6'-H), 7.45 (dd, $^3$J (5'-H, 6'-H) = 8.5 Hz, $^3$J (4'-H, 5'-H) = 8.5 Hz, 1H; 5'-H), 7.62 (d, $^3$J (6'-H, 7'-H) = 8.9 Hz, 1H; 7'-H), 7.76 (d, $^3$J (4'-H, 5'-H) = 8.9 Hz, 1H; 4'-H), 7.85 (dd, $^3$J (6-H, 5-H) = 8.5 Hz, $^3$J (4-H, 5-H) = 8.2 Hz, 1H; 5-H), 8.08 (dd, $^3$J (6-H, 7-H) = 8.5 Hz, $^3$J (5-H, 6-H) = 8.2 Hz, 1H; 6-H);

$^{13}$C NMR (100 MHz, CDCl$_3$): $\delta = 110$ (C-4), 120 (C-7), 121 (C-5'), 124 (C-6), 125 (C-5), 127 (C-6'), 128 (C-2'), 132 (C-5'), 132.4 (C-4'), 134 (C-7'), 141 (C-7''), 150 (C-3''), 161 ppm (C-2);

HRMS (EI, [M + H]$^+$) calculated for C$_{13}$H$_9$BrN$_2$O (273.9867); found (273.9862).

Synthesis of 2-(4-Chlorophenyl)benzo[d]oxazole (3q); known compound$^2$ using (Method A)

According to the general procedure, reactions between benzoazole 1b (1.0 mmol, 119 mg), 4-chlorophenylboronic acid 2e (1.0 mmol, 156 mg) were performed using FeCl$_3$ (0.05 mmol, 8.1 mg), 1,10-Phenanthroline (0.1 mmol, 18 mg), DCIB (1.3 mmol, 165 mg), Cs$_2$CO$_3$ (1.5
mmol 487 mg) and DMF (2 mL) to obtain the desired 2-(4-chlorophenyl)benzo[d]oxazole 3q in 74% (169 mg) yield as pale yellow solid.

**Figure 20.** $^1$H (400 MHz) NMR spectra of 3q in CDCl$_3$
Figure 21. $^{13}$C (100 MHz) NMR spectra of 3q in CDCl$_3$.

$^1$HNMR (400 MHz, CDCl$_3$): $\delta$ = 7.39 (dd, $^3$J (6-H, 7-H) = 8.5 Hz, $^4$J (5-H, 7-H) = 1.7 Hz, $^3$J (4-H, 5-H) = 8.5 Hz, $^4$J (4-H, 6-H) = 1.7 Hz, 2H; 4-H and 7-H), 7.53 (dd, $^3$J (3'-H, 4'-H) = 8.5 Hz, 2H; 4'-H and 6'-H), 7.61 (d, $^3$J (3'-H, 4'-H) = 8.9 Hz, 1H; 3'-H), 7.79 (d, $^3$J (6'-H, 7'-H) = 8.9 Hz, 1H; 7'-H), 8.22 (dd, $^3$J (6-H, 7-H) = 8.5 Hz, $^3$J (5-H, 6-H) = 8.2 Hz, $^3$J (4-H, 5-H) = 8.5 Hz, $^4$J (4-H, 5-H) = 8.5 Hz, 2H; 5-H and 6-H).

$^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ = 110 (C-4), 120 (C-7), 124 (C-5), 125 (C-4'), 125.6 (C-6'), 128 (C-7'), 128.4 (C-2'), 137 (C-5'), 142 (C-7'), 150 (C-3'), 162 ppm (C-2).

HRMS (EI, [M + H]$^+$) calculated for C$_{13}$H$_9$ClNO (230.0372); found (230.0365).
Synthesis of 5-bromo-2-(2-bromo-4-methylphenyl)benzo[d]oxazole (3r); unknown compound using (Method A)

According to the general procedure, reactions between 5-bromobenzo[d]oxazole 1c (1.0 mmol, 198 mg), 2-bromo-4-methylphenylboronic acid 2m (1.0 mmol, 215 mg) were performed using FeCl$_3$ (0.05 mmol, 8.1 mg), 1,10-Phenanthroline (0.1 mmol, 18 mg), DCIB (1.3 mmol, 165 mg), Cs$_2$CO$_3$ (1.5 mmol 487 mg) and DMF (2 mL) to obtain the desired 5-bromo-2-(2-bromo-4-methylphenyl)benzo[d]oxazole 3r in 67% (246 mg) yield as pale yellow solid.

Figure 22. $^1$H (400 MHz) NMR spectra of 3r in CDCl$_3$
$^1$HNMR (400 MHz, CDCl$_3$) $\delta = 2.45$ (s, 3H; 8′-H), 7.31 (s, 1H; 7-H), 7.51 (m, $^3$J (6′-H, 7′-H) = 8.9 Hz, 2H; 6′-H and 7′-H), 7.63 (s, 1H; 4′-H), 7.98 - 8.01 (m, $^3$J (4-H, 5-H) = 8.5 Hz, 2H; 4-H and 5-H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta = 110$ (C-4), 120 (C-7), 124 (C-5), 125 (C-4′), 125.6 (C-6′), 128 (C-7′), 128.4 (C-2′), 137 (C-5′), 142 (C-7″), 150 (C-3″), 162 ppm (C-2).

HRMS (EI, [M + H]$^+$) calculated for C$_{14}$H$_{10}$Br$_2$NO (365.9129); found (365.9124).

Synthesis of 2-(2-bromophenyl)-5-nitrobenzo[d]oxazole (3s); unknown compound using (Method A)

According to the general procedure, reactions between 5-nitrobenzo[d]oxazole 1d (1.0 mmol, 164 mg), 2-Bromophenylboronic acid 2n (1.0 mmol, 201 mg) were performed using FeCl$_3$ (0.05 mmol, 8.1 mg), 1,10-Phenanthroline (0.1 mmol, 18 mg), DCIB (1.3 mmol, 165 mg), Cs$_2$CO$_3$ (1.5 mmol 487 mg) and DMF (2 mL) to obtain the desired 2-(2-bromophenyl)-5-nitrobenzo[d]oxazole 3s in 69% (220 mg) yield as pale yellow solid.
Figure 23. $^1$H (400 MHz) NMR spectra of 3s in CDCl$_3$

Figure 24. $^{13}$C (100 MHz) NMR spectra of 3s in CDCl$_3$
^1HNMR (400 MHz, CDCl_3) δ = 7.46 (ddd, 3J (6′-H, 7′-H) = 8.1 Hz, 3J (5′-H, 6′-H) = 8.0 Hz, 4J (4′-H, 6′-H) = 0.8 Hz, 1H; 6′-H), 7.54 (ddd, 3J (4′-H, 5′-H) = 8.4 Hz, 3J (5′-H, 6′-H) = 8.3 Hz, 1H; 5′-H), 7.76 (d, 3J (4′-H, 5′-H) = 8.9 Hz, 1H; 4′-H), 7.84 (dd, 3J (6′-H, 7′-H) = 7.9Hz, 1H; 7′-H), 8.15 (dd, 3J (4-H, 5-H) = 8.0 Hz, 1H; 5-H), 8.41 (dd, 3J (4-H, 5-H) = 8.1 Hz, 1H; 4-H), 8.78 (d, 1H, 7-H); ^13C NMR (100 MHz, CDCl_3): δ = 100 (C-4), 111 (C-7), 116 (C-6), 121 (C-5), 122 (C-3′), 127 (C-5′), 132 (C-7′), 133 (C-4′), 135 (C-6′), 142 (C-2′), 145 (7a), 154 (3a), 164 ppm (C-2); HRMS (EI, [M + H]^+) calculated for C_{13}H_{8}BrN_{2}O_{3} (318.9718); found (318.9710).

**Synthesis of (E)-4-bromo-2-styrylbenzo[d]oxazole (3t)**; unknown compound using (Method A)

![3t](image)

According to the general procedure, reactions between 4-bromobenzo[d]oxazole 1e (1.0 mmol, 198 mg), (E)-styrylboronic acid 2o (1.0 mmol, 148 mg) were performed using FeCl_3 (0.05 mmol, 8.1 mg), 1,10-Phenanthroline (0.1 mmol, 18 mg), DCIB (1.3 mmol, 165 mg), Cs_2CO_3 (1.5 mmol 487 mg) and DMF (2 mL) to obtain the desired (E)-4-bromo-2-styrylbenzo[d]oxazole 3t in 63% (189 mg) yield as pale yellow solid.
Figure 25. $^1$H (400 MHz) NMR spectra of 3t in CDCl$_3$

$^1$HNMR (400 MHz, CDCl$_3$) $\delta = 7.17$ (d, $^3$J (8-H, 9-H) = 16 Hz, 1H; 9-H), 7.25 (t, $^3$J (8-H, 9-H) = 16 Hz, 1H; 8-H), 7.44 (m, 3H; 12-H, 13-H and 14-H), 7.52 (dd, $^3$J (5-H, 6-H) = 8.1 Hz, 2H; 5-H and 6-H), 7.63 (dd, $^3$J (11-H, 12-H) = 7.9 Hz, $^3$J (14-H, 15-H) = 8.2 Hz, 2H; 11-H and 15-H), 7.86 (d, $^3$J (4-H, 5-H) = 7.8 Hz, 1H; 4-H), HRMS (EI, [M + H]$^+$) calculated for C$_{15}$H$_{11}$BrNO (300.0023); found (300.0020).

Synthesis of 2-(4-chlorophenyl)benzo[d]thiazole (3u); known compound$^2$ using (Method A)

According to the general procedure, reactions between benzo[d]thiazole 1f (1.0 mmol, 135 mg), 4-chlorophenylboronic acid 2e (1.0 mmol, 156 mg) were performed using FeCl$_3$ (0.05 mmol, 8.1 mg), 1,10-Phenanthroline (0.1 mmol, 18 mg), DCIB (1.3 mmol, 165 mg), Cs$_2$CO$_3$
(1.5 mmol 487 mg) and DMF (2 mL) to obtain the desired 2-(4-chlorophenyl)benzo[d]thiazole 3u in 74% (181 mg) yield as pale yellow solid.

Figure 26. $^1$H (400 MHz) NMR spectra of 3u in CDCl$_3$
Figure 27. $^{13}$C (100 MHz) NMR spectra of 3u in CDCl$_3$

$^1$HNMR (400 MHz, CDCl$_3$) $\delta = 7.41$ (ddd, $^2$J (4-H, 5-H) = 8.4 Hz, $^3$J (5-H, 6-H) = 8.3 Hz, $^4$J (5-H, 7-H) = 1.7 Hz, 1H; 5-H), 7.47 (d, $^2$J (3'-H, 4'-H) = 7.9 Hz, 2H; 3'-H and 7'-H), 7.51 (ddd, $^3$J (5-H, 6-H) = 8.5 Hz, $^3$J (6-H, 7-H) = 8.4, $^4$J (4-H, 6-H) = 8.5 Hz, 1H; 6-H), 7.91 (d, $^3$J (4-H, 5-H) = 8.5 Hz, 1H; 4-H), 8.04 (d, $^3$J (3-H, 4-H) = 7.8 Hz, 2H; 4'-H and 6'-H), 8.08 (d, $^3$J (6-H, 7-H) = 7.8 Hz, 1H; 7-H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta = 121$ (C-4), 123 (C-7), 125 (C-6), 126 (C-5), 128 (C-3'), 129 (C-5'), 132 (7'), 135 (C-4'), 137 (C-2'), 154 (C-7'), 166 ppm (C-2); HRMS (El, [M + H]$^+$) calculated for C$_{13}$H$_9$N$_2$O$_2$S (246.0384); found (246.0378).

Synthesis of 2-(4-nitrophenyl)benzo[d]thiazole (3v); known compound$^2$ using (Method A)

According to the general procedure, reactions between benzo[d]thiazole 1f (1.0 mmol, 135 mg), 4-nitrophenylboronic acid 2k (1.0 mmol, 167 mg) were performed using FeCl$_3$ (0.05
mmol, 8.1 mg), 1,10-Phenanthroline (0.1 mmol, 18 mg), DCIB (1.3 mmol, 165 mg), Cs₂CO₃ (1.5 mmol 487 mg) and DMF (2 mL) to obtain the desired 2-(4-nitrophenyl)benzo[d]thiazole 3v in 71% (182 mg) yield as pale yellow solid.

Figure 28. ¹H (400 MHz) NMR spectra of 3v in CDCl₃
**Figure 29.** $^{13}$C (100 MHz) NMR spectra of 3v in CDCl$_3$

$^1$HNMR (400 MHz, CDCl$_3$) δ = 7.18 (d, $^3$J (6′-H, 7′-H) = 8.4 Hz, $^3$J (3′-H, 4′-H) = 8.3 Hz, 2H; 4′-H and 6′-H), 7.32 (ddd, $^3$J (4-H, 5-H) = 8.5 Hz, $^3$J (5-H, 6-H) = 8.4 Hz, $^4$J (5-H, 7-H) = 1.8 Hz, 1H; 5-H), 7.40 (ddd, $^3$J (5-H, 6-H) = 8.5 Hz, $^3$J (6-H, 7-H) = 8.3 Hz, $^4$J (4-H, 6-H) = 0.8 Hz, 1H; 6-H), 7.90 (d, $^3$J (4-H, 5-H) = 7.9 Hz, 1H; 4-H), 7.98 (d, $^3$J (3′-H, 4′-H) = 8.0 Hz, 2H; 3′-H and 7′-H), 8.09 (d, $^3$J (6-H, 7-H) = 8.2 Hz, 1H; 7-H); $^{13}$C NMR (100 MHz, CDCl$_3$): δ = 115 (C-4), 119 (C-7), 121 (C-6), 123 (C-5), 125 (C-3′), 126 (C-5′), 126.5 (7′), 128 (C-4′), 131 (C-2′), 137 (C-7″), 148 ppm (C-2); HRMS (EI, [M + H]$^+$) calculated for C$_{13}$H$_9$ClINS (257.0144); found (257.0140)
Synthesis of 2-(4-bromophenyl)naphtho[1,2-d]oxazole (3w); unknown compound using (Method B)

According to the general procedure, reactions between 1-nitrosonaphthalene-2-ol 4a (1.0 mmol, 173 mg), 4'-bromoacetophenone 5j (1.0 mmol, 199 mg) were performed using CBr$_4$ (0.5 mmol, 165 mg), Cs$_2$CO$_3$ (2.1 mmol, 682 mg) and 10 mL CH$_3$CN to obtain the desired 2-(4-bromophenyl)naphtho[1,2-d]oxazole 3w in 53% (172 mg) yield as yellow crystalline solid.

*Figure 30.* $^1$H (400 MHz) NMR spectra of 3w in CDCl$_3$
Figure 31. $^{13}$C (100 MHz) NMR spectra of 3w in CDCl$_3$

$^1$H NMR (400 MHz, CDCl$_3$): $\delta$ = 7.59 (ddd, $^3J$ (3-H, 4-H) = 7.0 Hz, $^3J$ (2-H, 3-H) = 7.0 Hz, $^4J$ (1-H, 3-H) = 0.8 Hz, 1H; 3-H), 7.69 - 7.78 (m, 4H; 8-H, 9-H, 11-H and 12-H), 7.85 (d, $^3J$ (3-H, 4-H) = 8.2 Hz, 1H; 4-H), 8.00 (d, $^3J$ (1-H, 2-H) = 7.0 Hz, 1H; 2-H), 8.22 (d, $^3J$ (5-H, 6-H) = 7.0 Hz, 2H; 5-H and 6-H), 8.60 (d, $^3J$ (1-H, 2-H) = 8.2 Hz, 1H; 1-H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ = 110 (C-6), 122.0 (C-14), 125.4 (C-15), 125.6 (C-1), 126.2 (C-5), 126.4 (C-2), 126.6 (C-3), 127 (C-4), 128.0 (C-18), 128.7 (C-11 and C-12), 131 (C-10), 132 (C-8 and C-9), 137.10 (C-19), 148.0 (C-16), 161.0 ppm (C-17); HRMS (EI, [M + H]$^+$) calculated for C$_{17}$H$_{11}$BrNO (324.0023); found (324.0015).
Synthesis of 2-(3-bromophenyl)naphtho[1,2-d]oxazole (3x); unknown compound using (Method B)

According to the general procedure, reactions between 1-nitronaphthalene-2-ol 4a (1.0 mmol, 173 mg), 3'-bromoacetophenone 5k (1.0 mmol, 199 mg) were performed using CBr₄ (0.5 mmol, 165 mg), Cs₂CO₃ (2.1 mmol, 682 mg) and 10 mL CH₃CN to obtain the desired 2-(3-bromophenyl)naphtho[1,2-d]oxazole 3x in 65% (211 mg) yield as yellow crystalline solid.

Figure 32. ¹H (400 MHz) NMR spectra of 3x in CDCl₃
1H NMR (400 MHz, CDCl₃): δ = 7.42 (ddd, ³J (3-H, 4-H) = 7.0 Hz, ³J (2-H, 3-H) = 7.0 Hz, ⁴J (1-H, 3-H) = 0.8 Hz, 1H; 3-H), 7.57 (ddd, ³J (10-H, 11-H) = 7.0 Hz, ⁴J (8-H, 10-H) = 0.8 Hz, ⁴J (10-H, 12-H) = 0.8 Hz, 1H; 11-H), 7.63 - 7.73 (m, 3H; 11-H, 12-H and 8-H), 7.83 (d, ³J (1-H, 2-H) = 8.2 Hz, 1H; 2-H), 7.98 (d, ³J (3-H, 4-H) = 7.0 Hz, 1H; 4-H), 8.26 (d, ³J (5-H, 6-H) = 7.0 Hz, 1H; 5-H), 8.49 (m, ³J (5-H, 6-H) = 7.0 Hz, 1H; 6-H), 8.60 (d, ³J (1-H, 2-H) = 8.2 Hz, 1H; 1-H); ¹³C NMR (100 MHz, CDCl₃): δ = 110 (C-6), 122.1 (C-14), 123 (C-15), 125.0 (C-1), 125.8 (C-5), 126 (C-2), 126.6 (C-3), 127 (C-4), 128 (C-18), 129 (C-8), 130 (C-9), 130.4 (C-11), 131 (C-12), 133 (C-10), 137.1 (C-19), 148.0 (C-16), 161.3 ppm (C-17); HRMS (EI, [M + H]+) calculated for C₁₇H₁₁BrNO (324.0023); found (324.0015).

7. References
