Supporting Information

Synthesis of 2-Isoxazolyl-2,3-Dihydrobenzofurans via Palladium-Catalyzed Cascade Cyclization of Alkenyl Ethers

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A. General Information

$^1$H and $^{13}$C NMR spectra were recorded using Bruker DRX-400 spectrometer or Bruker DRX-500 spectrometer using CDCl$_3$ as solvent. The chemical shifts are referenced to residual $^1$H and $^{13}$C signals of the deuterated solvents respectively ($\delta_1 = 7.26$, $\delta_C = 77.00$ for chloroform). Melting points were determined with a Buchi Melting Point B-545 instrument. IR spectra were obtained either as potassium bromide pellets or as liquid films between two potassium bromide pellets with a Bruker TENSOR 27 spectrometer. The data of HRMS was carried out on a high-resolution mass spectrometer (LCMSIT-TOF). TLC was performed by using commercially prepared 100-400 mesh silica gel plates and visualization was effected at 254 nm. Unless otherwise noted, all reagents and solvents were obtained from commercial suppliers and used without further purification.

B. General Procedure for the Preparation of Alkynyl Oxime Ethers 1

Alkynyl oxime ethers were prepared according to the previously reported procedure.$^1$

\[
\begin{align*}
\text{O} & \quad \text{PdCl}_2(\text{PPh}_3)_2 \quad \text{CuI, Et}_3\text{N} \\
\text{Cl} & \quad \text{RT, 12 h} \\
\text{O} & \quad \text{NH}_2\text{OMe} \\
\text{Cl} & \quad \text{anhydrous Na}_2\text{SO}_4 \\
\text{R}^1 & \quad \text{pyridine (3.5 mmol/1.5 mL)} \\
\text{R}^2 & \quad \text{MeOH, RT, 12 h} \\
\text{N} & \quad \text{1} \\
\text{O} & \quad \text{RT, 12 h}
\end{align*}
\]

**Step 1:** PdCl$_2$(PPh$_3$)$_2$ (0.02 mmol, 0.4 mol %, 14 mg), CuI (0.1 mmol, 2 mol %, 19 mg), and triethylamine (10 mL) were added to a 50 mL round-bottom flask. The flask was flushed with nitrogen for 3 min, and the terminal acetylene (5.0 mmol) was added to the stirred suspension, followed by immediate dropwise addition of acyl chloride (6.5 mmol). The mixture was stirred at room temperature overnight. After the fully consumption of starting material by TLC detection, the resulting solution was extracted with diethyl ether (3 × 20 mL). The organic layers were combined and dried over anhydrous MgSO$_4$. The solvent was removed under vacuum, and the residue was purified by flash column chromatography on silica gel using PE/EA as the eluent to obtain alkynone B (85-90% yields).

**Step 2:** Alkynone B (3.5 mmol), methoxylamine hydrochloride (7.0 mmol, 2.0 equiv, 581 mg), anhydrous Na$_2$SO$_4$ (7.0 mmol, 2.0 equiv, 994 mg), pyridine (1 mL), and methanol (10 mL) were added to a 50 mL round-bottom flask. The reaction mixture was stirred at room temperature overnight. The mixture was diluted with saturated NH$_4$Cl solution (25 mL) and extracted with EtOAc (3 × 25 mL). The organic layers were combined, washed with brine, and dried over anhydrous MgSO$_4$. The solvent was removed under vacuum, and the residue was purified by flash column chromatography on silica gel using PE/EA as the eluent to give the desired product 1 (45-85% yields).
C. General Procedure for the Preparation of Alkenyl Ethers 2

Alkenyl ethers were prepared according to the previously reported procedure.\(^2\)

\[
\begin{align*}
\text{C} & \xrightarrow{\text{K}_2\text{CO}_3, \text{acetone}} \text{D} \\
\text{C} & \xrightarrow{\text{t-BuOK, DMSO}} \text{D} \\
\end{align*}
\]

**Step 1:** To a solution of 2-iodophenol (5.0 mmol) and 1,2-dibromoethane (5.0 equiv) in acetone (50 mL) was added K\(_2\)CO\(_3\) (2.0 equiv). The resulting mixture was stirred at room temperature for 14 h and then reflux for 6 h. The reaction was quenched with water and extracted with CH\(_2\)Cl\(_2\). The organic layer was washed with brine, dried over Na\(_2\)SO\(_4\), and concentrated. The crude product was purified by a silica gel column chromatography (hexanes/EtOAc = 100:1) to give D (65-70\% yields).

**Step 2:** To a solution of D (3.0 mmol) in DMSO (20 mL) was added t-BuOK (1.5 equiv). The resulting mixture was stirred at room temperature for 24 h. The reaction mixture was filtered and washed with CH\(_2\)Cl\(_2\). The combined filtrate was concentrated and the residue was purified by a silica gel column chromatography (hexanes/EtOAc = 100:1) to give the desired products 2 (75-90\% yields).

D. General Procedure for the Synthesis of Products 3

To a 25 mL dried reaction tube was added the mixture of Pd(OAc)\(_2\) (15 mol \%), CuCl\(_2\) (2.5 equiv), TBAB (1.0 equiv), K\(_2\)CO\(_3\) (2.0 equiv), alkynyl oxime ethers 1 (0.2 mmol) and alkenyl ethers 2 (0.4 mmol) in THF (2.5 mL) successively. The mixture was stirred at 60 °C for 12 h under air atmosphere. After the reaction was completed, the mixture was cooled to room temperature and diluted with H\(_2\)O (15 mL), and extracted with EtOAc (3 \times 10 mL). Collected organic layers were dried over anhydrous MgSO\(_4\) and concentrated in vacuum. The resulting crude was purified by flash column chromatography on silica gel with petroleum ether/ethyl acetate (150:1~50:1) to give the desired products 3.

E. Optimization of the Reaction Conditions

I. Screening of Additives

<table>
<thead>
<tr>
<th>Entry</th>
<th>Additive (equiv)</th>
<th>Yield of 3a (%)(^a)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>TBAB</td>
<td>64</td>
</tr>
<tr>
<td>2</td>
<td>TBAI</td>
<td>27</td>
</tr>
</tbody>
</table>

\(^a\) Yield determined by 1H NMR in CDCl\(_3\).
II. Screening of Oxidants

![Chemical structure](image)

<table>
<thead>
<tr>
<th>Entry</th>
<th>Oxidant (equiv)</th>
<th>Yield of 3a (%)b</th>
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<tbody>
<tr>
<td>1</td>
<td>CuCl₂2H₂O</td>
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<tr>
<td>2</td>
<td>CuCl₂</td>
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</tr>
<tr>
<td>3</td>
<td>CuSO₄</td>
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<tr>
<td>4</td>
<td>CuBr₂</td>
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<td>CuF₂</td>
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<tr>
<td>6</td>
<td>CuO</td>
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<tr>
<td>7</td>
<td>Cu(OAc)₂</td>
<td>trace</td>
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<tr>
<td>8</td>
<td>Cu(OH)₂</td>
<td>n.d.</td>
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<tr>
<td>9</td>
<td>CuBr</td>
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<td>16</td>
<td>H₂O₂</td>
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<td>17</td>
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<td>PhI(OAc)₂</td>
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<td><strong>21</strong></td>
<td>CuCl₂(2.5)</td>
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<td>22</td>
<td>CuCl₂(3.0)</td>
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*Reaction conditions: 1a (0.20 mmol), 2a (0.40 mmol), Pd(OAc)₂ (15 mol %), CuCl₂ (1.0 equiv), K₂CO₃ (2.0 equiv), THF (2.5 mL) stirred at 110 °C for 4.5 h in sealed tube. Detected by NMR using CH₂Br₂ as internal standard.
III. Screening of Bases

<table>
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<tr>
<th>Entry</th>
<th>Base (equiv)</th>
<th>Yield of 3a (%)&lt;sup&gt;b&lt;/sup&gt;</th>
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<td>Na&lt;sub&gt;2&lt;/sub&gt;CO&lt;sub&gt;3&lt;/sub&gt;</td>
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<td>NaHCO&lt;sub&gt;3&lt;/sub&gt;</td>
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<td>Et&lt;sub&gt;3&lt;/sub&gt;N</td>
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<tr>
<td>12</td>
<td>K&lt;sub&gt;2&lt;/sub&gt;CO&lt;sub&gt;3&lt;/sub&gt; (4.0)</td>
<td>72</td>
</tr>
</tbody>
</table>

<sup>a</sup>Reaction conditions: 1a (0.20 mmol), 2a (0.40 mmol), Pd(OAc)<sub>2</sub> (15 mol %), CuCl<sub>2</sub> (2.5 equiv), TBAB (1.0 equiv), THF (2.5 mL) stirred at 110 °C for 4.5 h in sealed tube.

<sup>b</sup>Detected by NMR using CH<sub>2</sub>Br<sub>2</sub> as internal standard.

F. Synthetic Applications

I. Synthetic Procedure for 4

To a resealable Schlenk tube was added 3e (0.2 mmol), phenylboronic acid (1.5 equiv), Pd(PPh<sub>3</sub>)<sub>4</sub> (5 mol %), K<sub>2</sub>CO<sub>3</sub> (2.0 equiv), THF (3.0 mL) and a stir bar. The reaction vessel was fitted with a rubber septum, which was evacuated and back-filled with nitrogen. The reaction tube was sealed and immersed in a preheated oil bath at 80 °C for 12 h and the solution was stirred with the aid of a magnetic stirrer. After the reaction was completed (monitored by TLC), the resulting mixture was cooled to room temperature and extracted with ethyl acetate. The combined organic layers were evaporated under vacuum. The desired product 4 was obtained in 92% yield after purified by column chromatography on silica gel with a mixture of petroleum ether/ethyl acetate (v/v = 50/1).
II. Synthetic Procedure for 5

3-(4-Bromophenyl)-4-(2,3-dihydrobenzofuran-2-yl)-5-phenylisoxazole (3e, 0.20 mmol), phenylacetylene (2.0 equiv), Pd(PPh₃)₂Cl₂ (5 mol %), CuI (10 mol %) and Et₃N (3.0 mL) were added in a Schlenk tube under nitrogen atmosphere and stirred at 80 °C for 12 h. After the reaction was completed (monitored by TLC), the resulting mixture was cooled to room temperature and extracted with ethyl acetate. The combined organic layers were evaporated under vacuum. The desired product 5 was obtained in 87% yield after purified by column chromatography on silica gel with a mixture of petroleum ether/ethyl acetate (v/v = 100/1).

III. Synthetic Procedure for 6

Step 1: To a resealable Schlenk tube was added 3e (1 mmol), Pd(PPh₃)₂Cl₂ (5 mol %), CuI (5 mol %), Et₃N (5.0 mL) and a stir bar. The reaction vessel was fitted with a rubber septum, which was evacuated and back-filled with nitrogen and then stirred for 5 min. After trimethylsilylacetylene was added (1.4 equiv), the reaction tube was immersed in a preheated oil bath at 40 °C for 10 h and the solution was stirred with the aid of a magnetic stirrer. The resulting mixture was cooled to room temperature and extracted with dichloromethane. After the reaction solution was vacuumed, potassium carbonate (3.0 mmol) was added. The mixed solution of dichloromethane and methanol (1/1) was used as solvent stirred at room temperature for 2 h. After the reaction was completed (monitored by TLC), the resulting mixture was extracted with ethyl acetate. The combined organic layers were evaporated under vacuum. The terminal alkyne product was obtained in 78% yield after purified by column chromatography on silica gel with a mixture of petroleum ether/ethyl acetate (v/v = 80/1).

Step 2: To a test tube was added the terminal alkyne product (0.15 mmol), benzyl azide (0.1 mmol) and 25% THF aqueous solution and a stir bar. After stirring at room temperature for 10 min, the mixture was added CuSO₄ (0.05 mmol) and sodium ascorbate (0.05 mmol). The reaction tube was stirred at room temperature for 12 h. After the reaction was completed (monitored by TLC), the resulting mixture was...
extracted with ethyl acetate and combined organic layers were evaporated under vacuum. The desired product 6 was obtained in 87% yield after purified by column chromatography on silica gel with a mixture of petroleum ether/ethyl acetate (v/v = 50/1).

IV. Synthetic Procedure for 7

To a resealable Schlenk tube was added 3e’ (0.1 mmol), morpholine (1.2 equiv), Pd(OAc)$_2$ (20 mol %), t-BuOK (3.0 equiv), toluene (5.0 mL) and a stir bar. The reaction vessel was fitted with a rubber septum, which was evacuated and back-filled with nitrogen and then stirred for 5 min. After tri-tert-butylphosphine (TTBP, 1.0 equiv) was added dropwise, the reaction tube was immersed in a preheated oil bath at 120 °C for 8 h and the solution was stirred with the aid of a magnetic stirrer. The resulting mixture was cooled to room temperature and extracted with ethyl acetate. The combined organic layers were evaporated under vacuum. The product was obtained in 91% yield after purified by column chromatography on silica gel with a mixture of petroleum ether/ethyl acetate (v/v = 50/1).

V. Synthetic Procedure for 8

To a resealable Schlenk tube was added 3e’ (0.1 mmol), 1-methylpiperazine (1.2 equiv), Pd(OAc)$_2$ (20 mol %), t-BuOK (3.0 equiv), toluene (5.0 mL) and a stir bar. The reaction vessel was fitted with a rubber septum, which was evacuated and back-filled with nitrogen, and then stirred for 5 min. After TTBP (1.0 equiv) was added dropwise, the reaction tube was immersed in a preheated oil bath at 120 °C for 8 h and the solution was stirred with the aid of a magnetic stirrer. The resulting mixture was cooled to room temperature and extracted with ethyl acetate. The combined organic layers were evaporated under vacuum. The product was obtained in 81% yield after purified by column chromatography on silica gel with a mixture of ethyl acetate/ethanol (v/v = 20/1).

VI. Synthetic Procedure for 9
To a resealable Schlenk tube were added 3e’ (0.1 mmol), thiomorpholine (1.2 equiv), Pd(OAc)$_2$ (20 mol%), $t$-BuOK (3.0 equiv), toluene (5.0 mL) and a stir bar. The reaction vessel was fitted with a rubber septum, which was evacuated and back-filled with nitrogen and then stirred for 5 min. After TTBP (1.0 equiv) was added drop by dropwise, the reaction tube was immersed in a preheated oil bath at 120 °C for 8 h and the solution was stirred with the aid of a magnetic stirrer. The resulting mixture was cooled to room temperature and extracted with ethyl acetate. The combined organic layers were evaporated under vacuum. The product was obtained in 76% yield after purified by column chromatography on silica gel with a mixture of petroleum ether/ethyl acetate (v/v = 30/1).

G. Analytical Data for All Compounds

1aa-1ah, 1al-1an, 1ba-1b and 2ag-2ai are known compounds and the NMR data are in good agreement with the literature\cite{1, 3, 4}. 1ai, 1aj and 1ak are unknown compounds and the corresponding NMR spectra data are shown as bellow.

(Z)-1-(3-Fluorophenyl)-3-phenylprop-2-yn-1-one O-Methyl Oxime (1i): Yield: 607 mg (48%), red oil. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.89 – 7.60 (m, 4 H), 7.42 (m, 4 H), 7.16 (m, 1H), 4.22 (s, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 162.6 (d, $J =$ 244.2 Hz), 138.6 (d, $J =$ 3.1 Hz), 135.6 (d, $J =$ 8.0 Hz), 132.0, 129.8 (d, $J =$ 8.2 Hz), 129.5, 128.3, 122.1 (d, $J =$ 2.9 Hz), 121.4, 116.4 (d, $J =$ 21.3 Hz), 113.1(d, $J =$ 23.6 Hz), 101.4, 78.9, 63.1; $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -98.29 – -120.95 (m) ppm; IR (KBr) $\tilde{\nu}$max 3070, 2937, 2814, 2205, 1602, 1439, 1332, 1240, 1166, 1046, 893, 796, 686, 520 cm$^{-1}$; HRMS (ESI) Calcd for C$_{16}$H$_{13}$FNO, [M+H]$^+$: 254.0976, found 254.0978.

(E)-1-(2-Chlorophenyl)-3-phenylprop-2-yn-1-one O-Methyl Oxime (1j): Yield: 605 mg (45%), red oil. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.60 (m, 3 H), 7.49 (d, $J =$ 6.4 Hz, 1H), 7.37 (m, 5H), 4.21 (s, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 138.8, 133.1, 131.9, 130.8, 130.2, 129.4, 128.2, 126.7, 121.6, 101.7, 80.0, 62.9 ppm; IR (KBr) $\tilde{\nu}$max 3592, 3068, 2935, 2202, 1956, 1810, 1563, 1445, 1330, 1240, 1166, 1037, 903, 810, 692, 543, 453 cm$^{-1}$; HRMS (ESI) Calcd for C$_{16}$H$_{13}$ClNO, [M+H]$^+$: 270.0680, found 270.0685.
(Z)-1-(Naphthalen-2-yl)-3-phenylprop-2-yn-1-one O-Methyl Oxime (1k): Yield: 576 mg (40%), white solid. M.p.: 115-116 °C. 1H NMR (400 MHz, CDCl3) δ 8.40 (s, 1H), 8.13 (d, J = 8.8 Hz, 1H), 8.02 – 7.82 (m, 3H), 7.80 – 7.68 (m, 2H), 7.54 (m, 2H), 7.48 – 7.39 (m, 3H), 4.24 (s, 3H); 13C NMR (100 MHz, CDCl3) δ 140.0, 133.9, 133.0, 132.1, 131.1, 129.5, 128.6, 128.4, 128.1, 127.5, 127.1, 126.8, 126.4, 123.0, 121.8, 101.2, 79.4, 63.2 ppm; IR (KBr)νmax 3059, 2936, 2817, 2207, 1958, 1601, 1446, 1331, 1250, 1178, 1049, 909, 814, 753, 684, 592, 469 cm⁻¹; HRMS (ESI) Calcd for C20H16NO, [M+H]+: 286.1226, found 286.1228.

2-Iodo-4-methyl-1-(vinyloxy)benzene (2aa): Yield: 867 mg (67%), yellow oil. 1H NMR (400 MHz, CDCl3) δ 7.67 (s, 1H), 7.14 (d, J = 8.4 Hz, 1H), 6.90 (d, J = 8.2 Hz, 1H), 6.60 (m, 1H), 4.76 (d, J = 13.8 Hz, 1H), 4.51 (d, J = 5.8 Hz, 1H), 2.32 (s, 3H); 13C NMR (100 MHz, CDCl3) δ 153.4, 148.4, 139.7, 134.7, 129.9, 117.1, 94.8, 87.3, 20.0 ppm; IR (KBr)νmax 3042, 2929, 1783, 1631, 1479, 1384, 1240, 1143, 1044, 953, 693, 537 cm⁻¹; HRMS (ESI) Calcd for C9H10IO, [M+H]+: 261.9849, found 261.9853.

4-Bromo-2-iodo-1-(vinyloxy)benzene (2ab): Yield: 949 mg (58%), brown oil. 1H NMR (400 MHz, CDCl3) δ 7.92 (d, J = 2.2 Hz, 1H), 7.42 (m, 1H), 6.84 (d, J = 8.8 Hz, 1H), 4.79 (m, 1H), 4.55 (m, 1H); 13C NMR (100 MHz, CDCl3) δ 155.1, 147.6, 141.5, 132.4, 118.1, 116.5, 96.6, 88.1 ppm; IR (KBr)νmax 3481, 3073, 2930, 1734, 1640, 1553, 1368, 1231, 1132, 1036, 811, 691 cm⁻¹; HRMS (ESI) Calcd for C8H7BrIO, [M+H]+: 324.8719, found 324.8710.

2-Iodo-4-(trifluoromethyl)-1-(vinyloxy)benzene (2ac): Yield: 813 mg (52%), brown oil. 1H NMR (400 MHz, CDCl3) δ 7.60 (d, J = 8.4 Hz, 2H), 7.08 (d, J = 8.4 Hz, 2H), 4.90 (d, J = 13.6 Hz, 2H), 4.59 (d, J = 6.0 Hz, 2H); 13C NMR (100 MHz, CDCl3) δ 159.3, 146.8, 127.1 (q, J = 3.7 Hz), 125.5, 125.3, 124.9, 122.8, 116.7, 97.3; 19F NMR (376 MHz, CDCl3) δ -61.85 ppm; IR (KBr)νmax 2936, 2417, 1725, 1614, 1518, 1513, 1239, 1131, 937, 815, 696 cm⁻¹; HRMS (ESI) Calcd for C9H7F3IO, [M+H]+: 314.9410, found 314.9415.

4-((tert-Butyl)-2-iodo-1-(vinyloxy)benzene (2ad): Yield: 906 mg (60%), yellow oil. 1H NMR (400 MHz, CDCl3) δ 7.80 (d, J = 2.0 Hz, 1H), 7.33 (dd, J = 8.6, 2.0 Hz, 1H), 6.91 (d, J = 8.6 Hz, 1H), 6.62 – 6.52 (m, 1H), 4.74 (dd, J = 13.8, 1.2 Hz, 1H), 4.59 – 4.26 (m, 1H), 1.30 (s, 9H); 13C NMR (100 MHz, CDCl3) δ 153.5, 148.4, 136.6, 126.6, 116.9, 95.2, 87.4, 34.2, 31.3 ppm; IR (KBr)νmax 3060, 2955, 1745, 1635, 1481, 1380, 1249, 1148, 1040, 952, 835, 693, 604 cm⁻¹; HRMS (ESI) Calcd for C12H16IO, [M+H]+: 303.0240, found 303.0235.
4-Chloro-1-iodo-2-(vinyloxy)benzene (2ae): Yield: 599 mg (43%), brown oil. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.71 (d, $J = 8.4$ Hz, 1H), 6.96 (d, $J = 2.4$ Hz, 1H), 6.85 (dd, $J = 8.4$, 2.2 Hz, 1H), 6.55 (dd, $J = 13.6$, 6.0 Hz, 1H), 4.86 (dd, $J = 13.6$, 2.0 Hz, 1H), 4.61 (dd, $J = 6.0$, 2.0 Hz, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 156.4, 147.2, 140.1, 135.2, 125.1, 117.3, 97.5, 84.4 ppm; IR (KBr)$\nu_{\text{max}}$ 3580, 3497, 3413, 3062, 2253, 1732, 1641, 1562, 1461, 1382, 1236, 1135, 960, 856, 676, 525 cm$^{-1}$; HRMS (ESI) Calcd for C$_8$H$_7$ClIO, [M+H]$^+$: 280.9225, found 280.9221.

4-(2,3-Dihydrobenzofuran-2-yl)-3,5-diphenylisoxazole (3a): Yield: 54 mg (81%), colorless solid. M.p.: 130.2 – 131.1 ºC. $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 7.74 (d, $J = 7.0$ Hz, 2H), 7.65 (d, $J = 7.4$ Hz, 2H), 7.53 – 7.43 (m, 3H), 7.39 (t, $J = 7.2$ Hz, 1H), 7.33 (t, $J = 7.3$ Hz, 2H), 7.17 (t, $J = 7.7$ Hz, 1H), 6.96 (d, $J = 7.2$ Hz, 1H), 6.85 (m, 2H), 5.85 (t, $J = 10.1$ Hz, 1H), 3.13 (m, 2H); $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 169.6, 163.7, 158.7, 130.5, 129.6, 129.0, 128.9, 128.8, 128.4, 128.3, 127.5, 126.8, 124.5, 120.8, 112.8, 109.5, 75.5, 34.8 ppm; IR (KBr)$\nu_{\text{max}}$ 3359, 3056, 2926, 1604, 1460, 1230, 1017, 910, 726, 496 cm$^{-1}$; HRMS (ESI) Calcd for C$_{23}$H$_{18}$NO$_2$, [M+H]$^+$: 340.1332, found 340.1331.

4-(2,3-Dihydrobenzofuran-2-yl)-5-phenyl-3-(p-tolyl)isoxazole (3b): Yield: 56 mg (80%), colorless solid. M.p.: 139.5 – 140.3 ºC. $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 7.73 (d, $J = 7.0$ Hz, 2H), 7.56 (d, $J = 7.7$ Hz, 2H), 7.46 (m, 3H), 7.17 (m, 3H), 6.98 (d, $J = 7.2$ Hz, 1H), 6.86 (m, 2H), 5.84 (t, $J = 10.1$ Hz, 1H), 3.52 – 2.94 (m, 2H), 2.36 (s, 3H); $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 169.5, 163.6, 158.7, 139.7, 130.4, 129.2, 128.8, 128.7, 128.4, 128.3, 127.5, 126.9, 126.0, 124.6, 120.8, 112.5, 109.5, 75.6, 34.6, 21.3 ppm; IR (KBr)$\nu_{\text{max}}$ 3432, 3050, 2931, 1613, 1461, 1327, 1228, 1021, 913, 827, 744, 592, 503 cm$^{-1}$; HRMS (ESI) Calcd for C$_{24}$H$_{20}$NO$_2$, [M+H]$^+$: 354.1489, found 354.1484.

4-(2,3-Dihydrobenzofuran-2-yl)-3-(4-fluorophenyl)-5-phenylisoxazole (3c): Yield: 61 mg (87%), colorless solid. M.p.: 126.7 – 127.8 ºC. $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 7.73 (d, $J = 7.0$ Hz, 2H), 7.68 – 7.59 (m, 2H), 7.56 – 7.39 (m, 3H), 7.18 (t, $J = 8.0$ Hz, 1H), 6.99 (m, 3H), 6.85 (t, $J = 8.0$ Hz, 2H), 5.84 (t, $J = 10.0$ Hz, 1H), 3.13 (m, 2H); $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 169.7, 163.6 (d, $J = 248.3$ Hz), 162.8, 158.6, 130.8 (d, $J = 8.3$ Hz), 130.6, 128.9, 128.4, 128.3, 126.9 (d, $J = 8.4$ Hz), 125.1 (d, $J = 3.1$ Hz), 124.6, 120.9, 115.7, 115.5, 112.8, 109.5, 75.4, 34.8; $^{19}$F NMR (470 MHz, CDCl$_3$) $\delta$ -109.05 – -115.69 (m) ppm; IR (KBr)$\nu_{\text{max}}$ 3058, 2934, 1604, 1457, 1333, 1230, 920, 844, 742, 595 cm$^{-1}$; HRMS (ESI) Calcd for C$_{23}$H$_{16}$FNNaO$_2$, [M+Na]$^+$: 380.1057, found 380.1066.
3-(4-Chlorophenyl)-4-(2,3-dihydrobenzofuran-2-yl)-5-phenylisoxazole (3d): Yield: 61 mg (83%), colorless solid. M.p.: 105.3 – 106.2 °C. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.75 (d, $J = 6.8$ Hz, 2H), 7.61 (d, $J = 8.0$ Hz, 2H), 7.50 (d, $J = 6.6$ Hz, 3H), 7.31 (d, $J = 8.0$ Hz, 2H), 7.21 (t, $J = 7.6$ Hz, 1H), 7.01 (d, $J = 7.2$ Hz, 1H), 6.89 (t, $J = 6.4$ Hz, 2H), 5.86 (t, $J = 10.0$ Hz, 1H), 3.23 (m, 1H), 3.08 (m, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 169.8, 162.6, 158.6, 135.9, 130.6, 130.2, 128.9, 128.7, 128.5, 128.4, 127.5, 127.2, 126.6, 124.6, 124.6, 124.2, 121.0, 112.8, 109.5, 75.3, 34.8 ppm; IR (KBr) $\tilde{\nu}_{\text{max}}$ 3057, 2930, 1597, 1460, 1328, 1229, 1092, 1012, 917, 837, 747, 510 cm$^{-1}$; HRMS (ESI) Calcd for C$_{23}$H$_{16}$ClNNaO$_2$, [M+Na]$^+$: 396.0762, found 396.0762.

3-(4-Bromophenyl)-4-(2,3-dihydrobenzofuran-2-yl)-5-phenylisoxazole (3e): Yield: 65 mg (78%), colorless solid. M.p.: 119.7 – 120.5 °C. $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 7.72 (d, $J = 7.1$ Hz, 2H), 7.48 (m, 7H), 7.19 (t, $J = 7.6$ Hz, 1H), 6.99 (d, $J = 7.1$ Hz, 1H), 6.86 (t, $J = 8.0$ Hz, 2H), 5.84 (t, $J = 10.0$ Hz, 1H), 3.14 (m, 2H); $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 169.8, 162.6, 158.5, 131.7, 130.6, 130.4, 128.8, 128.4, 128.3, 128.0, 127.2, 126.5, 124.6, 124.2, 121.0, 112.7, 109.5, 75.3, 34.8 ppm; IR (KBr) $\tilde{\nu}_{\text{max}}$ 3359, 2925, 1623, 1461, 1231, 1084, 1008, 917, 837, 751, 500 cm$^{-1}$; HRMS (ESI) Calcd for C$_{23}$H$_{16}$BrNNaO$_2$, [M+Na]$^+$: 440.0257, found 440.0259.

4-(2,3-Dihydrobenzofuran-2-yl)-5-phenyl-3-(4-(trifluoromethyl)phenyl)isoxazole (3f): Yield: 60 mg (74%), colorless solid. M.p.: 133.1 – 134.3 °C. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.75 (t, $J = 7.6$ Hz, 4H), 7.53 (m, 5H), 7.18 (t, $J = 7.6$ Hz, 1H), 6.96 (d, $J = 7.2$ Hz, 1H), 6.85 (t, $J = 7.8$ Hz, 2H), 5.85 (t, $J = 10.0$ Hz, 1H), 3.14 (m, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 169.8, 162.5, 158.5, 132.6, 131.7, 130.6, 130.4, 128.8, 128.4, 128.3, 128.0, 127.2, 126.5, 124.6, 124.2, 121.0, 112.7, 109.5, 75.3, 34.8 ppm; IR (KBr) $\tilde{\nu}_{\text{max}}$ 2937, 1605, 1466, 1323, 1136, 923, 845, 753, 592, 487 cm$^{-1}$; HRMS (ESI) Calcd for C$_{24}$H$_{16}$F$_3$NNaO$_2$, [M+Na]$^+$: 430.1025, found 430.1033.

4-(2,3-Dihydrobenzofuran-2-yl)-5-phenyl-3-(4-((trifluoromethyl)thio)phenyl)isoxazole (3g): Yield: 67 mg (77%), colorless solid. M.p.: 160.2 – 161.3 °C. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.74 (d, $J = 6.8$ Hz, 2H), 7.68 (d, $J = 8.0$ Hz, 2H), 7.58 (d, $J = 8.0$ Hz, 2H), 7.51 (m, 3H), 7.18 (t, $J = 7.6$ Hz, 1H), 6.95 (d, $J = 7.2$ Hz, 1H), 6.85 (t, $J = 7.2$ Hz, 2H), 5.86 (t, $J = 10.0$ Hz, 1H), 5.85 (t, $J = 3.6$ Hz, 124.5, 123.7 (d, $J = 270.8$ Hz), 121.0, 113.2, 109.5, 75.1, 35.0; $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -62.86 ppm; IR (KBr) $\tilde{\nu}_{\text{max}}$ 2937, 1605, 1466, 1323, 1236, 1136, 923, 845, 753, 592, 487 cm$^{-1}$; HRMS (ESI) Calcd for C$_{24}$H$_{16}$F$_3$NNaO$_2$S, [M+Na]$^+$: 462.1025, found 462.0752.
4-(2,3-Dihydrobenzofuran-2-yl)-3-(3-methoxyphenyl)-5-phenylisoxazole (3h): Yield: 57 mg (78%), colorless solid. M.p.: 144.5 – 145.6 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.80 (d, J = 6.6 Hz, 2H), 7.51 (d, J = 5.2 Hz, 3H), 7.31 (m, 2H), 7.21 (m, 2H), 7.01 (m, 2H), 6.90 (m, 2H), 5.91 (t, J = 10.2 Hz, 1H), 3.58 (s, 3H), 3.19 (d, J = 10.2 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 169.8, 163.4, 159.5, 158.6, 130.4, 130.2, 129.6, 128.8, 128.3, 128.2, 127.3, 126.9, 126.4, 126.1, 121.1, 120.9, 116.6, 113.1, 112.2, 109.5, 75.5, 54.8, 34.4 ppm; IR (KBr) νmax 3488, 3059, 2937, 2840, 1594, 1467, 1309, 1232, 1163, 1034, 903, 750, 694, 528, 451 cm⁻¹; HRMS (ESI) Calcd for C₂₄H₂₀NO₃, [M+H]+: 370.1438, found 370.1445.

4-(2,3-Dihydrobenzofuran-2-yl)-3-(3-fluorophenyl)-5-phenylisoxazole (3i): Yield: 57 mg (81%), colorless solid. M.p.: 144.1 – 144.9 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.76 (d, J = 6.8 Hz, 2H), 7.58 – 7.38 (m, 5H), 7.31 (m, 1H), 7.21 (t, J = 8.0 Hz, 1H), 7.11 (t, J = 8.4 Hz, 1H), 7.01 (d, J = 7.2 Hz, 1H), 6.88 (m, 2H), 5.88 (t, J = 10.0 Hz, 1H), 3.18 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 169.7, 162.6 (d, J = 2.3 Hz), 162.5 (d, J = 245.7 Hz), 158.5, 130.9 (d, J = 8.3 Hz), 130.6, 130.1 (d, J = 8.2 Hz), 128.8, 128.4, 128.3, 127.2 126.5 124.7 (d, J = 3.0 Hz), 124.5, 120.9, 116.6 (d, J = 20.9 Hz), 116.0 (d, J = 23.1 Hz), 112.9, 109.5, 75.2, 34.9; ¹⁹F NMR (376 MHz, CDCl₃) δ -112.11 (dd, J = 14.8, 9.0 Hz) ppm; IR (KBr) νmax 3060, 2936, 1594, 1465, 1229, 895, 752, 507 cm⁻¹; HRMS (ESI) Calcd for C₂₃H₁₆FNNaO₂, [M+Na]+: 380.1057, found 380.1063.

3-(2-Chlorophenyl)-4-(2,3-dihydrobenzofuran-2-yl)-5-phenylisoxazole (3j): Yield: 50 mg (68%), colorless solid. M.p.: 102.8 – 103.7 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.80 (m, 2H), 7.57 – 7.45 (m, 3H), 7.39 (m, 2H), 7.34 – 7.25 (m, 1H), 7.19 (m, 1H), 7.07 (t, J = 7.6Hz, 1H), 6.93 (d, J = 7.2 Hz, 1H), 6.77 (t, J = 7.4 Hz, 1H), 6.66 (d, J = 8.0 Hz, 1H), 6.10 – 5.59 (t, J = 9.2, 1H), 3.28 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 168.2, 161.4, 158.6, 133.6, 131.8, 130.7, 130.4, 129.4, 128.8, 128.3, 128.2, 128.1, 127.3, 126.4, 126.1, 124.3, 120.6, 115.0, 109.2, 75.1, 35.3 ppm; IR (KBr) νmax 3583, 3490, 3385, 3284, 3050, 2936, 2845, 2549, 2417, 2255, 1589, 1448, 1222, 1033, 910, 730, 497 cm⁻¹; HRMS (ESI) Calcd for C₂₃H₁₆ClNNaO₂, [M+Na]⁺: 396.0762, found 396.0765.

4-(2,3-Dihydrobenzofuran-2-yl)-3-(naphthalen-2-yl)-5-phenylisoxazole (3k): Yield: 56 mg (78%), colorless solid. M.p.: 161.4 – 162.5 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.16 (s, 1H), 7.82 (m, 5H), 7.52 (m, 5H), 7.49 – 7.38 (m, 1H), 7.24 (t, J = 7.8 Hz, 1H), 6.95 (q, J = 8.0 Hz, 2H), 6.84 (t, J = 7.4 Hz, 1H), 5.97 (t, J = 10.0 Hz, 1H), 3.41 – 2.96 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 169.9, 163.5, 158.7, 133.6, 132.9, 130.5, 129.0, 128.9, 128.5, 128.4, 128.3, 127.5, 127.4, 126.9, 126.3, 125.7, 124.7, 120.9, 112.7, 109.6, 75.6, 34.7 ppm; IR (KBr) νmax 3411, 3223, 3053, 2938, 2251, 1594, 1460, 1228, 917, 750, 579, 480 cm⁻¹; HRMS (ESI) Calcd for C₂₇H₁₉NNaO₂, [M+Na]⁺: 412.1308, found 412.1313.
4-(2,3-Dihydrobenzofuran-2-yl)-3-(furan-2-yl)-5-phenylisoxazole (3l): Yield: 48 mg (75%), colorless solid. M.p.: 105.1 – 106.1 °C. \(^1^H\) NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.65 (d, \(J = 7.2\) Hz, 2H), 7.53 – 7.39 (m, 3H), 7.33 (s, 1H), 7.17 (m, 2H), 7.00 – 6.70 (m, 3H), 6.43 (s, 1H), 6.04 (t, \(J = 10.0\) Hz, 1H), 3.64 – 3.06 (m, 2H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 169.0, 159.0, 154.2, 143.4, 130.5, 128.7, 128.4, 128.3, 127.1, 126.8, 124.6, 120.8, 112.3, 111.8, 111.5, 109.5, 75.3, 35.8 ppm; IR (KBr) \(\nu\) max 3385, 3052, 2930, 1598, 1468, 1327, 1229, 1159, 1084, 1010, 906, 826, 749, 589 cm\(^{-1}\); HRMS (ESI) Calcd for C\(_{21}\)H\(_{15}\)N\(_2\)O\(_3\), [M+Na]\(^+\): 352.0944, found 352.0945.

3-Cyclohexyl-4-(2,3-dihydrobenzofuran-2-yl)-5-phenylisoxazole (3m): Yield: 35 mg (51%), red oil. \(^1^H\) NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.60 (m, 2H), 7.42 (d, \(J = 6.0\) Hz, 3H), 7.18 (t, \(J = 8.0\) Hz, 2H), 7.02 – 6.65 (m, 2H), 5.87 (t, \(J = 9.6\) Hz, 1H), 3.38 (m, 2H), 2.57 (t, \(J = 11.6\) Hz, 1H), 2.01 (m, 2H), 1.84 – 1.44 (m, 6H), 1.41 – 1.15 (m, 2H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 167.7, 167.0, 159.0, 130.0, 128.7, 128.5, 128.1, 127.8, 126.2, 124.6, 120.9, 113.4, 109.4, 75.3, 36.3, 32.6, 31.7, 26.4, 26.2, 25.8 ppm; IR (KBr) \(\nu\) max 3420, 3049, 2930, 1614, 1461, 1231,95, 750, 502 cm\(^{-1}\); HRMS (ESI) Calcd for C\(_{25}\)H\(_{23}\)N\(_2\)O\(_2\), [M+Na]\(^+\): 368.1621, found 368.1625.

4-(2,3-Dihydrobenzofuran-2-yl)-3-phenyl-5-(p-tolyli)saxazole (3n): Yield: 55 mg (79%), colorless solid. M.p.: 138.7 – 139.6 °C. \(^1^H\) NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.67 (m, 4H), 7.39 (m, 3H), 7.29 (d, \(J = 7.6\) Hz, 2H), 7.21 (t, \(J = 7.6\) Hz, 1H), 7.00 (d, \(J = 7.2\) Hz, 1H), 6.88 (m, 2H), 5.87 (t, \(J = 10.0\) Hz, 1H), 3.52 – 2.81 (m, 2H), 2.44 (s, 3H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 169.8, 163.7 158.7, 140.9, 129.6, 129.5, 129.1, 128.9, 128.5, 128.3, 128.2, 126.9, 124.7, 124.6, 120.8, 112.2, 109.6, 75.6, 34.6, 21.5 ppm; IR (KBr) \(\nu\) max 3049, 2932, 2850, 1607, 1464, 1318, 1229, 1097, 1021, 911, 825, 746, 506 cm\(^{-1}\); HRMS (ESI) Calcd for C\(_{21}\)H\(_{17}\)N\(_2\)O\(_2\), [M+H]\(^+\): 354.1489, found 354.1484.

4-(2,3-Dihydrobenzofuran-2-yl)-5-(4-methoxyphenyl)-3-phenylisoxazole (3o): Yield: 54 mg (74%), colorless solid. M.p.: 135.2 – 136.3 °C. \(^1^H\) NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.79 – 7.57 (m, 4H), 7.48 – 7.28 (m, 3H), 7.18 (t, \(J = 7.8\) Hz, 1H), 6.97 (t, \(J = 7.6\) Hz, 3H), 6.85 (m, 2H), 5.82 (t, \(J = 10.2\) Hz, 1H), 3.84 (s, 3H), 3.27 – 2.90 (m, 2H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 169.6, 163.6, 161.3, 158.7, 129.9, 129.5, 129.1, 128.8, 128.5, 128.3, 126.9, 124.6, 120.7, 120.0, 114.2, 111.6, 109.5, 75.7, 55.3, 34.5 ppm; IR (KBr) \(\nu\) max 3591, 3442, 3228, 2935, 2838, 2248, 1622, 1459, 1248, 1170, 1100, 1026, 910, 835, 529, 449 cm\(^{-1}\); HRMS (ESI) Calcd for C\(_{25}\)H\(_{20}\)NO\(_3\), [M+H]\(^+\): 370.1438, found 370.1441.

5-(4-Chlorophenyl)-4-(2,3-dihydrobenzofuran-2-yl)-3-phenylisoxazole (3p): Yield: 60 mg (81%), red oil. \(^1^H\) NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.66 (m, 4H), 7.39 (m, 5H), 7.19 (t, \(J = 7.6\) Hz, 1H), 6.98 (d, \(J = 7.2\) Hz, 1H), 6.86 (m, 2H), 5.80 (t, \(J = 10.0\) Hz, 1H), 3.14 (m, 2H); \(^{13}\)C NMR (100 MHz,
4-(2,3-Dihydrobenzofuran-2-yl)-3-phenyl-5-(m-tolyl)isoxazole (3q): Yield: 52 mg (75%), colorless solid. M.p.: 130.3 – 131.3 ºC. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.66 (d, $J$ = 7.6 Hz, 2H), 7.54 (d, $J$ = 7.6 Hz, 1H), 7.50 (s, 1H), 7.37 (m, 4H), 7.28 (s, 1H), 7.18 (t, $J$ = 7.8 Hz, 1H), 6.97 (d, $J$ = 7.2 Hz, 1H), 6.86 (m, 2H), 5.84 (t, $J$ = 10.0 Hz, 1H), 3.19 (m, 1H), 3.09 (m, 1H), 2.26 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 169.8, 163.7, 158.8, 138.7, 131.2, 129.6, 129.1, 129.0, 128.9, 128.7, 128.6, 128.4, 127.5, 127.0, 125.4, 124.5, 120.8, 112.8, 109.6, 75.4, 34.8 ppm; IR (KBr) $\nu_{\text{max}}$ 3582, 3472, 3058, 2931, 1606, 1472, 1318, 1230, 1161, 1094, 1017, 918, 832, 747, 507 cm$^{-1}$; HRMS (ESI) Calcd for C$_{23}$H$_{16}$ClNNaO$_2$, [M+Na]$^+$: 396.0762, found 396.0765.

4-(2,3-Dihydrobenzofuran-2-yl)-5-(2-fluorophenyl)-3-phenylisoxazole (3r): Yield: 48 mg (68%), red oil. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.77 – 7.47 (m, 4H), 7.45 – 7.19 (m, 5H), 7.13 (t, $J$ = 7.4 Hz, 1H), 6.97 (d, $J$ = 6.8 Hz, 1H), 6.88 – 6.64 (m, 2H), 5.79 (t, $J$ = 9.6 Hz, 1H), 3.19 (m, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 163.6 (d, $J$ = 93.2 Hz), 159.5 (d, $J$ = 250.5 Hz), 158.7, 132.6 (d, $J$ = 8.3 Hz), 131.3, 129.6, 128.9, 128.8, 128.5, 128.2, 126.5, 124.5, 120.7, 116.4, 116.2, 115.9, 115.8, 115.6, 109.4, 75.3, 35.2; $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -112.09 ppm; IR (KBr) $\nu_{\text{max}}$ 3058, 2934, 1602, 1468, 1321, 1293, 1093, 1020, 919, 750, 613, 533 cm$^{-1}$; HRMS (ESI) Calcd for C$_{23}$H$_{16}$FNNaO$_2$, [M+Na]$^+$: 380.1057, found 380.1060.

4-(2,3-Dihydrobenzofuran-2-yl)-3-phenyl-5-(4'-propyl-[1,1'-biphenyl]-4-yl)isoxazole (3s): Yield: 74 mg (81%), colorless solid. M.p.: 148.1 – 149.3 ºC. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.81 (d, $J$ = 8.4 Hz, 2H), 7.68 (d, $J$ = 7.8 Hz, 4H), 7.55 (d, $J$ = 8.0 Hz, 2H), 7.38 (m, 3H), 7.29 (d, $J$ = 8.0 Hz, 2H), 7.20 (t, $J$ = 7.6 Hz, 1H), 6.99 (d, $J$ = 6.8 Hz, 1H), 6.95 – 6.79 (m, 2H), 5.90 (t, $J$ = 10.0 Hz, 1H), 3.34 – 2.98 (m, 2H), 2.66 (t, $J$ = 7.6 Hz, 2H), 1.72 (m, 2H), 1.00 (t, $J$ = 7.6 Hz, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 169.4, 163.7, 158.7, 143.2, 142.7, 137.2, 129.6, 129.0, 128.9, 128.5, 128.3, 127.2, 126.9, 126.8, 125.9, 124.6, 120.8, 112.7, 109.5, 75.5, 37.6, 34.7, 24.4, 13.8 ppm; IR (KBr) $\nu_{\text{max}}$ 3485, 3387, 3049, 2935, 1610, 1489, 1319, 1229, 1097, 1016, 916, 826, 741, 515 cm$^{-1}$; HRMS (ESI) Calcd for C$_{32}$H$_{27}$NNaO$_2$, [M+Na]$^+$: 480.1934, found 480.1933.
7.48 (d, J = 5.0 Hz, 1H), 7.44 – 7.30 (m, 4H), 7.19 (t, J = 7.6 Hz, 1H), 7.03 (d, J = 7.2 Hz, 1H), 6.87 (t, J = 6.4 Hz, 2H), 5.86 (t, J = 10.4 Hz, 1H), 3.31 – 2.96 (m, 2H); 13C NMR (100 MHz, CDCl₃) δ 165.3, 163.5, 158.7, 129.6, 128.9, 128.8, 128.6, 128.2, 126.9, 126.8, 126.7, 126.6, 124.6, 121.0, 119.1, 109.6, 75.5, 34.8 ppm; IR (KBr) νmax 3550, 3093, 2931, 1706, 1601, 1460, 1349, 1227, 900, 742 cm⁻¹; HRMS (ESI) Calcd for C₂₁H₁₅NNaO₂, [M+Na]⁺: 368.0716, found 368.0718.

4-(2,3-Dihydrobenzofuran-2-yl)-3-phenyl-5-propylisoxazole (3u): Yield: 27 mg (45%), red oil. ¹H NMR (400 MHz, CDCl₃) δ 7.61 – 7.48 (m, 2H), 7.42 – 7.31 (m, 3H), 7.16 (t, J = 7.6 Hz, 1H), 7.08 (d, J = 7.2 Hz, 1H), 6.91 – 6.76 (m, 2H), 5.72 (t, J = 9.6 Hz, 1H), 3.39 (m, 1H), 3.18 – 2.96 (m, 2H); 13C NMR (101 MHz, CDCl₃) δ 171.9, 162.3, 158.9, 129.5, 129.2, 128.7, 128.6, 126.3, 124.6, 120.9, 113.6, 109.4, 75.5, 36.6, 28.3, 21.4, 13.8 ppm; IR (KBr) νmax 3499, 3396, 3299, 3054, 2932, 2682, 2590, 2499, 1693, 1588, 1454, 1329, 1224, 901, 746 cm⁻¹; HRMS (ESI) Calcd for C₂₀H₁₉NNaO₂, [M+Na]⁺: 328.1308, found 328.1309.

5-Butyl-4-(2,3-dihydrobenzofuran-2-yl)-3-phenylisoxazole (3v): Yield: 36 mg (57%), red oil. ¹H NMR (400 MHz, CDCl₃) δ 7.58 (d, J = 7.4 Hz, 2H), 7.44 – 7.31 (m, 3H), 7.16 (t, J = 7.6 Hz, 1H), 7.09 (d, J = 7.6 Hz, 1H), 6.85 (m, 2H), 5.73 (t, J = 9.4 Hz, 1H), 3.40 (m, 1H), 3.12 (m, 1H), 2.80 (m, 2H), 1.68 (m, 2H), 1.44 – 1.25 (m, 2H), 0.90 (t, J = 7.2 Hz, 3H); 13C NMR (100 MHz, CDCl₃) δ 172.1, 162.3, 158.9, 129.5, 129.1, 128.7, 128.6, 126.3, 124.6, 120.8, 113.5, 109.4, 75.4, 36.5, 30.0, 26.1, 22.3, 13.6 ppm; IR (KBr) νmax 3357, 3451, 3056, 2944, 1695, 1605, 1462, 1326, 1231, 1089, 913, 750 cm⁻¹; HRMS (ESI) Calcd for C₂₁H₂₁NNaO₂, [M+Na]⁺: 342.1464, found 342.1468.

4-(2,3-Dihydrobenzofuran-2-yl)-5-pentyl-3-phenylisoxazole (3w): Yield: 36 mg (56%), red oil. ¹H NMR (400 MHz, CDCl₃) δ 7.63 – 7.53 (m, 2H), 7.42 – 7.30 (m, 3H), 7.16 (t, J = 7.6 Hz, 1H), 7.09 (d, J = 7.2 Hz, 1H), 6.91 – 6.71 (m, 2H), 5.72 (t, J = 9.6 Hz, 1H), 3.39 (m, 1H), 3.26 – 3.02 (m, 1H), 2.79 (m, 2H), 1.78 – 1.52 (m, 2H), 1.40 – 1.16 (m, 4H), 0.90 (m, 3H); 13C NMR (100 MHz, CDCl₃) δ 172.1, 162.3, 158.9, 129.5, 129.1, 128.7, 128.6, 126.3, 124.6, 120.8, 113.5, 109.4, 75.4, 36.6, 31.3, 27.7, 26.4, 22.2, 13.9 ppm; IR (KBr) νmax 3424, 3058, 2938, 1705, 1602, 1460, 1320, 1231, 1152, 915, 750 cm⁻¹; HRMS (ESI) Calcd for C₂₂H₂₃NNaO₂, [M+Na]⁺: 356.1621, found 356.1619.

4-(2,3-Dihydrobenzofuran-2-yl)-5-hexyl-3-phenylisoxazole (3x): Yield: 35 mg (51%), red oil. ¹H NMR (400 MHz, CDCl₃) δ 7.57 (m, 2H), 7.42 – 7.30 (m, 3H), 7.16 (t, J = 7.6 Hz, 1H), 7.09 (d, J = 7.2 Hz, 1H), 6.90 – 6.75 (m, 2H), 5.72 (t, J = 9.2 Hz, 1H), 3.39 (m, 1H), 3.23 – 2.95 (m,
1H), 2.91 – 2.46 (m, 2H), 1.78 – 1.60 (m, 2H), 1.29 (m, 6H), 0.88 (m, 3H); 13C NMR (100 MHz, CDCl3) δ 172.2, 162.3, 158.9, 129.5, 129.2, 128.7, 128.6, 128.4, 126.3, 124.6, 120.9, 113.5, 109.4, 75.5, 36.6, 31.3, 28.9, 27.9, 26.5, 22.4, 13.9 ppm; IR (KBr)νmax 3561, 3055, 2935, 1693, 1596, 1462, 1330, 1231, 1088, 914, 749, 516 cm⁻¹; HRMS (ESI) Calcd for C25H28N2O2, [M+H]+: 348.1958, found 348.1956.

4-(2,3-Dihydrobenzofuran-2-yl)-5-heptyl-3-phenylisoxazole (3y): Yield: 37 mg (52%), red oil. 1H NMR (400 MHz, CDCl3) δ 7.58 (d, J = 7.0 Hz, 2H), 7.43 – 7.31 (m, 3H), 7.16 (t, J = 7.6 Hz, 1H), 7.09 (d, J = 7.6 Hz, 1H), 6.93 – 6.75 (m, 2H), 5.73 (t, J = 9.6 Hz, 1H), 3.40 (m, 1H), 3.12 (m, 1H), 2.79 (m, 2H), 1.69 (m, 2H), 1.40 – 1.15 (m, 8H), 0.88 (t, J = 6.6 Hz, 3H); 13C NMR (101 MHz, CDCl3) δ 172.1, 162.2, 158.9, 129.4, 129.1, 128.6, 128.5, 128.3, 126.2, 124.6, 120.8, 113.4, 109.3, 75.4, 36.5, 31.6, 29.1, 28.7, 28.0, 26.4, 22.5, 14.0 ppm; IR (KBr)νmax 3281, 3056, 2933, 2862, 2851, 2512, 1712, 1589, 1449, 1215, 1020, 903, 728, 626, 532, 451 cm⁻¹; HRMS (ESI) Calcd for C24H22NNaO2, [M+Na]+: 384.1934, found 384.1939.

5-Cyclopropyl-4-(5-methyl-2,3-dihydrobenzofuran-2-yl)-3-phenylisoxazole (3z): Yield: 34 mg (54%), yellow oil. 1H NMR (400 MHz, CDCl3) δ 7.54 – 7.41 (m, 2H), 7.20 – 7.06 (m, 4H), 6.90 – 6.78 (m, 2H), 5.77 (t, J = 9.6 Hz, 1H), 3.46 – 3.18 (m, 2H), 2.33 (s, 3H), 2.10 – 1.83 (m, 1H), 1.33 – 1.09 (m, 2H), 1.06 – 0.82 (m, 2H); 13C NMR (100 MHz, CDCl3) δ 171.1, 162.2, 159.1, 139.6, 129.4, 128.6, 128.4, 126.6, 126.1, 124.7, 120.8, 113.3, 109.4, 75.6, 36.3, 21.3, 8.5, 8.1, 8.7 ppm; IR (KBr)νmax 3574, 3489, 3334, 3178, 3049, 2932, 2851, 2421, 1712, 1512, 1499, 1215, 1020, 903, 728, 626, 532, 451 cm⁻¹; HRMS (ESI) Calcd for C24H22NNaO2, [M+H]+: 318.1489, found 318.1484.

4-(5-Methyl-2,3-dihydrobenzofuran-2-yl)-3,5-diphenylisoxazole (3aa): Yield: 33 mg (47%), colorless solid. M.p.: 124.8 – 125.5 ºC. 1H NMR (400 MHz, CDCl3) δ 7.74 (d, J = 7.2 Hz, 2H), 7.66 (d, J = 7.4 Hz, 2H), 7.46 (d, J = 6.6 Hz, 3H), 7.36 (m, 3H), 6.97 (d, J = 8.0 Hz, 1H), 6.81 – 6.68 (m, 2H), 5.81 (t, J = 10.0 Hz, 1H), 3.09 (q, J = 15.6 Hz, 2H), 2.26 (s, 3H); 13C NMR (100 MHz, CDCl3) δ 169.6, 156.6, 156.4, 130.1, 129.6, 129.0, 128.9, 128.8, 128.6, 128.5, 128.4, 128.5, 128.4, 128.4, 128.3, 126.5, 125.1, 112.7, 109.0, 99.9, 75.6, 34.8, 20.7 ppm; IR (KBr)νmax 3504, 3232, 3163, 3062, 2927, 2848, 2762, 2678, 2421, 2256, 2081, 1964, 1876, 1622, 1477, 1215, 1117, 1016, 910, 807, 714, 616, 525, 438 cm⁻¹; HRMS (ESI) Calcd for C34H20N2O2, [M+H]+: 548.1489, found 548.1490.

4-(5-Bromo-2,3-dihydrobenzofuran-2-yl)-3,5-diphenylisoxazole (3ab): Yield: 43 mg (52%), red oil. 1H NMR (400 MHz, CDCl3) δ 7.71 (d, J = 7.2 Hz, 2H), 7.60 (d, J = 7.6 Hz, 2H), 7.41 (m, 6H), 7.27 (d, J = 7.6 Hz, 1H), 7.04 (s, 1H), 6.73 (d, J = 8.4 Hz, 1H), 5.85 (t, J = 10.0 Hz, 1H), 3.11 (m, 2H); 13C NMR (100 MHz, CDCl3) δ 169.8, 163.6, 157.9, 131.2, 130.7, 129.8, 129.3, 129.0, 128.9, 128.6, 128.4, 127.5, 127.3, 112.6, 112.4, 111.1, 76.2, 34.6 ppm; IR (KBr)νmax 3573, 3469, 3365, 3202, 2924, 2846, 2419, 1630, 1462, 1231, 1160, 1008, 905, 912, 708, 532, 453 cm⁻¹; HRMS (ESI)
Calcd for C\textsubscript{23}H\textsubscript{16}BrNNaO\textsubscript{2}, [M+Na]\textsuperscript{+}: 440.0257, found 440.0259.

3,5-Diphenyl-4-(5-(trifluoromethyl)-2,3-dihydrobenzofuran-2-yl)isoxazole (3ac):

Yield: 32 mg (41%), colorless solid. M.p.: 114.4 – 115.2 °C. \(^1\)H NMR (400 MHz, CDCl\textsubscript{3}) \(\delta\) 7.78 (d, \(J = 5.2\) Hz, 2H), 7.67 (d, \(J = 6.0\) Hz, 2H), 7.55 (m, 5H), 7.42 (d, \(J = 8.4\) Hz, 2H), 6.73 (d, \(J = 8.4\) Hz, 2H), 5.59 (t, \(J = 6.8\) Hz, 1H), 3.67 (m, 2H); \(^13\)C NMR (100 MHz, CDCl\textsubscript{3}) \(\delta\) 169.7, 163.1, 158.9, 130.7 (d, \(J = 85.9\) Hz), 129.2, 129.1, 128.9, 128.4, 127.8 (d, \(J = 121.0\) Hz), 127.1 (q, \(J = 3.6\) Hz), 125.3, 124.8, 124.5, 124.1, 123.8, 122.7, 116.2, 110.8, 71.9, 31.0; \(^19\)F NMR (376 MHz, CDCl\textsubscript{3}) \(\delta\) -61.78 ppm; IR (KBr) \(\nu\)\textsubscript{max} 3508, 3386, 3059, 2922, 2847, 1611, 1511, 1416, 1323, 1242, 1119, 989, 913, 836, 748, 700, 615, 518, 449 cm\(^{-1}\); HRMS (ESI) Calcd for C\textsubscript{24}H\textsubscript{16}F\textsubscript{3}NNaO\textsubscript{2}, [M+Na]\textsuperscript{+}: 430.1025, found 430.1026.

4-(5-((tert-Butyl)-2,3-dihydrobenzofuran-2-yl)-3,5-diphenylisoxazole (3ad):

Yield: 44 mg (56%), colorless solid. M.p.: 163.1 – 164.2 °C. \(^1\)H NMR (400 MHz, CDCl\textsubscript{3}) \(\delta\) 7.74 (m, 4H), 7.58 – 7.32 (m, 6H), 7.24 (d, \(J = 8.0\) Hz, 1H), 7.03 (s, 1H), 6.84 (d, \(J = 8.0\) Hz, 1H), 5.98 – 5.58 (t, \(J = 10.0\) Hz, 1H), 3.16 (m, 2H), 1.33 (s, 9H); \(^13\)C NMR (100 MHz, CDCl\textsubscript{3}) \(\delta\) 169.5, 163.7, 156.5, 143.9, 130.4, 129.5, 129.0, 128.9, 128.5, 128.4, 126.5, 125.0, 121.5, 113.0, 108.7, 75.6, 34.9, 34.2, 31.6 ppm; IR (KBr) \(\nu\)\textsubscript{max} 3058, 2952, 1604, 1481, 1237, 1126, 915, 814, 702, 594, 501 cm\(^{-1}\); HRMS (ESI) Calcd for C\textsubscript{27}H\textsubscript{26}NO\textsubscript{2}, [M+H]\textsuperscript{+}: 396.1958, found 396.1949.

4-(6-Chloro-2,3-dihydrobenzofuran-2-yl)-3,5-diphenylisoxazole (3ae):

Yield: 38 mg (51%), red oil. \(^1\)H NMR (400 MHz, CDCl\textsubscript{3}) \(\delta\) 7.71 (d, \(J = 7.2\) Hz, 2H), 7.61 (d, \(J = 7.6\) Hz, 2H), 7.40 (m, 6H), 6.83 (m, 3H), 5.87 (t, \(J = 10.0\) Hz, 1H), 3.08 (m, 2H); \(^13\)C NMR (100 MHz, CDCl\textsubscript{3}) \(\delta\) 169.8, 163.6, 159.6, 133.6, 130.7, 129.7, 129.0, 128.9, 128.5, 128.4, 127.5, 126.5, 125.0, 121.5, 113.0, 108.7, 75.6, 34.9, 34.2, 31.6 ppm; IR (KBr) \(\nu\)\textsubscript{max} 3481, 3418, 3256, 3059, 2922, 2758, 2418, 2259, 1969, 1613, 1470, 1323, 1148, 1065, 918, 839, 705, 615, 439 cm\(^{-1}\); HRMS (ESI) Calcd for C\textsubscript{23}H\textsubscript{17}ClNO\textsubscript{2}, [M+H]\textsuperscript{+}: 374.0942, found 374.0941.

anti-4-(3-Methyl-2,3-dihydrobenzofuran-2-yl)-3,5-diphenylisoxazole (3ag):

Yield: 43 mg (62%), colorless solid. M.p.: 173.3 – 174.1 °C. \(^1\)H NMR (500 MHz, CDCl\textsubscript{3}) \(\delta\) 7.78 (d, \(J = 6.5\) Hz, 2H), 7.70 (d, \(J = 7.0\) Hz, 2H), 7.56 – 7.32 (m, 6H), 7.20 (t, \(J = 7.5\) Hz, 1H), 6.91 (m, 3H), 5.30 (d, \(J = 10.0\) Hz, 1H), 3.57 – 3.02 (m, 1H), 1.14 (d, \(J = 6.5\) Hz, 3H); \(^13\)C NMR (125 MHz, CDCl\textsubscript{3}) \(\delta\) 170.2, 164.0, 158.3, 132.0, 130.5, 129.6, 129.0, 128.9, 128.8, 128.6, 128.5, 128.3, 127.5, 123.4, 121.0, 111.7, 109.7, 83.4, 40.8, 17.6 ppm; IR (KBr) \(\nu\)\textsubscript{max} 3059, 2915, 1901, 1697, 1597, 1459, 1304, 1224, 1096, 1023, 934, 846, 711, 592, 500 cm\(^{-1}\); HRMS (ESI) Calcd for C\textsubscript{24}H\textsubscript{20}NO\textsubscript{2}, [M+H]\textsuperscript{+}: 354.1489, found 354.1481.
3-[(1,1'-Biphenyl]-4-yl)-4-(2,3-dihydrobenzofuran-2-yl)-5-phenylisoxazole (4): Yield: 76 mg (92%), colorless solid. M.p.: 150.2 – 151.1 °C. 1H NMR (500 MHz, CDCl_3) δ 7.75 (s, 4H), 7.64 – 7.33 (m, 10H), 7.20 (s, 1H), 6.98 (s, 1H), 6.54 – 6.70 (m, 2H), 5.90 (s, 1H), 3.19 (dd, J = 18.0, 10.0 Hz, 2H); 13C NMR (126 MHz, CDCl_3) δ 169.7, 163.4, 158.7, 142.4, 140.2, 130.5, 129.3, 128.9, 128.8, 128.4, 128.3, 127.9, 127.7, 127.5, 127.2, 127.1, 126.9, 124.6, 120.9, 112.8, 109.6, 75.5, 34.8 ppm; IR (KBr) ν max 3049, 2931, 2847, 1690, 1599, 1463, 1319, 1226, 1013, 911, 845, 698, 577, 499 cm⁻¹; HRMS (ESI) Calcd for C_{26}H_{22}NO_2, [M+H]^+: 416.1645, found 416.1635.

4-(2,3-Dihydrobenzofuran-2-yl)-5-phenyl-3-(4-(phenylethynyl)phenyl)isoxazole (5): Yield: 76 mg (87%), colorless solid. M.p.: 162.6 – 163.5 °C. 1H NMR (500 MHz, CDCl_3) δ 7.75 (d, J = 5.5 Hz, 2H), 7.67 (d, J = 7.5 Hz, 2H), 7.52 (dd, J = 20.9, 4.6 Hz, 7H), 7.36 (s, 3H), 7.21 (t, J = 7.1 Hz, 1H), 7.01 (d, J = 6.6 Hz, 1H), 6.89 (dd, J = 12.3, 7.2 Hz, 2H), 5.87 (t, J = 9.9 Hz, 1H), 3.16 (dt, J = 25.8, 15.3 Hz, 2H); 13C NMR (126 MHz, CDCl_3) δ 169.9, 163.1, 158.6, 131.7, 131.6, 130.6, 128.8, 128.7, 128.5, 128.4, 128.3, 127.3, 126.7, 124.7, 124.6, 122.9, 121.0, 112.7, 109.6, 90.9, 88.8, 75.5, 34.8 ppm; IR (KBr) ν max 3055, 2932, 2215, 1894, 1696, 1602, 1459, 1325, 1228, 1019, 916, 843, 741 cm⁻¹; HRMS (ESI) Calcd for C_{31}H_{22}NO_2, [M+H]^+: 440.1645, found 440.1634.

3-(4-(1-Benzyl-1H,1,2,3-triazol-4-yl)phenyl)-4-(2,3-dihydrobenzofuran-2-yl)-5-phenylisoxazole (6): Yield: 43 mg (87%), colorless solid. M.p.:175.4 – 176.5 °C. 1H NMR (400 MHz, CDCl_3) δ 7.84 – 7.63 (m, 7H), 7.55 – 7.43 (m, 3H), 7.42 – 7.35 (m, 3H), 7.31 (dd, J = 7.4, 2.2 Hz, 2H), 7.16 (t, J = 7.8, 1H), 6.99 – 6.93 (m, 1H), 6.89 – 6.78 (m, 2H), 5.85 (t, J = 10.2 Hz, 1H), 5.56 (s, 2H), 3.14 (t, J = 9.8 Hz, 2H); 13C NMR (100 MHz, CDCl_3) δ 169.8, 163.2, 158.6, 147.4, 134.5, 131.8, 130.6, 129.4, 129.1, 128.9, 128.8, 128.7, 128.5, 128.4, 128.1, 127.4, 126.8, 125.7, 124.7, 120.9, 119.9, 112.6, 109.6, 75.6, 54.2, 34.7; IR (KBr) ν max 3052, 2926, 2848, 1601, 1454, 1351, 1228, 1043, 909, 840, 735, 458 cm⁻¹; HRMS (ESI) Calcd for C_{32}H_{22}O_2S_2, [M+H]^+: 497.1972, found 496.1972.

4-(4-(2,3-Dihydrobenzofuran-2-yl)-3-phenylisoxazol-5-yl)phenyl)morpholine (7): Yield: 38 mg (91%), brown solid. M.p.:156.3 – 157.1 °C. 1H NMR (400 MHz, CDCl_3) δ 7.64 (t, J = 7.4 Hz, 4H), 7.35 (m, 3H), 7.17 (t, J = 7.6 Hz, 1H), 7.05 – 6.74 (m, 5H), 5.82 (t, J = 10.0 Hz, 1H), 3.86 (t, J = 4.7 Hz, 4H), 3.24 (t, J = 4.8 Hz, 4H), 3.13 (d, J = 10.2 Hz, 2H); 13C NMR (100 MHz, CDCl_3) δ 169.9, 163.7, 158.8, 152.4, 129.5, 129.4, 129.2, 128.9, 128.5, 128.3, 127.1, 126.4, 120.7, 118.2, 114.6, 111.0, 109.6, 75.9, 66.6, 48.0, 34.5 ppm; IR (KBr) ν max 3201, 3055, 2963, 2921, 2854, 1610, 1516, 1453, 1417, 1361, 1304, 1234, 1120, 977,928, 897, 749, 644, 525 cm⁻¹; HRMS (ESI) Calcd for C_{25}H_{23}N_2O_3, [M+H]^+: 425.1860, found 425.1855.

4-(2,3-Dihydrobenzofuran-2-yl)-5-(4-(4-methylpiperazin-1-yl)phenyl)-3-
phenyliso xazole (8): Yield: 35 mg (81%), brown solid. M.p.:162.7 – 163.6 °C. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.64 (d, 4H), 7.50 – 7.29 (m, 3H), 7.17 (t, \(J = 7.8\) Hz, 1H), 7.04 – 6.70 (m, 5H), 5.82 (t, \(J = 10.0\) Hz, 1H), 3.30 (t, \(J = 5.0\) Hz, 4H), 3.13 (d, \(J = 10.0\) Hz, 2H), 2.56 (t, \(J = 5.0\) Hz, 4H), 2.35 (s, 3H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 169.9, 163.7, 158.79, 152.3, 129.5, 129.4, 129.2, 128.9, 128.5, 128.2, 124.6, 120.7, 117.6, 114.8, 110.8, 109.5, 75.9, 54.8, 47.7, 46.1, 34.4 ppm; IR (KBr) \(\tilde{\nu}_{\text{max}}\) 3523, 3449, 3403, 3277, 2987, 2903, 2044, 1764, 1672, 1603, 1477, 1430, 1373, 1247, 1052, 1005, 931, 857, 704, 749, 650, 613, 512, 466 cm\(^{-1}\); HRMS (ESI) Calcd for C\(_{28}\)H\(_{28}\)N\(_3\)O\(_2\), [M+H]\(^+\): 438.2176, found 438.2171.

4-(2,3-Dihydrobenzofuran-2-yl)-3-phenyl-5-(4-thiomorpholinophenyl)isoxazole (9): Yield: 33 mg (76%), brown solid. M.p.:169.8 – 170.7 °C. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.80 – 7.57 (m, 4H), 7.48 – 7.29 (m, 3H), 7.20 – 7.10 (m, 1H), 6.93 – 6.77 (m, 4H), 5.82 (t, \(J = 10.2\) Hz, 1H), 3.81 – 3.52 (m, 4H), 3.14 (d, \(J = 10.2\) Hz, 2H), 2.82 – 2.60 (m, 4H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 169.9, 163.7, 158.8, 151.5, 129.7, 129.5, 129.2, 128.9, 128.5, 128.3, 127.1, 124.6, 120.7, 117.4, 115.3, 110.8, 109.6, 75.9, 50.7, 34.5, 26.1 ppm; IR (KBr) \(\tilde{\nu}_{\text{max}}\) 3049, 2919, 2851, 1608, 1515, 1416, 1385, 1359, 1286, 1226, 1193, 1100, 1018, 949, 895, 858, 822, 749, 699, 526, 453, 421 cm\(^{-1}\); HRMS (ESI) Calcd for C\(_{27}\)H\(_{25}\)N\(_2\)O\(_2\)S, [M+H]\(^+\): 441.1630, found 441.1630.

H. References

I. X-ray Crystallographic Analysis

I. X-ray Crystallographic Analysis for 3c

Table S1. Crystal data and structure refinement for 3c

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<th>Property</th>
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<td>Empirical formula</td>
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<td>$b = 11.2727(7)$ Å, $\beta = 83.916(2)^\circ$</td>
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<td>$c = 14.3335(8)$ Å, $\gamma = 83.801(2)^\circ$</td>
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<td>$R_1 = 0.0863, wR_2 = 0.1204$</td>
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II. X-ray Crystallographic Analysis for 3ag

![Chemical structure of 3ag]

CCDC: 2053026

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<td><strong>Final $R$ indices [$I &gt; 2\sigma(I)$]</strong></td>
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<td><strong>Final $R$ indices (all data)</strong></td>
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J. NMR Spectra for All the Compounds

(Z)-1-(3-Fluorophenyl)-3-phenylprop-2-yn-1-one O-Methyl Oxime (1i)
$^{19}$F NMR (376 MHz, CDCl$_3$)
\((E)-1-(2\text{-Chlorophenyl})-3\text{-phenylprop-2-yn-1-one} \ O\text{-Methyl Oxime} \ (1j)\)

\[\text{H NMR} \ (400 \text{ MHz, CDCl}_3)\]

\[\text{C NMR} \ (100 \text{ MHz, CDCl}_3)\]
(Z)-1-(Naphthalen-2-yl)-3-phenylprop-2-yn-1-one O-Methyl Oxime (1k)

$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (100 MHz, CDCl$_3$)
2-Iodo-4-methyl-1-(vinyl oxy)benzene (2aa)

$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (100 MHz, CDCl$_3$)
4-Bromo-2-iodo-1-(vinylloxy)benzene (2ab)

$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (100 MHz, CDCl$_3$)
2-Iodo-4-(trifluoromethyl)-1-(vinylxy)benzene (2ac)
$^{19}$F NMR (376 MHz, CDCl$_3$)
4-(\textit{tert}-Butyl)-2-iodo-1-(vinylxoy)benzene (2ad)
4-Chloro-1-iodo-2-(vinyloxy)benzene (2ae)

$^1$H NMR (100 MHz, CDCl$_3$)

$^{13}$C NMR (400 MHz, CDCl$_3$)
4-(2,3-Dihydrobenzofuran-2-yl)-3,5-diphenyloxazole (3a)
4-(2,3-Dihydrobenzofuran-2-yl)-5-phenyl-3-(p-tolyl)isoxazole (3b)

$^1$H NMR (500 MHz, CDCl$_3$)

$^{13}$C NMR (125 MHz, CDCl$_3$)
4-(2,3-Dihydrobenzofuran-2-yl)-3-(4-fluorophenyl)-5-phenylisoxazole (3c)
$^{19}F$ NMR (470 MHz, CDCl₃)
3-(4-Chlorophenyl)-4-(2,3-dihydrobenzofuran-2-yl)-5-phenylisoxazole (3d)

$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (100 MHz, CDCl$_3$)
3-(4-Bromophenyl)-4-(2,3-dihydrobenzofuran-2-yl)-5-phenylisoxazole (3e)

$^1$H NMR (500 MHz, CDCl$_3$)

$^{13}$C NMR (125 MHz, CDCl$_3$)
4-(2,3-Dihydrobenzofuran-2-yl)-5-phenyl-3-(4-(trifluoromethyl)phenyl)isoxazole (3f)

$^{1}\text{H NMR (400 MHz, CDCl}_3$)

$^{13}\text{C NMR (100 MHz, CDCl}_3$)
$^{19}F$ NMR (376 MHz, CDCl$_3$)
4-(2,3-Dihydrobenzofuran-2-yl)-5-phenyl-3-(4-((trifluoromethyl)thio)phenyl)isoxazole (3g)

$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (100 MHz, CDCl$_3$)
4-(2,3-Dihydrobenzofuran-2-yl)-3-(3-methoxyphenyl)-5-phenylisoxazole (3h)

$\text{H NMR (400 MHz, CDCl}_3$)

$\text{C NMR (100 MHz, CDCl}_3$)
4-(2,3-Dihydrobenzofuran-2-yl)-3-(3-fluorophenyl)-5-phenylisoxazole (3i)
$^1$H NMR (376 MHz, CDCl$_3$)
3-(2-Chlorophenyl)-4-(2,3-dihydrobenzofuran-2-yl)-5-phenylisoxazole (3j)

$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (100 MHz, CDCl$_3$)
4-(2,3-Dihydrobenzofuran-2-yl)-3-(naphthalen-2-yl)-5-phenylisoxazole (3k)

\[ \text{\textsuperscript{1}H NMR (400 MHz, CDCl\textsubscript{3})} \]

\[ \text{\textsuperscript{13}C NMR (100 MHz, CDCl\textsubscript{3})} \]
4-(2,3-Dihydrobenzofuran-2-yl)-3-(furan-2-yl)-5-phenylisoxazole (3l)

\[ \text{H NMR (400 MHz, CDCl}_3 \text{)} \]

\[ \text{C NMR (100 MHz, CDCl}_3 \text{)} \]
3-Cyclohexyl-4-(2,3-dihydrobenzofuran-2-yl)-5-phenylisoxazole (3m)

$^1$H NMR (400 MHz, CDC$_3$)

$^{13}$C NMR (100 MHz, CDC$_3$)
4-(2,3-Dihydrobenzofuran-2-yl)-3-phenyl-5-(p-tolyl)isoxazole (3n)

$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (100 MHz, CDCl$_3$)
4-(2,3-Dihydrobenzofuran-2-yl)-5-(4-methoxyphenyl)-3-phenylisoxazole (3o)

$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (100 MHz, CDCl$_3$)
5-(4-Chlorophenyl)-4-(2,3-dihydrobenzofuran-2-yl)-3-phenylisoxazole (3p)
4-(2,3-Dihydrobenzofuran-2-yl)-3-phenyl-5-(m-tolyl)isoxazole (3q)

$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (100 MHz, CDCl$_3$)
4-(2,3-Dihydrobenzofuran-2-yl)-5-(2-fluorophenyl)-3-phenylisoxazole (3r)

$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (100 MHz, CDCl$_3$)
$^1$H NMR (370 MHz, CDCl$_3$)
4-(2,3-Dihydrobenzofuran-2-yl)-3-phenyl-5-(4’-propyl-[1,1’-biphenyl]-4-yI)isoxazole (3s)

\[ \text{\^{1}H NMR (400 MHz, CDCl}_3\text{)} \]

\[ \text{\^{13}C NMR (100 MHz, CDCl}_3\text{)} \]
4-(2,3-Dihydrobenzofuran-2-yl)-3-phenyl-5-(thiophen-3-yl)isoxazole (3t)

$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (100 MHz, CDCl$_3$)

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4-(2,3-Dihydrobenzofuran-2-yl)-3-phenyl-5-propylisoxazole (3u)

\[ \text{\( ^1H \) NMR (400 MHz, CDCl\textsubscript{3})} \]

\[ \text{\( ^{13}C \) NMR (100 MHz, CDCl\textsubscript{3})} \]
5-Butyl-4-(2,3-dihydrobenzofuran-2-yl)-3-phenylisoxazole (3v)

$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (100 MHz, CDCl$_3$)
4-(2,3-Dihydrobenzofuran-2-yl)-5-pentyl-3-phenylisoxazole (3w)

$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (100 MHz, CDCl$_3$)
4-(2,3-Dihydrobenzofuran-2-yl)-5-hexyl-3-phenylisoxazole (3x)

$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (100 MHz, CDCl$_3$)
4-(2,3-Dihydrobenzofuran-2-yl)-5-heptyl-3-phenylisoxazole (3y)

$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (100 MHz, CDCl$_3$)
5-Cyclopropyl-4-(5-methyl-2,3-dihydrobenzofuran-2-yl)-3-phenylisoxazole (3z)

$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (100 MHz, CDCl$_3$)
4-(5-Methyl-2,3-dihydrobenzofuran-2-yl)-3,5-diphenyloxazole (3aa)
4-(5-Bromo-2,3-dihydrobenzofuran-2-yl)-3,5-diphenylisoxazole (3ab)
3,5-Diphenyl-4-(5-(trifluoromethyl)-2,3-dihydrobenzofuran-2-yl)isoxazole (3ac)

$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (100 MHz, CDCl$_3$)

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$^1$H NMR (376 MHz, CDCl$_3$)
4-(5-(tert-Butyl)-2,3-dihydrobenzofuran-2-yl)-3,5-diphenylisoxazole (3ad)
4-(6-Chloro-2,3-dihydrobenzofuran-2-yl)-3,5-diphenyloxazole (3ae)
anti-4-(3-Methyl-2,3-dihydrobenzofuran-2-yl)-3,5-diphenyloxazole (3ag)
3-([1,1'-Biphenyl]-4-yl)-4-(2,3-dihydrobenzofuran-2-yl)-5-phenylisoxazole (4)
4-(2,3-Dihydrobenzofuran-2-yl)-5-phenyl-3-(4-(phenylethynyl)phenyl)isoxazole (5)
3-(4-(1-Benzyl-1H-1,2,3-triazol-4-yl)phenyl)-4-(2,3-dihydrobenzofuran-2-yl)-5-phenylisoxazole (6)
4-(4-(4-(2,3-Dihydrobenzofuran-2-yl)-3-phenylisoxazol-5-yl)phenyl)morpholine (7)
4-(2,3-Dihydrobenzofuran-2-yl)-5-(4-(4-methylpiperazin-1-yl)phenyl)-3-phenylisoazole (8)
4-(2,3-Dihydrobenzofuran-2-yl)-3-phenyl-5-(4-thiomorpholinophenyl)isoxazole (9)