Supporting Information

Rhodium(III)-Catalyzed Cascade Reactions of Benzoic Acids with Dioxazolones: Discovery of 2,5-Substituted Benzoxazinones as AIE Molecules

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1. General Information

Catalytic reactions were carried out in Schlenk tubes using pre-dried glassware. 1,4,2-Dioxazol-5-ones 2a-4 were prepared according to previously described procedures (Xiong, H. et al. Org. Chem. Front. 2018, 5, 2880–2284). Other chemicals were obtained from commercial sources and used without further purification. Column chromatography purifications were performed using 200–300 mesh silica gel. Melting points were determined with a SGW X-4 digital melting point apparatus, and the thermometer was uncorrected. NMR spectra were mostly recorded for $^1$H NMR at 500 MHz, for $^{13}$C NMR at 125 MHz and for $^{19}$F NMR at 471 MHz. CDCl$_3$ and d$_6$-DMSO was used as solvent. Chemical shifts were referenced relative to residual solvent signal (CDCl$_3$, $^1$H NMR: δ 7.26 ppm, $^{13}$C NMR: δ 77.16 ppm; d$_6$-DMSO, $^1$H NMR: δ 2.50 ppm, $^{13}$C NMR: δ 39.99 ppm). The following abbreviations are used to describe peak patterns where appropriate: br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Coupling constants (J) are reported in Hertz (Hz). Infrared (IR) spectra were recorded on a Bruker Vector 22 infrared spectrometer and reported in cm$^{-1}$. HRMS were performed on Agilent Technologies 6224 TOF LC/MS apparatus (ESI). UV-Visible absorption spectra were measured using Shimadzu UV-1800 spectrophotometer. Fluorescence spectra were measured on a Shimadzu RF-5301PC spectrometer with a slit width 3 nm for emission. The water/THF mixtures with different water fractions were prepared by slowly adding distilled water into the THF solution of samples under ultrasound at room temperature. Fluorescence quantum yields of compounds in solution and in powders were measured on Absolutely Photoluminescence Quantum Yield Measurement System (HAMAMARSU, C11347-11Quantaurus-QY).

2. Optimization of Reaction Conditions

We embarked on our study with the optimization of reaction conditions first, using benzoic acid 1a and 1,4,2-dioxazolone 2a as the model substrates (Table S1). The reaction afforded no product with [Cp*RhCl$_2$]$_2$ as the catalyst and NaOAc as the base in THF at 120 °C (entry 1). However, an addition of 15% AgSbF$_6$ altered the result and led to the formation of desired product 3a in 40% isolated yield (entry 2), indicating the crucial role AgSbF$_6$ played as a halogen scavenger additive in this reaction. Next, we screened various solvents and found that THF was the most favorable among all to give desired product in good yield (entries 2–5). Several base candidates were then surveyed for the reaction and the uniformly decreased amount of products (entries 6–8) indicated NaOAc is the base of choice. Lowering temperature from 120 °C to 50 °C led to a continuous reduction of the product turnover (entries 9–10). Meanwhile, significant improvement in reaction yield (48%, entry 11) was observed when the concentration of AgSbF$_6$ was increased from 15% to 30%, although further densifying AgSbF$_6$ only resulted in a slight additional increase of the yield (50%, entry 12). In the presence of 30% AgSbF$_6$, we examined the base ratio and found that increasing the molarity of NaOAc from 0.1 to 0.2 mmol accelerated the reaction to afford more products (entries 13 and 14). However, further addition of NaOAc (0.4 mmol, entry 15) completely depleted the product. On the other hand, decreasing the amount of 1,4,2-dioxazolone 2a by half afforded less product 3a (42%, entry 16). Based on these results, we were able to determine the optimal reaction conditions as shown by entry 14.
### Table S1. Optimization of Reaction Conditions

<table>
<thead>
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<th>entry</th>
<th>catalyst system</th>
<th>base</th>
<th>solvent</th>
<th>yield&lt;sup&gt;ab&lt;/sup&gt;</th>
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<td>THF</td>
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<td>MeOH</td>
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<td>NaOAc</td>
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<tr>
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<td>NaOAc</td>
<td>THF</td>
<td>42%</td>
</tr>
</tbody>
</table>

<sup>a</sup>Reaction conditions: 1a (0.2 mmol), 2a (0.2 mmol), cat (5 mol%), AgSbF<sub>6</sub> (15 mol%), base (0.04 mmol), solvent (2 mL), 120 °C, 12 h. <sup>b</sup>Isolated yields calculated by dioxazolones 2. <sup>c</sup>80 °C. <sup>d</sup>50 °C. <sup>e</sup>AgSbF<sub>6</sub> (30 mol%). <sup>f</sup>AgSbF<sub>6</sub> (45 mol%). <sup>g</sup>AgSbF<sub>6</sub> (30 mol%), NaOAc (0.1 mmol). <sup>h</sup>AgSbF<sub>6</sub> (30 mol%), NaOAc (0.2 mmol). <sup>i</sup>AgSbF<sub>6</sub> (30 mol%), NaOAc (0.4 mmol). <sup>j</sup>2a (0.1 mmol).

### 3. General Procedure for the Synthesis and Characterization

#### 3.1 General procedure for the synthesis of 3-substituted-1,4,2-dioxazol-5-ones (2)

3-Substituted-1,4,2-dioxazol-5-ones 2 were prepared according to the methods given in the cited references (Xiong, H. et. al. Org. Chem. Front. 2018, 5, 2880–2284).

A flask was charged with hydroxylamine hydrochloride (1 equivalent), potassium carbonate (1 equivalent) and solvent (EA/H<sub>2</sub>O, 7:1). The reaction was cooled to 0 °C with vigorous stirring and
substituted acyl chloride (1 equivalent) was added dropwise. The reaction was stirred overnight, diluted with water and extracted with ethyl acetate. The combined organic layers were washed with brine, dried over anhydrous sodium sulfate and concentrated \textit{in vacuo}. The crude hydroxamic acid product was purified by recrystallization from EtOAc/Pentane.

To a slurry of hydroxamic acid (1 equivalent) in dichloromethane was added carbonyl diimidazole (CDI, 1.5 equivalents). The reaction was stirred for 30 minutes, diluted with 1M aqueous HCl and extracted with dichloromethane. The combined organic layers were dried over sodium sulfate, and concentrated \textit{in vacuo} to give dioxazolone 2. Purification by dissolving in toluene and filtration was performed in necessary.

### 3.2 General procedure for the synthesis of desired product 3

![Chemical structure of reaction](image)

Benzoic acid 1 (0.20 mmol), 1,4,2-dioxazol-5-one 2 (0.20 mmol), NaOAc (17 mg, 0.20 mmol), AgSbF$_6$ (20 mg, 0.06 mmol) and [Cp*RhCl$_2$]$_2$ (6 mg, 0.010 mmol) were placed into a 10 mL sealing tube. THF (2.0 mL) was then introduced and the reaction mixture was stirred at 120 °C for 12 h. After cooling to ambient temperature, a saturated NaHCO$_3$ solution was added to the reaction and the mixture was extracted three times with CHCl$_3$ followed by washing with water and saturated brine. Then it was concentrated under vacuum and the residue was loaded onto silica gel and purified by flash column chromatography (petroleum ether/chloroform/EtOAc) to afford the desired product 3.

### 3.3 Characterization data of 3

![Chemical structure of compound](image)

\textit{N-(4-Oxo-2-phenyl-4H-benzo[d][1,3]oxizin-5-yl)benzamide (3a)}

Compound 3a was prepared according to the 2.2 and was purified on silica gel to give a white solid in 60% yield (20.5 mg). Mp: 200.5–201.4 °C.

$^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 12.00 (1H, s), 8.97 (1H, dd, $J = 8.0, 1.0$ Hz), 8.27 (2H, m), 8.07 (2H, m), 7.82 (1H, t, $J = 8.0$ Hz), 7.57 (2H, m), 7.52 (4H, m), 7.37 (1H, dd, $J = 8.0, 1.0$ Hz); $^1$C NMR (125 MHz, CDCl$_3$): $\delta$ 165.9, 162.1, 156.2, 147.5, 141.5, 138.2, 134.2, 132.9, 129.6, 128.9, 128.8, 128.3, 127.5, 121.4, 118.5, 104.1; IR (KBr): 3303.0, 1726.1, 1678.2, 1645.6, 1625.0, 1572.0, 1542.0, 1294.0, 1261.3, 1181.6, 1127.5 cm$^{-1}$; HRMS (ESI) $m/z$ calcd for C$_{21}$H$_{14}$N$_2$O$_3$ [M+H]$^+$ 343.1083, found 343.1082.
4-Ethyl-N-(2-(4-ethylphenyl)-4-oxo-4H-benzo[d][1,3]oxazin-5-yl)benzamide (3b)

Compound 3b was prepared according to the 2.2 and was purified on silica gel to give a white solid in 68% yield (27.3 mg). Mp: 185.5−186.7 °C.

$^1$H NMR (500 MHz, CDCl$_3$): δ 11.94 (1H, s), 8.89 (1H, dd, $J = 8.5, 1.0$ Hz), 8.13 (2H, d, $J = 8.5$ Hz), 7.94 (2H, d, $J = 8.5$ Hz), 7.56 (1H, t, $J = 7.5$ Hz), 7.29 (5H, m), 2.67 (4H, q, $J = 7.5$ Hz), 1.22 (6H, t, $J = 8.0$ Hz);

$^{13}$C NMR (125 MHz, CDCl$_3$): δ 165.2, 161.5, 155.6, 149.2, 148.4, 144.9, 142.0, 141.1, 137.4, 130.9, 127.7, 126.9, 126.2, 120.4, 117.4, 114.4, 28.2, 12.5, 14.4;

IR (KBr): 3295.2, 2964.4, 1705.5, 1684.0, 1607.0, 1578.2, 1542.1, 1508.9, 1297.3, 1262.0, 1181.6, 1122.3;

HRMS (ESI) $m/z$ calcd for C$_{25}$H$_{22}$N$_2$O$_5$ [M+H]$^+$ 399.1709, found 399.1704.

4-Methoxy-N-(2-(4-methoxyphenyl)-4-oxo-4H-benzo[d][1,3]oxazin-5-yl)benzamide (3c)

Compound 3c was prepared according to the 2.2 and was purified on silica gel to give a white solid in 72% yield (29.0 mg). Mp: 182.8−183.6 °C.

$^1$H NMR (500 MHz, CDCl$_3$): δ 11.96 (1H, s), 8.93 (1H, d, $J = 8.5$ Hz), 8.24 (2H, d, $J = 9.0$ Hz), 8.06 (2H, d, $J = 9.0$ Hz), 7.81 (1H, t, $J = 8.0$ Hz), 7.34 (1H, d, $J = 8.0$ Hz), 7.02 (4H, m);

$^{13}$C NMR (125 MHz, CDCl$_3$): δ 165.5, 163.5, 163.9, 162.4, 156.2, 147.9, 142.0, 138.2, 130.3, 129.5, 126.6, 121.9, 120.8, 117.9, 114.3, 114.2, 103.7, 55.6, 55.5;

IR (KBr): 3307.6, 2923.6, 2850.9, 1716.1, 1680.8, 1602.4, 1569.7, 1541.4, 1507.7, 1293.4, 1268.9, 1110.4, 1180.6 cm$^{-1}$;

HRMS (ESI) $m/z$ calcd for C$_{23}$H$_{18}$N$_2$O$_5$ [M+H]$^+$ 403.1294, found 403.1290.

4-(tert-Butyl)-N-(2-(4-(tert-butyl)phenyl)-4-oxo-4H-benzo[d][1,3]oxazin-5-yl)benzamide (3d)

Compound 3d was prepared according to the 2.2 and was purified on silica gel to give a white solid in 63% yield (28.6 mg). Mp: 219.7−220.2 °C.

$^1$H NMR (500 MHz, CDCl$_3$): δ 12.02 (1H, s), 8.97 (1H, dd, $J = 8.0, 1.0$ Hz), 8.22(2H, d, $J = 7.5, 2.0$ Hz), 8.03 (2H, d, $J = 8.5, 2.0$ Hz), 7.83 (1H, t, $J = 8.5$ Hz), 7.56 (2H, d, $J = 5.5$ Hz), 7.545 (2H, d, $J = 5.5$ Hz), 7.39 (1H, dd, $J = 8.0, 0.5$ Hz)$^{13}$C NMR (125 MHz, CDCl$_3$): 166.0, 162.3, 156.8,
N-(4-Oxo-2-(4-(trifluoromethyl)phenyl)-4H-benzo[d][1,3]oxazin-5-yl)-4-
(trifluoromethyl)benzamide (3e)

Compound 3e was prepared according to the 2.2 and was purified on silica gel to give a white solid in 47% yield (22.5 mg). Mp: 197.4–198.2 °C.

$^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 12.04 (1H, s), 9.00 (1H, dd, $J = 8.5$, 1.0 Hz), 8.42 (2H, d, $J = 8.5$ Hz), 8.19 (2H, d, $J = 8.5$ Hz), 7.90 (1H, t, $J = 8.0$ Hz), 7.81 (4H, t, $J = 8.0$ Hz), 7.47 (1H, dd, $J = 8.0$, 1.0 Hz),

$^{13}$C NMR (125 MHz, CDCl$_3$): $\delta$ 164.5, 161.8, 154.9, 147.1, 141.4, 138.5, 137.3, 134.3 (q, $^2J_{C-F} = 38.8$Hz), 134.1 (q, $^2J_{C-F} = 38.8$Hz), 132.8, 128.6, 127.9, 126.0 (q, $^3J_{C-F} = 3.6$Hz), 125.9 (q, $^3J_{C-F} = 3.7$Hz), 124.7 (q, $^1J_{C-F} = 270.9$Hz), 122.5 (q, $^1J_{C-F} = 271.1$Hz), 121.1, 118.2, 103.2;

$^{19}$F NMR (471 MHz, CDCl$_3$): $\delta$ $-$63.02 (3F, s), $-$63.10 (3F, s); IR (KBr): 3297.6, 2961.8, 2924.1, 1720.7, 1694.1, 1606.3, 1574.8, 1541.4, 1294.7, 1261.9, 1170.8, 1113.8; HRMS (ESI) m/z calcd for C$_{29}$H$_{30}$N$_2$O$_3$ [M+H]$^+$ 455.2335, found 455.2331.

3-Methoxy-N-(2-(4-methoxyphenyl)-4-oxo-4H-benzo[d][1,3]oxazin-5-yl)benzamide (3f)

Compound 3f was prepared according to the 2.2 and was purified on silica gel to give a white solid in 62% yield (24.9 mg). Mp: 190.3–191.1 °C.

$^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 12.01 (1H, s), 8.97 (1H, dd, $J = 8.5$, 1.0 Hz), 7.89 (1H, m), 7.85 (1H, t, $J = 8.0$ Hz), 7.80 (1H, m), 7.65 (1H, m), 7.63 (1H, m), 7.42 (3H, m), 7.12 (2H, m), 3.92 (3H, s), 3.91 (3H, s); $^{13}$C NMR (125 MHz, CDCl$_3$): $\delta$ 165.8, 162.1, 160.1, 160.1, 156.1, 157.5, 141.8, 141.7, 138.2, 135.7, 130.9, 130.0, 129.9, 121.5, 120.9, 119.6, 119.4, 119.0, 118.5, 112.6, 112.4, 104.1, 55.6, 55.5; IR (KBr): 3302.4, 2923.9, 2850.7, 1716.2, 1682.2, 1603.1, 1573.1, 1541.3, 1294.8, 1261.8; HRMS (ESI) m/z calcd for C$_{23}$H$_{18}$N$_2$O$_3$ [M+H]$^+$ 403.1294, found 403.1297.
3-Methyl-N-(4-oxo-2-(p-tolyl)-4H-benzo[d][1,3]oxazin-5-yl)benzamide (3g)

Compound 3g was prepared according to the 2.2 and was purified on silica gel to give a white solid in 64% yield (23.7 mg). Mp: 194.4−195.6 °C.

$^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 11.99 (1H, s), 8.97 (1H, dd, $J = 8.5, 1.0$ Hz), 8.11 (1H, s), 8.09(1H, m ), 7.89 (2H, m), 7.84 (1H, t, $J = 8.5$ Hz), 7.41 (5H, m), 2.47 (3H, s), 2.46 (3H, s); $^{13}$C NMR (125 MHz, CDCl$_3$): $\delta$ 166.2, 162.3, 156.5, 147.6, 141.8, 138.9, 138.8, 138.3, 133.4, 133.3, 129.6, 128.9, 128.9, 128.8, 128.3, 125.6, 124.6, 121.4, 118.6, 104.2, 21.6, 21.5; IR (KBr): 3304.2, 2954.8, 2853.9, 1703.5, 1683.3, 1606.9, 1573.6, 1539.9, 1297.9, 1271.3, 1171.3, 1119.0; HRMS (ESI) m/z calcd for C$_{23}$H$_{18}$N$_2$O$_3$ [M+H]$^+$ 371.1396, found 371.1382.

![Chemical structure of 3g](image)

3-Chloro-N-(2-(4-chlorophenyl)-4-oxo-4H-benzo[d][1,3]oxazin-5-yl)benzamide (3h)

Compound 3h was prepared according to the 2.2 and was purified on silica gel to give a white solid in 47% yield (19.3 mg). Mp: 202.3−203.1 °C.

$^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 11.91 (1H, s), 8.92 (1H, dd, $J = 8.5, 0.5$ Hz), 8.25 (1H, t, $J = 1.5$ Hz), 8.18 (1H, m), 8.04 (1H, t, $J = 1.5$ Hz), 7.92 (1H, m), 7.83 (1H, t, $J = 8.0$ Hz), 7.53 (2H, m), 7.45 (2H, m), 7.39 (1H, dd, $J = 8.0, 1.0$ Hz); $^{13}$C NMR (125 MHz, CDCl$_3$): $\delta$ 163.4, 160.8, 154.0, 146.2, 140.5, 137.4, 134.9, 134.4, 134.2, 131.9, 131.5, 130.3, 129.2, 129.1, 127.4, 127.1, 125.3, 124.2, 120.8, 117.9, 103.1; IR (KBr): 3275.3, 1715.0, 1676.9, 1625.4, 1609.2, 1576.5, 1540.7, 1298.2, 1260.0, 1176.3, 1103.3, 1075.6 HRMS (ESI) m/z calcd for C$_{21}$H$_{12}$Cl$_2$N$_2$O$_3$ [M+H]$^+$ 411.0303, found 411.0306.

![Chemical structure of 3h](image)

N-(4-Oxo-2-((E)-styryl)-4H-benzo[d][1,3]oxazin-5-yl)cinnamamide (3i)

Compound 3i was prepared according to the 2.2 and was purified on silica gel to give a white solid in 60% yield (28.3 mg). Mp: 210.5–211.2 °C.

$^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 11.26 (1H, s), 8.87 (1H, dd, $J = 8.5, 0.5$ Hz), 7.82 (1H, d, $J = 16.5$ Hz), 7.77 (2H, m), 7.57 (4H, m), 7.40 (6H, m), 7.28 (1H, d, $J = 1.0$ Hz), 4.76 (1H, d, $J = 16.0$ Hz), 6.63 (1H, d, $J = 15.5$Hz); $^{13}$C NMR (125 MHz, CDCl$_3$): $\delta$ 164.7, 161.5, 156.5, 147.5, 143.1, 142.5, 141.8, 138.0, 134.5, 134.4, 128.4, 130.5, 130.2, 129.1, 128.9, 128.2, 128.1, 121.4, 121.0, 118.6, 118.2, 103.6; IR (KBr): 3283.7, 1721.0, 1686.4, 1628.9, 1601.3, 1569.1, 1530.6, 1278.1, 1199.5, 1158.6, 760.3, 722.8; HRMS (ESI) m/z calcd for C$_{25}$H$_{19}$N$_2$O$_3$ [M+H]$^+$ 395.1392, found 395.1392.

![Chemical structure of 3i](image)
$N$-(4-Oxo-2-((thiophen-2-yl)-4H-benzo[d][1,3]oxazin-5-yl)thiophene-2-carboxamide (3j)

Compound 3j was prepared according to the 2.2 and was purified on silica gel to give a yellow solid in 64% yield (16.3 mg). Mp: 189.4–190.2 °C.

$^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 11.87 (1H, s), 8.81 (1H, dd, $J = 8.5, 1.0$ Hz), 7.93 (1H, dd, $J = 4.0, 1.5$ Hz), 7.81 (1H, dd, $J = 4.0, 1.0$ Hz), 7.77 (1H, t, $J = 8.0$ Hz), 7.62 (1H, dd, $J = 5.0, 1.5$ Hz), 7.61 (1H, dd, $J = 5.0, 1.5$ Hz), 7.29 (1H, dd, $J = 8.0, 1.0$ Hz), 7.16 (2H, m); $^{13}$C NMR (125 MHz, CDCl$_3$): $\delta$ 161.6, 160.5, 152.8, 147.6, 141.6, 139.7, 138.3, 133.5, 132.9, 132.0, 129.0, 128.4, 128.1, 121.0, 118.1, 103.5; IR (KBr): 3350.5, 1720.5, 1673.2, 1578.3, 1569.8, 1493.5, 1269.1, 1219.2, 1171.1, 1079.2; HRMS (ESI) m/z calcd for C$_{17}$H$_{10}$N$_2$O$_3$S$_2$ [M+H$^+$] 355.0221, found 355.0225.

4-Methyl-$N$-(4-oxo-2-((p-tolyl)-4H-benzo[d][1,3]oxazin-5-yl)benzamide (3k)

Compound 3k was prepared according to the 2.2 and was purified on silica gel to give a white solid in 58% yield (22.2 mg). Mp: 196.2–196.8 °C.

$^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 11.95 (1H, s), 8.81 (1H, d, $J = 0.5$ Hz), 8.15 (2H, d, $J = 8.5$ Hz), 7.97 (2H, d, $J = 8.0$ Hz), 7.32 (4H, m), 7.18 (1H, d, $J = 1.0$ Hz), 2.52 (3H, s), 2.44 (6H, s); $^{13}$C NMR (125 MHz, CDCl$_3$): $\delta$ 165.9, 162.1, 156.5, 150.2, 147.5, 143.6, 143.0, 141.5, 131.5, 129.6, 129.6, 128.3, 127.5, 127.0, 121.6, 119.1, 101.7, 22.8, 21.8, 21.6; IR (KBr): 2956.2, 2869.6, 1714.1, 1688.8, 1673.0, 1610.8, 1569.1, 1292.6, 1265.3, 1181.5, 1149.6; HRMS (ESI) m/z calcd for C$_{24}$H$_{20}$N$_2$O$_3$ [M+H$^+$] 385.1552, found 385.1557.

4-Ethyl-$N$-(7-ethyl-2-((4-ethylphenyl)-4-oxo-4H-benzo[d][1,3]oxazin-5-yl)benzamide (3l)

Compound 3l was prepared according to the 2.2 and was purified on silica gel to give a white solid in 49% yield (20.8 mg). Mp: 194.4–195.3 °C.

$^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 11.99 (1H, s), 8.87 (1H, d, $J = 1.0$ Hz), 8.21 (2H, d, $J = 8.0$ Hz), 7.36 (4H, m), 7.25 (1H, s), 2.83 (2H, q, $J = 2.5$ Hz), 2.75 (4H, q, $J = 2.5$ Hz), 1.36 (3H, t, $J = 2.5$ Hz), 1.29 (6H, t, $J = 2.5$ Hz); $^{13}$C NMR (125 MHz, CDCl$_3$): $\delta$ 166.0, 162.2, 156.5, 156.2, 149.8, 149.1, 147.7, 141.7, 131.8, 128.4, 128.4, 128.4, 127.6, 127.2, 120.4, 118.2, 101.8, 29.9, 29.0, 28.9,
15.3, 15.2, 14.8; IR (KBr): 3306.9, 2958.3, 2869.8, 1733.4, 1702.7, 1688.7, 1611.3, 1567.3, 1540.5, 1508.2, 1283.7, 1262.6, 1183.8, 1138.6; HRMS (ESI) m/z calcd for C_{27}H_{27}N_{2}O_{3} [M+H]^+ 427.2022, found 427.2021.

N-(7-Methyl-4-oxo-2-phenyl-4H-benzo[d][1,3]oxazin-5-yl)benzamide (3m)

Compound 3m was prepared according to the 2.2 and was purified on silica gel to give a white solid in 80% yield (28.5 mg). Mp: 196.7−197.6 °C. 

$^1$H NMR (500 MHz, CDCl$_3$): δ 11.98 (1H, s), 8.83 (1H, s), 8.26 (2H, m), 8.07 (2H, m), 7.57 (2H, m), 7.52 (4H, m), 7.22 (1H, s), 2.53 (3H, s); $^{13}$C NMR (125 MHz, CDCl$_3$): δ 166.0, 162.1, 156.4, 150.3, 147.4, 141.5, 134.3, 132.9, 132.4, 129.8, 128.9, 128.4, 127.5, 122.0, 119.4, 101.8, 22.9; IR (KBr): 3304.7, 2923.3, 2853.3, 1715.6, 1673.9, 1612.8, 1571.4, 1542.1, 1294.7, 1264.8, 1178.8, 1145.8; HRMS (ESI) m/z calcd for C$_{27}$H$_{27}$N$_{2}$O$_{3}$ [M+H]$^+$ 427.2021, found 427.2021.

N-(7-Ethyl-4-oxo-2-phenyl-4H-benzo[d][1,3]oxazin-5-yl)benzamide (3n)

Compound 3n was prepared according to the 2.2 and was purified on silica gel to give a yellow solid in 74% yield (27.4 mg). Mp: 192.4−193.2 °C. 

$^1$H NMR (500 MHz, CDCl$_3$): δ 11.95 (1H, s), 8.83 (1H, d, J = 1.5 Hz), 8.23 (2H, dd, J = 7.5, 1.0 Hz), 8.07 (2H, dd, J = 7.5, 1.0 Hz), 7.53 (6H, m), 2.79 (2H, q, J = 7.5 Hz), 1.36 (3H, t, J = 7.5 Hz); $^{13}$C NMR (125 MHz, CDCl$_3$): δ 165.8, 162.0, 156.2, 147.4, 141.5, 134.2, 132.8, 132.3, 129.7, 128.9, 128.8, 128.2, 127.5, 120.6, 118.4, 101.9, 29.9, 14.7; IR (KBr): 3304.7, 2923.3, 2853.3, 1715.6, 1673.9, 1612.8, 1571.4, 1542.1, 1294.7, 1264.8, 1178.8, 1145.8; HRMS (ESI) m/z calcd for C$_{22}$H$_{19}$N$_{2}$O$_{3}$ [M+H]$^+$ 371.1392, found 371.1392.

N-(7-Fluoro-4-oxo-2-phenyl-4H-benzo[d][1,3]oxazin-5-yl)benzamide (3o)

Compound 3o was prepared according to the 2.2 and was purified on silica gel to give a white solid in 55% yield (19.9 mg). Mp: 205.7−206.4 °C. 

$^1$H NMR (500 MHz, CDCl$_3$): δ 12.087 (1H, s), 8.77 (1H, dd, J = 12, 2.5 Hz), 8.27 (2H, d, J = 7.5 Hz), 8.06 (2H, d, J = 7.5 Hz), 7.60 (2H, m), 7.53 (4H, m), 7.06 (1H, dd, J = 8.5, 2.5 Hz); $^{13}$C NMR (125 MHz, CDCl$_3$): δ 169.6 (d, $^3$J$_{C:F}$ = 279.8 Hz), 166.0, 161.4, 157.1, 149.8 (d, $^3$J$_{C:F}$ =15.4 Hz),
143.9 (d, $^{3}J_{CF} = 15.4$ Hz), 133.7, 133.3, 132.7, 129.2, 129.0, 128.9, 128.5, 127.3, 108.0 (d, $^{3}J_{CF} = 23.5$ Hz), 106.7 (d, $^{3}J_{CF} = 23.5$ Hz), 100.8 (d, $^{4}J_{CF} = 7.0$ Hz); $^{19}$F NMR (471 MHz, CDCl$_3$): $\delta$ -93.91 (1F, t, $J = 10.8$ Hz); IR (KBr): 3296.7, 1718.7, 1694.2, 1594.9, 1561.4, 1260.9, 1184.4; HRMS (ESI) m/z calcd for C$_{21}$H$_{13}$FN$_2$O$_3$ [M+H]$^+$ 361.0988, found 361.0983.

$\text{N-(7-Chloro-4-oxo-2-phenyl-4H-benzo[d][1,3]oxazin-5-yl)benzamide (3p)}$

Compound 3p was prepared according to the 2.2 and was purified on silica gel to give a white solid in 64% yield (24.1 mg). Mp: 209.4−209.9 °C.

$^{1}$H NMR (500 MHz, CDCl$_3$): $\delta$ 1.99 (1H, s), 9.03 (1H, d, $J = 2.0$ Hz), 8.26 (2H, dd, $J = 8.0$, 3.0 Hz), 8.07 (2H, dd, $J = 8.0$, 3.0 Hz), 7.62 (2H, td, $J = 7.5$, 1.5 Hz), 7.54 (4H, m), 7.38 (1H, d, $J = 3.0$ Hz); $^{13}$C NMR (125 MHz, CDCl$_3$): $\delta$ 165.8, 161.5, 157.2, 148.2, 144.8, 142.3, 133.7, 133.3, 132.7, 129.2, 129.0, 128.9, 128.5, 127.5, 121.3, 118.5, 102.4; IR (KBr): 3299.7, 1723.8, 1685.0, 1625.9, 1604.6, 1561.1, 1288.9, 1261.8, 1182.5; HRMS (ESI) m/z calcd for C$_{21}$H$_{13}$ClN$_2$O$_3$ [M+H]$^+$ 377.0693, found 377.0697.

$\text{N-(7-Bromo-4-oxo-2-phenyl-4H-benzo[d][1,3]oxazin-5-yl)benzamide (3q)}$

Compound 3q was prepared according to the 2.2 and was purified on silica gel to give a white solid in 55% yield (23.1 mg). Mp: 210.5–211.7 °C.

$^{1}$H NMR (500 MHz, CDCl$_3$): $\delta$ 11.96 (1H, s), 9.19 (1H, d, $J = 1.5$ Hz), 8.25 (2H, m), 8.06 (2H, m), 7.60 (2H, m), 7.53 (5H, m); $^{13}$C NMR (125 MHz, CDCl$_3$): $\delta$ 165.8, 161.6, 157.1, 148.0, 142.1, 133.7, 133.5, 133.3, 132.6, 129.2, 129.0, 128.9, 128.4, 127.5, 121.4, 102.7; IR (KBr): 3298.2, 1721.1, 1706.2, 1693.9, 1606.6, 1574.8, 1541.5, 1295.0, 1171.2, 1116.3; HRMS (ESI) m/z calcd for C$_{21}$H$_{13}$ClN$_2$O$_3$ [M+H]$^+$ 421.0188, found 421.0186.

$\text{N-(4-Oxo-2-phenyl-7-(trifluoromethyl)-4H-benzo[d][1,3]oxazin-5-yl)benzamide (3r)}$

Compound 3r was prepared according to the 2.2 and was purified on silica gel to give a yellow solid in 51% yield (20.9 mg). Mp: 200.4–201.7 °C.

$^{1}$H NMR (500 MHz, CDCl$_3$): $\delta$ 12.05 (1H, s), 9.31 (1H, d, $J = 0.5$ Hz), 8.31 (2H, m), 8.31 (2H, m), 7.66 (1H, d, $J = 1.5$ Hz), 7.63 (2H, m), 7.56 (4H, m); $^{13}$C NMR (125 MHz, CDCl$_3$): $\delta$ 167.0, 161.4,
157.3, 148.0, 139.3(q, $^2J_{CF}$=33.1Hz), 133.6, 133.5, 132.8, 129.1, 129.0, 128.3, 128.5, 122.9(q, $^2J_{CF}$=3.8Hz), 118.0(q, $^2J_{CF}$=3.8Hz), 114.7(q, $^2J_{CF}$=3.8Hz), 105.9; $^1$H NMR (471 MHz, CDCl$_3$): $^\delta$−64.00 (3F, s); IR (KBr): 3309.7, 1719.9, 1687.8, 1618.2, 1574.5, 1289.9, 1250.3, 1180.6, 1128.2; HRMS (ESI) m/z calcd for C$_{22}$H$_{14}$F$_3$N$_2$O$_3$[M+H]$^+$ 411.0957, found 411.0959.

3.4 General procedure for the synthesis of 4

![Chemical Reaction Diagram]

Benzoic acid 1 (0.20 mmol), 3-(4-(dimethylamino)phenyl)-1,4,2-dioxazol-5-one 2l (0.20 mmol), NaOAc (17 mg, 0.20 mmol), AgSbF$_6$ (20 mg, 0.06 mmol), [Cp*RhCl$_2$]$_2$ (6 mg, 0.010 mmol) and THF (2.0 mL) were placed into a 10 mL sealing tube. The reaction mixture was stirred at 120 °C for 12 h. After cooling to ambient temperature, a saturated NaHCO$_3$ solution was added to the reaction solution, and the mixture was extracted three times with CHCl$_3$. The combined organic layers were washed with brine, dried over anhydrous sodium sulfate and concentrated in vacuo. The mixture was purified by flash column chromatography on silica gel with Petroleum ether-chloroform-EA as the eluent to give the desired products 4.

3.5 Characterization data of 4

![Chemical Structure]

2-(4-(Dimethylamino)phenyl)-4H-benzo[d][1,3]oxazin-4-one (4a) (CAS Registry Number 95654-38-9)

Compound 4a was prepared according to the 2.4 and was purified on silica gel to give a yellow solid in 70% yield (37.2mg). Mp: 176.4−177.6 °C.

$^1$H NMR (500 MHz, CDCl$_3$): $^\delta$ 8.19 (3H, m), 7.76 (1H, td, $J$ = 8.5, 1.5 Hz), 7.62 (1H, d, $J$ = 8.0, 1.5 Hz), 7.42 (1H, t, $J$ = 8.0 Hz), 7.37 (2H, d, $J$ = 9.0 Hz s), 3.09 (6H, s); $^1$C NMR (125 MHz, CDCl$_3$): $^\delta$ 159.1, 157.0, 151.9, 146.8, 135.4, 129.1, 127.5, 125.9, 125.5, 116.1, 116.1, 115.4, 110.6, 39.3; IR (KBr): 2911.7, 2856.7, 1738.5, 1593.8, 1557.9, 1528.4, 1270.1, 1185.1; HRMS (ESI) m/z calcd for C$_{16}$H$_{14}$N$_2$O$_2$ [M+H]$^+$ 267.1134, found 267.1138.

![Chemical Structure]

2-(4-(Dimethylamino)phenyl)-7-methoxy-4H-benzo[d][1,3]oxazin-4-one (4b)

Compound 4b was prepared according to the 2.4 and was purified on silica gel to give a yellow...
solid in 82% yield (48.5mg). Mp: 181.9–182.4 °C.

1H NMR (500 MHz, CDCl3): δ 8.16 (2H, d, J = 9.0 Hz), 8.05 (1H, d, J = 9.0), 7.00 (1H, d, J = 2.5 Hz, 6.94 (1H, dd, J = 9.0, 2.0 Hz), 6.70 (2H, d, J = 9.0 Hz), 3.92 (3H, s), 3.06 (6H, s); 13C NMR (125 MHz, CDCl3): δ 166.2, 159.9, 158.9, 153.1, 150.3, 130.1, 130.08, 116.8, 116.2, 111.3, 109.3, 108.0, 55.8, 40.1; IR (KBr): 2908.7, 2819.3, 1737.6, 1595.4, 1557.6, 1530.6, 1270.7, 1186.7; HRMS (ESI) m/z calcd for C17H16N2O3 [M+H]+ 297.1239, found 297.1235.

2-(4-(Dimethylamino)phenyl)-6-methyl-4H-benzo[d][1,3]oxazin-4-one (4c)

Compound 4c was prepared according to the 2.4 and was purified on silica gel to give a yellow solid in 72% yield (40.3mg). Mp: 184.5–185.8 °C.

1H NMR (500 MHz, CDCl3): δ 8.15 (2H, d, J = 9.0 Hz), 7.92 (1H, d, J = 1.0 Hz), 7.50 (1H, d, J = 8.5 Hz), 6.73 (2H, d, J = 8.0 Hz), 3.07 (6H, s), 2.45 (3H, s); 13C NMR (125 MHz, CDCl3): δ 159.4, 156.3, 151.9, 144.7, 136.6, 136.1, 128.8, 127.0, 125.3, 116.0, 115.1, 110.3, 39.1, 20.2; IR (KBr): 2956.3, 2923.7, 2869.8, 2850.6, 1733.1, 1596.0, 1570.3, 1521.1, 1261.6, 1188.8, 1159.9; HRMS (ESI) m/z calcd for C17H16N2O2 [M+H]+ 281.1290, found 281.1288.

6-Chloro-2-(4-(dimethylamino)phenyl)-4H-benzo[d][1,3]oxazin-4-one (4d)

Compound 4d was prepared according to the 2.4 and was purified on silica gel to give a yellow solid in 43% yield (25.8mg). Mp: 192.2–193.5 °C.

1H NMR (500 MHz, CDCl3): δ 8.09 (3H, m), 7.65 (1H, dd, J = 8.5, 2.5 Hz), 7.50 (1H, d, J = 8.5 Hz), 6.82 (2H, d, J = 8.5 Hz), 3.06 (6H, s); 13C NMR (125 MHz, CDCl3): δ 159.2, 158.2, 153.1, 146.5, 136.5, 132.1, 130.1, 128.1, 127.7, 117.4, 116.4, 111.3, 40.1; IR (KBr): 2955.6, 2869.4, 1737.8, 1595.9, 1557.8, 1530.8, 1270.6, 1187.1; HRMS (ESI) m/z calcd for C16H13ClN2O2 [M+H]+ 301.0744, found 301.0748.

3.6 Procedure for the synthesis of 4e

Under argon atmosphere, 2-amino-4-methylbenzoic acid (302.0mg, 2.0 mmol) was dissolved in 10 ml of dry pyridine at room temperature and the solution was cooled to 0°C. Subsequently, benzoyl chloride (560.0 mg, 4.0 mmol) in pyridine (2.0 ml) was added slowly to this solution. The
reaction mixture was stirred at 0°C for 1 h and then at room temperature for 2 h. After completion, the mixture was neutralized with NaHCO₃ solution and poured into ice water. The precipitate was collected by filtration and dried to yield the desired compounds. The crude product was purified by recrystallization from EtOAc/Pentane to give a yellow solid 4e in 82% yield (388.7 mg). ¹H NMR (500 MHz, CDCl₃): δ 8.29 (2H, m), 8.10 (1H, d, J = 8.0 Hz), 7.56 (1H, td, J = 8.5, 1.5 Hz), 7.50 (3H, m), 7.31 (1H, dd, J = 8.0, 1.0 Hz), 2.51 (3H, s); ¹³C NMR (125 MHz, CDCl₃): δ 158.6, 156.2, 147.1, 146.0, 131.5, 128.6, 127.7, 127.4, 127.2, 126.2, 113.4, 21.1; HRMS (ESI) m/z calcd for C₁₅H₁₂NO₂ [M+H]+ 238.0863, found 238.0862.

3.7 Procedure for the synthesis of 5a and 5b

To a solution of anthranilic acid (1.1 mmol) in anhydrous THF (4 mL) was added 1.0 mmol of the appropriate benzoyl chloride at room temperature. After cooling the solution using ice-water bath, 1.5 mmol of triethylamine was added dropwise and reaction was stirred at room temperature for additional 4–12 h. The mixture was poured into a 20–30 mL cold solution of 1.0 M HCl, and the precipitate was collected by filtration. Recrystallization from THF-hexane solution afforded the desired compound in quantitative yield of compound 5a (90%) and 5b (78%).

Compound 5a (459.1 mg): ¹H NMR (500 MHz, d₆-DMSO): δ 13.68 (1H, s), 12.25 (1H, s), 8.61 (1H, s), 7.96 (3H, m), 7.66 (1H, m), 7.60 (2H, m), 7.03 (1H, dd, J = 8.0, 1.0 Hz), 2.40 (3H, s); ¹³C NMR (125 MHz, d₆-DMSO): δ 170.6, 165.1, 145.4, 141.7, 135.03, 131.7, 129.5, 127.4, 124.2, 120.5, 114.1, 22.2; HRMS (ESI) m/z calcd for C₁₅H₁₄NO₃ [M+H]+ 256.0968, found 256.0964.

Compound 5b (496.1 mg): ¹H NMR (500 MHz, d₆-DMSO): δ 13.39 (1H, s), 12.29 (1H, s), 8.48 (1H, d, J = 2.5 Hz), 8.00 (1H, d, J = 9.0 Hz), 7.82 (2H, d, J = 9.0 Hz), 6.81 (2H, d, J = 9.0 Hz), 6.71 (1H, d, J = 9.0 Hz), 3.86 (3H, s), 3.02 (6H, s); ¹³C NMR (125 MHz, d₆-DMSO): δ 165.2, 153.1, 144.2, 133.5, 129.0, 121.1, 111.7, 108.3, 104.3, 55.8; HRMS (ESI) m/z calcd for C₁₇H₁₄N₂O₄ [M+H]+ 315.1339, found 315.1338.
4. Kinetic Isotope Effect (KIE) Experiment

4.1 Competition KIE experiment

Benzoic acid 1 (0.20 mmol), [D]-1a (0.20 mmol), 3-phenyl-1,4,2-dioxazol-5-one 2a (0.40 mmol), NaOAc (34 mg, 0.40 mmol), AgSbF₆ (40 mg, 0.12 mmol) and [Cp*RhCl₂]₂ (12 mg, 0.020 mmol) were placed into a 10 ml sealing tube. THF (4.0 mL) was introduced and the reaction mixture was stirred at 120 °C for 2.5 h. After cooling to ambient temperature, a saturated NaHCO₃ solution was added to the reaction solution, and the mixture was extracted three times with CHCl₃ followed by washing with water and saturated brine. Then it was concentrated and loaded onto silica gel for purification by flash column chromatography (Petroleum ether/ chloroform/ EtOAc) to afford the desired product.
4.2 Parallel KIE experiment

Reaction A: Benzoic acid [D]-1a (0.20 mmol), 3-phenyl-1,4,2-dioxazol-5-one 2a (0.20 mmol), NaOAc (17 mg, 0.20 mmol), AgSbF₆ (20 mg, 0.06 mmol) and [Cp*RhCl₂]₂ (6 mg, 0.01 mmol) were placed into a 10 ml sealing tube. THF (2.0 mL) was introduced and the reaction mixture was stirred at 120 °C for 2.5 h.

Reaction B: Benzoic acid 1a (0.20 mmol), 3-phenyl-1,4,2-dioxazol-5-one 2a (0.20 mmol), NaOAc (17 mg, 0.20 mmol), AgSbF₆ (20 mg, 0.06 mmol) and [Cp*RhCl₂]₂ (6 mg, 0.01 mmol) were placed into a 10 ml tube sealing. THF (2.0 mL) was introduced and the reaction mixture was stirred at 120 °C for 2.5 h.

After cooling to ambient temperature, reaction A and B were mixed and a saturated NaHCO₃ solution was added to the mixture. The mixture was extracted three times with CHCl₃, washed with water and saturated brine. Then it was concentrated in vacuum and loaded onto silica gel for purification by flash column chromatography (Petroleum ether/chloroform/EtOAc) to afford the mixed desired product D-3a and 3a.
5. Optical properties of compound 3

**Figure S1.** UV absorption (up) and emission (down) spectra of 3a (concentration: 10 µM) in THF/water mixtures with different water fractions.
**Figure S2.** UV absorption (left, THF, 10 µM) and emission spectra (right) of 3b in THF (blue line, 10 µM) and in 95% water/THF mixture (red line, 10 µM).

**Figure S3.** UV absorption (left, THF, 10 µM) and emission spectra (right) of 3c in THF (blue line, 10 µM) and in 95% water/THF mixture (red line, 10 µM).

**Figure S5.** UV absorption (left, THF, 10 µM) and emission spectra (right) of 3d in THF (blue line, 10 µM) and in 95% water/THF mixture (red line, 10 µM).
**Figure S6.** UV absorption (left, THF, 10 µM) and emission spectra (right) of 3e in THF (blue line, 10 µM) and in 95% water/THF mixture (red line, 10 µM).

**Figure S7.** UV absorption (left, THF, 10 µM) and emission spectra (right) of 3f in THF (blue line, 10 µM) and in 95% water/THF mixture (red line, 10 µM).

**Figure S8.** UV absorption (left, THF, 10 µM) and emission spectra (right) of 3g in THF (blue line, 10 µM) and in 95% water/THF mixture (red line, 10 µM).
**Figure S9.** UV absorption (left, THF, 10 µM) and emission spectra (right) of 3h in THF (blue line, 10 µM) and in 95% water/THF mixture (red line, 10 µM).

**Figure S10.** UV absorption (left, THF, 10 µM) and emission spectra (right) of 3i in THF (blue line, 10 µM) and in 95% water/THF mixture (red line, 10 µM).

**Figure S11.** UV absorption (left, THF, 10 µM) and emission spectra (right) of 3j in THF (blue line, 10 µM) and in 95% water/THF mixture (red line, 10 µM).
**Figure S12.** UV absorption (left, THF, 10 µM) and emission spectra (right) of 3l in THF (blue line, 10 µM) and in 95% water/THF mixture (red line, 10 µM).

**Figure S13.** UV absorption (left, THF, 10 µM) and emission spectra (right) of 3n in THF (blue line, 10 µM) and in 95% water/THF mixture (red line, 10 µM).

**Figure S14.** UV absorption (left, THF, 10 µM) and emission spectra (right) of 3o in THF (blue line, 10 µM) and in 95% water/THF mixture (red line, 10 µM).
**Figure S15.** UV absorption (left, THF, 10 µM) and emission spectra (right) of 3p in THF (blue line, 10 µM) and in 95% water/THF mixture (red line, 10 µM).

**Figure S16.** UV absorption (left, THF, 10 µM) and emission spectra (right) of 3q in THF (blue line, 10 µM) and in 95% water/THF mixture (red line, 10 µM).

**Figure S17.** UV absorption (left, THF, 10 µM) and emission spectra (right) of 3r in THF (blue line, 10 µM) and in 95% water/THF mixture (red line, 10 µM).
6. NMR spectroscopic data

N-(4-oxo-2-phenyl-4H-benzo[d][1,3]oxazin-5-yl)benzamide (3a)
4-ethyl-N-(2-(4-ethylphenyl)-4-oxo-4H-benzo[d][1,3]oxazin-5-yl)benzamide (3b)
4-methoxy-N-(2-(4-methoxyphenyl)-4-oxo-4H-benzo[d][1,3]oxazin-5-yl)benzamide (3c)
4-(tert-butyl)-N-(2-(4-(tert-butyl)phenyl)-4-oxo-4H-benzo[d][1,3]oxazin-5-yl)benzamide (3d)
N-(4-oxo-2-(4-(trifluoromethyl)phenyl)-4H-benzo[d][1,3]oxazin-5-yl)-4-(trifluoromethyl)benzamide (3e)
3-methoxy-N-(2-(4-methoxyphenyl)-4-oxo-4H-benzo[d][1,3]oxazin-5-yl)benzamide (3f)
3-methyl-N-(4-oxo-2-(p-tolyl)-4H-benzo[d][1,3]oxazin-5-yl)benzamide (3g)
3-chloro-N-(2-(4-chlorophenyl)-4-oxo-4H-benzo[d][1,3]oxazin-5-yl)benzamide (3h)
N-(4-oxo-2-((E)-styryl)-4H-benzo[d][1,3]oxazin-5-yl)cinnamamide (3i)
N-(4-oxo-2-(thiophen-2-yl)-4H-benzo[d][1,3]oxazin-5-yl)thiophene-2-carboxamide (3j)
4-methyl-N-(4-oxo-2-(p-tolyl)-4H-benzo[d][1,3]oxazin-5-yl)benzamide (3k)
4-ethyl-N-(7-ethyl-2-(4-ethylphenyl)-4-oxo-4H-benzo[d][1,3]oxazin-5-yl)benzamide (3l)
N-(7-methyl-4-oxo-2-phenyl-4H-benzo[1,3]oxazin-5-yl)benzamide (3m)
N-(7-ethyl-4-oxo-2-phenyl-4H-benzo[d][1,3]oxazin-5-yl)benzamide (3n)
N-(7-fluoro-4-oxo-2-phenyl-4H-benzo[d][1,3]oxazin-5-yl)benzamide (3o)
N-(7-chloro-4-oxo-2-phenyl-4H-benzo[d][1,3]oxazin-5-yl)benzamide (3p)
N-(7-bromo-4-oxo-2-phenyl-4H-benzo[d][1,3]oxazin-5-yl)benzamide (3q)
N-(4-oxo-2-phenyl-7-(trifluoromethyl)-4H-benzo[d][1,3]oxazin-5-yl)benzamide (3r)

3r
2-(4-(dimethylamino)phenyl)-4H-benzo[d][1,3]oxazin-4-one (4a)
2-(4-(dimethylamino)phenyl)-7-methoxy-4H-benzo[d][1,3]oxazin-4-one (4b)
2-(4-(dimethylamino)phenyl)-6-methyl-4H-benzo[d][1,3]oxazin-4-one (4c)
6-chloro-2-(4-(dimethylamino)phenyl)-4H-benzo[d][1,3]oxazin-4-one (4d)
7-methyl-2-phenyl-4H-benzo[d][1,3]oxazin-4-one (4e)
2-benzamido-4-methylbenzoic acid (5a)
2-(4-(dimethylamino)benzamido)-4-methoxybenzoic acid (5b)