Supporting Information

Palladium-Catalyzed Site-Selective Direct Olefination of 6- Electron-Withdrawing Group Substitued 3-Arylbenzo[d]isoxazoles

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1. General Information

Unless otherwise indicated, all reagents were obtained from commercial sources and used as received without further purification. All solvents were only dried over 4 Å molecular sieves. Reaction products were purified via column chromatography on silica gel (300–400 mesh). Melting points were determined using an open capillaries and uncorrected. NMR spectra were determined on Bruker AV400 in CDCl$_3$ with TMS as internal standard for $^1$H NMR (400 MHz) and $^{13}$C NMR (100 MHz), respectively. HRMS were measured on a QSTAR Pulsar I LC/TOF MS mass spectrometer or Micromass GCTTM gas chromatograph-mass spectrometer.

2. General Procedures and Characterization Data of the Products

2.1 Table 1  Optimization of the reaction conditions

<table>
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<tr>
<th>Entry</th>
<th>Catalyst</th>
<th>Oxidant</th>
<th>Solvent</th>
<th>Additive</th>
<th>Yield$^b$</th>
</tr>
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<tbody>
<tr>
<td>1</td>
<td>Pd(OAc)$_2$</td>
<td>AgOAc</td>
<td>dioxane</td>
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</tr>
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<td>2</td>
<td>Pd(OAc)$_2$</td>
<td>AgOAc</td>
<td>DCE</td>
<td>–</td>
<td>23%</td>
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<tr>
<td>3</td>
<td>Pd(OAc)$_2$</td>
<td>AgOAc</td>
<td>t-AmyOH</td>
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<td>4</td>
<td>Pd(OAc)$_2$</td>
<td>AgOAc</td>
<td>TFA</td>
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<tr>
<td>5</td>
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<td>AgOAc</td>
<td>DMF</td>
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<td>AgOAc</td>
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<td>7</td>
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<td>–</td>
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<td>DMF/DMSO (9:1)</td>
<td>EudCOOH</td>
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</tr>
<tr>
<td>20</td>
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<td>–</td>
<td>DMF/DMSO (9:1)</td>
<td>EudCOOH</td>
<td>7%</td>
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</table>

$^a$ Reaction conditions: 1a (0.2 mmol), 2a (0.4 mmol), catalyst (10 mol%), oxidant (2.0 equiv), additive (3.0 equiv), solvent (2 mL), 100 °C, 12 h. $^b$ Isolated yield of 3aa. DCE = 1,2-dichloroethane; t-AmyOH = 2-methyl-2-butanol; PivOH = pivalic acid; 2-PBA = 2-phenylbenzoic acid; BQ = 1,4-benzoquinone; MesCOOH = 2,4,6-trimethylbenzoic acid; EudCOOH = 3,4,5-trimethoxybenzoic acid.

General procedure: A mixture of substrate 1a (43 mg, 0.2 mmol), 2a (43 μL, 0.94 g/mL, 0.4 mmol), Pd catalyst (10 mol %), oxidant (2.0 equiv) and additive (3.0 equiv) in solvent (2 mL) was stirred, and then the mixture was heated to 100 °C for 12 h. Upon completion of the reaction, to
the mixture were added saturated brine (20 mL) and dichloromethane (20 mL), then the aqueous layer was extracted with dichloromethane (20 mL × 2). The combined organic layer was dried over anhydrous MgSO₄. Finally, the solution was concentrated \textit{in vacuo} to provide a crude product, which was further purified via a column chromatography on silica gel (eluents: petroleum ether/ethyl acetate = 20:1) to supply the product 3a.

\[ \text{Ethyl (E)-3-(6-fluoro-3-phenylbenzo[d]isoxazol-7-yl)acrylate (3a): white solid, the best result: 46 mg (74\% yield), m.p. 108–109 °C; } ^1\text{H NMR (400 MHz, CDCl}_3, \text{ppm): } \delta \text{ 8.02 (d, } J = 16.4 \text{ Hz, 1H), 7.92–7.90 (m, 2H), 7.84 (dd, } J_1 = 8.8 \text{ Hz, } J_2 = 4.8 \text{ Hz, 1H), 7.59–7.56 (m, 3H), 7.23 (d, } J = 16.4 \text{ Hz, 1H), 7.20 (t, } J = 8.8 \text{ Hz, 1H), 4.32 (q, } J = 7.2 \text{ Hz, 2H), 1.38 (t, } J = 7.2 \text{ Hz, 3H); } ^{13}\text{C NMR (100 MHz, CDCl}_3, \text{ppm): } \delta \text{ 166.8, 162.7 (d, } J_{CF} = 8.0 \text{ Hz), 162.3 (d, } J_{CF} = 256.8 \text{ Hz), 157.4, 130.7, 130.4 (d, } J_{CF} = 4.5 \text{ Hz), 129.3 (2C), 128.2 (2C), 127.9, 125.1, 124.0 (d, } J_{CF} = 11.7 \text{ Hz), 117.8, 113.6 (d, } J_{CF} = 25.8 \text{ Hz), 107.9 (d, } J_{CF} = 16.5 \text{ Hz), 60.8, 14.3; HRMS (EI): } m/z \text{ [M}^+\text{] calcd. for C}_{18}\text{H}_{14}\text{FNO}_3: 311.0958; \text{ found: 311.0956.} \]
2.2 Substrate scope of 3-arylbenzo[d]isoxazoles and alkenes

(1) **Table 2** Substrate scope of 3-arylbenzo[d]isoxazoles

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<th>R1</th>
<th>R2</th>
<th>Product</th>
<th>Yield (%)</th>
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<td>F</td>
<td>3a</td>
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<tr>
<td>Me</td>
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<td>OEt</td>
<td>3n</td>
<td>0%</td>
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</table>

*Reaction conditions: 1 (0.2 mmol), 2a (0.4 mmol), Pd(OAc)$_2$ (10 mol%), Ag$_2$O (2.0 equiv), EudCOOH (3.0 equiv), DMF/DMSO (9:1, 2 mL), 100 °C, 12 h. Isolated yield.*
Table 3  Substrate scope of alkenes$^{a,b}$

| Reaction conditions: 1a (0.2 mmol), 2 (0.4 mmol), Pd(OAc)$_2$ (10 mol%), Ag$_2$O (2.0 equiv), EudCOOH (3.0 equiv), DMF/DMSO (9:1, 2 mL), 100 °C, 12 h. $^b$ Isolated yield. | General procedure: A mixture of substrate 1 (0.2 mmol), 2 (0.4 mmol), Pd(OAc)$_2$ (4.5 mg, 10 mol %), Ag$_2$O (93 mg, 2.0 equiv) and EudCOOH (127 mg, 3.0 equiv) in DMF/DMSO (9:1, 2 mL) was stirred, and then the mixture was heated to 100 °C for 12 h. Upon completion of the reaction, to the mixture were added saturated brine (20 mL) and dichloromethane (20 mL), then the aqueous layer was extracted with dichloromethane (20 mL × 2). The combined organic layer was dried over anhydrous MgSO$_4$. Finally, the solution was concentrated in vacuo to provide a crude product, which was further purified via a column chromatography on silica gel (eluents: petroleum ether/ethyl acetate = 20:1) to supply the product 3 or 4. |

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Ethyl (E)-3-(6-fluoro-3-(p-tolyl)benzo[d]isoxazol-7-yl)acrylate (3b): white solid, 49 mg (76% yield), m.p. 89–90 °C; $^1$H NMR (400 MHz, CDCl$_3$, ppm): δ 8.02 (d, $J$ = 16.4 Hz, 1H), 7.84 (dd, $J$, ...)
= 8.4 Hz, $J_2 = 4.8$ Hz, 1H), 7.80 (d, $J = 8.0$ Hz, 2H), 7.38 (d, $J = 8.0$ Hz, 2H), 7.23 (d, $J = 16.4$ Hz, 1H), 7.19 (t, $J = 8.8$ Hz, 1H), 4.32 (q, $J = 7.2$ Hz, 2H), 2.46 (s, 3H), 1.38 (t, $J = 7.2$ Hz, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$, ppm): $\delta$ 166.8, 162.6 (d, $J_{CF} = 8.1$ Hz), 162.3 (d, $J_{CF} = 256.8$ Hz), 157.3, 141.0, 130.4 (d, $J_{CF} = 4.5$ Hz), 130.3 (2C), 128.0 (2C), 125.1, 124.9, 124.1 (d, $J_{CF} = 11.6$ Hz), 117.9, 113.4 (d, $J_{CF} = 25.9$ Hz), 107.9 (d, $J_{CF} = 16.4$ Hz), 60.8, 21.5, 14.3; HRMS (EI): $m/z$ [M$^+$] calcd. for C$_{19}$H$_{16}$FNO$_2$: 325.1114; found: 325.1113.

![Ethyl (E)-3-(3-(4-tert-butyl)phenyl)-6-fluorobenzo[d]isoxazol-7-yl)acrylate (3c)](image)

Ethyl (E)-3-(3-(4-tert-butyl)phenyl)-6-fluorobenzo[d]isoxazol-7-yl)acrylate (3c): white solid, 55 mg (75% yield), m.p. 91–92 °C; $^1$H NMR (400 MHz, CDCl$_3$, ppm): $\delta$ 8.02 (d, $J = 16.4$ Hz, 1H), 7.86 (d, $J = 8.8$ Hz, 1H), 7.84 (d, $J = 8.4$ Hz, 2H), 7.59 (d, $J = 8.4$ Hz, 2H), 7.23 (d, $J = 16.4$ Hz, 1H), 7.17 (d, $J = 8.8$ Hz, 1H), 4.32 (q, $J = 7.2$ Hz, 2H), 1.39 (s, 9H), 1.38 (t, $J = 7.2$ Hz, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$, ppm): $\delta$ 166.8, 162.6 (d, $J_{CF} = 8.1$ Hz), 162.3 (d, $J_{CF} = 256.8$ Hz), 157.2, 154.1, 130.4 (d, $J_{CF} = 4.5$ Hz), 127.9 (2C), 126.3 (2C), 125.0, 124.9, 124.2 (d, $J_{CF} = 11.6$ Hz), 117.9, 113.4 (d, $J_{CF} = 25.8$ Hz), 107.8 (d, $J_{CF} = 16.6$ Hz), 60.8, 35.0, 31.2 (3C), 14.3; HRMS (EI): $m/z$ [M$^+$] calcd. for C$_{22}$H$_{23}$FNO$_3$: 367.1584; found: 367.1582.

![Ethyl (E)-3-(6-fluoro-3-(4-fluorophenyl)benzo[d]isoxazol-7-yl)acrylate (3d)](image)

Ethyl (E)-3-(6-fluoro-3-(4-fluorophenyl)benzo[d]isoxazol-7-yl)acrylate (3d): white solid, 53 mg (80% yield), m.p. 118–119 °C; $^1$H NMR (400 MHz, CDCl$_3$, ppm): $\delta$ 8.02 (d, $J = 16.4$ Hz, 1H), 7.90 (dd, $J_1 = 8.8$ Hz, $J_2 = 5.2$ Hz, 2H), 7.81 (dd, $J_1 = 8.8$ Hz, $J_2 = 4.8$ Hz, 1H), 7.28 (d, $J = 8.8$ Hz, 2H), 7.22 (d, $J = 16.4$ Hz, 1H), 7.21 (t, $J = 8.8$ Hz, 1H), 4.32 (q, $J = 7.2$ Hz, 2H), 1.38 (t, $J = 7.2$ Hz, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$, ppm): $\delta$ 166.7, 164.2 (d, $J_{CF} = 250.0$ Hz), 162.7 (d, $J_{CF} = 8.0$ Hz), 162.3 (d, $J_{CF} = 257.0$ Hz), 156.5, 130.3 (d, $J_{CF} = 4.4$ Hz), 130.1 (d, $J_{CF} = 8.1$ Hz, 2C), 125.2 (d, $J_{CF} = 4.1$ Hz), 124.0, 123.7 (d, $J_{CF} = 11.7$ Hz), 117.6, 116.5 (d, $J_{CF} = 21.9$ Hz, 2C), 113.7 (d, $J_{CF} = 25.9$ Hz), 108.0 (d, $J_{CF} = 16.6$ Hz), 60.9, 14.3; HRMS (EI): $m/z$ [M$^+$] calcd. for C$_{18}$H$_{13}$F$_2$NO$_3$: 329.0863; found: 329.0864.

![Ethyl (E)-3-(3-(4-chlorophenyl)-6-fluorobenzo[d]isoxazol-7-yl)acrylate (3e)](image)

Ethyl (E)-3-(3-(4-chlorophenyl)-6-fluorobenzo[d]isoxazol-7-yl)acrylate (3e): white solid, 54 mg (78% yield), m.p. 133–134 °C; $^1$H NMR (400 MHz, CDCl$_3$, ppm): $\delta$ 8.02 (d, $J = 16.4$ Hz, 1H), 7.85 (d, $J = 8.4$ Hz, 2H), 7.81 (dd, $J_1 = 8.8$ Hz, $J_2 = 4.8$ Hz, 1H), 7.56 (d, $J = 8.4$ Hz, 2H), 7.22 (d, $J = 16.4$ Hz, 1H), 7.21 (t, $J = 8.8$ Hz, 1H), 4.32 (q, $J = 7.2$ Hz, 2H), 1.38 (t, $J = 7.2$ Hz, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$, ppm): $\delta$ 166.7, 162.8 (d, $J_{CF} = 8.0$ Hz), 162.3 (d, $J_{CF} = 257.3$ Hz), 156.4, 137.0, 130.2 (d, $J_{CF} = 4.4$ Hz), 129.6 (2C), 129.4 (2C), 126.4, 125.3, 123.7 (d, $J_{CF} = 11.6$ Hz), 117.5, 113.8 (d, $J_{CF} = 26.0$ Hz), 108.0 (d, $J_{CF} = 16.7$ Hz), 60.9, 14.3; HRMS (EI): $m/z$ [M$^+$] calcd. for C$_{18}$H$_{13}$ClFNO$_3$: 345.0568; found: 345.0566.
Ethyl (E)-3-(6-fluoro-3-(m-toly)benz|d|isoxazol-7-yl)acrylate (3f): white solid, 47 mg (72% yield), m.p. 85–86 °C; 1H NMR (400 MHz, CDCl₃, ppm): δ 8.02 (d, J = 16.4 Hz, 1H), 7.84 (dd, J₁ = 8.8 Hz, J₂ = 4.8 Hz, 1H), 7.72 (s, 1H), 7.68 (d, J = 7.6 Hz, 1H), 7.46 (t, J = 7.6 Hz, 1H), 7.38 (d, J = 7.6 Hz, 1H), 7.22 (d, J = 16.4 Hz, 1H), 7.19 (t, J = 8.8 Hz, 1H), 4.32 (q, J = 7.2 Hz, 2H), 2.48 (s, 3H), 1.38 (t, J = 7.2 Hz, 3H); 13C NMR (100 MHz, CDCl₃, ppm): δ 166.8, 162.7 (d, J CF = 8.1 Hz), 162.3 (d, J CF = 257.4 Hz), 157.5, 139.2, 131.5, 130.4 (d, J CF = 4.6 Hz), 129.2, 128.7, 127.7, 125.3, 124.1 (d, J CF = 11.6 Hz), 117.8, 113.5 (d, J CF = 26.0 Hz), 107.8 (d, J CF = 16.7 Hz), 6.8, 21.5, 14.7; HRMS (EI): m/z [M⁺] calcd. for C₁₉H₁₆FNO₃: 325.1114; found: 325.1115.

Ethyl (E)-3-(3-(3-chlorophenyl)-6-fluorobenzo|d|isoxazol-7-yl)acrylate (3g): white solid, 56 mg (81% yield), m.p. 93–94 °C; 1H NMR (400 MHz, CDCl₃, ppm): δ 8.02 (d, J = 16.4 Hz, 1H), 7.90 (s, 1H), 7.83 (dd, J₁ = 8.8 Hz, J₂ = 4.8 Hz, 1H), 7.80 (d, J = 7.6 Hz, 1H), 7.55 (d, J = 7.6 Hz, 1H), 7.51 (d, J = 7.6 Hz, 1H), 7.23 (t, J = 8.8 Hz, 1H), 7.22 (d, J = 16.4 Hz, 1H), 4.32 (q, J = 7.2 Hz, 2H), 1.38 (t, J = 7.2 Hz, 3H); 13C NMR (100 MHz, CDCl₃, ppm): δ 166.7, 162.8 (d, J CF = 8.1 Hz), 162.3 (d, J CF = 257.4 Hz), 156.2, 135.3, 130.8, 130.6, 130.2 (d, J CF = 4.4 Hz), 129.6, 128.1, 126.3, 125.3, 123.6 (d, J CF = 11.6 Hz), 117.4, 113.9 (d, J CF = 26.1 Hz), 108.1 (d, J CF = 16.5 Hz), 60.9, 14.3; HRMS (EI): m/z [M⁺] calcd. for C₁₈H₁₃ClFNO₃: 345.0568; found: 345.0565.

Ethyl (E)-3-(6-fluoro-3-(3-nitrophenyl)benzo|d|isoxazol-7-yl)acrylate (3h): yellow solid, 58 mg (81% yield), m.p. 143–144 °C; 1H NMR (400 MHz, CDCl₃, ppm): δ 8.79 (s, 1H), 8.44 (d, J = 8.0 Hz, 1H), 8.02 (d, J = 16.4 Hz, 1H), 7.90 (s, 1H), 7.83 (dd, J₁ = 8.8 Hz, J₂ = 4.8 Hz, 1H), 7.80 (t, J = 8.0 Hz, 1H), 7.29 (t, J = 8.8 Hz, 1H), 7.23 (d, J = 16.4 Hz, 1H), 4.33 (q, J = 7.2 Hz, 2H), 1.39 (t, J = 7.2 Hz, 3H); 13C NMR (100 MHz, CDCl₃, ppm): δ 166.6, 163.0 (d, J CF = 8.0 Hz), 162.5 (d, J CF = 258.1 Hz), 155.5, 148.7, 133.9, 130.6, 130.0 (d, J CF = 4.3 Hz), 129.7, 125.6, 125.3, 123.2 (d, J CF = 11.0 Hz), 123., 117.0, 114.4 (d, J CF = 26.1 Hz), 108.3 (d, J CF = 16.8 Hz), 61.0, 14.3; HRMS (EI): m/z [M⁺] calcd. for C₁₉H₁₃FN₂O₃: 356.0808; found: 356.0810.

Ethyl (E)-3-(6-fluoro-3-(2-chlorophenyl)benzo|d|isoxazol-7-yl)acrylate (3i): yellow solid, 58 mg (84% yield), m.p. 125–126 °C; 1H NMR (400 MHz, CDCl₃, ppm): δ 8.08 (d, J = 16.0 Hz, 1H), 7.68–7.63 (m, 2H), 7.62 (dd, J₁ = 8.8 Hz, J₂ = 4.8 Hz, 1H), 7.52 (dt, J₁ = 7.6 Hz, J₂ = 1.6 Hz, 1H),
7.48 (dd, \( J_1 = 7.6 \) Hz, \( J_2 = 1.6 \) Hz, 1H), 7.43 (d, \( J = 16.0 \) Hz, 1H), 6.93 (t, \( J = 8.8 \) Hz, 1H), 4.30 (q, \( J = 7.2 \) Hz, 2H), 1.36 (t, \( J = 7.2 \) Hz, 3H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\), ppm): \( \delta 167.2, 164.5, 162.5 \) (d, \( \frac{1}{3} J_{CF} = 261.1 \) Hz), 156.1 (d, \( \frac{3}{3} J_{CF} = 7.8 \) Hz), 133.0, 132.2, 131.7, 131.1 (d, \( \frac{3}{3} J_{CF} = 5.2 \) Hz), 131.0, 127.3, 126.5, 125.2, 125.1, 117.4 (d, \( \frac{2}{2} J_{CF} = 31.1 \) Hz), 114.8, 108.0 (d, \( \frac{2}{2} J_{CF} = 14.6 \) Hz), 60.6, 14.3; HRMS (EI): \( m/z \) \([M^+]\) calcd. for C\(_{18}\)H\(_{13}\)ClFNO\(_3\): 345.0568; found: 345.0569.

**Ethyl (E)-3-(6-fluoro-3-(thiophen-2-yl)benzo[d]isoxazol-7-yl)acrylate (3j):** white solid, 52 mg (82% yield), m.p. 136–137 °C; \(^1\)H NMR (400 MHz, CDCl\(_3\), ppm): \( \delta 7.92 \) (dd, \( J_1 = 8.8 \) Hz, \( J_2 = 4.8 \) Hz, 1H), 7.78 (d, \( J = 15.6 \) Hz, 1H), 7.71 (d, \( J = 3.6 \) Hz, 1H), 7.36–7.33 (m, 2H), 7.19 (dt, \( J_1 = 8.8 \) Hz, \( J_2 = 2.0 \) Hz, 1H), 6.36 (d, \( J = 15.6 \) Hz, 1H), 4.28 (q, \( J = 7.2 \) Hz, 2H), 1.35 (t, \( J = 7.2 \) Hz, 3H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\), ppm): \( \delta 166.4, 164.5 \) (d, \( \frac{1}{3} J_{CF} = 13.4 \) Hz), 164.3 (d, \( \frac{3}{3} J_{CF} = 250.8 \) Hz), 151.6, 142.1, 136.1, 131.5, 131.1, 128.9, 122.7 (d, \( \frac{2}{2} J_{CF} = 10.9 \) Hz), 119.1, 116.3, 113.6 (d, \( \frac{2}{2} J_{CF} = 25.2 \) Hz), 97.7 (d, \( \frac{2}{2} J_{CF} = 26.6 \) Hz), 60.8, 14.3; HRMS (EI): \( m/z \) \([M^+]\) calcd. for C\(_{16}\)H\(_{12}\)SFNO\(_3\): 317.0522; found: 317.0520.

**Ethyl (E)-3-(6-chloro-3-(4-ethoxyphenyl)benzo[d]isoxazol-7-yl)acrylate (3k):** white solid, 52 mg (70% yield), m.p. 148–149 °C; \(^1\)H NMR (400 MHz, CDCl\(_3\), ppm): \( \delta 8.16 \) (d, \( J = 16.4 \) Hz, 1H), 7.83 (d, \( J = 8.8 \) Hz, 2H), 7.77 (d, \( J = 8.4 \) Hz, 1H), 7.36–7.33 (m, 2H), 7.19 (dt, \( J_1 = 8.8 \) Hz, \( J_2 = 2.0 \) Hz, 1H), 6.36 (d, \( J = 15.6 \) Hz, 1H), 4.28 (q, \( J = 7.2 \) Hz, 2H), 4.11 (q, \( J = 6.8 \) Hz, 2H), 1.47 (t, \( J = 6.8 \) Hz, 3H), 1.37 (t, \( J = 7.2 \) Hz, 3H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\), ppm): \( \delta 166.9, 164.5 \) (d, \( \frac{3}{3} J_{CF} = 13.4 \) Hz), 164.3 (d, \( \frac{1}{3} J_{CF} = 250.8 \) Hz), 151.6, 142.1, 136.1, 131.5, 131.1, 128.9, 122.7 (d, \( \frac{2}{2} J_{CF} = 10.9 \) Hz), 119.1, 116.3, 113.6 (d, \( \frac{2}{2} J_{CF} = 25.2 \) Hz), 97.7 (d, \( \frac{2}{2} J_{CF} = 26.6 \) Hz), 60.8, 14.3; HRMS (EI): \( m/z \) \([M^+]\) calcd. for C\(_{20}\)H\(_{18}\)ClNO\(_4\): 371.0924; found: 371.0925.

**Ethyl (E)-3-(6-bromo-3-(4-methoxyphenyl)benzo[d]isoxazol-7-yl)acrylate (3l):** white solid, 54 mg (67% yield), m.p. 169–170 °C; \(^1\)H NMR (400 MHz, CDCl\(_3\), ppm): \( \delta 8.13 \) (d, \( J = 16.0 \) Hz, 1H), 7.85 (d, \( J = 8.8 \) Hz, 2H), 7.70 (d, \( J = 8.4 \) Hz, 1H), 7.62 (d, \( J = 8.4 \) Hz, 1H), 7.32 (d, \( J = 16.0 \) Hz, 1H), 7.08 (d, \( J = 8.8 \) Hz, 2H), 4.32 (q, \( J = 7.2 \) Hz, 2H), 3.90 (s, 3H), 1.38 (t, \( J = 7.2 \) Hz, 3H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\), ppm): \( \delta 166.9, 162.7, 161.0, 156.9, 137.4, 134.5, 129.5 \) (2C), 126.3, 126.1, 123.4, 120.4, 120.0, 117.7, 115.2 (2C), 63.7, 60.9, 14.8, 14.3; HRMS (EI): \( m/z \) \([M^+]\) calcd. for C\(_{19}\)H\(_{16}\)BrNO\(_4\): 401.0263; found: 401.0267.
Ethyl (E)-3-(3-(4-ethoxyphenyl)-6-nitrobenzo[d]isoxazol-7-yl)acrylate (3m): yellow solid, 60 mg (79% yield), m.p. 152–153 °C; 1H NMR (400 MHz, CDCl₃, ppm): δ 8.02 (d, J = 16.0 Hz, 1H), 7.99 (d, J = 8.8 Hz, 1H), 7.92 (d, J = 8.8 Hz, 1H), 7.86 (d, J = 8.8 Hz, 2H), 7.29 (d, J = 16.0 Hz, 1H), 7.10 (d, J = 8.8 Hz, 2H), 4.33 (q, J = 7.2 Hz, 2H), 4.14 (q, J = 7.2 Hz, 2H), 1.42 (t, J = 7.2 Hz, 3H), 1.38 (t, J = 7.2 Hz, 3H); 13C NMR (100 MHz, CDCl₃, ppm): δ 166.0, 161.5, 161.3, 157.3, 149.5, 131.9, 129.6 (2C), 128.9, 124.3, 123.3, 120.5, 119.1, 115.4 (2C), 114.5, 63.8, 61.2, 14.7, 14.3; HRMS (EI): m/z [M⁺] calcd. for C₂₀H₁₈N₂O₆: 382.165; found: 382.1166.

Ethyl (E)-3-(6-fluoro-3-methylbenzo[d]isoxazol-7-yl)acrylate (3p): white solid, 37 mg (74% yield), m.p. 66–68 °C; 1H NMR (400 MHz, CDCl₃, ppm): δ 7.97 (d, J = 16.4 Hz, 1H), 7.56 (dd, J₁ = 8.8 Hz, J₂ = 4.8 Hz, 1H), 7.16 (d, J = 16.4 Hz, 1H), 7.13 (t, J = 8.8 Hz, 1H), 4.30 (q, J = 7.2 Hz, 2H), 2.59 (s, 3H), 1.36 (t, J = 7.2 Hz, 3H); 13C NMR (100 MHz, CDCl₃, ppm): δ 166.8, 162.4 (d, JₐCF = 256.1 Hz), 161.8 (d, J₃CF = 8.1 Hz), 159.7, 130.5 (d, J₃CF = 4.8 Hz), 124.9, 123.0 (d, J₃CF = 11.7 Hz), 119.5, 112.9 (d, J₂CF = 26.0 Hz), 107.8 (d, J₂CF = 14.7 Hz), 60.8, 14.3, 9.8; HRMS (EI): m/z [M⁺] calcd. for C₁₃H₁₂FNO₃: 249.0801; found: 249.0799.

Ethyl (E)-3-(3-ethyl-6-fluorobenzo[d]isoxazol-7-yl)acrylate (3q): white solid, 41 mg (77% yield), m.p. 72–74 °C; 1H NMR (400 MHz, CDCl₃, ppm): δ 7.97 (d, J = 16.4 Hz, 1H), 7.59 (dd, J₁ = 8.4 Hz, J₂ = 4.8 Hz, 1H), 7.16 (d, J = 16.4 Hz, 1H), 7.11 (t, J = 8.4 Hz, 1H), 4.30 (q, J = 7.2 Hz, 2H), 3.01 (q, J = 7.6 Hz, 2H), 1.45 (t, J = 7.6 Hz, 3H), 1.36 (t, J = 7.2 Hz, 3H); 13C NMR (100 MHz, CDCl₃, ppm): δ 166.8, 162.3 (d, JₐCF = 256.1 Hz), 161.9 (d, J₃CF = 8.2 Hz), 157.4, 130.5 (d, J₃CF = 11.7 Hz), 118.7, 112.8 (d, J₂CF = 26.2 Hz), 107.8 (d, J₂CF = 16.6 Hz), 60.8, 18.7, 14.3, 12.1; HRMS (EI): m/z [M⁺] calcd. for C₁₄H₁₄FNO₃: 263.0958; found: 263.0957.

Butyl (E)-3-(6-fluoro-3-phenylbenzo[d]isoxazol-7-yl)acrylate (4a): white solid, 53 mg (78% yield), m.p. 64–65 °C; 1H NMR (400 MHz, CDCl₃, ppm): δ 8.02 (d, J = 16.0 Hz, 1H), 7.92–7.90 (m, 2H), 7.85 (dd, J₁ = 8.4 Hz, J₂ = 4.8 Hz, 1H), 7.60–7.56 (m, 3H), 7.24 (d, J = 16.0 Hz, 1H), 7.20 (t, J = 8.8 Hz, 1H), 4.27 (t, J = 6.8 Hz, 2H), 1.73 (quint, J = 6.8 Hz, 2H), 1.47 (m, 2H), 0.99 (t, J = 7.6 Hz, 3H); 13C NMR (100 MHz, CDCl₃, ppm): δ 166.9, 162.7 (d, JₐCF = 8.2 Hz), 162.3 (d, J₁CF = 257.1 Hz), 157.4, 130.7, 130.3 (d, J₃CF = 4.7 Hz), 129.3 (2C), 128.2 (2C), 127.9, 125.1, 124.0 (d, J₂CF = 11.7 Hz), 117.8, 113.6 (d, J₂CF = 25.9 Hz), 107.9 (d, J₂CF = 16.6 Hz), 64.7, 30.7, 19.2, 13.8; HRMS (EI): m/z [M⁺] calcd. for C₂₀H₁₈FNO₃: 339.1271; found: 339.1270.
**Isobutyl (E)-3-(6-fluoro-3-phenylbenzo[d]isoxazol-7-yl)acrylate (4b):** white solid, 55 mg (81% yield), m.p. 87–88 °C; \(^1\)H NMR (400 MHz, CDCl\(_3\), ppm): \(\delta \) 8.03 (d, \(J = 16.4 \text{ Hz}, 1\)H), 7.92–7.90 (m, 2H), 7.85 (dd, \(J_1 = 8.8 \text{ Hz}, J_2 = 4.8 \text{ Hz}, 1\)H), 7.60–7.56 (m, 3H), 7.25 (d, \(J = 16.4 \text{ Hz}, 1\)H), 7.20 (t, \(J = 8.8 \text{ Hz}, 1\)H), 4.04 (q, \(J = 6.8 \text{ Hz}, 2\)H), 2.11–2.10 (m, 1H), 1.01 (d, \(J = 6.8 \text{ Hz}, 6\)H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\), ppm): \(\delta \) 166.9, 162.7 (d, \(3J_{CF} = 8.0 \text{ Hz}\)), 162.3 (d, \(^1J_{CF} = 256.9 \text{ Hz}\)), 157.4, 130.7, 130.4 (d, \(^3J_{CF} = 4.6 \text{ Hz}\)), 129.3 (2C), 128.2 (2C), 127.9, 125.1, 124.0 (d, \(^1J_{CF} = 11.6 \text{ Hz}\)), 117.8, 113.6 (d, \(^2J_{CF} = 25.8 \text{ Hz}\)), 107.9 (d, \(^2J_{CF} = 16.5 \text{ Hz}\)), 71.0, 27.8, 19.2 (2C); HRMS (EI): \(m/z\) [M+] calcd. for C\(_{20}\)H\(_{18}\)FNO\(_3\): 339.1271; found: 339.1269.

**tert-Butyl (E)-3-(6-fluoro-3-phenylbenzo[d]isoxazol-7-yl)acrylate (4c):** white solid, 54 mg (80% yield), m.p. 148–149 °C; \(^1\)H NMR (400 MHz, CDCl\(_3\), ppm): \(\delta \) 7.93 (d, \(J = 16.4 \text{ Hz}, 1\)H), 7.92–7.90 (m, 2H), 7.83 (dd, \(J_1 = 8.8 \text{ Hz}, J_2 = 4.8 \text{ Hz}, 1\)H), 7.59–7.57 (m, 3H), 7.20 (d, \(J = 16.4 \text{ Hz}, 1\)H), 7.17 (t, \(J = 8.8 \text{ Hz}, 1\)H), 1.57 (s, 9H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\), ppm): \(\delta \) 166.1, 162.7 (d, \(3J_{CF} = 8.2 \text{ Hz}\)), 162.2 (d, \(^1J_{CF} = 256.6 \text{ Hz}\)), 157.3, 130.7, 129.3, 129.2 (2C), 128.2 (2C), 127.9, 127.1, 123.7 (d, \(^3J_{CF} = 11.6 \text{ Hz}\)), 117.7, 113.6 (d, \(^2J_{CF} = 26.1 \text{ Hz}\)), 108.1 (d, \(^2J_{CF} = 16.7 \text{ Hz}\)), 81.0, 28.2 (3C); HRMS (EI): \(m/z\) [M+] calcd. for C\(_{20}\)H\(_{18}\)FNO\(_3\): 339.1270; found: 339.1270.

**Phenyl (E)-3-(6-fluoro-3-phenylbenzo[d]isoxazol-7-yl)acrylate (4d):** white solid, 50 mg (70% yield), m.p. 151–152 °C; \(^1\)H NMR (400 MHz, CDCl\(_3\), ppm): \(\delta \) 8.21 (d, \(J = 16.4 \text{ Hz}, 1\)H), 7.94–7.91 (m, 2H), 7.90 (dd, \(J_1 = 8.8 \text{ Hz}, J_2 = 4.8 \text{ Hz}, 1\)H), 7.60–7.58 (m, 3H), 7.44 (d, \(J = 6.8 \text{ Hz}, 2\)H), 7.43 (t, \(J = 8.4 \text{ Hz}, 2\)H), 7.28 (d, \(J = 7.2 \text{ Hz}, 1\)H), 7.24–7.22 (m, 3H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\), ppm): \(\delta \) 165.2, 162.8 (d, \(3J_{CF} = 8.0 \text{ Hz}\)), 162.5 (d, \(^1J_{CF} = 256.6 \text{ Hz}\)), 157.3, 130.7, 129.3 (2C), 128.2 (2C), 127.8, 125.9, 124.6 (d, \(^3J_{CF} = 11.7 \text{ Hz}\)), 124.1, 121.6 (2C), 117.9, 113.6 (d, \(^2J_{CF} = 25.9 \text{ Hz}\)), 107.7 (d, \(^2J_{CF} = 16.3 \text{ Hz}\)); HRMS (EI): \(m/z\) [M+] calcd. for C\(_{20}\)H\(_{18}\)FNO\(_3\): 359.0958; found: 359.0961.

**Benzyl (E)-3-(6-fluoro-3-phenylbenzo[d]isoxazol-7-yl)acrylate (4e):** white solid, 57 mg (76% yield), m.p. 149–150 °C; \(^1\)H NMR (400 MHz, CDCl\(_3\), ppm): \(\delta \) 8.07 (d, \(J = 16.4 \text{ Hz}, 1\)H), 7.92–7.89 (m, 2H), 7.85 (dd, \(J_1 = 8.8 \text{ Hz}, J_2 = 4.8 \text{ Hz}, 1\)H), 7.59–7.56 (m, 3H), 7.46 (d, \(J = 6.8 \text{ Hz}, 2\)H), 7.41 (t, \(J = 6.8 \text{ Hz}, 2\)H), 7.36 (d, \(J = 7.2 \text{ Hz}, 1\)H), 7.28 (d, \(J = 16.4 \text{ Hz}, 1\)H), 7.20 (t, \(J = 8.8 \text{ Hz}, 1\)H), 5.32 (s, 2H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\), ppm): \(\delta \) 166.6, 163.7 (d, \(^3J_{CF} = 7.9 \text{ Hz}\)), 162.3
(d, $^1J_{CF} = 263.1$ Hz), 157.4, 135.9, 131.0 (d, $^3J_{CF} = 4.6$ Hz), 130.9, 130.7, 129.2 (2C), 128.6 (2C), 128.3 (2C), 128.2 (2C), 127.9, 124.7, 124.2 (d, $^3J_{CF} = 11.6$ Hz), 117.8, 113.6 (d, $^2J_{CF} = 20.8$ Hz), 107.8 (d, $^2J_{CF} = 16.6$ Hz), 66.6; HRMS (EI): $m/z$ [M$^+$] calcd. for C$_{23}$H$_{16}$FNO$_3$: 373.1114; found: 373.1113.

Methyl 2-((6-fluoro-3-phenylbenzo[d]isoxazol-7-yl)methyl)acrylate (4f): white solid, 44 mg (71% yield), m.p. 39–40 ºC; $^1$H NMR (400 MHz, CDCl$_3$, ppm): $\delta$ 7.93–7.90 (m, 2H), 7.76 (dd, $J_1 = 8.8$ Hz, $J_2 = 4.8$ Hz, 1H), 7.58–7.55 (m, 3H), 7.16 (t, $J = 8.8$ Hz, 1H), 6.31 (s, 1H), 5.50 (s, 1H), 4.01 (s, 2H), 3.79 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$, ppm): $\delta$ 166.9, 163.7 (d, $^3J_{CF} = 10.2$ Hz), 162.0 (d, $^1J_{CF} = 249.5$ Hz), 157.5, 136.5, 130.4, 129.2 (2C), 128.5, 128.1 (2C), 126.6, 121.1 (d, $^3J_{CF} = 11.2$ Hz), 116.9, 113.4 (d, $^2J_{CF} = 26.1$ Hz), 109.0 (d, $^2J_{CF} = 21.4$ Hz), 52.1, 25.7; HRMS (EI): $m/z$ [M$^+$] calcd. for C$_{18}$H$_{14}$FNO$_3$: 311.0958; found: 311.0960.

Cyclohexyl 2-((6-fluoro-3-phenylbenzo[d]isoxazol-7-yl)methyl)acrylate (4g): yellow solid, 52 mg (69% yield), m.p. 88–89 ºC; $^1$H NMR (400 MHz, CDCl$_3$, ppm): $\delta$ 7.93–7.90 (m, 2H), 7.75 (dd, $J_1 = 8.8$ Hz, $J_2 = 4.8$ Hz, 1H), 7.56–7.55 (m, 3H), 7.15 (t, $J = 8.8$ Hz, 1H), 6.31 (s, 1H), 4.88–4.82 (m, 1H), 4.00 (s, 2H), 1.87–1.70 (m, 4H), 1.54–1.25 (m, 6H); $^{13}$C NMR (100 MHz, CDCl$_3$, ppm): $\delta$ 165.8, 163.7 (d, $^3J_{CF} = 10.4$ Hz), 162.0 (d, $^1J_{CF} = 249.4$ Hz), 157.5, 137.2, 130.4, 129.2 (2C), 128.5, 128.1 (2C), 126.3, 121.0 (d, $^3J_{CF} = 11.1$ Hz), 116.9, 113.4 (d, $^2J_{CF} = 26.3$ Hz), 109.3 (d, $^2J_{CF} = 21.6$ Hz), 73.3, 31.5 (2C), 25.8, 25.4, 23.7 (2C); HRMS (EI): $m/z$ [M$^+$] calcd. for C$_{23}$H$_{22}$FNO$_3$: 379.1584; found: 379.1586.

Methyl 2-(6-fluoro-3-phenylbenzo[d]isoxazol-7-yl)cyclopent-2-ene-1-carboxylate (4h): yellow oil, 42 mg (63% yield), $^1$H NMR (400 MHz, CDCl$_3$, ppm): $\delta$ 7.91–7.89 (m, 2H), 7.68 (dd, $J_1 = 8.4$ Hz, $J_2 = 4.8$ Hz, 1H), 7.56–7.54 (m, 3H), 7.12 (t, $J = 8.8$ Hz, 1H), 7.08–7.07 (m, 1H), 4.81 (t, $J = 8.4$ Hz, 1H), 3.59 (s, 3H), 3.08–3.01 (m, 1H), 2.73–2.59 (m, 2H), 2.23–2.14 (m, 1H) $^{13}$C NMR (100 MHz, CDCl$_3$, ppm): $\delta$ 164.8, 163.1 (d, $^3J_{CF} = 10.1$ Hz), 161.4 (d, $^1J_{CF} = 248.5$ Hz), 157.3, 146.0, 135.8, 130.3, 129.2 (2C), 128.6, 128.1 (2C), 120.4 (d, $^3J_{CF} = 11.4$ Hz), 117.1, 115.3 (d, $^2J_{CF} = 18.9$ Hz), 113.5 (d, $^2J_{CF} = 27.0$ Hz), 51.4, 39.6, 32.9, 30.7; HRMS (EI): $m/z$ [M$^+$] calcd. for C$_{20}$H$_{16}$FNO$_3$: 337.1114; found: 337.1111.

(E)-1-(6-Fluoro-3-phenylbenzo[d]isoxazol-7-yl)pent-1-en-3-one (4i): yellow solid, 39 mg (66%
yield), m.p. 136–137 °C; ¹H NMR (400 MHz, CDCl₃, ppm): δ 7.91 (d, J = 16.4 Hz, 1H), 7.92–7.90 (m, 2H), 7.85 (dd, J₁ = 8.8 Hz, J₂ = 4.8 Hz, 1H), 7.59–7.57 (m, 3H), 7.53 (d, J = 16.4 Hz, 1H), 7.20 (t, J = 8.8 Hz, 1H), 2.77 (q, J = 7.2 Hz, 2H), 1.21 (t, J = 7.2 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃, ppm): δ 200.8, 162.7 (d, J₁CF = 8.0 Hz), 162.6 (d, J₁CF = 256.9 Hz), 157.4, 131.6 (d, J₁CF = 4.7 Hz), 130.7, 129.3 (2C), 128.2 (2C), 127.9, 127.7, 124.1 (d, J₁CF = 11.6 Hz), 117.8, 113.7 (d, J₁CF = 26.0 Hz), 108.2 (d, J₁CF = 16.5 Hz), 35.3, 8.1; HRMS (EI): m/z [M⁺] calcd. for C₁₈H₁₄FNO₂: 295.1099; found: 295.1098.

![Image of 4j](image-url)

**(E)-3-(6-Fluoro-3-phenylbenzo[d]isoxazol-7-yl)-N,N-dimethylacrylamide (4j):** white solid, 42 mg (68% yield), m.p. 195–196 °C; ¹H NMR (400 MHz, CDCl₃, ppm): δ 8.00 (d, J = 15.6 Hz, 1H), 7.91–7.90 (m, 2H), 7.82 (dd, J₁ = 8.8 Hz, J₂ = 4.8 Hz, 1H), 7.73 (d, J = 15.6 Hz, 1H), 7.59–7.57 (m, 3H), 7.19 (t, J = 8.8 Hz, 1H), 3.27 (s, 3H), 3.12 (s, 3H); ¹³C NMR (100 MHz, CDCl₃, ppm): δ 166.4, 162.7 (d, J₁CF = 8.1 Hz), 162.2 (d, J₁CF = 256.5 Hz), 157.4, 130.7, 129.3 (2C), 128.2 (2C), 128.1, 127.9, 124.3, 123.2 (d, J₁CF = 11.5 Hz), 117.6, 113.7 (d, J₁CF = 26.1 Hz), 108.1 (d, J₁CF = 16.7 Hz), 37.5, 36.0; HRMS (EI): m/z [M⁺] calcd. for C₁₈H₁₄FNO₂: 310.1118; found: 310.1119.

![Image of 4k](image-url)

**Diethyl (E)-(2-(6-fluoro-3-phenylbenzo[d]isoxazol-7-yl)vinyl)phosphonate (4k):** white solid, 43 mg (57% yield), m.p. 83–85 °C; ¹H NMR (400 MHz, CDCl₃, ppm): δ 7.91–7.89 (m, 2H), 7.85 (dd, J₁ = 8.4 Hz, J₂ = 4.8 Hz, 1H), 7.81 (d, J = 18.0 Hz, 1H), 7.59–7.56 (m, 3H), 7.20 (t, J = 8.4 Hz, 1H), 7.11 (d, J = 18.0 Hz, 1H), 4.23–4.16 (m, 4H), 1.39 (t, J = 7.2 Hz, 6H); ¹³C NMR (100 MHz, CDCl₃, ppm): δ 162.6 (d, J₁CP = 8.0 Hz), 162.0 (d, J₁CP = 256.9 Hz), 157.4, 134.4 (dd, J₁CF = 7.4 Hz, J₁CP = 5.3 Hz), 130.7, 129.3 (2C), 128.2 (2C), 127.8, 124.1 (d, J₁CF = 11.6 Hz), 122.3 (d, J₁CP = 186.0 Hz), 117.9, 113.7 (d, J₁CP = 26.1 Hz), 108.4 (dd, J₁CP = 25.1 Hz, J₁CP = 8.9 Hz), 62.1 (d, J₁CP = 5.3 Hz, 2C), 16.4 (d, J₁CP = 6.3 Hz, 2C); HRMS (EI): m/z [M⁺] calcd. for C₁₉H₁₅NO₄PF: 375.1036; found: 375.1031.

![Image of 4l](image-url)

**(E)-6-fluoro-3-phenyl-7-styrylbenzo[d]isoxazole (4l):** white solid, 43 mg (68% yield), m.p. 148–150 °C; ¹H NMR (400 MHz, CDCl₃, ppm): δ 7.97 (d, J = 16.4 Hz, 1H), 7.95–7.93 (m, 2H), 7.71 (dd, J₁ = 8.8 Hz, J₂ = 4.8 Hz, 1H), 7.65 (d, J = 7.6 Hz, 2H), 7.60–7.58 (m, 3H), 7.44–7.40 (m, 2H), 7.43 (d, J = 16.4 Hz, 1H), 7.33 (t, J = 7.6 Hz, 1H), 7.19 (t, J = 8.8 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃, ppm): δ 162.4 (d, J₁CF = 8.9 Hz), 161.0 (d, J₁CF = 252.0 Hz), 157.4, 137.3, 136.0, 130.5, 129.2 (2C), 128.8 (2C), 128.5, 128.4, 128.2 (2C), 126.9 (2C), 120.7, 117.5, 115.1, 113.6 (d, J₁CF = 26.4 Hz), 110.5 (d, J₁CF = 16.6 Hz); HRMS (EI): m/z [M⁺] calcd. for C₁₉H₁₄FNO₃: 315.1059; found: 315.1060.
(E)-6-fluoro-7-(4-methylstyryl)-3-phenylbenzo[d]isoxazole (4m): white solid, 43 mg (66% yield), m.p. 124–126 °C; 1H NMR (400 MHz, CDCl₃, ppm): δ 7.95–7.92 (m, 2H), 7.94 (d, J = 16.8 Hz, 1H), 7.68 (dd, J₁ = 8.4 Hz, J₂ = 4.8 Hz, 1H), 7.60–7.57 (m, 3H), 7.55 (d, J = 8.0 Hz, 2H), 7.38 (d, J = 16.8 Hz, 1H), 7.22 (d, J = 8.0 Hz, 2H), 7.17 (t, J = 8.8 Hz, 1H), 2.39 (s, 3H); 13C NMR (100 MHz, CDCl₃, ppm): δ 162.4 (d, 3JCF = 8.9 Hz), 160.9 (d, 1JCF = 251.7 Hz), 157.3, 138.5, 136.0, 134.5, 130.5, 129.5 (2C), 129.2 (2C), 128.4, 128.2 (2C), 126.9 (2C), 120.3 (d, 3JCF = 11.2 Hz), 117.5, 114.0, 113.6 (d, 2JCF = 26.3 Hz), 110.6 (d, 2JCF = 16.6 Hz), 21.4; HRMS (EI): m/z [M⁺] calcd. for C₂₂H₁₆FNO: 329.1216; found: 329.1217.

(E)-7-(4-chlorostyryl)-6-fluoro-3-phenylbenzo[d]isoxazole (4n): yellow solid, 54 mg (77% yield), m.p. 182–184 °C; 1H NMR (400 MHz, CDCl₃, ppm): δ 7.95–7.92 (m, 2H), 7.91 (d, J = 16.8 Hz, 1H), 7.72 (dd, J₁ = 8.8 Hz, J₂ = 4.8 Hz, 1H), 7.60–7.58 (m, 3H), 7.56 (d, J = 8.4 Hz, 2H), 7.39 (d, J = 16.8 Hz, 1H), 7.38 (d, J = 8.4 Hz, 2H), 7.18 (t, J = 8.8 Hz, 1H); 13C NMR (100 MHz, CDCl₃, ppm): δ 162.3 (d, 3JCF = 8.8 Hz), 161.0 (d, 1JCF = 252.5 Hz), 157.4, 135.7, 134.6, 134.1, 130.6, 129.3 (2C), 129.0 (2C), 128.3, 128.2 (2C), 128.1 (2C), 121.0 (d, 2JCF = 11.3 Hz), 117.6, 115.6, 113.6 (d, 2JCF = 26.3 Hz), 110.1 (d, 2JCF = 16.5 Hz); HRMS (EI): m/z [M⁺] calcd. for C₂₁H₁₃FClNO: 349.0670; found: 349.0672.

Methyl (E)-4-(2-(6-fluoro-3-phenylbenzo[d]isoxazol-7-yl)vinyl)benzoate (4o): yellow solid, 62 mg (83% yield), m.p. 208–210 °C; 1H NMR (400 MHz, CDCl₃, ppm): δ 8.08 (d, J = 8.4 Hz, 2H), 7.98 (d, J = 16.8 Hz, 1H), 7.95–7.92 (m, 2H), 7.75 (dd, J₁ = 8.8 Hz, J₂ = 4.8 Hz, 1H), 7.70 (d, J = 8.4 Hz, 2H), 7.60–7.58 (m, 3H), 7.53 (d, J = 16.8 Hz, 1H), 7.20 (t, J = 8.8 Hz, 1H), 3.94 (s, 3H); 13C NMR (100 MHz, CDCl₃, ppm): δ 166.8, 162.4 (d, 3JCF = 8.7 Hz), 161.2 (d, 1JCF = 253.0 Hz), 157.4, 141.6, 134.75, 134.71, 130.6, 130.1 (2C), 129.6, 129.3 (2C), 128.2 (2C), 126.7 (2C), 121.4 (d, 3JCF = 11.3 Hz), 117.6, 117.4, 113.6 (d, 2JCF = 26.3 Hz), 110.0 (d, 2JCF = 16.6 Hz), 52.2; HRMS (EI): m/z [M⁺] calcd. for C₂₃H₁₅FNO₃: 373.1114; found: 373.1115.
2.3 Single crystal structure of 3a

Identification code cd17297
Empirical formula C18 H14 F N O3
Formula weight 311.30
Temperature 293(2) K
Wavelength 0.71073 Å
Crystal system Triclinic
Space group P 1
Unit cell dimensions
\[ a = 7.5115(19) \text{ Å} \quad \alpha = 79.433(4)°. \]
\[ b = 13.839(4) \text{ Å} \quad \beta = 89.551(5)°. \]
\[ c = 14.941(4) \text{ Å} \quad \gamma = 89.948(5)°. \]
Volume 1526.7(7) Å³
Z 4
Density (calculated) 1.354 Mg/m³
Absorption coefficient 0.101 mm⁻¹
F(000) 648
Crystal size 0.200 x 0.100 x 0.050 mm³
Theta range for data collection 1.497 to 25.000°.
Index ranges -8<=h<=8, -16<=k<=16, -14<=l<=17
Reflections collected 8493
Independent reflections 6735 \[ R(\text{int}) = 0.0300 \]
Completeness to theta = 25.242° 98.2 %
Absorption correction Semi-empirical from equivalents
Max. and min. transmission 0.7456 and 0.5272
Refinement method Full-matrix least-squares on F²
Data / restraints / parameters 6735 / 3 / 834
Goodness-of-fit on F² 1.036
Final R indices [I>2sigma(I)]
\[ R1 = 0.0659, \quad wR2 = 0.1673 \]
R indices (all data)
\[ R1 = 0.0788, \quad wR2 = 0.1826 \]
Absolute structure parameter 1.6(10)
Extinction coefficient n/a
Largest diff. peak and hole 0.366 and -0.476 e.Å⁻³
3. Deuterium Incorporation Studies (Scheme 2)

**General procedure:** A mixture of substrate 1 (0.2 mmol), Pd(OAc)$_2$ (4.5 mg, 10 mol %), Ag$_2$O (93 mg, 2.0 equiv), K$_2$CO$_3$ (55 mg, 2.0 equiv) and D$_2$O (0.46 mL, 1.493 g/mL, 6.0 mmol) in DMF/DMSO (9:1, 2 mL) or CF$_3$COOD (2 mL) was stirred, and then the mixture was heated to 100 °C for 12 h. Upon completion of the reaction, to the mixture were added saturated brine (20 mL) and dichloromethane (20 mL), then the aqueous layer was extracted with dichloromethane (20 mL × 2). The combined organic layer was dried over anhydrous MgSO$_4$. Finally, the solution was concentrated *in vacuo* to provide a crude product, which was further purified via a column chromatography on silica gel (eluents: petroleum ether/ethyl acetate = 20:1) to recover the substrate 1. The deuterations were analyzed by $^1$H NMR, see: 4.2 Copies of the spectra for Scheme 2.
4. All Copies of Spectra
4.1 Copies of the spectra for Tables 2 and 3
**Elemental Composition Report**

**Single Mass Analysis**
- Tolerance = 5.0 mDa /
- DBE: min = -1.5, max = 50.0
- Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
119 formula(e) evaluated with 14 results within limits (up to 50 closest results for each mass)
Elements Used:
- C: 0-18
- H: 0-14
- N: 0-1
- O: 0-3
- F: 0-1

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**Diagram**

1. [Diagram of molecule 3a with elemental composition and mass analysis results.]
2. [Diagram of molecule 3b with mass spectrum and chemical shifts.]
Elemental Composition Report

**Single Mass Analysis**

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
139 formula(e) evaluated with 16 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-19   H: 0-16   N: 0-1   O: 0-3   F: 0-1

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Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
345 formula(e) evaluated with 29 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-22  H: 0-22  N: 0-1  O: 0-3  F: 0-1

Minimum:  3.00  -1.5
Maximum:  100.00  5.0  10.0  50.0

Mass  RA  Calc. Mass  mDa  PPM  DBE  I-FIT  Formula
367.1582  11.69  367.1584  -0.2  -0.5  12.0  67.8  C22H22N O3 F
**Elemental Composition Report**

**Single Mass Analysis**
Tolerance = 5.0 mDa /  DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
177 formula(e) evaluated with 17 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-18  H: 0-13  N: 0-1  O: 0-3  F: 0-2

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Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
689 formula(e) evaluated with 44 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-18  H: 0-13  N: 0-1  O: 0-3  F: 0-1  35Cl: 0-1  37Cl:0-1

Minimum: 3.00  -1.5
Maximum: 100.00  5.0  10.0  50.0

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Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
148 formula(e) evaluated with 16 results within limits (up to 50 closest results for each mass)

Elements Used:
C: 0-19  H: 0-16  N: 0-1  O: 0-3  F: 0-1

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Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa /
DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
718 formula(e) evaluated with 44 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-19   H: 0-13   N: 0-1   O: 0-3   F: 0-1   35Cl: 0-1   37Cl: 0-1

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26
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron ions
731 formula(e) evaluated with 60 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-18  H: 0-13  N: 0-2  O: 0-5  F: 0-1

Minimum: 3.00  5.00  -1.5
Maximum: 100.00  5.00  10.0  50.0

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Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
362 formula(e) evaluated with 188 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-18  H: 0-13  N: 0-1  O: 0-3  35Cl: 0-1  37Cl: 0-1  F: 0-1

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29
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
710 formula(e) evaluated with 38 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-20  H: 0-18  N: 0-1  O: 0-4  35Cl: 0-1  37Cl: 0-1

Minimum: 3.00  Maximum: 100.00  5.0  10.0  50.0
Mass  RA  Calc. Mass  mDa  PPM  DBE  i-FIT  Formula
371.0925  19.95  371.0924  0.1  0.3  12.0  6.8  C20 H18 N O4  35C
## Elemental Composition Report

### Single Mass Analysis

**Tolerance** = 5.0 mDa / **DBE**: min = -1.5, max = 50.0  
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions  
1056 formula(s) evaluated with 37 results within limits (up to 50 closest results for each mass)  
Elements Used:

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### Minimum and Maximum Values

- **Minimum**: 3.00 to -1.5  
- **Maximum**: 100.00 to 50.0

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**Elemental Composition Report**

**Single Mass Analysis**
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
500 formula(e) evaluated with 28 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-20 H: 0-18 N: 0-2 O: 0-6

Minimum: 3.00
Maximum: 100.00
5.0 10.0 50.0

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**Elemental Composition Report**

**Single Mass Analysis**

Tolerance = 5.0 mDa /  DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
440 formula(e) evaluated with 46 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-13  H: 0-12  N: 0-1  O: 0-3  F: 0-1

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Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa /  DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
440 formula(e) evaluated with 46 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-14   H: 0-14   N: 0-1   O: 0-3   F: 0-1

Minimum: 3.00
Maximum: 100.00

Mass  RA  Calc. Mass  mDa  PPM  DBE  i-FIT  Formula
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Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
172 formula(s) evaluated with 17 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-20  H: 0-18  N: 0-1  O: 0-3  F: 0-1

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<td>20.0</td>
<td>20.5</td>
<td>C20 H18 N O3 F</td>
</tr>
</tbody>
</table>
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
287 formula(e) evaluated with 27 results within limits (up to 50 closest results for each mass)

Elements Used:
C: 0-20  H: 0-18  N: 0-1  O: 0-3  F: 0-1

<table>
<thead>
<tr>
<th>Mass</th>
<th>RA</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>339.1269</td>
<td>4.04</td>
<td>339.1271</td>
<td>-0.2</td>
<td>-0.6</td>
<td>12.0</td>
<td>150.4</td>
<td>C20 H18 N O3 F</td>
</tr>
</tbody>
</table>
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
258 formula(e) evaluated with 25 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-20  H: 0-18  N: 0-1  O: 0-3  F: 0-1

<table>
<thead>
<tr>
<th>Mass</th>
<th>RA</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>339.1270</td>
<td>6.07</td>
<td>339.1271</td>
<td>-0.1</td>
<td>-0.3</td>
<td>12.0</td>
<td>7.8</td>
<td>C20 H18 N O3 F</td>
</tr>
</tbody>
</table>
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
631 formula(e) evaluated with 71 results within limits (up to 50 closest results for each mass
Elements Used:
C: 0-22  H: 0-14  N: 0-1  O: 0-3  F: 0-1

<table>
<thead>
<tr>
<th>Mass</th>
<th>RA</th>
<th>Calc. Mass</th>
<th>pDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>359.0961</td>
<td>1.12</td>
<td>359.0958</td>
<td>0.3</td>
<td>0.8</td>
<td>16.0</td>
<td>2773.5</td>
<td>C22 H14 N O3 F</td>
</tr>
</tbody>
</table>
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa  
DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
446 formula(e) evaluated with 46 results within limits (up to 1000 closest results for each mass
Elements Used:
C: 0-23   H: 0-16   N: 0-1   O: 0-3   F: 0-1

Minimum:  3.00  
Maximum:  100.00  5.0  10.0  -1.5  50.0

Mass   RA   Calc. Mass   mDa  PPM  DBE  I-FIT  Formula
373.1113  12.25  373.1114  -0.1  -0.3  16.0  85.5  C23 H16 N O3 F
### Elemental Composition Report

#### Single Mass Analysis

- **Tolerance**: 5.0 mDa
- **DBE**: min = -1.5, max = 50.0
- **Element prediction**: Off

Monoisotopic Mass, Odd and Even Electron Ions

220 formula(e) evaluated with 24 results within limits (up to 50 closest results for each mass)

Elements Used:
- C: 0-18
- H: 0-14
- N: 0-1
- O: 0-3
- F: 0-1

<table>
<thead>
<tr>
<th>Mass</th>
<th>RA</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>311.0960</td>
<td>17.35</td>
<td>311.9688</td>
<td>0.2</td>
<td>0.6</td>
<td>12.0</td>
<td>13.9</td>
<td>C18 H14 N O3 F</td>
</tr>
</tbody>
</table>
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa /  DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
774 formula(e) evaluated with 60 results within limits (up to 50 closest results for each mass);
Elements Used:
C: 0-23    H: 0-22    N: 0-1    O: 0-3    F: 0-1

<table>
<thead>
<tr>
<th>Mass</th>
<th>RA</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>379.1586</td>
<td>3.34</td>
<td>378.1584</td>
<td>0.2</td>
<td>0.5</td>
<td>13.0</td>
<td>79.2</td>
<td>C23 H22 N O3 F</td>
</tr>
</tbody>
</table>
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
577 formula(e) evaluated with 58 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-20  H: 0-16  N: 0-1  O: 0-3  F: 0-1

<table>
<thead>
<tr>
<th>Mass</th>
<th>RA</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>337.1111</td>
<td>50.32</td>
<td>337.1114</td>
<td>-0.3</td>
<td>-0.9</td>
<td>13.0</td>
<td>576.7</td>
<td>C20 H16 N O3 F</td>
</tr>
</tbody>
</table>
Single Mass Analysis
Tolerance = 5.0 mDa /  DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
98 formula(e) evaluated with 14 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-18  H: 0-14  N: 0-1  O: 0-2  F: 0-1
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron ions
295 formula(e) evaluated with 25 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-18  H: 0-15  N: 0-2  O: 0-2  F: 0-1

<table>
<thead>
<tr>
<th>Mass</th>
<th>RA</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>310.1119</td>
<td>40.90</td>
<td>310.1118</td>
<td>0.1</td>
<td>0.3</td>
<td>12.0</td>
<td>0.4</td>
<td>C18 H15 N2 O2 F</td>
</tr>
</tbody>
</table>
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
1021 formula(e) evaluated with 67 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-19  H: 0-19  N: 0-4  O: 0-4  P: 0-1  F: 0-1

Minimum:  3.00
Maximum:  100.00  5.0  10.0  -1.5  50.0

<table>
<thead>
<tr>
<th>Mass</th>
<th>RA</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>375.1031</td>
<td>19.04</td>
<td>375.1036</td>
<td>-0.5</td>
<td>-1.3</td>
<td>11.0</td>
<td>1.0</td>
<td>C19 H19 N O4 P F</td>
</tr>
</tbody>
</table>
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
184 formula(e) evaluated with 29 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-21  H: 0-14  N: 0-1  O: 0-1  F: 0-1

<table>
<thead>
<tr>
<th>Mass</th>
<th>RA</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>315.1060</td>
<td>100.00</td>
<td>315.1059</td>
<td>0.1</td>
<td>0.3</td>
<td>15.0</td>
<td>202.2</td>
<td>C21 H14 N O F</td>
</tr>
</tbody>
</table>
### Elemental Composition Report

**Single Mass Analysis**

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

190 formula(e) evaluated with 29 results within limits (up to 50 closest results for each mass)

Elements Used:

<table>
<thead>
<tr>
<th>C</th>
<th>H</th>
<th>O</th>
<th>N</th>
<th>F</th>
</tr>
</thead>
<tbody>
<tr>
<td>0-22</td>
<td>0-16</td>
<td>0-1</td>
<td>0-1</td>
<td>0-1</td>
</tr>
</tbody>
</table>

---

| Minimum: | 3.00  | 5.00 | 10.00 | -1.5 |
| Maximum: | 100.00 | 5.0  | 10.0  | 50.0 |

<table>
<thead>
<tr>
<th>Mass</th>
<th>RA</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>329.1217</td>
<td>100.00</td>
<td>329.1216</td>
<td>0.1</td>
<td>0.3</td>
<td>15.0</td>
<td>135.4</td>
<td>C22 H16 N O F</td>
</tr>
</tbody>
</table>
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
77 formula(e) evaluated with 48 results within limits (up to 50 closest results for each mass).
Elements Used:
C: 0-21 H: 0-13 N: 0-1 O: 0-1 F: 0-1 35Cl: 0-1 37Cl: 0-1

Minimum: 3.00
Maximum: 1.00 5.0 10.0 -1.5 50.0

<table>
<thead>
<tr>
<th>Mass</th>
<th>RA</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>349.0672</td>
<td>100.00</td>
<td>349.0670</td>
<td>0.2</td>
<td>0.6</td>
<td>15.0</td>
<td>281.5</td>
<td>C21 H13 N O 35Cl F</td>
</tr>
</tbody>
</table>

[Images of mass spectrometry and NMR spectra are present.]
### Elemental Composition Report

#### Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
482 formula(e) evaluated with 38 results within limits (up to 50 closest results for each mass)
Elements Used:

- C: 0-23
- H: 0-16
- N: 0-1
- O: 0-3
- F: 0-1

---

<table>
<thead>
<tr>
<th>Mass</th>
<th>RA</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>I-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>373.1115</td>
<td>100.00</td>
<td>373.1114</td>
<td>0.1</td>
<td>0.3</td>
<td>16.0</td>
<td>601.1</td>
<td>C23 H16 N O3 F</td>
</tr>
</tbody>
</table>
4.2 Copies of the spectra for Scheme 2

$^1$H NMR spectra for Scheme 2A

$^1$H NMR spectra for Scheme 2B
$^1$H NMR spectra for Scheme 2C

$^1$H NMR spectra for Scheme 2D
$^1$H NMR spectra for Scheme 2E

$^1$H NMR spectra for Scheme 2F
$^1$H NMR spectra for Scheme 2G