

Structure-Activity Relationship for the Oxadiazole Class of Antibiotics

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Experimental Procedures

General procedure for synthesis of benzoyl chlorides

This has been previously described.¹

General procedure for synthesis of heteroaryl acyl chlorides

The carboxylic acid (1.0 equiv) was dissolved in thionyl chloride (25.0 equiv), and the mixture was heated to reflux for 2.5 h. The excess thionyl chloride was removed *in vacuo*, and the resulting solid was used without further purification.

General procedure for synthesis of diphenyl ethers, Method A (nucleophilic aromatic substitution)

A 4-fluorobenzonitrile derivative (1.0 equiv.), a phenol derivative (1.0 equiv.), and K_2CO_3 (2.0 equiv.) were dissolved in either DMSO or DMF, and the mixture was stirred at 100 °C for 16 h. The mixture was cooled to room temperature and was diluted with water (2x volume of DMSO or DMF used), then it was extracted with ethyl acetate (3x). The combined organic layer was washed with water (3x), then once with brine, and dried (anhydrous Na_2SO_4). After being concentrated *in vacuo*, the crude material was purified by column chromatography on silica gel.

General procedure for synthesis of diphenyl ethers, Method B (Ullmann coupling)

This has been previously described.¹

General procedure for nitro reduction using Fe/HCl

This has been previously described.¹

General procedure for nitro reduction using $SnCl_2 \cdot H_2O$

Using an adaptation of a literature procedure,² the starting material (1.0 equiv.) was dissolved in ethanol (6.0 mL/mmol starting material), and $SnCl_2 \cdot 2H_2O$ (5.0 equiv.) was added. The mixture was stirred at 70 °C for 4 h, then cooled to room temperature and poured onto ice. The pH was adjusted to ~7-8 with saturated $NaHCO_3$, and the aqueous layer was extracted 3x with ethyl

acetate. The combined organic layers were dried (anhydrous Na₂SO₄), and the solvent was removed *in vacuo*. The crude product was purified by column chromatography on silica gel.

General procedure for synthesis of *N*'-hydroxybenzimidamides

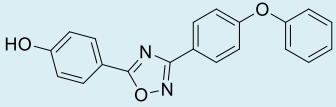
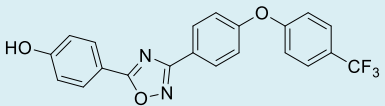
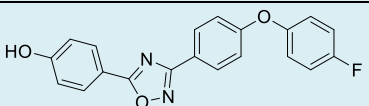
This was previously described.¹

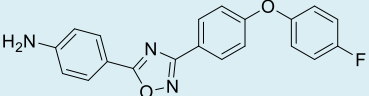
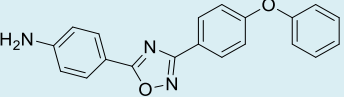
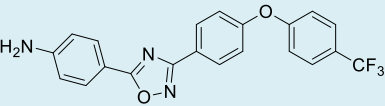
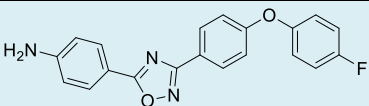
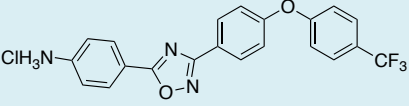
General procedure for synthesis of allyl-protected phenols

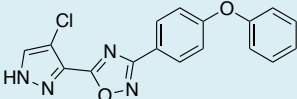
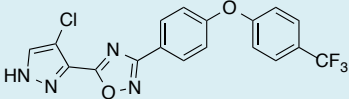
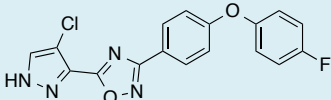
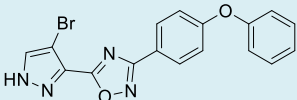
Allyl-protected phenols **9**,³ **12**,⁴ **13**,⁵ and **20**,⁶ are known compounds, and were synthesized using previously described procedures.³

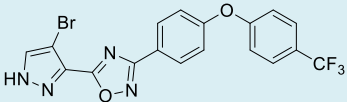
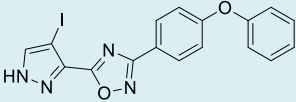
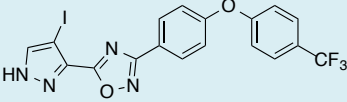
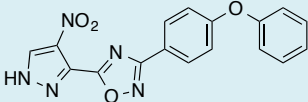
Compounds **52**, **14**, and **15** were synthesized using previously described procedures.^{1,7}

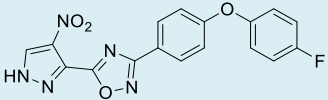
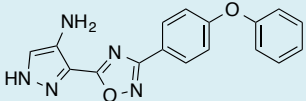
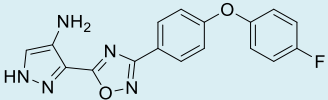
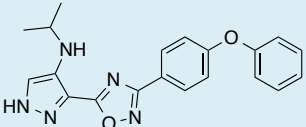
Table S1. Spectral data of final compounds

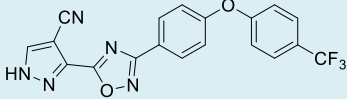
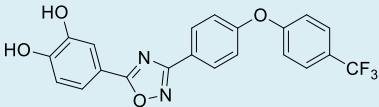
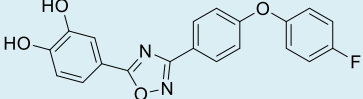
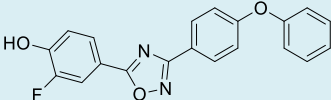
Compound Number	Structure and data
57a	 Lit. ¹
57b	 Lit. ¹
57c	
¹ H NMR	(500 MHz, DMSO- <i>d</i> ₆) δ 6.99 (d, <i>J</i> = 8.6 Hz, 2H), 7.14 (d, <i>J</i> = 8.6 Hz, 2H), 7.19-7.22 (m, 2H), 7.28-7.32 (m, 2H), 8.02 (d, <i>J</i> = 8.6 Hz, 2H), 8.06 (d, <i>J</i> = 8.6 Hz, 2H).
¹³ C NMR	(125 MHz, DMSO- <i>d</i> ₆) δ 114.1, 116.3, 116.9 (d, <i>J</i> _{CF} = 23.3 Hz), 117.8, 121.0, 121.9 (d, <i>J</i> _{CF} = 8.6 Hz), 129.2, 130.1, 151.3, 158.9 (d, <i>J</i> _{CF} = 239.4 Hz), 160.1, 162.1, 167.5, 175.4.
¹⁹ F NMR	(282 MHz, DMSO- <i>d</i> ₆) δ -118.89.
HRMS (ESI)	calcd for C ₂₁ H ₁₄ FN ₂ O ₃ 349.0983, found 349.0978 [MH] ⁺

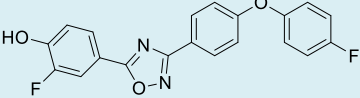
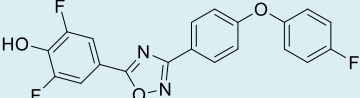
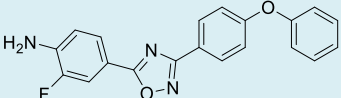
58	
¹ H NMR	(600 MHz, CDCl ₃) δ 4.13 (s, 2H), 6.71 (d, <i>J</i> = 8.5 Hz, 2H), 7.04-7.10 (m, 6H), 8.00 (d, <i>J</i> = 8.5 Hz, 2H), 8.11 (d, <i>J</i> = 8.5 Hz, 2H).
¹³ C NMR	(125 MHz, DMSO- <i>d</i> ₆) δ 114.0, 114.5, 116.6, 117.8, 121.3, 122.0, 129.3, 130.0, 150.6, 151.9, 158.3, 160.2, 168.1, 175.9.
HRMS (ESI)	calcd for C ₂₀ H ₁₅ FN ₃ O ₂ 348.1143, found 348.11563 [MH] ⁺
58a	
¹ H NMR	(600 MHz, acetone- <i>d</i> ₆) δ 5.63 (br s, 2H), 6.84 (d, <i>J</i> = 8.8 Hz, 2H), 7.13 (d, <i>J</i> = 7.5 Hz, 2H), 7.14 (d, <i>J</i> = 8.8 Hz, 2H), 7.22 (t, <i>J</i> = 7.5 Hz, 1H), 7.45 (t, <i>J</i> = 7.5 Hz, 2H), 7.92 (d, <i>J</i> = 8.8 Hz, 2H), 8.13 (d, <i>J</i> = 8.8 Hz, 2H).
¹³ C NMR	(150 MHz, acetone- <i>d</i> ₆) δ 112.4, 114.8, 119.2, 120.6, 123.2, 125.2, 130.0, 130.7, 131.1, 154.2, 157.2, 161.0, 168.7, 177.2.
HRMS (ESI)	calcd for C ₂₀ H ₁₅ N ₃ O ₂ 330.1237, found 330.1234 [MH] ⁺
58b	 Lit. ¹
58c	
¹ H NMR	(600 MHz, CDCl ₃) δ 4.13 (s, 2H), 6.71 (d, <i>J</i> = 8.5 Hz, 2H), 7.04-7.10 (m, 6H), 8.00 (d, <i>J</i> = 8.5 Hz, 2H), 8.11 (d, <i>J</i> = 8.5 Hz, 2H).
¹³ C NMR	(125 MHz, DMSO- <i>d</i> ₆) δ 114.0, 114.5, 116.6, 117.8, 121.3, 122.0, 129.3, 130.0, 150.6, 151.9, 158.3, 160.2, 168.1, 175.9.
¹⁹ F NMR	(282 MHz, CDCl ₃) δ -119.3
HRMS (ESI)	calcd for C ₂₀ H ₁₅ FN ₃ O ₂ 348.1143, found 348.11563 [MH] ⁺
59b	

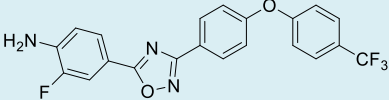
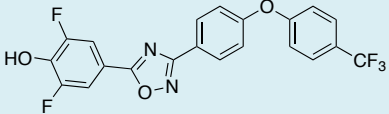
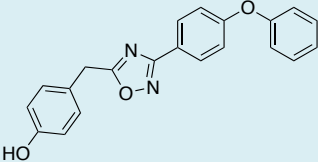
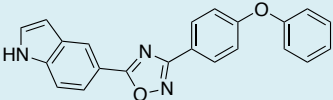
¹ H NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 5.90 (br s, 3H), 6.81 (d, <i>J</i> = 8.6 Hz, 2H), 7.28 (d, <i>J</i> = 9.0 Hz, 2H), 7.29 (d, <i>J</i> = 8.6 Hz, 2H), 7.79 (d, <i>J</i> = 8.6 Hz, 2H), 7.88 (d, <i>J</i> = 8.6 Hz, 2H), 8.11 (d, <i>J</i> = 9.0 Hz, 2H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 110.7, 114.5, 119.1, 119.8, 124.1 (q, <i>J</i> _{CF} = 286.8 Hz), 124.2 (q, <i>J</i> _{CF} = 32.5 Hz), 127.6 (q, <i>J</i> _{CF} = 3.8 Hz), 129.3, 129.6, 157.9, 159.3, 167.2, 175.9.
HRMS (ESI)	calcd for C ₂₁ H ₁₄ F ₃ N ₃ O ₂ 398.1111, found 398.1131 [MH] ⁺
60a	
¹ H NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 7.16-7.20 (m, 4H), 7.26 (t, <i>J</i> = 7.4 Hz, 1H), 7.48 (t, <i>J</i> = 7.6 Hz, 2H), 8.11 (d, <i>J</i> = 8.4 Hz, 1H), 8.39 (s, 1H), 14.27 (s, 1H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 110.3, 118.3, 119.7, 120.6, 124.5, 129.3, 130.3 (2C), 133.5, 155.4, 159.8, 167.5, 169.3.
HRMS (ESI)	calcd for C ₁₇ H ₁₁ ClN ₄ O ₂ 339.0643, found 339.0652 [MH] ⁺
60b	
¹ H NMR	(400 MHz, CDCl ₃) δ 7.16-7.19 (m, 4H), 7.66 (d, <i>J</i> = 8.8 Hz, 2H), 8.02 (s, 1H), 8.17-8.20 (m, 2H), 13.58 (br s, 1H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 110.8, 119.8, 120.6, 122.6, 124.8, 125.1, 128.3 (q, <i>J</i> _{CF} = 3.6 Hz), 130.1, 130.9, 134.1, 158.8, 159.9, 168.0, 170.2.
HRMS (ESI)	calcd for C ₁₈ H ₁₁ ClF ₃ N ₄ O ₂ 407.0517, found 407.0540 [MH] ⁺
60c	
¹ H NMR	(400 MHz, CDCl ₃) δ 7.07-7.13 (m, 6H), 7.91 (s, 1H), 8.16 (d, <i>J</i> = 9.2 Hz, 2H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 110.1, 116.8, 117.0, 117.9, 120.6, 121.8, 121.9, 129.3, 130.3, 133.5, 151.2, 151.3, 157.6, 160.0, 160.2, 167.4, 169.4.
HRMS (ESI)	calcd for C ₁₇ H ₁₁ ClFN ₄ O ₂ 357.0549, found 357.0544 [MH] ⁺
61a	

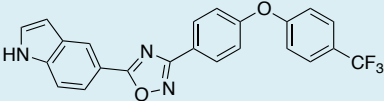
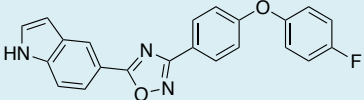
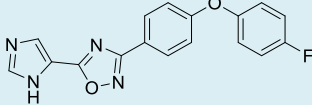
¹ H NMR	(400 MHz, CDCl ₃) δ 7.10–7.14 (m, 4H), 7.20–7.22 (m, 1H), 7.39–7.44 (m, 2H), 7.97 (s, 1H), 8.15–8.18 (m, 2H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 94.1, 117.9, 118.4, 119.7, 120.6, 124.5, 129.3, 130.0, 130.3, 132.7, 155.4, 159.8, 167.4.
HRMS (ESI)	calcd for C ₁₇ H ₁₂ BrN ₄ O ₂ 383.0138, found 383.0120 [MH] ⁺
61b	
¹ H NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 7.28–7.34 (m, 4H), 7.80 (d, <i>J</i> = 8.8 Hz, 2H), 8.14–8.16 (m, 2H), 8.38 (s, 1H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 94.2, 119.1, 120.0, 122.0, 124.1, 124.4, 127.7 (q, <i>J</i> _{CF} = 3.6), 129.5, 132.7, 135.1, 158.2, 159.2, 167.4, 169.8.
HRMS (ESI)	calcd for C ₁₈ H ₁₁ BrF ₃ N ₄ O ₂ 451.0012, found 450.9986 [MH] ⁺
62a	
¹ H NMR	(400 MHz, CDCl ₃) δ 7.11–7.15 (m, 4H), 7.18–7.22 (m, 1H), 7.39–7.44 (m, 2H), 8.05 (s, 1H), 8.05–8.18 (m, 2H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 60.7, 119.0, 120.3, 121.2, 125.3, 129.9, 131.0, 138.2, 138.9, 156.0, 160.5, 168.1, 170.7.
HRMS (ESI)	calcd for C ₁₇ H ₁₂ IN ₄ O ₂ 430.9999, found 430.9982 [MH] ⁺
62b	
¹ H NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 7.29–7.36 (m, 4H), 7.80 (d, <i>J</i> = 8.8 Hz, 2H), 8.16 (d, <i>J</i> = 8.4 Hz, 2H), 8.31 (s, 1H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 60.4, 119.1, 120.0, 122.1, 122.8, 124.1, 124.4, 125.5, 127.6 (q, <i>J</i> _{CF} = 3.5 Hz), 129.4, 137.4, 138.3, 158.1, 159.2, 167.3, 170.4.
HRMS (ESI)	calcd for C ₁₈ H ₁₁ F ₃ IN ₄ O ₂ 498.9873, found 498.9879 [MH] ⁺
63a	

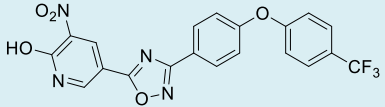
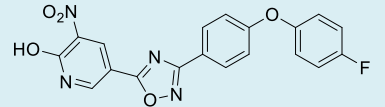
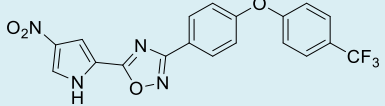
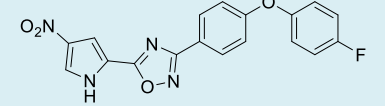
¹ H NMR	(400 MHz, CD ₃ OD) δ 7.12-7.14 (m, 4H), 7.20-7.24 (m, 1H), 7.41-7.45 (m, 2H), 8.12-8.15 (m, 2H), 8.82(s, 1H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 119.0, 120.5, 120.8, 125.3, 130.0, 131.0, 133.0, 134.8, 155.9, 160.8, 168.4, 169.2.
HRMS (ESI)	calcd for C ₁₇ H ₁₁ N ₅ O ₄ 372.0703, found 372.0707.
63c	
¹ H NMR	(500 MHz, DMSO- <i>d</i> ₆) δ 7.12-7.33 (m, 6H), 8.08 (<i>t</i> , <i>J</i> = 8.8 Hz, 2H), 9.2 (s, 1H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 116.8, 117.0, 117.9, 120.1, 122.0, 129.3, 132.5, 134.1, 151.2, 157.7, 160.1, 160.4, 167.7, 168.5
HRMS (ESI)	calcd for C ₁₇ H ₁₁ FN ₅ O ₄ 368.0790, found 368.0790 [MH] ⁺
64a	
¹ H NMR	(400 MHz, CDCl ₃) δ 4.31 (br s, 2H), 7.09-7.12 (m, 4H), 7.18-7.22 (m, 1H), 7.39-7.43 (m, 3H), 8.12-8.14 (m, 2H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 115.1, 118.3, 119.7, 121.0, 124.3, 124.5, 129.3, 130.3, 133.8, 155.5, 159.7, 166.8, 171.1.
HRMS (ESI)	calcd for C ₁₇ H ₁₄ N ₅ O ₂ [M+H] ⁺ 320.1142, found 320.1158.
64c	
¹ H NMR	(400 MHz, CDCl ₃) δ 6.79 (d, <i>J</i> = 8.8 Hz, 2H), 6.99-7.09 (m, 4H), 7.21 (s, 1H), 7.76 (d, <i>J</i> = 8.8 Hz, 2H).
¹³ C NMR	(400 MHz, CDCl ₃) δ 116.7, 116.9, 117.5, 118.1, 121.0, 121.6, 121.7, 124.1, 129.3, 132.3, 151.6, 151.7, 158.3, 160.4, 160.7, 167.4, 169.9.
HRMS (ESI)	calcd for C ₁₇ H ₁₃ FN ₅ O ₂ 338.1048, found 338.1038 [MH] ⁺
65a	

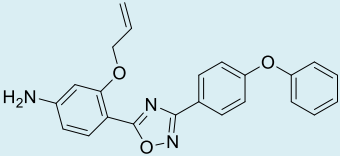
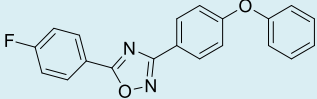
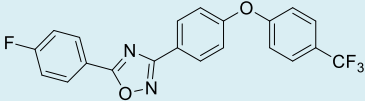
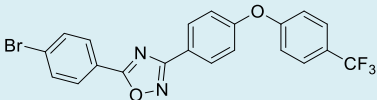
¹ H NMR	(400 MHz, CDCl ₃) δ 1.32 (s, 3H), 1.33 (s, 3H), 3.48-3.55 (m, 1H), 7.10-7.12 (m, 4H), 7.18-7.21 (m, 1H), 7.38-7.43 (m, 2H), 7.49 (s, 1H), 8.12-8.15 (m, 2H)
¹³ C NMR	(100 MHz, CDCl ₃) δ 23.2, 47.8, 115.9, 118.4, 120.0, 121.5, 123.0, 124.4, 129.5, 130.1, 135.5, 156.2, 160.5, 167.8, 170.5.
HRMS (ESI)	calcd for C ₂₀ H ₂₀ N ₅ O ₂ [M+H] ⁺ 362.1612, found 362.1630.
67b	
¹ H NMR	(400 MHz, CDCl ₃) δ 7.14-7.19 (m, 4H), 7.63-7.66 (m, 2H), 8.21-8.23 (m, 2H), 8.33 (s, 1H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 95.4, 111.4, 119.3, 119.8, 121.7, 126.1, 126.4, 127.6 (q, <i>J</i> _{CF} = 4 Hz), 130.0, 137.4, 139.4, 159.3, 159.5, 167.9, 168.8.
HRMS (ESI)	calcd for C ₁₉ H ₁₁ F ₃ N ₅ O ₂ 398.0859, found 398.0824 [MH] ⁺
69b	
¹ H NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 6.96 (d, <i>J</i> = 8.4 Hz, 1H), 7.16-7.18 (m, 2H), 7.27-7.29 (m, 2H), 7.51-7.55 (m, 2H), 7.99-8.01 (m, 2H), 8.10-8.12 (m, 2H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 114.9, 115.4, 117.0, 119.8, 120.5, 121.2, 123.2, 123.5, 124.8, 125.1, 126.2, 126.3 (q, <i>J</i> = 3.6 Hz), 130.0, 146.6, 151.4, 158.7, 160.0, 168.1, 176.4.
HRMS (ESI)	calcd for C ₂₁ H ₁₃ F ₃ N ₂ O ₄ 415.0900, found 415.0900 [MH] ⁺
69c	
¹ H NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 6.95 (d, <i>J</i> = 8.4 Hz, 1H), 7.11-7.14 (m, 2H), 7.19-7.23 (m, 2H), 7.28-7.32 (m, 2H), 7.50-7.54 (m, 2H), 8.04-8.06 (m, 2H), 9.68 (br s, 1H), 10.06 (br s, 1H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 114.3, 114.7, 116.3, 116.8, 117.0, 117.8, 120.5, 121.1, 121.8, 121.9, 129.2, 146.0, 150.7, 151.3, 151.4, 157.6, 160.0, 167.5, 175.6.
HRMS (ESI)	calcd for C ₂₀ H ₁₄ FN ₂ O ₄ 365.0932, found 365.0929 [MH] ⁺
70a	

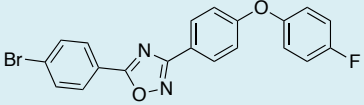
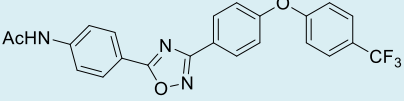
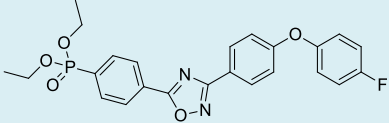
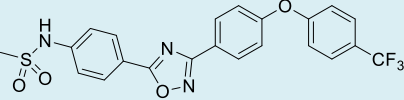
¹ H NMR	(500 MHz, CDCl ₃) δ 7.07-7.11 (m, 3H), 7.14 (t, <i>J</i> = 8.5 Hz, 1H), 7.18 (t, <i>J</i> = 7.4 Hz, 1H), 7.37-7.41 (m, 3H), 7.89-7.94 (m, 2H), 8.11 (d, <i>J</i> = 8.8 Hz, 2H).
HRMS (ESI)	calcd for C ₂₀ H ₁₄ FN ₂ O ₃ 349.0983, found 349.0974 [MH] ⁺
70c	
¹ H NMR	(500 MHz, CD ₃ OD) δ 7.03 (d, <i>J</i> = 9.0 Hz, 2H), 7.06-7.11 (m, 3H), 7.13-7.17 (m, 2H), 7.81-7.84 (m, 2H), 8.04 (d, <i>J</i> = 9.0 Hz, 2H).
¹³ C NMR	(125 MHz, DMSO- <i>d</i> ₆) δ 116.0, 117.0, 117.7, 118.9, 119.6, 122.8, 122.9, 126.5, 130.4, 151.4, 152.9, 153.4, 161.0, 162.2, 169.6, 176.4.
¹⁹ F NMR	(282 MHz, CD ₃ OD) δ -121.2, -137.9.
HRMS (ESI)	calcd for C ₂₀ H ₁₃ F ₂ N ₂ O ₃ 367.0889, found 367.0889 [MH] ⁺
71c	
¹ H NMR	(500 MHz, CD ₃ OD) δ 7.09 (d, <i>J</i> = 8.5 Hz, 2H), 7.13-7.17 (m, 4H), 7.78 (d, <i>J</i> = 8.5 Hz, 2H), 8.10 (d, <i>J</i> = 9.0 Hz, 2H).
¹³ C NMR	(125 MHz, CD ₃ OD) δ 113.1, 115.4 (t, <i>J</i> _{CF} = 9.6 Hz), 115.8 (d, <i>J</i> _{CF} = 23.8 Hz), 119.0, 122.6, 122.9 (d, <i>J</i> _{CF} = 8.3 Hz), 130.5, 140.6, 154.1 (dd, <i>J</i> _{CF} = 242.8, 7.0 Hz), 153.4 (d, <i>J</i> _{CF} = 2.5 Hz), 161.0 (d, <i>J</i> _{CF} = 240.3 Hz), 162.3, 169.8, 175.7.
¹⁹ F NMR	(282 MHz, CD ₃ OD) δ -121.2, -134.0.
HRMS (ESI)	calcd for C ₂₀ H ₁₂ F ₃ N ₂ O ₃ 385.0795, found 385.0770 [MH] ⁺
72a	
¹ H NMR	(500 MHz, CDCl ₃) δ 4.23 (br s, 2H), 6.85 (t, <i>J</i> = 8.6 Hz, 1H), 7.07-7.10 (m, 4H), 7.17 (t, <i>J</i> = 7.4 Hz, 1H), 7.38 (dd, <i>J</i> = 8.6, 7.6 Hz, 2H), 7.80-7.84 (m, 2H), 8.10 (d, <i>J</i> = 9.0 Hz, 2H).
¹³ C NMR	(125 MHz, CDCl ₃) δ 114.2 (d, <i>J</i> _{CF} = 8.2 Hz), 115.4 (d, <i>J</i> _{CF} = 20.6 Hz), 116.3 (d, <i>J</i> _{CF} = 3.3 Hz), 118.5, 119.9, 121.9, 124.3, 125.6 (d, <i>J</i> _{CF} = 3.3 Hz), 129.4, 130.1, 139.4 (d, <i>J</i> _{CF} = 12.3 Hz), 150.8 (d, <i>J</i> _{CF} = 240.3 Hz), 156.3, 160.2, 168.4, 175.2.
¹⁹ F NMR	(282 MHz, CDCl ₃) δ -135.26 (dd, <i>J</i> = 11.0, 8.6 Hz).
HRMS (ESI)	

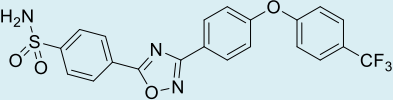
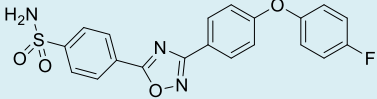
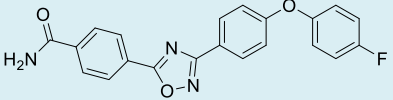
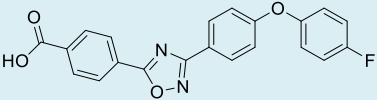
	calcd for C ₂₀ H ₁₅ FN ₃ O ₂ 348.1143, 348.1117 found [MH] ⁺
72b	
¹ H NMR	(500 MHz, CDCl ₃) δ 4.25 (br s, 2H), 6.85 (t, <i>J</i> = 8.6 Hz, 1H), 7.12-7.16 (m, 4H), 7.62 (d, <i>J</i> = 8.6 Hz, 2H), 7.80-7.84 (m, 2H), 8.16 (d, <i>J</i> = 8.8 Hz, 2H).
¹³ C NMR	(125 MHz, CDCl ₃) δ 114.1 (d, <i>J</i> _{CF} = 8.2 Hz), 115.4 (d, <i>J</i> _{CF} = 21.4 Hz), 116.3 (d, <i>J</i> _{CF} = 4.1 Hz), 118.9, 119.7, 123.3, 124.3 (q, <i>J</i> _{CF} = 271.6 Hz), 125.6 (d, <i>J</i> _{CF} = 2.5 Hz), 125.9 (q, <i>J</i> _{CF} = 32.9 Hz), 129.7, 139.5 (d, <i>J</i> _{CF} = 12.3 Hz), 150.8 (d, <i>J</i> _{CF} = 240.3 Hz), 158.6, 159.7 (d, <i>J</i> _{CF} = 1.6 Hz), 168.3, 175.4 (d, <i>J</i> _{CF} = 2.5 Hz).
¹⁹ F NMR	(282 MHz, CDCl ₃) δ -135.22 (dd, 1F, <i>J</i> = 12.2, 8.6 Hz), -62.21 (s, 3F).
73b	
¹ H NMR	(400 MHz, CDCl ₃) δ 7.13-7.17 (m, 4H), 7.64 (d, <i>J</i> = 8.5 Hz, 2H), 7.78 (dd, <i>J</i> = 6.7, 1.5 Hz, 2H), 8.16 (d, <i>J</i> = 9.0 Hz, 2H).
¹³ C NMR	(100 MHz, CDCl ₃) δ 112.3 (m), 119.0, 119.7, 122.8, 124.8, 126.0 (q, <i>J</i> _{CF} = 32.9 Hz) 127.6 (q, <i>J</i> _{CF} = 3.8 Hz), 129.7, 138.2, 139.1 (d, <i>J</i> _{CF} = 15.8 Hz), 148.1, 152.7 (dd, <i>J</i> _{CF} = 244.4, 6.8 Hz), 158.9, 168.5.
HRMS (ESI)	calcd for C ₂₁ H ₁₁ F ₅ N ₂ O ₃ 435.0763, found 435.0735 [MH] ⁺
74a	
¹ H NMR	(400 MHz, CDCl ₃) δ 4.18 (s, 2H), 6.36 (s, 1H), 6.74 (d, <i>J</i> = 8.6 Hz, 2H), 7.01-7.06 (m, 4H), 7.12-7.18 (m, 3H), 7.36 (m, 2H), 8.00 (d, 2H).
¹³ C NMR	(100 MHz, CDCl ₃) δ 32.4, 116.1, 118.5, 120.0, 121.1, 124.4, 125.3, 129.4, 130.2, 130.4, 155.6, 156.1, 160.5, 168.0, 178.8.
HRMS (ESI)	calcd for C ₂₁ H ₁₆ N ₂ O ₃ 345.1234, found 345.1211 [MH] ⁺
75a	

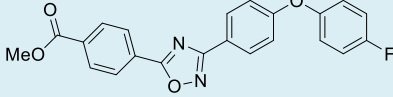
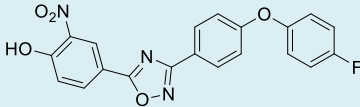
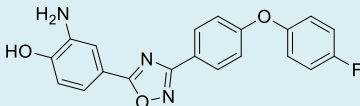
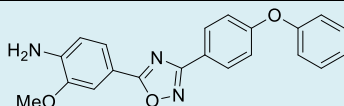
¹ H NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 6.68 (m, 1H), 7.14–7.18 (m, 4H), 7.24 (tt, <i>J</i> = 7.5, 1.2 Hz), 7.47 (m, 2H), 7.55 (t, <i>J</i> = 2.8 Hz, 1H), 7.63 (d, <i>J</i> = 8.5 Hz, 1H), 7.91 (dd <i>J</i> = 8.5, 1.7 Hz), 8.11 (d, <i>J</i> = 8.9 Hz), 8.46 (m, 1H), 11.64 (s, 1H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 102.7, 112.5, 114.2, 118.3, 119.7, 120.6, 121.2, 121.2, 124.5, 127.8, 129.2, 130.3, 138.4, 155.4, 159.7, 167.6, 170.9, 176.8.
HRMS (ESI)	calcd for C ₂₂ H ₁₅ N ₃ O ₂ 354.1237, found 354.1273 [MH] ⁺
75b	
¹ H NMR	(400 MHz, CDCl ₃) δ 6.71 (m, 1H), 7.13 (d, <i>J</i> = 8.7 Hz, 2H), 7.16 (d, <i>J</i> = 8.9 Hz, 2H), 7.32 (d, <i>J</i> = 8.7 Hz, 2H), 7.52 (d, <i>J</i> = 8.6 Hz, 1H), 7.63 (d, <i>J</i> = 8.9 Hz, 2H), 8.06 (d,d, <i>J</i> = 8.6, 1.61 Hz, 1H), 8.22 (d, <i>J</i> = 8.9 Hz, 2H), 8.52 (s, 1H), 8.57 (t, <i>J</i> = 0.8 Hz, 1H).
¹³ C NMR	(100 MHz, CDCl ₃) δ 104.3, 119.9, 116.3, 118.9, 119.8, 122.2, 122.4, 123.5, 124.3 (q, <i>J</i> _{CF} = 272.2 Hz), 125.9 (q, <i>J</i> _{CF} = 33.2 Hz), 126.2, 127.52 (q, <i>J</i> _{CF} = 3.8 Hz), 128.2, 129.7, 138.3, 158.5, 159.8, 168.3, 177.4.
¹⁹ F NMR	(376 MHz, CDCl ₃) δ 99.90 (s, 3F).
HRMS (ESI)	calcd for C ₂₃ H ₁₄ F ₃ N ₃ O ₂ 422.1111, found 422.1146 [MH] ⁺
75c	
¹ H NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 6.68 (m, 1H), 7.15 (d, <i>J</i> = 8.8 Hz, 2H), 7.12–7.16 (m, 2H), 7.29–7.33 (m, 2H), 7.55 (t, <i>J</i> = 2.8 Hz, 1H), 7.66 (d, <i>J</i> = 8.5 Hz, 1H), 7.91 (dd <i>J</i> = 8.5, 1.6 Hz), 8.10 (d, <i>J</i> = 8.8 Hz, 2H), 8.46 (m, 1H), 11.64 (s, 1H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 102.7, 112.5, 114.1, 116.8, 117.0, 117.9, 120.5, 121.1, 121.2, 121.9 (d, <i>J</i> _{CF} = 8.6 Hz), 127.8, 129.2, 138.4, 151.4, 160.0, 167.5, 176.8.
HRMS (ESI)	calcd for C ₂₂ H ₁₄ FN ₃ O ₂ 371.1143, found 372.1166 [MH] ⁺
76c	

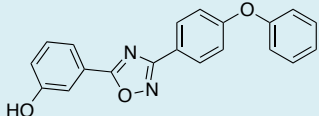
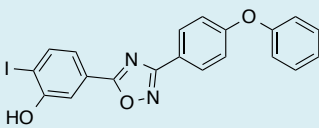
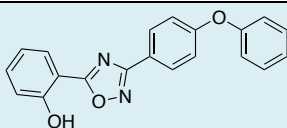
¹ H NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 7.12-7.14 (m, 2H), 7.19-7.22 (m, 2H), 7.28-7.32 (m, 2H), 7.98 (s, 1H), 8.04-8.06 (m, 2H), 8.23 (s, 1H), 12.98 (s, 1H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 116.8, 117.0, 117.8, 121.0, 121.8, 121.9, 122.8, 125.9, 129.2, 138.2, 151.3, 151.4, 157.7, 160.0, 167.3, 171.9.
HRMS (ESI)	calcd for C ₁₇ H ₁₂ FN ₄ O ₂ 323.0939, found 323.0948 [MH] ⁺
77b	
¹ H NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 7.29–7.31 (m, 4H), 7.81 (d, <i>J</i> = 8.8 Hz, 2H), 8.13 (d, <i>J</i> = 8.8 Hz, 2H), 8.78 (d, <i>J</i> = 2.4 Hz, 1H), 8.90 (d, <i>J</i> = 2.4 Hz, 1H), 13.76 (br s, 1H);
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 101.3, 119.3, 119.8, 121.7, 124.2, 124.5, 127.70 (q, <i>J</i> _{CF} = 4.0 Hz), 129.5, 136.9, 138.0, 145.0, 154.1, 158.3, 159.1, 167.5, 172.2.
HRMS (ESI)	calcd for C ₂₀ H ₁₂ F ₃ N ₄ O ₅ 445.0754, found 445.0742 [MH] ⁺
77c	
¹ H NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 7.09-7.33 (m, 6H), 8.03-8.08 (m, 2H), 8.73-8.90 (m, 2H), 13.73 (br s, 1H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 101.9, 117.5, 117.7, 118.4, 121.0, 122.6, 122.7, 129.9, 137.5, 138.6, 145.6, 151.8, 151.9, 154.8, 158.3, 160.7, 161.0, 168.2, 172.7.
HRMS (ESI)	calcd for C ₁₉ H ₁₂ FN ₄ O ₅ 395.0786, found 395.0779 [MH] ⁺
78b	
¹ H NMR	(400 MHz, CDCl ₃) δ 7.14-7.18 (m, 4H), 7.64-7.67 (m, 3H), 7.91-7.92 (m, 1H), 8.11-8.15 (m, 2H), 9.66 (br, 1H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 109.8, 117.6, 120.0, 120.4, 122.4, 123.5, 124.9, 125.3, 126.1, 126.2, 128.3 (q, <i>J</i> _{CF} = 3.6 Hz), 130.1, 138.3, 159.0, 159.8, 168.1, 169.1.
HRMS (ESI)	calcd for C ₁₉ H ₁₁ F ₃ N ₄ O ₄ 417.0805, found 417.0805 [MH] ⁺
78c	

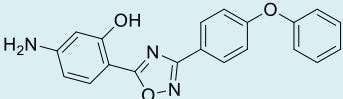
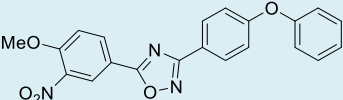
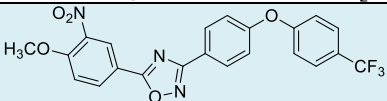
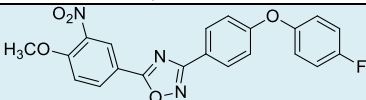
¹ H NMR	(400 MHz, CDCl ₃) δ 7.05-7.11 (m, 6H), 7.62-7.63 (m, 1H), 7.89-7.91 (m, 1H), 8.04-8.07 (m, 2H), 9.66 (br, 1H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 109.7, 117.4, 117.6(2C), 118.4, 121.1, 122.5, 122.6, 126.0, 129.8, 138.2, 151.8, 151.9, 158.3, 160.7, 160.9, 168.1, 168.9.
HRMS (ESI)	calcd for C ₂₀ H ₁₁ FN ₄ O ₄ Na 389.0657, found 389.0654 [MNa] ⁺
79a	
¹ H NMR	(600 MHz, CDCl ₃) δ 4.12 (br s, 2H), 4.65-4.67 (m, 2H), 5.36 (ddd, <i>J</i> = 10.9, 3.2, 1.8 Hz, 1H), 5.72 (ddd, <i>J</i> = 17.3, 3.5, 1.8 Hz, 1H), 6.12 (ddd, <i>J</i> = 17.3, 10.9, 4.7 Hz, 1H), 6.27 (d, <i>J</i> = 2.2 Hz, 1H), 6.37 (dd, <i>J</i> = 8.5, 2.2 Hz, 1H), 7.07-7.09 (m, 4H), 7.17 (dt, <i>J</i> = 7.5, 1.2 Hz, 1H), 7.37-7.40 (m, 2H), 8.00 (d, <i>J</i> = 8.5 Hz, 1H), 8.13 (d, <i>J</i> = 8.8 Hz, 2H).
¹³ C NMR	(150 MHz, CDCl ₃) δ 69.4, 98.9, 104.1, 107.7, 117.6, 118.5, 119.9, 122.5, 124.2, 129.4, 130.1, 132.6, 133.4, 152.2, 156.5, 159.5, 159.9, 167.7, 175.5.
HRMS (ESI)	calcd for C ₂₃ H ₁₉ N ₃ NaO ₃ 408.1319, found 408.1319 [MNa] ⁺
80a	
¹ H NMR	(600 MHz, acetone- <i>d</i> ₆) δ 7.12-7.16 (m, 2H), 7.15 (d, <i>J</i> = 9.0 Hz, 2H), 7.23 (tt, <i>J</i> = 7.4, 1.0 Hz, 1H), 7.42-7.47 (m, 4H), 8.14 (d, <i>J</i> = 9.0 Hz, 2H), 8.29 (dd, <i>J</i> = 8.8, 5.3 Hz, 2H).
¹³ C NMR	(125 MHz, acetone- <i>d</i> ₆) δ 117.5 (d, <i>J</i> _{CF} = 22.4 Hz), 119.2, 120.7, 121.7 (d, <i>J</i> _{CF} = 2.8 Hz), 122.4, 125.3, 130.1, 131.1, 131.7 (d, <i>J</i> _{CF} = 9.5 Hz), 157.0, 161.4, 166.5 (d, <i>J</i> _{CF} = 253.0 Hz), 169.2, 175.7.
HRMS (ESI)	calcd for C ₂₀ H ₁₄ FN ₂ O ₂ 333.1034, found 333.1004 [MH] ⁺
80b	 Lit. ¹
81b	

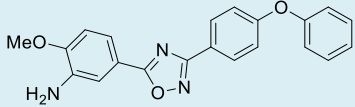
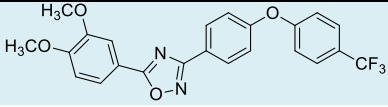
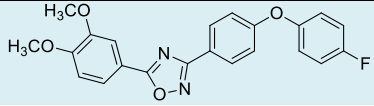
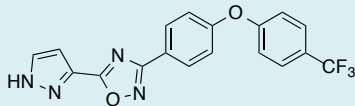
¹ H NMR	(600 MHz, acetone- <i>d</i> ₆) δ 7.28-7.30 (m, 4H), 7.79 (d, <i>J</i> = 8.2 Hz, 2H), 7.86 (d, <i>J</i> = 8.2 Hz, 2H), 8.15 (d, <i>J</i> = 8.8 Hz, 2H), 8.20 (d, <i>J</i> = 8.8 Hz, 2H).
¹³ C NMR	(150 MHz, acetone- <i>d</i> ₆) δ 120.1, 120.7, 123.7, 124.2, 125.4 (q, <i>J</i> _{CF} = 271.0), 126.0, 128.3, 128.5 (q, <i>J</i> _{CF} = 3.9 Hz), 130.4, 130.7, 133.6, 159.7, 160.7, 169.2, 176.0.
HRMS (ESI)	calcd for C ₂₁ H ₁₃ BrF ₃ N ₂ O ₂ 461.0107, found 461.0091 [MH] ⁺
81c	
¹ H NMR	(400 MHz, CDCl ₃) δ 7.00–7.05 (m, 6H), 7.65 (d, <i>J</i> = 8.4 Hz, 2H), 8.01–8.08 (m, 4H).
¹³ C NMR	(100 MHz, CDCl ₃) δ 116.7, 116.9, 118.0, 121.5, 121.6, 121.7, 123.4, 127.9, 129.6, 129.8, 132.7, 151.9 (2C), 158.4, 160.9, 168.7, 175.0.
HRMS (ESI)	calcd for C ₂₀ H ₁₂ BrFN ₂ O ₂ 411.0139, found 411.0139 [MH] ⁺
83b	
¹ H NMR	(600 MHz, acetone- <i>d</i> ₆) δ 2.15 (s, 3H, CH ₃), 7.29-7.32 (m, 4H, ArH),
HRMS (ESI)	calcd for C ₂₃ H ₁₇ F ₃ N ₃ O ₃ 440.1217, found 440.1233 [MH] ⁺
85c	
¹ H NMR	(400 MHz, CDCl ₃) δ 1.35 (t, <i>J</i> = 7.2 Hz, 6H), 4.10-4.19 (m, 4H), 7.04-7.09 (m, 6H), 7.97-8.02 (m, 2H), 8.10-8.14 (m, 2H), 8.28-8.31 (m, 2H).
¹³ C NMR	(100 MHz, CDCl ₃) δ 16.2, 16.3, 62.4, 62.5, 116.4, 116.7, 117.7, 121.1, 121.3, 121.4, 127.4, 127.8, 129.3, 132.2, 132.3, 132.4, 134.1, 151.6, 158.1, 160.5, 160.6, 168.5, 174.6.
HRMS (ESI)	calcd for C ₂₄ H ₂₃ FN ₂ O ₅ P 469.1323, found 469.1324 [MH] ⁺
86b	
¹ H NMR	(600 MHz, CDCl ₃) δ 3.14 (s, 3H), 6.76 (s, 1H), 7.14 (d, <i>J</i> = 8.5 Hz, 2H), 7.16 (d, <i>J</i> = 8.8 Hz, 2H), 7.37 (d, <i>J</i> = 8.8 Hz, 2H), 7.64 (d, <i>J</i> = 8.5 Hz, 2H), 8.18 (d, <i>J</i> = 8.8 Hz, 2H), 8.22 (d, <i>J</i> = 8.8 Hz, 2H).
HRMS (ESI)	calcd for C ₂₂ H ₁₇ F ₃ N ₃ O ₄ S 476.0886, found 476.0909 [MH] ⁺

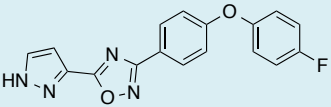
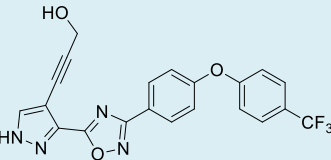
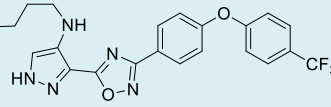
87b	
¹ H NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 7.30–7.34 (m, 4H), 7.66 (s, 2H), 7.82 (d, <i>J</i> = 9.2 Hz, 2H), 8.08 (d, <i>J</i> = 8.4 Hz, 2H), 8.16–8.18 (m, 2H), 8.40 (d, <i>J</i> = 8.0 Hz, 2H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 120.0, 120.5, 122.5, 124.9, 126.2, 126.7, 127.5, 128.4 (q, <i>J</i> _{CF} = 4.0 Hz), 129.5, 130.2, 148.6, 159.0, 159.8, 168.6, 175.1.
HRMS (ESI)	calcd for C ₂₁ H ₁₅ F ₃ N ₃ O ₄ S 462.0730, found 462.0752 [MH] ⁺
87c	
¹ H NMR	(400 MHz, CD ₃ OD) δ 7.06–7.18 (m, 6H), 8.10–8.12 (m, 4H), 8.35 (d, <i>J</i> = 6.8 Hz, 2H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 116.9, 117.1, 117.9, 120.5, 122.0, 122.1, 126.1, 126.9, 128.8, 129.4, 147.9, 151.3, 151.3, 157.8, 160.2, 160.4, 168.0, 174.4.
HRMS (ESI)	calcd for C ₂₀ H ₁₅ FN ₃ O ₄ S 412.0762, found 412.0755 [MH] ⁺
88c	
¹ H NMR	(500 MHz, DMSO- <i>d</i> ₆) δ 6.41 (s, 2H), 7.16 (d, <i>J</i> = 8.8 Hz, 2H), 7.21–7.24 (m, 2H), 7.30–7.33 (m, 2H), 8.10–8.13 (m, 4H), 8.26 (d, <i>J</i> = 8.2 Hz, 2H).
¹³ C NMR	(125 MHz, DMSO- <i>d</i> ₆) δ 116.9 (d, <i>J</i> _{CF} = 23.9 Hz), 117.9, 120.5, 121.9 (d, <i>J</i> _{CF} = 8.2 Hz), 125.5, 127.9, 128.6, 129.3, 138.3, 151.2 (d, <i>J</i> _{CF} = 2.5 Hz), 158.9 (d, <i>J</i> _{CF} = 241.1), 160.3, 166.8, 167.9, 174.8.
HRMS (ESI)	calcd for C ₂₁ H ₁₅ FN ₃ O ₃ 376.1092, found 376.1091 [MH] ⁺
89c	
¹ H NMR	(500 MHz, DMSO- <i>d</i> ₆) δ 7.15 (d, <i>J</i> = 9.0 Hz, 2H), 7.13 (dd, <i>J</i> = 8.9, 4.5 Hz, 2H), 7.31 (t, <i>J</i> = 8.9 Hz, 2H), 8.10 (d, <i>J</i> = 9.0 Hz, 2H), 8.18 (d, <i>J</i> = 8.8 Hz, 2H), 8.30 (d, <i>J</i> = 8.8 Hz, 2H).
¹³ C NMR	(125 MHz, DMSO- <i>d</i> ₆) δ 116.9, 117.9, 120.5, 121.9, 126.8, 128.2, 129.3, 130.3, 134.7, 151.2, 158.9, 160.3, 166.4, 167.9, 174.6.
¹⁹ F NMR	(282 MHz, DMSO- <i>d</i> ₆): δ -118.8.

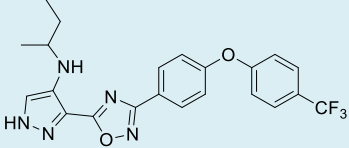
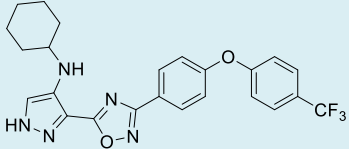
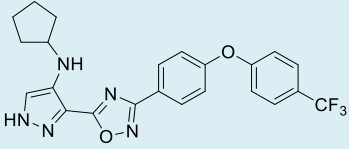
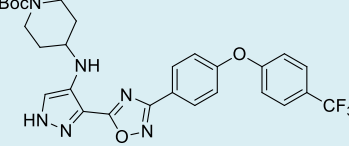
HRMS (ESI)	calcd for C ₂₁ H ₁₂ FN ₂ Na ₂ O ₄ 421.0571, found 421.0572 [MH] ⁺
90c	
¹ H NMR	(500 MHz, CDCl ₃) δ 3.98 (s, 3H), 7.05-7.11 (m, 6H), 8.14 (d, <i>J</i> = 9.0 Hz, 2H), 8.22 (d, <i>J</i> = 8.4 Hz, 2H), 8.29 (d, <i>J</i> = 8.4 Hz, 2H).
¹³ C NMR	(125 MHz, DMSO- <i>d</i> ₆) δ 52.5, 116.6, 117.8, 121.2, 121.4, 127.9, 128.1, 129.4, 130.2, 133.7, 151.7, 159.3, 160.6, 166.0, 168.6, 174.7.
¹⁹ F NMR	(282 MHz, CDCl ₃): δ -119.0.
HRMS (ESI)	calcd for C ₂₂ H ₁₆ FN ₂ O ₄ 391.1089, found 391.1099 [MH] ⁺
91c	
¹ H NMR	(400 MHz, CDCl ₃) δ 7.06-7.13 (m, 6H), 7.36-7.39 (m, 1H), 8.12-8.15 (m, 2H), 8.40-8.42 (m, 1H), 9.00-9.01 (m, 1H), 10.95 (s, 1H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 114.9, 117.4, 117.7, 118.5, 121.0, 121.2, 122.5, 122.6, 126.1, 129.9, 134.5, 138.0, 152.0, 156.4, 158.3, 160.7, 160.8, 168.4, 174.4.
HRMS (ESI)	calcd for C ₂₀ H ₁₃ FN ₃ O ₅ 394.0834, found 394.0834 [MH] ⁺
92c	
¹ H NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 5.02 (br, 2H), 6.84 (d, <i>J</i> = 8.4 Hz, 1H), 7.12-7.14 (m, 2H), 7.19-7.22 (m, 2H), 7.27-7.33 (m, 3H), 7.42 (d, <i>J</i> = 2.0 Hz, 1H), 8.03-8.06 (m, 2H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 113.3, 115.1(2C), 117.4, 117.7, 118.0, 118.5, 121.8, 122.5, 122.6, 129.8, 138.3, 149.5, 152.0 (2C), 158.3, 160.7 (2C), 168.1, 176.8.
HRMS (ESI)	calcd for C ₂₀ H ₁₅ FN ₃ O ₃ 364.1097, found 364.1099 [MH] ⁺
94a	

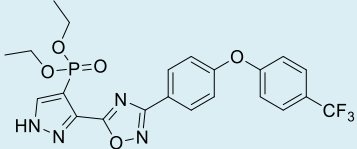
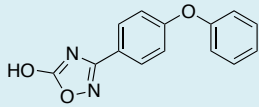
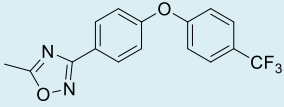
¹ H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 3.98 (s, 3H), 4.30 (s, 2H), 6.77 (d, <i>J</i> = 8.2 Hz, 1H), 7.08-7.11 (m, 4H), 7.17 (tt, <i>J</i> = 7.5, 1.0 Hz, 1H), 7.39 (dd, <i>J</i> = 7.5, 1.0 Hz, 2H), 7.58 (d, <i>J</i> = 1.8 Hz, 1H), 7.70 (dd, <i>J</i> = 8.2, 1.8 Hz, 1H), 8.12 (d, <i>J</i> = 9.1 Hz, 2H).
¹³ C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 56.0, 109.8, 113.8, 114.0, 118.6, 119.8, 122.2, 122.8, 124.2, 129.5, 130.1, 141.2, 146.8, 156.4, 160.1, 168.4, 176.3.
HRMS (ESI)	calcd for C ₂₁ H ₁₈ N ₃ O ₃ 360.1343, found 360.1362 [MH] ⁺
95a	
¹ H NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 7.12 (m, 1H), 7.14-7.19 (m, 4H), 7.25 (tt, <i>J</i> = 7.5, 1.1 Hz, 1H), 7.45-7.50 (m, 3H), 7.56 (m, 1H), 7.62 (m, 1H), 8.09 (d, <i>J</i> = 8.9 Hz), 10.10 (s, H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 114.1, 118.3, 118.6, 119.8, 120.5, 120.8, 124.4, 124.6, 129.2, 130.4, 130.9, 155.4, 158.0, 160.0, 167.8, 175.4.
HRMS (ESI)	calcd for C ₂₀ H ₁₄ N ₂ O ₃ 331.1077, found 331.1104 [MH] ⁺
96a	
¹ H NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 7.14-7.18 (m, 4H), 7.25 (t, d, <i>J</i> = 7.3, 0.8 Hz, 1H), 7.38 (dd, <i>J</i> = 8.2, 1.9 Hz, 1H), 7.48 (t, <i>J</i> = 7.7 Hz, 2H), 7.64 (d, <i>J</i> = 1.9 Hz, 1H), 7.98 (td, <i>J</i> = 8.2 Hz, 1H), 8.08 (d, <i>J</i> = 8.8 Hz, 2H).
¹³ C NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 91.8, 113.0, 118.3, 119.8, 119.9, 120.6, 123.19, 124.3, 124.6, 129.2, 130.4, 140.3, 159.9, 170.7.
HRMS (ESI)	calcd for C ₂₀ H ₁₃ IN ₂ O ₃ 457.0044, found 457.0082 [MH] ⁺
97a	
¹ H NMR	(400 MHz, CDCl ₃) δ 7.05 (m, 1H), 7.09-7.14 (m, 4H), 7.15 (m, 1H), 7.20 (tt, <i>J</i> = 7.4, 1.1 Hz, 1H), 7.38-7.43 (m, 2H), 7.53 (m, 1H), 8.00 (dd, <i>J</i> = 8.0, 1.7 Hz, 1H), 8.09 (d, <i>J</i> = 9.0 Hz), 10.53 (s, 1H).
¹³ C NMR	(100 MHz, CDCl ₃) δ 108.4, 118.0, 118.6, 120.2, 120.4, 122.5, 124.6, 128.1, 129.6, 130.3, 135.5, 156.1, 158.4, 160.9, 166.9, 174.4.
HRMS (ESI)	calcd for C ₂₀ H ₁₄ N ₂ O ₃ 323.1077, found 323.1105 [MH] ⁺

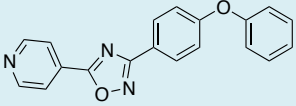
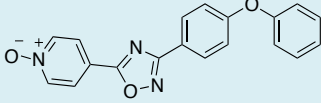
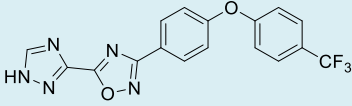
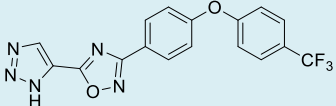
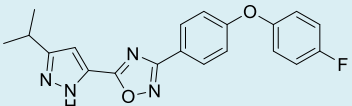
98a	
¹ H NMR	(600 MHz, CDCl ₃) δ 4.17 (s, 2H), 6.31-6.33 (m, 2H), 7.08-7.10 (m, 4H), 7.19 (t, <i>J</i> = 7.4 Hz, 1H), 7.40 (dd, <i>J</i> = 7.4, 1.2 Hz, 2H), 7.76 (d, <i>J</i> = 8.8 Hz, 1H), 8.06 (d, <i>J</i> = 8.8 Hz, 2H), 10.59 (s, 1H).
¹³ C NMR	(150 MHz, CDCl ₃) δ 99.3, 101.3, 108.1, 118.5, 120.0, 120.9, 124.5, 129.5, 129.7, 130.2, 153.2, 156.2, 160.3, 160.6, 166.4, 174.5.
HRMS (ESI)	calcd for C ₂₀ H ₁₆ N ₃ O ₃ 346.1186, found 346.1196 [MH] ⁺
99a	
¹ H NMR	(500 MHz, CDCl ₃) δ 4.08 (s, 3H), 7.08-7.11 (m, 2H), 7.10 (d, <i>J</i> = 9.0 Hz, 2H), 7.19 (tt, <i>J</i> = 7.5, 1.1 Hz, 1H), 7.27 (d, <i>J</i> = 8.8 Hz, 1H), 7.40 (dd, <i>J</i> = 7.4, 1.1 Hz, 2H), 8.12 (d, <i>J</i> = 9.0 Hz, 2H), 8.37 (dd, <i>J</i> = 8.8, 2.2 Hz, 1H), 8.71 (d, <i>J</i> = 2.2 Hz, 1H).
¹³ C NMR	(150 MHz, CDCl ₃) δ 57.2, 105.2, 114.3, 117.1, 118.5, 120.0, 121.2, 121.3, 124.5, 126.0, 129.5, 130.2, 133.7, 156.0, 160.6, 168.8, 173.6.
HRMS (ESI)	calcd for C ₂₁ H ₁₆ N ₃ O ₅ 390.1084, found 390.1068 [MH] ⁺
99b	
¹ H NMR	(400 MHz, CDCl ₃) δ 4.09 (s, 3H), 7.14-7.19 (m, 4H), 7.27-7.29 (m, 1H), 7.64-7.66 (m, 2H), 8.17-8.20 (m, 2H), 8.38 (dd, <i>J</i> = 2.0 Hz, 1H), 8.72 (d, <i>J</i> = 2.4 Hz, 1H).
¹³ C NMR	(100 MHz, CDCl ₃) δ 57.2, 114.3, 117.0, 119.1, 119.7, 122.7, 122.9, 125.6, 126.0, 126.3, 127.6 (q, <i>J</i> = 3.6 Hz), 129.8, 133.7, 140.2, 156.1, 159.0, 159.6, 168.7, 173.8.
HRMS (ESI)	calcd for C ₂₂ H ₁₅ F ₃ N ₃ O ₅ 458.0958, found 458.0960 [MH] ⁺
99c	
¹ H NMR	(400 MHz, CDCl ₃) δ 4.13 (s, 3H), 7.09-7.17 (m, 5H), 7.30-7.33 (m, 2H), 8.15-8.18 (m, 2H), 8.41-8.43 (m, 1H), 8.76 (d, <i>J</i> = 2.0 Hz, 1H).
¹³ C NMR	(100 MHz, CDCl ₃) δ 57.2, 114.3, 116.7, 116.9, 117.1, 118.1, 121.4, 121.6, 121.7, 125.9, 129.6, 133.6, 140.2, 151.9, 152.0, 156.0, 158.4,

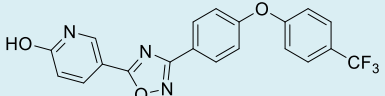
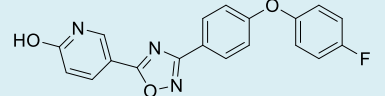
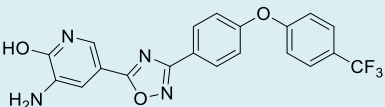
HRMS (ESI)	160.8, 160.9, 168.8, 173.6. calcd for C ₂₁ H ₁₄ FN ₃ NaO ₅ 430.0810, found 430.0840 [MNa] ⁺
100a	
¹ H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 3.88 (s, 3H), 7.02 (d, <i>J</i> = 8.5 Hz, 1H), 7.14-7.17 (m, 4H), 7.24 (tt, <i>J</i> = 7.4, 1.1 Hz, 1H), 7.39-7.41 (m, 1H), 7.45-7.49 (m, 3H), 8.06 (d, 2H, <i>J</i> = 8.8 Hz).
¹³ C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 55.6, 110.6, 111.7, 115.8, 116.8, 118.2, 119.8, 121.1, 124.5, 129.1, 130.3, 138.6, 150.2, 155.4, 160.0, 167.5, 175.9.
HRMS (ESI)	calcd for C ₂₁ H ₁₈ N ₃ O ₃ 360.1343, found 360.1355 [MH] ⁺
101b	
¹ H NMR	(400 MHz, CDCl ₃) δ 3.99 (s, 3H), 4.03 (s, 3H), 7.02 (d, <i>J</i> = 8.8 Hz, 1H), 7.13-7.19 (m, 4H), 7.62-7.65 (m, 2H), 7.70 (d, <i>J</i> = 2.0 Hz, 1H), 7.85 (dd, <i>J</i> = 2.0 Hz, 1H), 8.19-8.21 (m, 2H).
¹³ C NMR	(100 MHz, CDCl ₃) δ 56.3, 56.4, 110.8, 111.4, 117.1, 118.9, 119.7, 122.3, 122.9, 123.3, 125.7, 125.8, 126.1, 127.5 (q, <i>J</i> = 3.8 Hz), 129.7, 149.6, 153.2, 158.6, 159.7, 168.4, 175.9.
HRMS (ESI)	calcd for C ₂₃ H ₁₈ F ₃ N ₂ O ₄ 443.1213, found 443.1235 [MH] ⁺
101c	
¹ H NMR	(400 MHz, CDCl ₃) δ 3.96 (s, 3H), 3.99 (s, 3H), 6.98 (d, <i>J</i> = 8.4 Hz, 1H), 7.03-7.10 (m, 5H), 7.67 (d, <i>J</i> = 2.0 Hz, 1H), 7.82 (dd, <i>J</i> = 2.0 Hz, 1H), 8.10-8.13 (m, 2H).
¹³ C NMR	(100 MHz, CDCl ₃) δ 56.3, 56.4, 110.7, 111.3, 116.7, 116.9, 117.1, 118.1, 121.5, 121.6, 121.9, 122.3, 129.5, 149.5, 152.0, 152.1, 153.1, 158.3, 160.6, 160.7, 168.5, 175.7.
HRMS (ESI)	calcd for C ₂₂ H ₁₈ FN ₂ O ₄ 393.1245, found 393.1264 [MH] ⁺
102b	

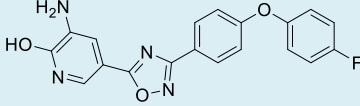
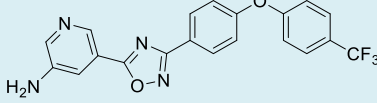
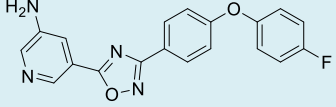
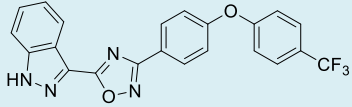
¹ H NMR	(400 MHz, CDCl ₃) δ 7.15-7.19 (m, 5H), 7.65 (d, <i>J</i> = 8.8, 2H), 8.04 (d, <i>J</i> = 2.4 Hz, 1H), 8.20-8.22 (m, 2H).
¹³ C NMR	(100 MHz, CDCl ₃) δ 107.5, 119.2, 119.7, 122.7, 126.0, 126.3, 127.6 (q, <i>J</i> _{CF} = 3.0 Hz), 129.8, 131.8, 137.6, 159.0, 159.5, 168.5, 170.9.
HRMS (ESI)	calcd for C ₁₈ H ₁₂ F ₃ N ₄ O ₂ 373.0907, found 373.0907 [MH] ⁺
102c	
¹ H NMR	(400 MHz, CD ₃ OD) δ 7.07-7.16 (m, 7H), 7.90 (s, 1H), 8.09-8.12 (m, 2H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 106.8, 116.8, 117.0, 117.8, 120.7, 121.9, 122.0, 129.2, 131.1, 136.8, 151.3, 157.6, 160.0, 160.2, 167.5, 171.3.
HRMS (ESI)	calcd for C ₁₇ H ₁₂ FN ₄ O ₂ 323.0939, found 323.0941 [MH] ⁺
103b	
¹ H NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 4.37 (d, <i>J</i> = 6.0 Hz, 2H), 5.38 (t, <i>J</i> = 6.0 Hz, 1H), 7.29-7.33 (m, 4H), 7.81 (d, <i>J</i> = 8.4 Hz, 2H), 8.16 (d, <i>J</i> = 8.4 Hz, 2H), 8.37 (s, 1H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 49.6, 73.9, 93.7, 103.5, 119.3, 119.8, 122.1, 124.2, 124.5, 127.7 (q, <i>J</i> _{CF} = 3.5 Hz), 129.5, 134.6, 137.2, 158.2, 159.2, 167.4, 170.3.
HRMS (ESI)	calcd for C ₂₁ H ₁₄ F ₃ N ₄ O ₃ 427.1013, found 427.1013 [MH] ⁺
104b	
¹ H NMR	(400 MHz, CDCl ₃) δ 0.98-1.01 (m, 3H), 1.44-1.50 (m, 2H), 1.67-1.75 (m, 2H), 3.20 (t, <i>J</i> = 8.0 Hz, 2H), 4.81 (br s, 1H), 7.14-7.18 (m, 4H), 7.43 (s, 1H), 7.64 (d, <i>J</i> = 8.0 Hz, 2H), 8.15-8.19 (m, 2H).
¹³ C NMR	(100 MHz, CDCl ₃) δ 14.1, 20.5, 31.9, 46.6, 119.1, 119.2, 119.6, 122.9, 125.9, 126.2, 127.6 (q, <i>J</i> _{CF} = 3.6 Hz), 129.8, 136.9, 158.8, 159.5, 159.6, 167.6, 170.6.
HRMS (ESI)	calcd for C ₂₂ H ₂₁ F ₃ N ₅ O ₂ 444.1642, found 444.1668 [MH] ⁺

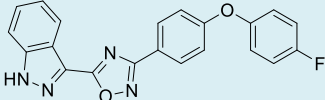
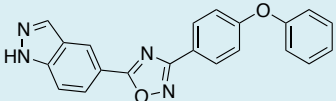
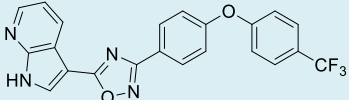
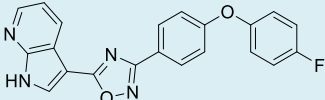
<p>105b</p> <p>¹H NMR</p> <p>¹³C NMR</p> <p>HRMS (ESI)</p>	 <p>(400 MHz, CDCl₃) δ 1.02 (t, <i>J</i> = 7.2 Hz, 3H), 1.29 (d, <i>J</i> = 6.4 Hz, 4H), 1.58-1.76 (m, 2H), 3.28-3.33 (m, 1H), 7.14-7.18 (m, 4H), 7.45 (s, 1H), 7.64 (d, <i>J</i> = 8.4 Hz, 2H), 8.17-8.19 (m, 2H).</p> <p>(100 MHz, CDCl₃) δ 10.4, 20.5, 29.8, 53.5, 116.3, 119.1, 119.7, 122.5, 122.9, 125.6, 125.9, 126.2, 127.6 (q, <i>J</i>_{CF} = 3.6 Hz), 129.8, 135.9, 158.9, 159.5, 167.6, 170.5.</p> <p>calcd for C₂₂H₂₁F₃N₅O₂ 444.1642, found 444.1647 [MH]⁺</p>
<p>106b</p> <p>¹H NMR</p> <p>¹³C NMR</p> <p>HRMS (ESI)</p>	 <p>(400 MHz, CDCl₃) δ 1.36-1.45 (m, 5H), 1.64-1.82 (m, 3H), 2.10 (d, <i>J</i> = 10.4 Hz, 2H), 3.18 (br s, 1H), 4.90 (d, <i>J</i> = 3.2 Hz, 1H), 7.14-7.19 (m, 3H), 7.37 (s, 1H), 7.63-7.65 (m, 2H), 8.16-8.20 (m, 2H).</p> <p>(150 MHz, CDCl₃) δ 24.8, 26.1, 33.4, 54.9, 115.9, 119.1, 119.6, 122.9, 125.6, 125.9, 126.2, 127.5 (q, <i>J</i>_{CF} = 3.6 Hz), 129.7, 135.6, 158.9, 159.5, 167.6, 170.7.</p> <p>calcd for C₂₄H₂₃F₃N₅O₂ 470.1798, found 470.1812 [MH]⁺</p>
<p>107b</p> <p>¹H NMR</p> <p>¹³C NMR</p> <p>HRMS (ESI)</p>	 <p>(400 MHz, CDCl₃) δ 1.59-1.71 (m, 4H), 1.77-1.82 (m, 2H), 2.01-2.07 (m, 2H), 3.73-3.75 (m, 1H), 4.87-4.88 (m, 1H), 7.14-7.17 (m, 3H), 7.36 (d, <i>J</i> = 1.2 Hz, 1H), 7.64 (d, <i>J</i> = 8.8 Hz, 2H), 8.15-8.18 (m, 2H).</p> <p>(100 MHz, CDCl₃) δ 24.3, 33.7, 57.7, 116.4, 119.1, 119.6, 122.8, 125.6, 125.9, 126.2, 127.6 (q, <i>J</i>_{CF} = 3.7 Hz), 129.8, 136.2, 158.9, 159.5, 167.6, 170.5.</p> <p>calcd for C₂₃H₂₁F₃N₅O₂ 456.1642, found 456.1679 [MH]⁺</p>
<p>110b</p>	

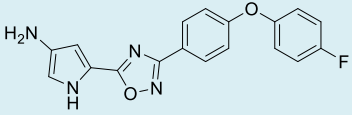
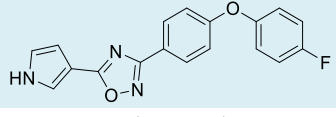
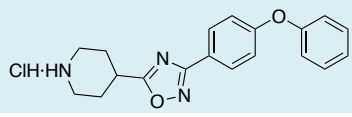
¹ H NMR	(400 MHz, CDCl ₃) δ 1.45-1.54 (m, 2H), 1.47 (s, 9H), 2.09-2.12 (m, 2H), 3.00-3.06 (m, 2H), 3.32-3.37 (m, 1H), 4.03 (br, 2H), 7.14-7.19 (m, 4H), 7.40 (s, 1H), 7.63-7.65 (m, 2H), 8.14-8.16 (m, 2H).
¹³ C NMR	(100 MHz, CDCl ₃) δ 28.7, 32.4, 53.2, 80.0, 119.1, 119.2, 119.6, 122.6, 122.7, 122.9, 125.6, 126.0, 126.4, 127.6 (q, <i>J</i> = 4.4 Hz), 129.7, 134.9, 155.0, 159.0, 159.5, 167.6, 170.4.
HRMS (ESI)	calcd for C ₂₈ H ₃₀ F ₃ N ₆ O ₄ 571.2275, found 571.2261 [MH] ⁺
111b	
¹ H NMR	(400 MHz, CDCl ₃) δ 1.23-1.26 (m, 6H), 4.09-4.20 (m, 4H), 7.02-7.10 (m, 4H), 7.60 (d, <i>J</i> = 8.4, 2H), 8.03-8.09 (m, 3H).
¹³ C NMR	(100 MHz, CDCl ₃) δ 16.5, 16.6, 63.2, 63.3, 108.1, 110.3, 119.2, 119.7, 122.5, 122.9, 125.6, 126.0, 126.3, 127.6 (q, <i>J</i> _{CF} = 3.6 Hz), 129.8, 138.8, 139.0, 159.0, 159.5, 168.4, 170.1.
HRMS (ESI)	calcd for C ₂₂ H ₂₁ F ₃ N ₄ O ₅ P 509.1196, found 509.1206 [MH] ⁺
112a	
¹ H NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 7.11-7.16 (m, 4H), 7.25 (tt, <i>J</i> = 7.4, 1.1 Hz, 1H), 7.44-7.49 (m, 2H), 7.82 (d, <i>J</i> = 8.8 Hz, 2H), 12.94 (s, 1H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 117.7, 118.2, 119.8, 124.7, 128.2, 130.4, 155.1, 156.9, 160.0, 160.2.
HRMS (ESI)	calcd for C ₁₄ H ₁₀ N ₂ O ₃ 255.0784, found 255.0785 [MH] ⁺
113b	
¹ H NMR	(600 MHz, acetone- <i>d</i> ₆) δ 2.66 (s, 3H), 7.25 (d, <i>J</i> = 8.8 Hz, 2H), 7.27 (d, <i>J</i> = 8.5 Hz, 2H), 7.78 (d, <i>J</i> = 8.5 Hz, 2H), 8.11 (d, <i>J</i> = 8.8 Hz, 2H).
¹³ C NMR	(150 MHz, acetone- <i>d</i> ₆) δ 12.3, 120.0, 120.7, 124.1, 125.4 (q, <i>J</i> _{CF} = 271.0 Hz), 126.1 (q, <i>J</i> _{CF} = 32.5 Hz), 128.4 (q, <i>J</i> _{CF} = 3.7 Hz), 130.2, 159.4, 160.8 (q, <i>J</i> _{CF} = 1.5 Hz), 168.5, 178.2.
HRMS (ESI)	calcd for C ₁₆ H ₁₂ F ₃ N ₂ O ₂ 321.0845, found 321.0847 [MH] ⁺

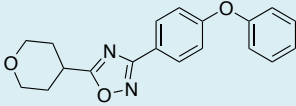
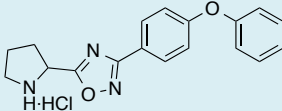
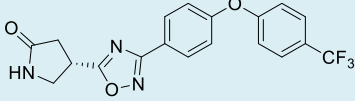
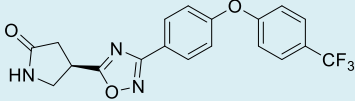
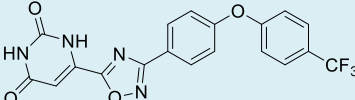
114a	
¹ H NMR	(400 MHz, CDCl ₃) δ 7.09-7.12 (m, 4H), 7.20 (t, <i>J</i> = 7.5 Hz, 1H), 7.48-7.43 (m, 2H), 8.06 (d, <i>J</i> = 6.1 Hz, 2H), 8.13 (m, 2H), 8.89 (d, <i>J</i> = 6.1 Hz, 2H).
¹³ C NMR	(100 MHz, CDCl ₃) δ 118.6, 120.1, 121.0, 121.7, 124.5, 129.6, 130.2, 148.8, 151.1 (2C), 156.1, 160.8, 169.2.
HRMS (ESI)	calcd for C ₁₉ H ₁₃ N ₃ O ₂ 316.1081, found 316.1103 [MH] ⁺
115a	
¹ H NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 7.09-7.28 (m, 5H), 7.39-7.55 (m, 2H), 7.94-8.20 (m, 4H), 8.43 (m, 2H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 118.3, 119.8, 120.3, 124.5, 125.2, 129.2, 130.3, 140.0, 151.1, 155.2, 160.0, 168.0, 172.7.
HRMS (ESI)	calcd for C ₁₉ H ₁₃ N ₃ O ₃ 332.1030, found 332.1028 [MH] ⁺
116b	
¹ H NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 7.09 (d, <i>J</i> = 7.2 Hz, 4H), 7.54 (d, <i>J</i> = 7.2 Hz, 2H), 7.71 (d, <i>J</i> = 6.8 Hz, 2H), 8.77 (s, 1H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 117.8, 120.6, 120.7, 121.5, 123.4, 123.6, 123.9, 126.1, 128.0 (q, <i>J</i> _{CF} = 3.1 Hz), 137.4, 149.7, 153.3, 161.8.
HRMS (ESI)	calcd for C ₁₇ H ₁₁ F ₃ N ₅ O ₂ 374.0859, found 374.0859 [MH] ⁺
117b	
¹ H NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 7.29-7.33 (m, 4H), 7.81 (d, <i>J</i> = 8.8 Hz, 2H), 8.13-8.16 (m, 2H), 8.99 (d, <i>J</i> = 7.2, 1H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 120.0, 120.4, 122.5, 124.9, 125.2, 126.2, 128.3 (q, <i>J</i> _{CF} = 3.6), 130.1, 159.0, 159.8, 159.8, 168.2, 170.1.
HRMS (ESI)	calcd for C ₁₁ H ₁₁ F ₃ N ₅ O ₂ 374.0859, found 374.0831 [MH] ⁺
119c	

¹ H NMR	(400 MHz, CDCl ₃) δ 1.37 (s, 3H), 1.39 (s, 3H), 3.10-3.17 (m, 1H), 6.82 (s, 1H), 6.83-7.12 (m, 5H), 8.13-8.16 (m, 2H), 10.76 (br s, 1H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 103.7, 116.7, 116.9, 117.9, 121.4, 121.6, 121.7, 129.5, 151.8, 151.9, 153.1, 158.3, 160.6, 160.7, 168.3, 171.1.
HRMS (ESI)	calcd for C ₂₀ H ₁₈ FN ₄ O ₂ 365.1408, found 365.1429 [MH] ⁺
120b	
¹ H NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 6.54 (d, <i>J</i> = 9.6 Hz, 1H), 7.27-7.30 (m, 4H), 7.80 (d, <i>J</i> = 8.4 Hz, 2H), 8.01-8.04 (m, 1H), 8.08-8.11 (m, 2H), 8.35 (d, <i>J</i> = 2.8 Hz, 1H), 12.46 (s, 1H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 102.6, 119.2, 119.8, 120.7, 122.1, 124.1, 124.5, 127.7 (q, <i>J</i> _{CF} = 4.0 Hz), 129.4, 138.0, 139.4, 158.1, 159.2, 162.0, 167.3, 173.5.
HRMS (ESI)	calcd for C ₂₀ H ₁₃ FN ₃ O ₃ 400.0904, found 400.0892 [MH] ⁺
120c	
¹ H NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 6.52-6.55 (m, 1H), 7.11-7.14 (m, 2H), 7.19-7.22 (m, 2H), 7.27-7.32 (m, 2H), 8.00-8.05 (m, 3H), 8.34 (d, <i>J</i> = 2.0 Hz, 1H), 12.45 (s, 1H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 102.6, 116.8, 117.0, 117.8, 120.7, 121.8, 121.9, 129.2, 138.0, 139.3, 151.2, 151.3, 157.6, 160.0, 160.1, 162.0, 167.4, 173.3.
HRMS (ESI)	calcd for C ₁₉ H ₁₃ FN ₃ O ₃ 350.0935, found 350.0935 [MH] ⁺
121b	
¹ H NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 5.56 (s, 2H), 7.02 (d, <i>J</i> = 2.4 Hz, 1H), 7.28-7.30 (m, 4H), 7.64 (d, <i>J</i> = 1.6 Hz, 1H), 7.80 (d, <i>J</i> = 8.4 Hz, 2H), 8.08-8.11 (m, 2H), 12.10 (s, 1H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 104.7, 106.3, 119.9, 120.4, 123.0, 123.5, 124.5, 124.8, 125.2, 126.2, 128.3 (q, <i>J</i> _{CF} = 3.8 Hz), 130.0, 139.9, 158.5, 158.8, 159.9, 167.9, 175.0.
HRMS (ESI)	calcd for C ₂₀ H ₁₄ F ₃ N ₄ O ₃ 415.1013, found 415.0997 [MH] ⁺

121c	
¹ H NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 5.55 (s, 2H), 7.01 (d, <i>J</i> = 2.4 Hz, 1H), 7.10-7.13 (m, 2H), 7.18-7.22 (m, 2H), 7.23-7.32 (m, 2H), 7.62 (d, <i>J</i> = 2.0 Hz, 1H), 8.01-8.04 (m, 2H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 104.0, 105.6, 116.8, 117.0, 117.8, 120.6, 121.8, 121.9, 139.2, 151.2, 151.3, 157.6, 157.8, 160.0, 160.1, 167.3, 174.2.
HRMS (ESI)	calcd for C ₁₉ H ₁₄ FN ₄ O ₃ 365.1044, found 365.1031 [MH] ⁺
122b	
¹ H NMR	(400 MHz, CDCl ₃) δ 4.01 (br, 2H), 7.14-7.19 (m, 4H), 7.63-7.65 (m, 2H), 7.73-7.74 (m, 1H), 8.17-8.20 (m, 2H), 8.31 (d, <i>J</i> = 2.4 Hz, 1H), 8.83 (d, <i>J</i> = 1.6 Hz, 1H).
¹³ C NMR	(100 MHz, CDCl ₃) δ 119.1, 119.7, 120.8, 122.7, 125.6, 125.9, 127.6 (q, <i>J</i> _{CF} = 3.0 Hz), 129.8, 139.1, 141.1, 142.8, 158.9, 159.5, 168.5, 174.4.
HRMS (ESI)	calcd for C ₂₀ H ₁₄ F ₃ N ₄ O ₂ 399.1063, found 399.1057 [MH] ⁺
122c	
¹ H NMR	(400 MHz, CDCl ₃) δ 3.99 (br, 2H), 7.05-7.12 (m, 6H), 7.72-7.73 (m, 1H), 8.10-8.14 (m, 2H), 8.30 (d, <i>J</i> = 2.4 Hz, 1H), 8.82 (d, <i>J</i> = 1.6 Hz, 1H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 116.7, 117.0, 118.0, 119.7, 120.9, 121.4, 121.6, 121.7, 129.6, 139.2, 141.1, 142.8, 151.9, 160.8, 160.9, 168.7, 174.3.
HRMS (ESI)	calcd for C ₁₉ H ₁₄ FN ₄ O ₂ 349.1095, found 349.1098 [MH] ⁺
123b	
¹ H NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 7.29-7.36 (m, 4H), 7.43-7.46 (m, 1H), 7.54-7.58 (m, 1H), 7.76-7.82 (m, 3H), 8.23-8.25 (m, 2H), 8.34 (d, <i>J</i> = 8.4 Hz, 1H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 111.4, 119.1, 119.9, 120.5, 121.4, 122.2, 123.4, 124.1, 124.4, 127.4, 127.6 (q, <i>J</i> _{CF} = 3.6 Hz), 129.5, 129.8, 141.0, 158.1, 159.2, 159.3, 167.4, 170.9.
HRMS (ESI)	calcd for C ₂₂ H ₁₄ F ₃ N ₄ O ₂ 423.1063, found 423.1050 [MH] ⁺

123c	
¹ H NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 7.17–7.24 (m, 4H), 7.29–7.34 (m, 2H), 7.42–7.46 (m, 1H), 7.54–7.76 (m, 1H), 7.77 (d, <i>J</i> = 8.4 Hz, 1H), 8.17–8.19 (m, 2H), 8.33 (d, <i>J</i> = 8.4 Hz, 1H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 111.4, 116.8, 117.0, 117.9, 120.5, 120.8, 121.4, 121.7, 121.8, 123.4, 127.4, 129.3, 129.9, 141.0, 151.3, 151.4, 157.6, 160.0, 160.1, 167.5, 170.8.
HRMS (ESI)	calcd for C ₂₁ H ₁₄ FN ₄ O ₂ 373.1095, found 373.1112 [MH] ⁺
124a	
¹ H NMR	(400 MHz, CDCl ₃) δ 7.09–7.13 (m, 4H), 7.19 (tt, <i>J</i> = 7.4, 1.1 Hz, 1H), 7.40 (dd, <i>J</i> = 8.6, 8.4 Hz, 2H), 7.66 (d, <i>J</i> = 8.8 Hz, 1H), 8.16 (d, <i>J</i> = 8.8 Hz, 2H), 8.24–8.27 (m, 2H), 8.72 (s, 1H).
¹³ C NMR	(100 MHz, CDCl ₃) δ 110.8, 118.0, 118.6, 120.0, 121.8, 122.9, 123.6, 124.4, 126.7, 129.5, 130.2, 136.7, 141.7, 156.4, 160.4, 168.7, 176.1.
HRMS (ESI)	calcd for C ₂₁ H ₁₄ N ₄ O ₂ 377.1009, found 377.1012 [MNa] ⁺
125b	
¹ H NMR	(400 MHz, CDCl ₃) δ 7.15–7.21 (m, 4H), 7.41–7.44 (m, 1H), 7.65 (d, <i>J</i> = 8.4 Hz, 2H), 8.23–8.26 (m, 2H), 8.35 (s, 1H), 8.52–8.54 (m, 1H), 8.76–8.78 (m, 1H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 98.7, 116.9, 118.1, 119.1, 119.9, 122.6, 124.0, 124.4, 127.7 (q, <i>J</i> _{CF} = 3.0 Hz), 128.7, 129.4, 131.4, 144.7, 148.8, 157.9, 159.4, 167.1, 172.6.
HRMS (ESI)	calcd for C ₂₂ H ₁₄ F ₃ N ₄ O ₂ 423.1063, found 423.1082 [MH] ⁺
125c	

¹ H NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 7.13-7.16 (m, 2H), 7.19-7.23 (m, 2H), 7.28-7.33 (m, 2H), 7.35-7.38 (m, 1H), 8.11 (d, <i>J</i> = 2.4 Hz, 1H), 8.14 (s, 1H), 8.42-8.43 (m, 1H), 8.55 (d, <i>J</i> = 8.0 Hz, 1H), 8.60 (d, <i>J</i> = 2.4 Hz, 1H), 12.87 (s, 1H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 98.7, 116.7, 116.8, 117.0, 117.9, 118.0, 121.2, 121.7, 121.8, 128.6, 129.2, 131.3, 144.7, 148.8, 151.4 (2C), 157.6, 159.9, 160.0, 167.2, 172.5.
HRMS (ESI)	calcd for C ₂₁ H ₁₄ FN ₄ O ₂ 373.1095, found 373.1093 [MH] ⁺
126c	
¹ H NMR	(400 MHz, CDCl ₃) δ 3.21 (br s, 2H), 6.61 (s, 1H), 6.69 (s, 1H), 7.02-7.09 (m, 6H), 8.01-8.06 (m, 2H), 9.01 (s, 1H).
¹³ C NMR	(100 MHz, CDCl ₃) δ 106.1, 111.1, 115.6, 116.7, 116.9, 118.0, 121.5, 121.6, 121.7, 129.3, 129.4, 133.8, 151.9, 158.4, 160.6, 160.7, 167.8, 169.5.
HRMS (ESI)	calcd for C ₁₈ H ₁₄ FN ₄ O ₂ 337.1095, found 337.1093 [MH] ⁺
127c	
¹ H NMR	(400 MHz, CDCl ₃) δ 6.40-6.43 (m, 1H), 7.03-7.16 (m, 7H), 8.06-8.10 (m, 2H), 9.34 (br s, 1H).
¹³ C NMR	(100 MHz, CDCl ₃) δ 111.6, 114.9, 116.7, 116.9, 117.3, 118.0, 121.5, 121.6, 121.7, 123.8, 129.5, 151.9, 152.0, 158.3, 160.6, 160.7, 167.9, 169.7.
HRMS (ESI)	calcd for C ₁₈ H ₁₃ FN ₃ O ₂ 322.0986, found 322.0984 [MH] ⁺
128a	
¹ H NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 1.98-2.28 (m, 4H), 3.03-3.36 (m, 4H), 3.51 (m, 1H), 7.12-7.15 (m, 4H), 7.24 (tt, <i>J</i> = 7.4, 1.1 Hz), 7.47 (m, 2H), 8.01 (d, <i>J</i> = 8.9 Hz), 9.06 (m, 2H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 25.55, 31.19, 41.97, 118.27, 119.77, 120.69, 124.57, 129.13, 130.34, 155.29, 159.80, 167.00, 180.81.
HRMS (ESI)	calcd for C ₁₉ H ₁₉ N ₃ O ₂ 322.1550, found 322.1552 [MH] ⁺

131a	
¹ H NMR	(400 MHz, CDCl ₃) δ 2.02-2.10 (m, 4H), 3.25 (m, 1H), 3.58 (m, 2H), 4.07 (m, 2H), 7.05-7.09 (m, 4H), 7.18 (tt, <i>J</i> = 7.4, 1.1 Hz, 1H), 7.39 (m, 2H), 8.04 (d, <i>J</i> = 8.9 Hz, 2H).
¹³ C NMR	(100 MHz, CDCl ₃) δ 29.6, 33.8, 67.1, 118.6, 119.9, 121.6, 124.4, 129.4, 130.2, 156.3, 160.3, 168.0, 181.4.
HRMS (ESI)	calcd for C ₁₉ H ₁₈ N ₂ O ₃ 323.1390, found 323.1403 [MH] ⁺
132a	
¹ H NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 2.22 (s, 2H), 2.44 (s, 1H), 2.58 (s, 1H), 3.65 (m, 2H), 5.18, (s, 1H), 7.01-7.06 (m, 4H), 7.17 (t, <i>J</i> = 7.5 Hz, 1H), 7.37 (t, <i>J</i> = 7.8 Hz, 2H), 8.00 (d, <i>J</i> = 8.3 Hz, 2H), 10.23 (s, 1H), 11.14 (s, 1H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 23.7, 30.1, 46.1, 54.0, 118.5, 120.0, 120.4, 124.5, 129.7, 130.2, 156.1, 160.7, 168.2, 174.2.
HRMS (ESI)	calcd for C ₁₈ H ₁₈ N ₃ O ₂ 308.1394, found 308.1403 [MH] ⁺
133b	
¹ H NMR	(500 MHz, CDCl ₃) δ 2.43-2.53 (m, 2H), 2.57-2.64 (m, 1H), 2.68-2.76 (m, 1H), 5.05-5.06 (m, 1H), 6.83 (s, 1H), 7.12 (d, <i>J</i> = 8.5 Hz, 4H), 7.62 (d, <i>J</i> = 8.5 Hz, 2H), 8.07 (d, <i>J</i> = 8.5 Hz, 2H).
¹³ C NMR	(125 MHz, CDCl ₃) δ 26.4, 29.1, 50.4, 119.1, 119.7, 122.2, 126.0, 126.3, 127.6 (q, <i>J</i> _{CF} = 3.6 Hz), 129.8, 159.1, 159.4, 168.1, 178.0, 178.9.
134b	
¹ H NMR	(500 MHz, CDCl ₃) δ 2.42-2.51 (m, 2H), 2.57-2.63 (m, 1H), 2.66-2.74 (m, 1H), 5.04-5.07 (m, 1H), 7.11 (d, <i>J</i> = 8.5 Hz, 4H), 7.62 (d, <i>J</i> = 8.5 Hz, 2H), 8.06 (d, <i>J</i> = 8.5 Hz, 2H).
¹³ C NMR	(125 MHz, CDCl ₃) δ 26.4, 29.2, 50.5, 119.1, 119.7, 122.3, 125.3, 126.0, 126.3, 127.5 (q, <i>J</i> _{CF} = 3.5 Hz), 129.8, 159.1, 159.4, 168.1, 178.3, 179.0.
135b	

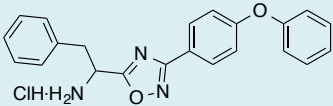
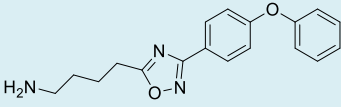
¹ H NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 6.40 (d, <i>J</i> = 1.6 Hz, 1H), 7.29-7.34 (m, 4H), 7.81 (d, <i>J</i> = 8.8 Hz, 2H), 8.13-8.15 (m, 2H), 11.56 (s, 1H), 11.87 (s, 1H).
HRMS (ESI)	calcd for C ₁₉ H ₁₁ F ₃ N ₄ O ₄ 417.0805, found 417.0805 [MH] ⁺
136a	
¹ H NMR	(400 MHz, DMSO- <i>d</i> ₆) δ 3.29-3.33 (m, 1H), 3.50-3.54 (m, 1H), 5.15-5.18 (m, 1H), 7.13-7.16 (m, 4H), 7.21-7.32 (m, 6H), 7.47 (t, <i>J</i> = 8.3 Hz, 2H), 7.99 (d, <i>J</i> = 8.6 Hz, 2H), 9.34 (s, 3H).
¹³ C NMR	(100 MHz, DMSO- <i>d</i> ₆) δ 37.3, 48.0, 118.3, 119.9, 124.6, 127.4, 128.6, 129.2, 129.3, 130.3, 134.2, 155.1, 160.1, 167.1, 175.8.
HRMS (ESI)	calcd for C ₂₂ H ₂₀ N ₃ O ₂ 358.1550, found 358.1547 [MH] ⁺
137a	
¹ H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 1.49 (quint, <i>J</i> = 7.4 Hz, 2H), 1.81 (quint, <i>J</i> = 7.4 Hz, 2H), 2.63 (t, <i>J</i> = 7.4 Hz, 2H), 3.00 (t, <i>J</i> = 7.4 Hz, 2H), 7.12-7.14 (m, 4H), 7.24 (t, <i>J</i> = 7.4 Hz, 1H), 7.46 (t, <i>J</i> = 7.4 Hz, 2H), 8.00 (d, <i>J</i> = 8.8 Hz, 2H).
¹³ C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 23.3, 25.6, 30.5, 40.1, 118.3, 119.7, 120.9, 124.5, 129.1, 130.3, 155.3, 159.7, 167.0, 180.2.
HRMS (ESI)	calcd for C ₁₈ H ₂₀ N ₃ O ₂ 310.1550, found 310.1523 [MH] ⁺

Table S2. Minimal-Inhibitory concentrations (MICs)

Compound Number	<i>E. faecium</i> NCTC 7171	<i>S. aureus</i> ATCC 29213
	MIC (μg/mL)	MIC (μg/mL)
57a	1	1
57b	1	1
57c	1	1
58a	2	4

58b	2	1
58c	>128	>128
59b	2	1
60a	>128	1
60c	8	0.5
60b	2	1
61a	16	1
61b	>128	1
62a	32	1
62b	32	2
63a	4	2
63b	2	2
63c	4	1
64a	32	16
64b	16	4
64c	32	16
65a	>128	0.5
65b	>128	0.5
66b	>128	0.25
67b	>128	2
68b	128	4
69b	128	2
69c	8	4
70a	4	4

70b	2	2
70c	2	2
71b	2	2
71c	4	8
72a	>32	>128
72b	2	2
73a	4	8
73b	4	4
74a	8	8
75a	2	2
75b	2	4
75c	2	2
76b	4	2
76c	128	>128
77b	4	8
77c	4	8
78b	64	8
78c	128	>128
79a	>128	8
80a	-	>128
80b	-	>128
81b	-	>128
81c	>128	>128
82a	>32	>32

82b	-	>128
83b	-	256
84c	32	>128
85c	>128	>128
86b	32	>128
87b	128	>128
87c	>128	>128
88c	64	>128
89c	128	>128
90c	>128	>128
91c	>128	>128
92c	128	>128
93b	>128	>128
94a	>128	>128
95a	>128	>128
96a	32	>128
97a	>128	>128
98a	>128	>128
99a	128	>128
99b	>128	>128
99c	>128	>128
100a	>128	>128
101b	>128	>128
101c	>128	>128

102b	64	>128
102c	32	>128
103b	>128	>128
104b	>128	>128
105b	128	>128
106b	128	>128
107b	>128	>128
108b	16	>128
109b	>128	>128
110b	>128	>128
111b	>128	>128
112a	>128	>128
113a	-	>128
114a	64	>128
115a	64	>128
116b	>128	>128
117b	>128	16
118c	>128	>128
119c	64	>128
120b	32	>128
120c	64	>128
121b	64	>128
121c	128	>128
122b	>128	>128

122c	128	>128
123b	>128	>128
123c	16	>128
124a	64	>128
125b	32	>128
125c	64	>128
126c	64	128
127c	>128	>128
128a	16	32
129a	>128	>128
129c	>128	>128
130c	>128	>128
131a	>128	>128
132a	64	64
133b	>128	>128
134b	>128	>128
135b	>128	>128
136a	>128	>128
137a	32	64

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