One-Pot Synthesis of Benzazoles and Quinazolinones via Iron Pentacarbonyl Mediated Carbonylation of Aryl Iodides under Microwave Irradiation

Wun-Huei Lin a, Wen-Chun Wu a, Manikandan Selvaraju a and Chung-Ming Sun* a,b

a Department of Applied Chemistry, National Chiao-Tung University, 1001, Ta-Hseuh Road, Hsinchu 300-10, Taiwan, ROC
b Department of Medicinal and Applied Chemistry, Kaohsiung Medical University, 100, Shih-Chuan 1st Road, Kaohsiung 807-08, Taiwan, ROC

Email: cmsun@mail.nctu.edu.tw

Table of contents

General remarks  S2
Experimental procedure for the synthesis of 6a & 8a  S2
Spectral data of compounds 6, 7, 8 and 11  S3
Spectra (1H NMR, 13C, LR-MS, HRMS, IR) of compounds 6, 7, 8 and 11  S12
General Remarks
Solvents were distilled before use. All reactions were performed under an inert atmosphere with unpurified reagents and dry solvents. Analytical thin-layer chromatography (TLC) was performed using 0.25 mm silica gel coated Kieselgel 60 F254 plates. All the microwave experiments were conducted in Biotage initiator under optimized reaction condition of power and pressure. Flash chromatography was performed using the indicated solvent and silica gel 60 (Merck, 230-400 mesh). $^1$H NMR (300 & 400 MHz) and $^{13}$C NMR (75 MHz) spectra were recorded on a Bruker DX-300 spectrometer. Chemical shifts are reported in parts per million (ppm) on the δ scale from an internal standard. High-resolution mass spectra (HRMS) were recorded on a JEOL TMS-HX 110 mass spectrometer.

Experimental Section

Experimental procedure for the synthesis of 2-phenylbenzo[d]oxazole (6a).

A microwave vial (5 mL) was charged with iodobenzene 1a (0.1 g, 0.49 mmol) and 2-nitrophenol 2a (0.102 g, 0.735 mmol), Pd(OAc)$_2$ (0.011g, 0.049 mmol), Fe(CO)$_5$ (0.144 g, 0.735 mmol) and molecular sieves (0.1 g) in ethanol (3 mL). The vial was sealed immediately and subjected to microwave irradiation at 110 °C for 20 minutes. After cooling, the reaction mixture was filtered through celite pad, and the solvent was removed under reduced pressure. The crude product was purified by silica-gel column chromatography using 20 % EtOAc/ Hexane to obtain the pure product 6a (0.081 g, 88 %).

Experimental procedure for the synthesis of 2-phenylquinazolin-4(3H)-one (11a).

A microwave vial (5 mL) was charged with iodobenzene 1a (0.1 g, 0.49 mmol) and 2-nitrobenzamide 9a (0.122 g, 0.735 mmol), PdCl$_2$ (0.0086 g, 0.049 mmol), Xantphos (0.056g, 0.098 mmol), Fe(CO)$_5$ (0.144 g, 0.735 mmol) and molecular sieves (0.1 g) in ethanol (3 mL). The vial was sealed immediately and subjected to microwave irradiation at 110 °C for 30 minutes. After cooling, the reaction mixture was filtered through celite pad, and the solvent was removed under reduced pressure. The crude product was purified by silica-gel column chromatography using 8 % EtOAc/ Hexane to obtain the pure product 11a (0.101 g, 87 %).
Spectral data of compounds 6, 7, 8 and 11:

2-phenylbenzo[d]oxazole (6a)

$^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 8.30-8.27 (m, 2H), 7.83 (m, 1H), 7.62-7.54 (m, 4H), 7.39-7.36 (m, 2H); $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 163.0, 150.7, 142.1, 131.5, 128.9, 127.6, 127.1, 125.1, 124.5, 120.0, 110.6; MS (ESI-MS) m/z: 196 (M+H)$^+$; HRMS: calcd for C$_{13}$H$_9$NO (M+H): 196.0757, Found 196.0752; IR (cm$^{-1}$, neat): 3058, 1616, 1552, 1488.

5-chloro-2-phenylbenzo[d]oxazole (6b)

$^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 8.28-8.24 (m, 2H), 7.77 (s, 1H), 7.57-7.51 (m, 4H), 7.34 (dd, $J$ = 8.6, 2.1 Hz, 1H); $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 164.3, 149.3, 143.2, 131.9, 130.0, 129.0, 127.7, 126.7, 125.3, 119.9, 111.3; MS (ESI-MS) m/z: 230 (M+H)$^+$; HRMS: calcd for C$_{13}$H$_8$ClNO(M+H)$^+$: 230.0367, Found 230.0367; IR (cm$^{-1}$, neat): 3063, 1553, 1451.

6-methyl-2-phenylbenzo[d]oxazole (6c)

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.25-8.23 (m, 2H), 7.64 (d, $J$ = 8.1 Hz, 1H), 7.57-7.50 (m, 3H), 7.38 (s, 1H), 7.16 (d, $J$ = 8.1 Hz, 1H), 2.50 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 162.5, 151.0, 139.8, 135.5, 131.2, 128.8, 127.4, 126.4, 125.8, 119.3, 110.7, 21.7; MS (ESI-MS) m/z: 210 (M+H)$^+$; HRMS: calcd for C$_{14}$H$_{11}$NO(M+H)$^+$: 210.0913, Found 210.0909; IR (cm$^{-1}$, neat): 3055, 3028, 2916, 1616, 1554, 1481.

5-(tert-butyl)-2-phenylbenzo[d]oxazole (6d)

$^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 8.30-8.26 (m, 2H), 7.85 (s, 1H), 7.55-7.51 (m, 3H), 7.49 (m, 1H), 7.45 (m, 1H), 1.43 (s, 9H); $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 163.1, 148.7, 148.1, 142.0, 131.3, 128.8, 127.5, 127.3, 122.8, 116.5, 109.7, 34.9, 31.8; MS (ESI-MS) m/z: 252 (M+H)$^+$; HRMS: calcd for C$_{17}$H$_{17}$NO(M+H)$^+$: 252.1383, Found 252.1383; IR (cm$^{-1}$, neat): 3066, 2961, 2906, 1616, 1555, 1480.

2-phenoxazolo[4,5-b]pyridine (6e)

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.56 (d, $J$ = 8.1, 1H), 8.31-8.29 (m, 2H), 7.85 (d, $J$ = 8.1, 1H), 7.57-7.51 (m, 3H), 7.49 (m, 1H), 7.45 (m, 1H), 1.43 (s, 9H); $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 165.6, 156.3, 146.6, 143.0, 132.4, 128.9, 128.0, 126.4, 120.0, 118.1; MS (ESI-MS) m/z: 197 (M+H)$^+$; HRMS: calcd for C$_{12}$H$_8$N$_2$O(M+H)$^+$: 197.0709, Found 197.0708; IR (cm$^{-1}$, neat): 3072, 3025, 2916, 1613, 1551, 1481.

2-(o-tolyl)benzo[d]oxazole (6f)

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.19 (m, 1H), 7.80 (dd, $J$ = 7.2, 2.2 Hz, 1H), 7.58 (dd, $J$ = 7.2, 2.2 Hz, 1H), 7.45 (m, 1H), 2.38 (s, 3H); $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 165.6, 156.3, 146.6, 143.0, 132.4, 128.9, 128.0, 126.4, 120.0, 118.1; MS (ESI-MS) m/z: 197 (M+H)$^+$; HRMS: calcd for C$_{12}$H$_8$N$_2$O(M+H)$^+$: 197.0709, Found 197.0708; IR (cm$^{-1}$, neat): 3072, 3025, 2916, 1613, 1551, 1481.
Hz, 1H), 7.42-7.32 (m, 5H), 2.81 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 163.3, 150.2, 142.1, 138.8, 131.7, 130.8, 129.9, 126.2, 126.0, 124.9, 124.3, 120.1, 110.4, 22.1; MS (ESI-MS) m/z: 210 (M+H)$^+$; HRMS: calcd for C$_{14}$H$_{11}$NO (M+H)$^+$: 210.0913, Found 210.0911; IR (cm$^{-1}$, neat): 3061, 2966, 2916, 1615, 1548, 1452.

2-(m-toly)benzo[d]oxazole (6g)

$^1$H NMR (400 MHz, CDCl$_3$) δ 8.09 (s, 1H), 8.04 (d, J = 7.7 Hz, 1H), 7.78(m, 1H), 7.56 (dd, J = 7.2, 2.2 Hz, 1H), 7.39 (t, J = 7.6 Hz, 1H), 7.36 – 7.31 (m, 3H), 2.44 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 163.2, 150.7, 142.0, 138.6, 132.3, 128.7, 128.1, 126.9, 124.9, 124.7, 119.9, 110.5, 21.3; MS (ESI-MS) m/z: 210 (M+H)$^+$; HRMS: calcd for C$_{14}$H$_{11}$NO (M+H)$^+$: 210.0913, Found 210.0914; IR (cm$^{-1}$, neat): 3055, 2913, 1615, 1552, 1453.

2-(p-toly)benzo[d]oxazole (6h)

$^1$H NMR (400 MHz, CDCl$_3$) δ 8.14 (d, J = 8.2 Hz, 2H), 7.77 (m, 1H), 7.57 (m, 1H), 7.34 – 7.30 (m, 4H), 2.42 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 163.2, 150.6, 142.1, 142.0, 129.6, 127.5, 124.8, 124.4, 124.3, 119.8, 110.4, 21.6; MS (ESI-MS) m/z: 210 (M+H)$^+$; HRMS: calcd for C$_{14}$H$_{11}$NO (M+H)$^+$: 210.0913, Found 210.0916; IR (cm$^{-1}$, neat): 3063, 2963, 1622, 1555, 1550, 1452.

2-(3-methoxyphenyl)benzo[d]oxazole (6i)

$^1$H NMR (300 MHz, CDCl$_3$) δ 7.89 (m, 1H), 7.82-7.78 (m, 2H), 7.62 (m, 1H), 7.47-7.36 (m, 3H), 7.12 (m, 1H), 3.93 (s, 3H); $^{13}$C NMR (75 MHz, CDCl$_3$) δ 162.9, 159.9, 150.7, 142.0, 130.0, 128.3, 125.1, 124.6, 120.1, 120.0, 118.3, 111.8, 110.6, 55.5; MS (ESI-MS) m/z: 226 (M+H)$^+$; HRMS: calcd for C$_{14}$H$_{11}$NO$_2$ (M+H)$^+$: 226.0863; Found 226.0861; IR (cm$^{-1}$, neat): 3069, 2949, 2837, 1602, 1583, 1489.

2-(thiophen-2-yl)benzo[d]oxazole (6j)

$^1$H NMR (400 MHz, CDCl$_3$) δ 7.92 (m, 1H), 7.76 (m, 1H), 7.58 – 7.52 (m, 2H), 7.34-7.32 (m, 2H), 7.20 (m, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 159.0, 150.4, 141.9, 130.2, 129.9, 129.6, 128.2, 125.0, 124.6, 119.7, 110.4; MS (ESI-MS) m/z: 202 (M+H)$^+$; HRMS: calcd for C$_{11}$H$_7$NOS (M+H)$^+$: 202.0248, Found 202.0319; IR (cm$^{-1}$, neat): 3069, 2949, 2837, 1602, 1583, 1489.

5-chloro-2-(3-methoxyphenyl)benzo[d]oxazole (6k)

$^1$H NMR (400 MHz, CDCl$_3$) δ 7.76 (d, J = 7.7 Hz, 1H), 7.69 (s, 2H), 7.42 (d, J = 8.6 Hz, 1H), 7.37 (t, J = 8.0 Hz, 1H), 7.26 (dd, J = 8.6, 1.7 Hz, 1H), 7.06 (m, 1H), 3.86 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 164.1, 159.8, 149.2, 143.1, 129.9, 127.7, 125.3, 120.1, 119.8, 118.5, 112.0,
111.2, 55.4; MS (ESI-MS) m/z: 260 (M+H)⁺; HRMS : calcd for C₁₄H₁₀ClNO₂(M+H)⁺: 260.0473, Found 260.0473; IR (cm⁻¹, neat): 3069, 2960, 1596, 1578, 1474

2-phenyl-1H-benzo[d]imidazole (7a)

1H NMR (400 MHz, CD₃OD) δ 8.07 (d, J = 7.3 Hz, 2H), 7.59 (dd, J = 7.2, 1.8 Hz, 2H), 7.54 – 7.46 (m, 3H), 7.26 – 7.21 (m, 2H); 1³C NMR (100 MHz, CD₃OD) δ 151.9, 129.9, 129.5, 128.7, 126.3, 122.4; MS (ESI-MS) m/z: 195 (M+H)⁺; HRMS: calcd for C₁₃H₁₀N₂(M+H)⁺: 195.0917, Found 195.0921; IR (cm⁻¹, neat): 3255, 3043, 1659, 1595, 1533, 1456

Methyl 2-phenyl-1H-benzo[d]imidazole-5-carboxylate (7b)

1H NMR (300 MHz, CDCl₃) δ 8.30 (s, 1H), 8.13 (d, J = 7.8, 2H), 7.93 (d, J = 8.5, 1H), 7.59 (m, 1H), 7.42–7.33 (m, 3H), 3.91 (s, 3H); 1³C NMR (75 MHz, CDCl₃) δ 167.9, 154.6, 130.6, 129.2, 129.07, 128.9, 127.0, 124.5, 124.3, 52.1; MS (ESI) m/z: 253 (M+H)⁺; HRMS (ESI) calcd for C₁₅H₁₂N₂O₂ (M+H)⁺: 253.0972, Found 253.0977.

Methyl 1-phenethyl-2-phenyl-1H-benzo[d]imidazole-5-carboxylate (7c)

1H NMR (400 MHz, CDCl₃) δ 8.53 (s, 1H), 8.04 (d, J = 8.5 Hz, 1H), 7.51 – 7.43 (m, 5H), 7.41 (d, J = 8.5 Hz, 1H), 7.23 – 7.08 (m, 3H), 6.87 – 6.84 (m, 2H), 4.47 (t, J = 7.3 Hz, 2H), 3.96 (s, 3H), 3.04 (t, J = 7.3 Hz, 2H); 1³C NMR (100 MHz, CDCl₃) δ 167.6, 155.6, 142.6, 138.5, 136.9, 130.0, 129.7, 129.2, 128.8, 128.6, 128.5, 127.0, 124.7, 124.4, 122.3, 109.8, 52.1, 46.3, 35.8; MS (ESI) m/z: 357.3 (M+H)⁺; HRMS (ESI) calcd for C₂₃H₂₀N₂O₂ (M+H)⁺: 257.1598, Found 257.1603.

Methyl 1-(furan-2-ylmethyl)-2-phenyl-1H-benzo[d]imidazole-5-carboxylate (7d)

1H NMR (400 MHz, CDCl₃) δ 8.53 (s, 1H), 8.03 (d, J = 8.5 Hz, 1H), 7.84 – 7.80 (m, 2H), 7.58 – 7.52 (m, 3H), 7.49 (d, J = 8.6 Hz, 1H), 7.40 (s, 1H), 6.35 (d, J = 3.1 Hz, 1H), 6.25 (d, J = 3.1 Hz, 1H), 3.04 (s, 3H); 1³C NMR (100 MHz, CDCl₃) δ 167.5 , 155.5 , 148.8 , 143.1 , 142.6 , 139.0 , 130.3 , 129.6 , 129.5 , 128.8 , 124.9 , 124.6 , 122.2 , 110.6 , 110.1 , 108.8 , 52.1 , 42.3; MS (ESI) m/z: 333.2 (M+H)⁺; HRMS (ESI) calcd for C₂₀H₁₆N₂O₃ (M+H)⁺: 322.1234, Found 322.1238.

Methyl 1-(2-(cyclohex-1-en-1-yl)ethyl)-2-phenyl-1H-benzo[d]imidazole-5-carboxylate (7e)

1H NMR (400 MHz, CDCl₃) δ 8.52 (d, J = 1.5 Hz, 1H), 8.04 (dd, J = 8.5, 1.5 Hz, 1H), 7.75 – 7.71 (m, 2H), 7.55 – 7.52 (m, 3H), 7.43 (d, J = 8.5 Hz, 1H), 5.19 (t, J = 3.6 Hz, 1H), 4.33 (t, J = 7.5, 2H), 3.96 (s, 3H), 2.36 (t, J = 7.5 Hz, 2H), 1.86 – 1.70 (m, 4H), 1.49 – 1.40 (m, 4H); 1³C NMR (100 MHz, CDCl₃) δ 167.7 , 155.5 , 142.6 , 138.8 , 133.0 , 130.2 , 130.0 , 129.3 , 128.8,
124.7, 124.5, 124.2, 122.3, 109.9, 52.1, 43.8, 37.8, 28.2, 25.1, 22.5, 21.9; MS (ESI) m/z: 361.3 (M+H)^+; HRMS (ESI) calcd for C_{23}H_{24}N_{2}O_{5} (M+H)^+: 361.1911, Found 361.1914

Methyl 1-pentyl-2-phenyl-1H-benzo[d]imidazole-5-carboxylate (7f)

^1^H NMR (400 MHz, CDCl\textsubscript{3}) \(\delta\) 8.52 (dd, \(J = 1.6, 0.6\) Hz, 1H), 8.04 (dd, \(J = 8.5, 0.6\) Hz, 1H), 7.76 – 7.67 (m, 2H), 7.61 – 7.49 (m, 3H), 7.43 (dd, \(J = 8.5, 0.6\) Hz, 1H), 4.24 (t, \(J = 7.2\) Hz, 2H), 3.96 (s, 3H), 1.81 (p, \(J = 7.4\) Hz, 2H), 1.29 – 1.17 (m, 4H), 0.83 (t, \(J = 7.1\) Hz, 3H); ^1^C NMR (100 MHz, CDCl\textsubscript{3}) \(\delta\) 167.6, 155.4, 142.7, 138.8, 130.2, 130.0, 129.3, 128.8, 124.5, 124.2, 122.3, 109.7, 52.1, 44.9, 29.4, 28.7, 22.0, 13.8; MS (ESI) m/z: 323.3 (M+H)^+; HRMS (ESI) calcd for C\(_{20}\)H\(_{22}\)N\(_2\)O\(_2\) (M+H)^+: 323.1754, Found 323.1759.

6-chloro-1-(2-methoxyethyl)-2-(p-tolyl)-1H-benzo[d]imidazole (7g)

^1^H NMR (400 MHz, Acetone-\textit{d}_6) \(\delta\) 7.83 – 7.72 (m, 2H), 7.70 (d, \(J = 2.0\) Hz, 1H), 7.64 (d, \(J = 8.6\) Hz, 1H), 7.38 (d, \(J = 8.4\) Hz, 2H), 7.24 (dd, \(J = 8.6, 2.0\) Hz, 1H), 4.50 (t, \(J = 5.4\) Hz, 2H), 3.79 (t, \(J = 5.4\) Hz, 2H), 3.21 (s, 3H), 2.43 (s, 3H); ^1^C NMR (100 MHz, Acetone-\textit{d}_6) \(\delta\) 155.1, 142.1, 139.7, 137.0, 129.6, 129.1, 127.8, 127.3, 122.2, 120.3, 111.0, 70.5, 58.0, 44.7, 20.5; MS (ESI) m/z: 301.3 (M+H)^+; HRMS (ESI) calcd for C\(_{17}\)H\(_{17}\)ClN\(_2\)O (M+H)^+: 301.1102, Found 301.1106.

6-chloro-1-(2-methoxyethyl)-2-phenyl-1H-benzo[d]imidazole (7h)

^1^H NMR (400 MHz, Acetone-\textit{d}_6) \(\delta\) 7.90 – 7.87 (m, 2H), 7.73 (d, \(J = 2.0\) Hz, 1H), 7.67 (d, \(J = 8.6\) Hz, 1H), 7.59 – 7.54 (m, 3H), 7.26 (dd, \(J = 8.6, 2.0\) Hz, 1H), 4.52 (t, \(J = 5.3\) Hz, 2H), 3.79 (t, \(J = 5.3\) Hz, 2H), 3.20 (s, 3H); ^1^C NMR (100 MHz, Acetone-\textit{d}_6) \(\delta\) 155.0, 142.0, 136.9, 130.6, 129.8, 129.7, 128.5, 127.5, 122.4, 120.4, 111.1, 70.5, 58.0, 44.7; MS (ESI) m/z: 287.2 (M+H)^+; HRMS (ESI) calcd for C\(_{16}\)H\(_{15}\)ClN\(_2\)O (M+H)^+: 287.0946, Found 287.0950.

6-chloro-1-(2-methoxyethyl)-2-(thiophen-2-yl)-1H-benzo[d]imidazole (7i)

^1^H NMR (400 MHz, Acetone-\textit{d}_6) \(\delta\) 7.84 (dd, \(J = 4.2, 1.1\) Hz, 1H), 7.73 (dd, \(J = 4.5, 1.0\) Hz, 1H), 7.68 (d, \(J = 1.3\) Hz, 1H), 7.63 – 7.60 (m, 1H), 7.27 – 7.22 (m, 2H), 4.68 (t, \(J = 5.3\) Hz, 2H), 3.90 (t, \(J = 5.3\) Hz, 2H), 3.28 (s, 3H); ^1^C NMR (100 MHz, Acetone-\textit{d}_6) \(\delta\) 148.9, 141.8, 137.3, 132.6, 129.1, 128.6, 127.9, 127.6, 122.6, 120.1, 110.8, 70.8, 58.2, 44.9; MS (ESI) m/z: 293.2 (M+H)^+; HRMS (ESI) calcd for C\(_{14}\)H\(_{13}\)ClN\(_2\)OS (M+H)^+: 293.0510, Found 293.0510.

6-chloro-1-(2-methoxyethyl)-2-(4-methoxyphenyl)-1H-benzo[d]imidazole (7j)

56
$^1$H NMR (400 MHz, Acetone-$d_6$) δ 7.84 (d, $J = 8.8$ Hz, 2H), 7.68 (d, $J = 1.5$ Hz, 1H), 7.62 (d, $J = 8.5$ Hz, 1H), 7.23 (dd, $J = 8.5$, 1.9 Hz, 1H), 7.11 (d, $J = 8.8$ Hz, 2H), 4.50 (t, $J = 5.3$ Hz, 2H), 3.90 (s, 3H), 3.81 (t, $J = 5.3$ Hz, 2H), 3.23 (s, 3H); $^{13}$C NMR (100 MHz, Acetone-$d_6$) δ 160.9, 142.1, 137.0, 131.2, 127.1, 122.2, 122.2, 120.2, 113.9, 110.9, 70.5, 58.1, 54.8, 44.7; MS (ESI) m/z: 317.2 (M+H)$^+$; HRMS (ESI) calcd for C$_{17}$H$_{17}$ClN$_2$O$_2$ (M+H)$^+$ m/z: 317.1051, Found 317.1056.

2-phenylbenzo[d]thiazole (8a)
$^1$H NMR (400 MHz, CDCl$_3$) δ 8.14 – 8.07 (m, 3H), 7.90 (m, 1H), 7.51 – 7.46 (m, 4H), 7.39 (m, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 168.0, 154.0, 135.0, 133.5, 131.0, 129.0, 127.5, 126.3, 125.2, 123.2, 121.6; MS (ESI-MS) m/z: 212 (M+H)$^+$; HRMS: calcd for C$_{13}$H$_9$NS (M+H)$^+$: 212.0528, Found 212.0524; IR (cm$^{-1}$, neat): 3066, 3016, 1506, 1477.

2-phenyl-5-(trifluoromethyl)benzo[d]thiazole (8b)
$^1$H NMR (400 MHz, CDCl$_3$) δ 8.34 (s, 1H), 8.11-8.09 (m, 2H), 8.01 (d, $J = 8.4$ Hz, 1H), 7.62 (d, $J = 8.4$ Hz, 1H), 7.53-7.52 (m, 3H); $^{13}$C NMR (75 MHz, CDCl$_3$) δ 170.1, 153.8, 138.5, 133.1, 128.8, 126.0, 122.2, 121.6, 121.5, 120.5, 120.3; MS (ESI-MS) m/z: 280 (M+H)$^+$; HRMS: calcd for C$_{14}$H$_8$F$_3$NS (M+H)$^+$: 280.0402, Found 280.0405; IR (cm$^{-1}$, neat): 3061, 1653, 1603, 1483.

2-(o-tolyl)benzo[d]thiazole (8c)
$^1$H NMR (400 MHz, CDCl$_3$) δ 8.12 (d, $J = 7.7$ Hz, 1H), 7.94 (d, $J = 7.7$ Hz, 1H), 7.77 (d, $J = 7.0$ Hz, 1H), 7.52 (t, $J = 7.0$ Hz, 1H), 7.46 – 7.29 (m, 4H), 2.67 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 168.0, 153.8, 137.2, 135.6, 133.1, 131.5, 130.5, 126.1, 125.1, 123.4, 121.4, 21.4; MS (ESI-MS) m/z: 226 (M+H)$^+$; HRMS: calcd for C$_{14}$H$_{11}$NS (M+H)$^+$: 226.0685; Found 226.0684; IR (cm$^{-1}$, neat): 3063, 2957, 1725, 1600, 1486.

2-(m-tolyl)benzo[d]thiazole (8d)
$^1$H NMR (400 MHz, CDCl$_3$) δ 8.12 (d, $J = 8.1$ Hz, 1H), 7.95 (s, 1H), 7.87-7.82 (m, 2H), 7.49 (m, 1H), 7.33 (t, $J = 7.6$ Hz, 2H), 7.25 (d, $J = 7.6$ Hz, 1H), 2.41 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 168.2, 154.1, 138.7, 135.0, 133.4, 131.8, 128.9, 127.9, 126.2, 125.1, 124.8, 123.1, 121.6, 21.3; MS (ESI-MS) m/z: 226 (M+H)$^+$; HRMS: calcd for C$_{14}$H$_{11}$NS (M+H)$^+$: 226.0607, Found 226.0686; IR (cm$^{-1}$, neat): 3049, 2916, 1606, 1502, 1483.

2-(p-tolyl)benzo[d]thiazole (8e)
$^1$H NMR (400 MHz, CDCl$_3$) δ 8.10 (d, $J = 8.1$ Hz, 1H), 7.99-7.97 (m, 2H), 7.83 (d, $J = 8.1$, 1H),
7.50 (m, 1H), 7.36 (m, 1H), 7.25 (d, J = 7.9 Hz, 2H), 2.38 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 168.2, 154.2, 141.3, 134.9, 130.9, 129.6, 127.4, 126.2, 124.9, 123.0, 121.5, 21.5; MS (ESI-MS) m/z: 226 (M+H)+; HRMS: calcd for C₁₄H₁₁NS(M+H)+: 226.0685; Found 226.0685; IR (cm⁻¹, neat): 3052, 3022, 2919, 2860, 1612, 1483.

2-(3-methoxyphenyl)benzo[d]thiazole (8f)
¹H NMR (400 MHz, CDCl₃) δ 8.10 (d, J = 8.1 Hz, 1H), 7.89 (d, J = 8.1 Hz, 1H), 7.70 (s, 1H), 7.64 (d, J = 7.7 Hz, 1H), 7.52 (m, 1H), 7.39 (t, J = 7.9 Hz, 2H), 7.04 (dd, J = 8.0, 2.2 Hz, 1H), 3.87 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 168.0, 160.0, 153.7, 134.9, 134.6, 130.0, 126.3, 125.3, 123.1, 121.6, 120.2, 117.4, 112.0, 55.5; MS (ESI-MS) m/z: 242 (M+H)+; HRMS: calcd for C₁₄H₁₁NOS(M+H)+: 242.0634; Found 242.0634; IR (cm⁻¹, neat): 3058, 2934, 1600, 1469.

2-(thiophen-2-yl)benzo[d]thiazole (8g)
¹H NMR (400 MHz, CDCl₃) δ 8.03 (d, J = 8.1 Hz, 1H), 7.79 (d, J = 8.1 Hz, 1H), 7.60 (d, J = 8.1 Hz, 1H), 7.48 – 7.42 (m, 2H), 7.35 (m, 1H), 7.08 (m, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 161.3, 153.6, 137.3, 134.6, 129.3, 128.6, 128.0 126.4, 125.2, 122.9, 121.4; MS (ESI-MS) m/z: 218 (M+H)+; HRMS: calcd for C₁₁H₇N₂(M+H)+: 218.0093; Found 218.0089; IR (cm⁻¹, neat): 3105, 3063, 1541, 1476.

2-phenylquinazolin-4(3H)-one (11a).
¹H NMR (400 MHz, Acetone-d₆) δ 8.33 – 8.25 (m, 2H), 8.20 (d, J = 8.0 Hz, 1H), 7.84 – 7.80 (m, 1H), 7.74 (d, J = 8.2 Hz, 1H), 7.60 – 7.48 (m, 4H); ¹³C NMR (100 MHz, DMSO-d₆) δ 162.7, 152.8, 135.0, 133.1, 131.8, 129.0, 128.2, 127.9, 127.0, 126.3, 121.4; MS (ESI) m/z: 223.2 (M+H)+, HRMS (ESI) calcd for C₁₄H₁₀N₂O(M+H)+: 223.0866; Found 223.0870.

2-(p-tolyl)quinazolin-4(3H)-one (11b)
¹H NMR (400 MHz, DMSO-d₆) δ 8.11 (d, J = 7.9 Hz, 1H), 8.06 (d, J = 8.2 Hz, 2H), 7.78 (t, J = 8.3 Hz, 1H), 7.68 (d, J = 8.0 Hz, 1H), 7.46 (t, J = 7.9 Hz, 1H), 7.31 (d, J = 8.1 Hz, 2H), 2.35 (s, 3H); ¹³C NMR (100 MHz, DMSO-d₆) δ 162.2, 152.6, 149.2, 141.9, 135.0, 130.3, 129.6, 128.1, 127.8, 126.8, 126.3, 121.3, 21.4; MS (ESI) m/z: 237.3 (M+H)+; HRMS (ESI) calcd for C₁₅H₁₂N₂O (M+H)+/m/z : 237.1029, Found 237.1022.

2-(o-tolyl)quinazolin-4(3H)-one (11c)
¹H NMR (400 MHz, CDCl₃) δ 8.28 (d, J = 7.5 Hz, 1H), 7.80 (s, 1H), 7.79 (s, 1H), 7.56 (d, J = 7.2 Hz, 1H), 7.54 – 7.49 (m, 1H), 7.42 (d, J =7.0 Hz, 1H), 7.35 (d, J = 7.2 Hz, 2H), 2.53 (s, 3H); ¹³C
NMR (100 MHz, CDCl$_3$) $\delta$ 162.6, 153.2, 149.1, 136.8, 134.9, 133.6, 131.5, 130.6, 128.5, 127.9, 127.0, 126.4, 126.3, 120.8, 20.1; MS (ESI) m/z: 237.2 (M+H)$^+$; HRMS (ESI) calcd for C$_{15}$H$_{12}$N$_2$O (M+H)$^+$ m/z: 273.1022, Found 273.1021.

2-(m-toly)quinazolin-4(3H)-one (11d)
$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.32 (d, $J = 7.9$ Hz, 1H), 7.96 (s, 1H), 7.88 (d, $J = 7.7$ Hz, 1H), 7.86 – 7.78 (m, 2H), 7.50 (d, $J = 7.8$ Hz, 1H), 7.45 (d, $J = 7.7$ Hz, 1H), 7.40 (d, $J = 7.6$ Hz, 1H), 2.50 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 163.89, 151.96, 149.55, 138.85, 134.83, 132.41, 128.91, 128.03, 127.95, 127.43, 126.68, 126.28, 124.52, 120.84, 21.51; MS (ESI) m/z: 237.2 (M+H)$^+$; HRMS (ESI) calcd for C$_{15}$H$_{12}$N$_2$O (M+H)$^+$: 273.1022, Found 273.1026.

2-(4-isopropylphenyl)quinazolin-4(3H)-one (11e)
$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.33 (d, $J = 7.8$ Hz, 1H), 8.12 (d, $J = 8.1$ Hz, 2H), 7.87 – 7.74 (m, 2H), 7.50 (t, $J = 7.8$ Hz, 1H), 7.43 (d, $J = 8.2$ Hz, 2H), 3.02 (hept, $J = 7.3$ Hz, 1H), 1.32 (s, 3H), 1.31 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 163.5, 153.0, 151.6, 149.6, 134.8, 130.3, 127.9, 127.2, 127.2, 126.6, 126.4, 120.8, 34.2, 23.8; MS (ESI) m/z: 265.3 (M+H)$^+$; HRMS (ESI) calcd for C$_{17}$H$_{16}$N$_2$O (M+H)$^+$: 265.1335, Found 265.1341.

2-(4-methoxyphenyl)quinazolin-4(3H)-one (11f)
$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.33 – 8.28 (m, 1H), 8.16 – 8.08 (m, 2H), 7.81 – 7.77 (m, 2H), 7.47 (td, $J = 5.5$, 2.6 Hz, 1H), 7.10 – 7.04 (m, 2H), 3.91 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 163.4, 162.5, 151.2, 149.6, 134.8, 128.8, 127.8, 126.4, 126.4, 125.0, 120.6, 114.5, 55.5; MS (ESI) m/z: 253.2 (M+H)$^+$; HRMS (ESI) calcd for C$_{15}$H$_{12}$N$_2$O$_2$ (M+H)$^+$: 253.0972, Found 253.0972.

2-(3-methoxyphenyl)quinazolin-4(3H)-one (11g)
$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.32 (d, $J = 7.8$ Hz, 1H), 7.87 – 7.73 (m, 4H), 7.52 (d, $J = 8.0$ Hz, 1H), 7.48 (d, $J = 8.0$ Hz, 1H), 7.13 (d, $J = 7.7$ Hz, 1H), 3.96 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 163.5, 160.2, 151.5, 149.4, 134.9, 134.1, 130.1, 128.0, 126.9, 126.3, 120.9, 119.4, 118.2, 112.1, 55.6; MS (ESI) m/z: 253.3 (M+H)$^+$; HRMS (ESI) calcd for C$_{15}$H$_{12}$N$_2$O$_2$ (M+H)$^+$: 253.0972, Found 253.0972.

2-(4-fluorophenyl)quinazolin-4(3H)-one (11h)
$^1$H NMR (400 MHz, DMSO-d$_6$) $\delta$ 8.27 – 8.20 (m, 2H), 8.20 – 8.10 (m, 1H), 7.81 (d, $J = 8.2$ Hz, 1H), 7.72 (d, $J = 8.2$ Hz, 1H), 7.59 – 7.46 (m, 1H), 7.38 (t, $J = 8.2$ Hz, 2H); $^{13}$C NMR (100 MHz, DMSO-d$_6$) $\delta$ 164.5 (d, $^1J_{CF} = 248$ Hz), 151.8, 149.0, 135.1, 130.9, 130.8, 129.7, 128.2, 127.1,
126.3, 121.3, 116.2, 116.0; HRMS (ESI) calcd for C_{23}H_{20}N_{2}O_{2} (M+H)^+ m/z: 241.0772, Found 241.0771.

2-(thiophen-2-yl)quinazolin-4(3H)-one (11i)
{\textsuperscript{1}}H NMR (400 MHz, CDCl\textsubscript{3}) \( \delta 8.20 \) (d, \( J = 7.9 \) Hz, 1H), 8.11 (d, \( J = 3.7 \) Hz, 1H), 7.68 (d, \( J = 3.7 \) Hz, 2H), 7.52 – 7.48 (m, 1H), 7.40 – 7.34 (m, 1H), 7.11 (t, \( J = 3.8 \) Hz, 1H); \({\textsuperscript{13}}C\) NMR (100 MHz, CDCl\textsubscript{3}) \( \delta 163.2, 149.3, 147.7, 137.7, 134.5, 130.9, 128.6, 128.3, 127.4, 127.4, 126.2, 121.0; MS (ESI) m/z: 229.2 (M+H)^+; HRMS (ESI) calcd for C_{12}H_{8}N_{2}OS (M+H)^+: 229.0430, Found 229.0433.

7-chloro-2-phenylquinazolin-4(3H)-one (11j)
{\textsuperscript{1}}H NMR (400 MHz, CDCl\textsubscript{3}) \( \delta 8.24 \) (d, \( J = 8.5 \) Hz, 1H), 8.13 (d, \( J = 7.0 \) Hz, 1H), 7.61 – 7.56 (m, 3H), 7.45 (d, \( J = 8.5 \) Hz, 1H); \({\textsuperscript{13}}C\) NMR (100 MHz, CDCl\textsubscript{3}) \( \delta 161.9, 153.1, 149.5, 139.5, 131.9, 130.9, 128.0, 127.1, 127.0, 126.4, 126.1, 119.0; MS (ESI) m/z: 257.2 (M+H)^+; HRMS (ESI) calcd for C_{14}H_{9}ClN_{2}O m/z : 257.0476 (M+H)^+; Found 257.0473.

6-chloro-2-phenylquinazolin-4(3H)-one (11k)
{\textsuperscript{1}}H NMR (400 MHz, CDCl\textsubscript{3}) \( \delta 8.87 \) (dd, \( J = 8.5, 1.0 \) Hz, 1H), 8.01 (dd, \( J = 8.5, 1.0 \) Hz, 2H), 7.56 – 7.49 (m, 5H); \({\textsuperscript{13}}C\) NMR (100 MHz, CDCl\textsubscript{3}) \( \delta 167.3, 158.5, 155.0, 144.9, 137.5, 136.3, 133.4, 132.6, 132.4, 131.8, 131.5, 124.6; MS (ESI) m/z: 257.2 (M+H)^+; HRMS (ESI) calcd for C_{23}H_{20}N_{2}O_{2}(M+H)^+ m/z: 257.0476, Found 257.0474

8-chloro-2-phenylquinazolin-4(3H)-one (11l)
{\textsuperscript{1}}H NMR (400 MHz, CDCl\textsubscript{3}) \( \delta 8.52-8.22 \) (m, 5H), 7.89 (d, \( J = 7.7 \) Hz, 1H), 7.65 – 7.55 (m, 3H), 7.42 (t, \( J = 7.8 \) Hz, 1H); \({\textsuperscript{13}}C\) NMR (100 MHz, CDCl\textsubscript{3}) \( \delta 167.5, 157.7, 150.6, 139.3, 137.5, 136.7, 136.4, 133.5, 132.7, 131.1, 129.8, 127.6, 110.0; MS (ESI) m/z: 257.2 (M+H)^+; HRMS (ESI) calcd for C_{14}H_{9}ClN_{2}O m/z : 257.0476 (M+H)^+; Found 257.0475.

6,7-difluoro-2-phenylquinazolin-4(3H)-one (11m)
{\textsuperscript{1}}H NMR (400 MHz, CDCl\textsubscript{3}) \( \delta 8.11 – 8.04 \) (m, 2H), 7.50 – 7.46 (m, 1H), 7.37 – 7.32 (m, 4H); \({\textsuperscript{13}}C\) NMR (100 MHz, DMSO-d\textsubscript{6}) \( \delta 169.7, 165.0, 151.5 \) (d, \( J_{CF} = 248 \) Hz), 144.5 (d, \( J_{CF} = 228 \) Hz), 138.4, 138.4, 138.3, 138.3, 134.4, 132.8, 129.4, 127.4, 118.3, 118.1, 116.1, 116.1, 109.3, 109.1; MS (ESI) m/z: 259.2 (M+H)^+; HRMS (ESI) calcd for C_{23}H_{20}N_{2}O_{2} m/z: 259.0677 (M+H)^+, Found 259.0679.
6-methyl-2-phenylquinazolin-4(3H)-one (11n)

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.19 (dd, $J$ = 8.3, 2.1 Hz, 2H), 8.10 (s, 1H), 7.75 (d, $J$ = 8.3 Hz, 1H), 7.62 (dd, $J$ = 8.3, 2.0 Hz, 1H), 7.60 – 7.55 (m, 3H), 2.52 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 163.4, 150.9, 147.2, 137.1, 136.4, 132.7, 131.6, 129.1, 127.7, 127.2, 125.8, 120.5, 21.4; MS (ESI) m/z: 237.2 (M+H)$^+$; HRMS (ESI) calcd for C$_{15}$H$_{12}$N$_2$O(M+H)$^+$: 273.1022, Found 273.1025.

6-methoxy-2-phenylquinazolin-4(3H)-one (11o)

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 10.65 (S, 1H), 8.13 – 7.10 (m, 2H), 7.83 – 7.74 (m, 1H), 7.71 – 7.66 (m, 1H), 7.61 – 7.50 (m, 3H), 7.44 – 7.37 (m, 1H), 3.95 (s, 3H); $^{13}$C NMR (100 MHz, DMSO-$d_6$) $\delta$ 162.4, 158.1, 150.5, 143.6, 133.2, 131.4, 129.6, 129.1, 127.9, 124.5, 122.2, 106.3, 56.1; MS (ESI) m/z: 253.2 (M+H)$^+$; HRMS (ESI) calcd for C$_{23}$H$_{20}$N$_2$O$_2$(M+H)$^+$ m/z: 253.0972; Found 253.0973.
$^1$H NMR spectrum (300 MHz) of compound 6a in CDCl$_3$
$\text{13}^\text{C}$ spectrum (75 MHz) of compound 6a in CDCl$_3$
**Chemical Formula:**

$C_{13}H_{10}NO$

**Exact Mass:** 195.0684

**Molecular Weight:** 195.2167

ESI Mass spectrum of compound 6a
HRMS Mass spectrum of compound 6a

Chemical Formula:
C_{13}H_{9}NO

Exact Mass: 195.0684
Molecular Weight: 195.2167
IR spectrum of compound 6a
$^1$H NMR spectrum (300 MHz) of compound 6b in CDCl$_3$
$^{13}$C spectrum (75 MHz) of compound 6b in CDCl$_3$
Chemical Formula: C$_{13}$H$_8$ClNO

Exact Mass: 229.0294

m/z: 229.0294 (100.0%), 231.0265 (32.0%),
230.0328 (14.1%), 232.0298 (4.5%)
HRMS Mass spectrum of compound 6b

Chemical Formula: C_{13}H_{8}ClNO

Exact Mass: 229.0294

m/z: 229.0294 (100.0%), 231.0265 (32.0%),
  230.0328 (14.1%), 232.0298 (4.5%)
IR spectrum of compound 6b
$^1$H NMR spectrum (400 MHz) of compound 6c in CDCl$_3$
$^{13}$C spectrum (100 MHz) of compound 6c in CDCl$_3$
Chemical Formula: C_{14}H_{11}NO
Exact Mass: 209.0841
m/z: 209.0841 (100.0%), 210.0874 (15.1%), 211.0908 (1.1%)
HRMS Mass spectrum of compound 6c

Chemical Formula: C₁₄H₁₁NO
Exact Mass: 209.0841
m/z: 209.0841 (100.0%), 210.0874 (15.1%), 211.0908 (1.1%)
IR spectrum of compound 6c
$^1$H NMR spectrum (300 MHz) of compound 6d in CDCl$_3$
$^{13}$C spectrum (75 MHz) of compound 6d in CDCl$_3$
Chemical Formula: C_{17}H_{17}NO
Exact Mass: 251.1310
m/z: 251.1310 (100.0%), 252.1344 (18.4%),
253.1377 (1.6%)

ESI Mass spectrum of compound 6d
HRMS Mass spectrum of compound 6d

Chemical Formula: C_{17}H_{17}NO
Exact Mass: 251.1310
m/z: 251.1310 (100.0%), 252.1344 (18.4%), 253.1377 (1.6%)
IR spectrum of compound 6d
\(^1\)H NMR spectrum (400 MHz) of compound 6e in CDCl\(_3\)

S32
$^{13}$C spectrum (100 MHz) of compound 6e in CDCl$_3$
Chemical Formula: $C_{12}H_8N_2O$

Exact Mass: 196.0637

m/z: 196.0637 (100.0%), 197.0670 (13.0%)
Chemical Formula: C_{12}H_{9}N_{2}O

Exact Mass: 196.0637

m/z: 196.0637 (100.0%), 197.0670 (13.0%)

HRMS Mass spectrum of compound 6e
IR spectrum of compound 6e
$^1$H NMR spectrum (400 MHz) of compound $6f$ in CDCl$_3$
$^{13}$C spectrum (100 MHz) of compound 6f in CDCl$_3$
Chemical Formula: C_{14}H_{11}NO

Exact Mass: 209.0841

m/z: 209.0841 (100.0%), 210.0874 (15.1%), 211.0908 (1.1%)

6f

ESI Mass spectrum of compound 6f
HRMS Mass spectrum of compound 6f

Chemical Formula: C_{14}H_{11}NO
Exact Mass: 209.0841
m/z: 209.0841 (100.0%), 210.0874 (15.1%), 211.0908 (1.1%)
IR spectrum of compound 6f
$^1$H NMR spectrum (400 MHz) of compound 6g in CDCl$_3$
$^{13}$C spectrum (100 MHz) of compound 6g in CDCl$_3$
Chemical Formula: C_{14}H_{11}NO

Exact Mass: 209.0841

m/z: 209.0841 (100.0%), 210.0874 (15.1%), 211.0908 (1.1%)

ESI Mass spectrum of compound 6g
Chemical Formula: C_{14}H_{11}NO

Exact Mass: 209.0841

m/z: 209.0841 (100.0%), 210.0874 (15.1%), 211.0908 (1.1%)

HRMS Mass spectrum of compound 6g
IR spectrum of compound 6g
$^{1}$H NMR spectrum (400 MHz) of compound $6h$ in CDCl$_3$
$^{13}$C spectrum (100 MHz) of compound 6h in CDCl$_3$
Chemical Formula: C_{14}H_{11}NO
Exact Mass: 209.0841
m/z: 209.0841 (100.0%), 210.0874 (15.1%), 211.0908 (1.1%)
HRMS Mass spectrum of compound 6h

Chemical Formula: C\textsubscript{14}H\textsubscript{11}NO

Exact Mass: 209.0841

m/z: 209.0841 (100.0%), 210.0874 (15.1%),
211.0908 (1.1%)
IR spectrum of compound 6h
$^1$H NMR spectrum (300 MHz) of compound 6i in CDCl$_3$
$^{13}$C spectrum (75 MHz) of compound 6i in CDCl$_3$
Chemical Formula: C_{14}H_{11}NO_{2}

Exact Mass: 225.0790

m/z: 225.0790 (100.0%), 226.0823 (15.1%), 227.0857 (1.1%)
HRMS Mass spectrum of compound 6i

Chemical Formula: C_{14}H_{11}NO_{2}
Exact Mass: 225.0790
m/z: 225.0790 (100.0%), 226.0823 (15.1%), 227.0857 (1.1%)
IR spectrum of compound 6i
$^1$H NMR spectrum (400 MHz) of compound 6j in CDCl$_3$
$^{13}$C spectrum (100 MHz) of compound 6j in CDCl$_3$
Chemical Formula: C_{11}H_{7}NOS  
Exact Mass: 201.0248  
m/z: 201.0248 (100.0%), 202.0282 (11.9%), 203.0206 (4.5%)  

ESI Mass spectrum of compound 6j
HRMS Mass spectrum of compound 6j

Chemical Formula: C_{11}H_{7}NOS

Exact Mass: 201.0248

m/z: 201.0248 (100.0%), 202.0282 (11.9%), 203.0206 (4.5%)

6j
IR spectrum of compound 6j
$^1$H NMR spectrum (400 MHz) of compound 6k in CDCl$_3$
$^{13}$C spectrum (100 MHz) of compound 6k in CDCl$_3$
Chemical Formula: C_{14}H_{10}ClNO_{2}

Exact Mass: 259.0400

m/z: 259.0400 (100.0%), 261.0371 (32.0%), 260.0434 (15.1%), 262.0404 (4.8%), 261.0467 (1.1%)

ESI Mass spectrum of compound 6k
HRMS Mass spectrum of compound 6k

Chemical Formula: C_{14}H_{10}ClNO_{2}

Exact Mass: 259.0400

m/z: 259.0400 (100.0%), 261.0371 (32.0%), 260.0434 (15.1%), 262.0404 (4.8%), 261.0467 (1.1%)
IR spectrum of compound 6k
$^1$H NMR spectrum (400 MHz) of compound 7a in CD$_3$OD
$^{13}$C spectrum (100 MHz) of compound 7a in CD$_3$OD
Chemical Formula: $C_{13}H_{10}N_{2}$

Exact Mass: 194.0844

m/z: 194.0844 (100.0%), 195.0878 (14.1%)

7a
HRMS Mass spectrum of compound 7a

Chemical Formula: C_{13}H_{10}N_{2}

Exact Mass: 194.0844

m/z: 194.0844 (100.0%), 195.0878 (14.1%)

7a
IR spectrum of compound 7a
$^1$H NMR spectrum (300 MHz) of compound 7b in CDCl$_3$
$^{13}\text{C}$ spectrum (75 MHz) of compound 7b in CDCl$_3$
Chemical Formula: C_{15}H_{12}N_{2}O_{2}
Exact Mass: 252.0899
m/z: 252.0899 (100.0%), 253.0932 (16.2%),
254.0966 (1.2%)

7b

ESI Mass spectrum of compound 7b
Chemical Formula: C_{15}H_{12}N_{2}O_{2}

Exact Mass: 252.0899

m/z: 252.0899 (100.0%), 253.0932 (16.2%), 254.0966 (1.2%)

HRMS Mass spectrum of compound 7b
IR spectrum of compound 7b
$^{1}$H NMR (400MHz) spectrum of compound 7c in CDCl$_3$
$^{13}$C NMR (100MHz) spectrum of compound 7c in CDCl$_3$
ESI$^+$ Mass spectrum of compound 7c
High resolution mass (ESI+) spectrum of compound 7c
$^1$H NMR (400MHz) spectrum of compound 7d in CDCl$_3$
$^{13}$C NMR (100MHz) spectrum of compound 7d in CDCl$_3$
ESI$^+$ Mass spectrum of compound 7d
HRMS Mass spectrum of compound 7d
$^1$H NMR (400MHz) spectrum of compound 7e in CDCl$_3$
$^{13}$C NMR (100MHz) spectrum of compound $7e$ in CDCl$_3$
ESI+ Mass spectrum of compound 7e
High resolution mass (ESI⁺) spectrum of compound 7e
$^{1}$H NMR (400MHz) spectrum of compound 7f in CDCl$_3$
13C NMR (100MHz) spectrum of compound 7f in CDCl₃
ESI\textsuperscript{+} Mass spectrum of compound \textit{7f}
High resolution mass (ESI⁺) spectrum of compound 7f
$^1$H NMR (400MHz) spectrum of compound 7g in Acetone-$d_6$
$^{13}$C NMR (100MHz) spectrum of compound 7g in Acetone-$d_6$
ESI\textsuperscript{+} Mass spectrum of compound 7g
High resolution mass (ESI⁺) spectrum of compound 7g
$^1$H NMR (400MHz) spectrum of compound 7h in Acetone-$d_6$
$^{13}$C NMR (100MHz) spectrum of compound $7h$ in Acetone-$d_6$
ESI$^+$ Mass spectrum of compound 7h
High resolution mass (ESI\(^+\)) spectrum of compound 7h
$^1$H NMR (400MHz) spectrum of compound 7i in Acetone-$d_6$
$^{13}$C NMR (100MHz) spectrum of compound 7i in Acetone-$d_6$
ESI+ Mass spectrum of compound 7i
HRMS Mass spectrum of compound 7i
H NMR (400MHz) spectrum of compound 7j in Acetone-$d_6$
$^{13}$C NMR (100MHz) spectrum of compound 7j in Acetone-$d_6$
ESI$^+$ Mass spectrum of compound 7j
HRMS Mass spectrum of compound 7j
$^1$H NMR spectrum (400 MHz) of compound 8a in CDCl$_3$
$^{13}$C spectrum (100 MHz) of compound 8a in CDCl$_3$
ESI Mass spectrum of compound 8a

H-19
20140509015 19 (0.668) Cn (Cen,2, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,40.00 ); Cm (19:20-2:15x3.000) Scan ES+ 7.88e7
Chemical Formula: $C_{13}H_9NS$

Exact Mass: 211.0456

m/z: 211.0456 (100.0%), 212.0489 (14.1%), 213.0414 (4.5%)

HRMS Mass spectrum of compound 8a
IR spectrum of compound 8a
$^1$H NMR spectrum (400 MHz) of compound 8b in CDCl$_3$
$^{13}$C spectrum (75 MHz) of compound 8b in CDCl$_3$
Chemical Formula: C_{14}H_{8}F_{3}NS
Exact Mass: 279.0330
m/z: 279.0330 (100.0%), 280.0363 (15.1%),
281.0288 (4.5%), 281.0397 (1.1%)

ESI Mass spectrum of compound 8b
HRMS Mass spectrum of compound 8b

Chemical Formula: C_{14}H_{9}F_{3}NS
Exact Mass: 279.0330
m/z: 279.0330 (100.0%), 280.0363 (15.1%), 281.0288 (4.5%), 281.0397 (1.1%)

8b
IR spectrum of compound 8b
$^{1}$H NMR spectrum (400 MHz) of compound 8c in CDCl$_3$
$^{13}$C spectrum (100 MHz) of compound 8c in CDCl$_3$
Chemical Formula: C_{14}H_{11}NS
Exact Mass: 225.0612
m/z: 225.0612 (100.0%), 226.0646 (15.1%), 227.0570 (4.5%), 227.0679 (1.1%)

ESI Mass spectrum of compound 8c
HRMS Mass spectrum of compound 8c

Chemical Formula: C$_{14}$H$_{11}$NS

Exact Mass: 225.0612

m/z: 225.0612 (100.0%), 226.0646 (15.1%), 227.0570 (4.5%), 227.0679 (1.1%)
IR spectrum of compound **8c**
$^1$H NMR spectrum (400 MHz) of compound 8d in CDCl$_3$
$^{13}$C spectrum (100 MHz) of compound 8d in CDCl$_3$
Chemical Formula: C$_{14}$H$_{11}$NS
Exact Mass: 225.0612
m/z: 225.0612 (100.0%), 226.0646 (15.1%),
227.0570 (4.5%), 227.0679 (1.1%)

ESI Mass spectrum of compound 8d
HRMS Mass spectrum of compound 8d
IR spectrum of compound 8d
\textsuperscript{1}H NMR spectrum (400 MHz) of compound 8e in CDCl\textsubscript{3}
$^{13}$C spectrum (100 MHz) of compound 8e in CDCl$_3$
Chemical Formula: C_{14}H_{11}NS
Exact Mass: 225.0612
m/z: 225.0612 (100.0%), 226.0646 (15.1%), 227.0570 (4.5%), 227.0679 (1.1%)
HRMS Mass spectrum of compound 8e
IR spectrum of compound 8e
$^1$H NMR spectrum (400 MHz) of compound 8f in CDCl$_3$
$^{13}$C spectrum (100 MHz) of compound 8f in CDCl$_3$
Chemical Formula: $C_{14}H_{11}NO_S$

Exact Mass: 241.0561

m/z: 241.0561 (100.0%), 242.0595 (15.1%), 243.0519 (4.5%), 243.0628 (1.1%)
HRMS Mass spectrum of compound 8f

Chemical Formula: C_{14}H_{11}NO

Exact Mass: 241.0561

m/z: 241.0561 (100.0%), 242.0595 (15.1%), 243.0519 (4.5%), 243.0628 (1.1%)
IR spectrum of compound 8f
$^1$H NMR spectrum (400 MHz) of compound $8g$ in CDCl$_3$
$\begin{array}{c}
\text{13C spectrum (100 MHz) of compound 8g in CDCl$_3$}
\end{array}$

S140
Chemical Formula: C_{11}H_{7}NS_{2}

Exact Mass: 217.0020

m/z; 217.0020 (100.0%), 218.0053 (11.9%), 218.9978 (9.0%), 218.0014 (1.6%), 220.0011 (1.1%)

ESI Mass spectrum of compound 8g
HRMS Mass spectrum of compound 8g

Chemical Formula: C_{11}H_{17}NS_{2}
Exact Mass: 217.0020
m/z: 217.0020 (100.0%), 218.0053 (11.9%), 218.9978 (9.0%), 218.0014 (1.6%), 220.0011 (1.1%)
IR spectrum of compound 8g
\(^1\text{H NMR (400MHz) spectrum of compound 11a in acetone-}\text{d}_6\)
$^{13}$C NMR (100MHz) spectrum of compound 11a in DMSO-$d_6$
ESI$^+$ Mass spectrum of compound 11a
High resolution mass (ESI$^+$) spectrum of compound 11a
$^1$H NMR (400MHz) spectrum of compound 11b in DMSO-$d_6$
$^{13}$C NMR (100MHz) spectrum of compound 11b in DMSO-$d_6$
ESI$^+$ Mass spectrum of compound 11b
High resolution mass (ESI+) spectrum of compound 11b
$^1$H NMR (400MHz) spectrum of compound 11c in CDCl$_3$
$^{13}$C NMR (100MHz) spectrum of compound 11c in CDCl$_3$
ESI$^+$ Mass spectrum of compound 11c
High resolution mass (ESI\(^+\)) spectrum of compound \textbf{11c}
$^1$H NMR (400MHz) spectrum of compound 11d in CDCl$_3$
$^{13}$C NMR (100MHz) spectrum of compound 11d in CDCl$_3$
ESI^+ Mass spectrum of compound 11d
High resolution mass (ESI+) spectrum of compound 11d
$^{1}$H NMR (400MHz) spectrum of compound 11e in CDCl$_3$
$^{13}$C NMR (100MHz) spectrum of compound 11e in CDCl$_3$
Scan ES+ 4.73e7

ESI+ Mass spectrum of compound 11e
High resolution mass (ESI⁺) spectrum of compound 11e
$^1$H NMR (400MHz) spectrum of compound 11f in CDCl$_3$
$^{13}$C NMR (100MHz) spectrum of compound 11f in CDCl$_3$
ESI\(^+\) Mass spectrum of compound 11f
High resolution mass (ESI⁺) spectrum of compound 11f
$^1$H NMR (400MHz) spectrum of compound 11g in CDCl$_3$
$^{13}$C NMR (100MHz) spectrum of compound 11g in CDCl$_3$
ESI+ Mass spectrum of compound 11g
High resolution mass (ESI⁺) spectrum of compound **11g**
$\text{H NMR (400MHz) spectrum of compound 11h in DMSO-$d_6$}$
$^{13}$C NMR (100 MHz) spectrum of compound 11h in DMSO-$d_6$
ESI$^+$ Mass spectrum of compound 11h
High resolution mass (ESI$^+$) spectrum of compound 11h
$^1$H NMR (400MHz) spectrum of compound 11i in CDCl$_3$
$^{13}$C NMR (100MHz) spectrum of compound 11i in CDCl$_3$/DMSO-$d_6$ (10:1)
ESI$^+$ Mass spectrum of compound 11i
High resolution mass (ESI⁺) spectrum of compound **11i**
\(^1\text{H NMR (400MHz) spectrum of compound 11j in CDCl}_3\)
$^{13}$C NMR (100MHz) spectrum of compound 11j in CDCl$_3$/DMSO-$d_6$ (10:1)
ESI$^+$ Mass spectrum of compound **11j**
High resolution mass (ESI+) spectrum of compound 11j
$^1$H NMR (400MHz) spectrum of compound 11k in CDCl$_3$
$^{13}$C NMR (100MHz) spectrum of compound 11k in CDCl$_3$
ESI$^+$/Mass spectrum of compound 11k

2P65
201601220022 15 (1.027) Cn (Cen,3, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,50.00); Cm (14:18-4:11)

Scan ES+ 3.09e6
HRMS spectrum of compound 11k
$^1$H NMR (400MHz) spectrum of compound 11l in CDCl$_3$
$^{13}$C NMR (100MHz) spectrum of compound 11l in CDCl$_3$/DMSO-$d_6$ (10:3)
ESI$^+$ Mass spectrum of compound 111
High resolution mass (ESI\(^+\)) spectrum of compound 111
$^1$H NMR (400MHz) spectrum of compound 11m in CDCl$_3$
$^{13}$C NMR (100 MHz) spectrum of compound 11m in DMSO-$d_6$
Mass spectrum of compound 11m

ESI+ Mass spectrum of compound 11m
HRMS spectrum of compound 11m
$^{1}$H NMR (400MHz) spectrum of compound 11n in CDCl$_3$
$^{13}$C NMR (100MHz) spectrum of compound 11n in CDCl$_3$
ESI$^+$ Mass spectrum of compound 11n
High resolution mass (ESI+) spectrum of compound 11n
$^1$H NMR (400MHz) spectrum of compound 11o in CDCl$_3$
$^{13}$C NMR (100MHz) spectrum of compound 11o in DMSO-$d_6$
ESI$^+$ Mass spectrum of compound 11o
HRMS spectrum of compound 11o