Iron-catalyzed oxidative synthesis of N-heterocycles from primary alcohols

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General information

All manipulations were carried out under air atmosphere unless otherwise specified. Melting points were measured with an X-4 melting point apparatus (Bei Jing Taike Co., Ltd.) and were uncorrected. $^1$H-NMR and $^{13}$C-NMR were determined in CDCl$_3$ or DMSO-$d_6$ on a Bruker DPX 300 MHz or a Bruker AVANCE III 400 MHz spectrometer at room temperature, respectively, and tetramethylsilane (TMS) served as an internal standard. Spin multiplicities are given as s (singlet), d (doublet), t (triplet), q (quartet) and m (multiplet) as well as brs (broad). Coupling constants ($J$) are given in hertz (Hz). ESI-MS was carried out on a LCMS-2020 (Shimadzu, Japan). HRMS were recorded on a LTQ-Orbitrap XL (Thermofisher, U.S.A.). All experiments were monitored by thin layer chromatography (TLC). TLC was performed on pre-coated silica gel plates (Qingdao Haiyang Chemical Co., Ltd).

Experimental section

**General procedure for the synthesis of quinazolin-4(3H)-ones 3a–k:**

A mixture of benzyl alcohol 1 (1.5 mmol), $o$-aminobenzamide 2 (0.5 mmol), 0.01 mmol FeCl$_3$ (0.1 M in DMSO, 100 μL) and 1.5 mmol TBHP (5.5 M in decane, 270 μL) in 2 mL DMSO was stirred in a Schlenk tube at 60 °C. After stirring for 7 h, the reaction mixture was cooled to the room temperature, and diluted with ethyl acetate, washed with brine, dried over anhydrous Na$_2$SO$_4$ and concentrated in vacuo. The residue was then purified by chromatography on silica gel with a eluent of petroleum ether and ethyl acetate. Products were characterized by Mp, $^1$H-, $^{13}$C-NMR and MS (ESI).

**General procedure for the synthesis of quinazolines 5a–j:**

A mixture of benzyl alcohol 1 (1.5 mmol), 0.01 mmol FeCl$_3$ (0.1 M in DMSO, 100 μL) and 1.5 mmol TBHP (5.5 M in decane, 270 μL) in 1 mL DMSO was stirred in a Schlenk tube at 60 °C under N$_2$. $O$-aminobenzylamine 4 (0.5 mmol) in 1mL DMSO was slowly added by syringe pump over 3h at 60 °C. After stirring for 6 h, the reaction mixture was cooled to the room temperature, and diluted with ethyl acetate, washed with brine, dried over anhydrous Na$_2$SO$_4$ and concentrated in vacuo. The residue was then purified by chromatography on silica gel with a eluent of petroleum ether and ethyl acetate. Products were characterized by Mp, $^1$H-, $^{13}$C-NMR and MS (ESI).

**General procedure for the synthesis of 3,4-dihydro-2H-1,2,4-benzothiadiazine 1,1-dioxides 7a–k:**

A mixture of benzyl alcohol 1 (1.5 mmol), $o$-aminobenzenesulfonamide 6 (0.5 mmol), 0.01 mmol FeCl$_3$ (0.1 M in DMSO, 100 μL) and 1.5 mmol TBHP (5.5 M in decane, 270 μL) in 2 mL DMSO was stirred in a Schlenk tube at 60 °C. After stirring for 12 h, the reaction mixture was cooled to the room temperature, and diluted with ethyl acetate, washed with brine, dried over anhydrous Na$_2$SO$_4$ and concentrated in vacuo. The residue was then purified by chromatography on silica gel with a eluent of dichloromethane and ethyl acetate. Products were characterized by Mp, $^1$H-, $^{13}$C-NMR and MS (ESI).
Product characterizations

2-phenylquinazolin-4(3H)-one (3a). white solid, 93% yield, mp. 235 – 237 °C. $^1$H NMR (300 MHz, DMSO-$d_6$) δ 12.53 (brs, 1H), 8.16 (t, $J = 7.7$ Hz, 3H), 7.83 (t, $J = 7.1$ Hz, 1H), 7.73 (d, $J = 8.0$ Hz, 1H), 7.65 – 7.41 (m, 4H); $^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 162.2, 152.3, 148.7, 134.6, 132.7, 131.4, 128.6, 127.7, 127.5, 126.5, 125.8, 121.0; MS (ESI): 223.00 [M+H]$^+$.  

2-(o-tolyl)quinazolin-4(3H)-one (3b). white solid, 57% yield, mp. 216 – 218 °C. $^1$H NMR (300 MHz, DMSO-$d_6$) δ 12.43 (brs, 1H), 8.16 (d, $J = 7.9$ Hz, 1H), 7.87 – 7.76 (m, 1H), 7.67 (d, $J = 8.0$ Hz, 1H), 7.59 – 7.46 (m, 2H), 7.45 – 7.37 (m, 1H), 2.37 (s, 3H); $^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 161.7, 154.3, 148.7, 136.1, 134.4, 134.2, 130.5, 129.9, 129.1, 127.3, 126.6, 125.8, 125.7, 121.0, 19.5; MS (ESI): 236.95 [M+H]$^+$.  

2-(p-tolyl)quinazolin-4(3H)-one (3c). white solid, 66% yield, mp. 241 – 243 °C. $^1$H NMR (300 MHz, DMSO-$d_6$) δ 12.44 (brs, 1H), 8.13 (dd, $J = 7.9$, 1.0 Hz, 1H), 8.08 (d, $J = 8.2$ Hz, 2H), 7.70 (d, $J = 7.8$ Hz, 1H), 7.53 – 7.41 (m, 1H), 7.33 (d, $J = 8.1$ Hz, 2H), 2.37 (s, 3H); $^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 162.3, 154.3, 148.7, 136.1, 134.4, 134.5, 129.9, 129.1, 127.6, 127.4, 126.3, 125.8, 120.9, 20.9; MS (ESI): 237.00 [M+H]$^+$.  

2-(4-methoxyphenyl)quinazolin-4(3H)-one (3d). white solid, 37% yield, mp. 248 – 251 °C. $^1$H NMR (300 MHz, DMSO-$d_6$) δ 12.39 (brs, 1H), 8.18 (d, $J = 8.9$ Hz, 2H), 8.12 (dd, $J = 7.9$, 1.1 Hz, 1H), 7.86 – 7.75 (m, 1H), 7.69 (d, $J = 7.7$ Hz, 1H), 7.52 – 7.41 (m, 1H), 7.07 (d, $J = 8.9$ Hz, 2H), 3.83 (s, 3H); $^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 162.3, 161.8, 151.8, 148.9, 134.5, 129.4, 127.3, 126.1, 125.8, 124.8, 120.7, 114.0, 55.4; MS (ESI): 253.00 [M+H]$^+$.  

2-(4-methoxyphenyl)quinazolin-4(3H)-one (3e).
2-(4-fluorophenyl)quinazolin-4(3H)-one (3e). white solid, 40% yield, mp. 284 – 287 °C. \(^1\)H NMR (300 MHz, DMSO-\(d_6\)) \(\delta\) 12.56 (brs, 1H), 8.30 – 8.19 (m, 2H), 8.14 (dd, \(J = 7.9\, \text{Hz},\, 1\text{H})\), 7.87 – 7.78 (m, 1H), 7.72 (d, \(J = 7.7\, \text{Hz},\, 1\text{H})\), 7.56 – 7.45 (m, 1H), 7.38 (t, \(J = 8.9\, \text{Hz},\, 2\text{H})\); \(^1\)C NMR (100 MHz, DMSO-\(d_6\)) \(\delta\) 164.0 (d, \(J_{C_4'-F} = 249.5\, \text{Hz}\, ,\, C_4')\), 162.2, 151.4, 148.6, 134.6, 130.3 (d, \(J_{C_2'-F} = 9.0\, \text{Hz}\, ,\, C_2')\), 129.2 (d, \(J_{C_1'-F} = 2.9\, \text{Hz}\, ,\, C_1')\), 127.4, 126.6, 125.8, 120.9, 115.6 (d, \(J_{C_3'-F} = 21.9\, \text{Hz}\, ,\, C_3')\); MS (ESI): 240.95 [M+H]+.

2-(4-chlorophenyl)quinazolin-4(3H)-one (3f). white solid, 45% yield, mp. 298 – 300 °C. \(^1\)H NMR (300 MHz, DMSO-\(d_6\)) \(\delta\) 12.58 (brs, 1H), 8.28 – 8.08 (m, 3H), 7.83 (t, \(J = 7.4\, \text{Hz},\, 1\text{H})\), 7.73 (d, \(J = 7.7\, \text{Hz},\, 1\text{H})\), 7.61 (d, \(J = 8.2\, \text{Hz},\, 2\text{H})\), 7.52 (t, \(J = 7.3\, \text{Hz},\, 1\text{H})\); \(^1\)C NMR (100 MHz, DMSO-\(d_6\)) \(\delta\) 162.2, 151.4, 148.5, 136.3, 134.6, 131.6, 129.6, 128.7, 127.4, 126.7, 125.9, 121.0; MS (ESI): 256.95 [M+H]+.

2-(2-bromophenyl)quinazolin-4(3H)-one (3g). white solid, 84% yield, mp. 165 – 167 °C. \(^1\)H NMR (300 MHz, DMSO-\(d_6\)) \(\delta\) 12.61 (brs, 1H), 8.17 (dd, \(J = 7.9\, \text{Hz},\, 1\text{H})\), 7.84 (dd, \(J = 8.5\, \text{Hz},\, 1\text{H})\), 7.76 (dd, \(J = 7.8\, \text{Hz},\, 1\text{H})\), 7.70 (d, \(J = 7.7\, \text{Hz},\, 1\text{H})\), 7.64 (dd, \(J = 7.4\, \text{Hz},\, 1\text{H})\), 7.59 – 7.41 (m, 3H); \(^1\)C NMR (100 MHz, DMSO-\(d_6\)) \(\delta\) 161.4, 153.3, 148.5, 136.3, 131.6, 129.6, 128.7, 127.4, 126.7, 125.9, 121.0; MS (ESI): 300.85 [M+H]+.

2-(2-iodophenyl)quinazolin-4(3H)-one (3h). yellow solid, 67% yield, mp. 217 – 219 °C. \(^1\)H NMR (300 MHz, DMSO-\(d_6\)) \(\delta\) 12.55 (brs, 1H), 8.21 – 8.07 (m, 1H), 7.97 (d, \(J = 8.0\, \text{Hz},\, 1\text{H})\), 7.89 – 7.78 (m, 1H), 7.69 (d, \(J = 8.0\, \text{Hz},\, 1\text{H})\), 7.61 – 7.47 (m, 3H), 7.27 (td, \(J = 7.5\, \text{Hz},\, 1\text{H})\); \(^1\)C NMR (100 MHz, DMSO-\(d_6\)) \(\delta\) 161.5, 155.2, 148.5, 139.6, 138.8, 134.5, 131.4, 129.8, 128.1, 127.4, 126.9, 125.8, 121.2, 96.4; MS (ESI): 348.85 [M+H]+; HRMS (ESI) m/z calcld for C\(_{14}\)H\(_{10}\)IN\(_2\)O [M+H]+ 348.9832, found 348.9833.

2-(furan-2-yl)quinazolin-4(3H)-one (3i). yellow solid, 76% yield, mp. 218 – 221 °C. \(^1\)H NMR (300 MHz, DMSO-\(d_6\)) \(\delta\) 12.48 (brs, 1H), 8.11 (d, \(J = 7.5\, \text{Hz},\, 1\text{H})\), 7.99 (s, 1H), 7.80 (t, \(J = 7.1\, \text{Hz},\, 1\text{H})\), 7.67 (d, \(J = 8.0\, \text{Hz},\, 1\text{H})\), 7.62 (d, \(J = 3.5\, \text{Hz},\, 1\text{H})\), 7.48 (t, \(J = 7.5\, \text{Hz},\, 1\text{H})\), 6.74 (dd, \(J = 3.4\, \text{Hz},\, 1\text{H})\);
$^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 161.5, 148.6, 146.5, 146.1, 144.0, 134.6, 127.2, 126.4, 125.9, 121.1, 114.5, 112.5; MS (ESI): 212.95 [M+H]$^+$. 

2-methylquinazolin-4(3H)-one (3j$^\dagger$). white solid, 42% yield, mp. 237 – 239 °C. $^1$H NMR (300 MHz, DMSO-$d_6$) δ 12.17 (brs, 1H), 8.05 (dd, $J = 7.9$, 1.0 Hz, 1H), 7.81 – 7.68 (m, 1H), 7.55 (d, $J = 8.1$ Hz, 1H), 7.43 (t, $J = 7.5$ Hz, 1H), 2.33 (s, 3H); $^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 161.7, 154.2, 148.9, 134.2, 126.5, 125.8, 125.6, 120.6, 21.4; MS (ESI): 161.05 [M+H]$^+$. 

2-heptylquinazolin-4(3H)-one (3k$^\dagger$). white solid, 60% yield, mp. 133 – 135 °C. $^1$H NMR (300 MHz, DMSO-$d_6$) δ 12.14 (brs, 1H), 8.11 – 8.00 (m, 1H), 7.80 – 7.67 (m, 1H), 7.57 (d, $J = 8.0$ Hz, 1H), 7.43 (t, $J = 7.5$ Hz, 1H), 2.66 – 2.52 (m, 2H), 1.81 – 1.63 (m, 2H), 1.34 – 1.11 (m, 8H), 0.83 (t, $J = 6.6$ Hz, 3H); $^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 161.8, 157.5, 148.9, 134.2, 126.7, 125.8, 125.6, 120.8, 34.5, 31.1, 28.4, 28.3, 26.7, 22.0, 13.9; MS (ESI): 245.05 [M+H]$^+$. 

2-phenylquinazoline (5a$^\ddagger$). white solid, 70% yield, mp. 94 – 95 °C. $^1$H NMR (300 MHz, CDCl$_3$) δ 9.47 (s, 1H), 8.71 – 8.54 (m, 2H), 8.16 – 8.04 (m, 1H), 7.97 – 7.86 (m, 2H), 7.66 – 7.58 (m, 1H), 7.58 – 7.46 (m, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 161.1, 160.5, 150.8, 138.1, 134.1, 130.6, 128.7, 128.6, 127.3, 127.1, 123.6; MS (ESI): 207.10 [M+H]$^+$. 

2-(o-tolyl)quinazoline (5b$^\ddagger$). yellow solid, 60% yield, mp. 36 – 37 °C. $^1$H NMR (300 MHz, CDCl$_3$) δ 9.50 (s, 1H), 8.10 (d, $J = 8.5$ Hz, 1H), 8.01 – 7.86 (m, 3H), 7.75 – 7.56 (m, 1H), 7.44 – 7.29 (m, 3H), 2.62 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 164.0, 160.1, 150.4, 138.6, 137.4, 134.1, 131.3, 130.7, 129.3, 128.6, 127.5, 127.1, 126.0, 122.9, 21.1; MS (ESI): 221.10 [M+H]$^+$. 

2-(p-tolyl)quinazoline (5c$^\ddagger$). yellow solid, 71% yield, mp. 103 – 104 °C. $^1$H NMR (300 MHz, CDCl$_3$) δ 9.45 (s, 1H), 8.52 (d, $J = 8.2$ Hz, 2H), 8.07 (d, $J = 8.5$ Hz, 1H), 7.89 (t, $J = 7.9$ Hz, 2H), 7.59 (t, $J = 7.5$ Hz, 1H), 7.35 (d, $J = 8.2$ Hz, 2H), 2.45 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 161.2, 160.4, 150.8,
2-(4-methoxyphenyl)quinazoline (5d). yellow solid, 71% yield, mp. 86 – 87 °C. $^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 9.42 (s, 1H), 8.75 – 8.45 (m, 2H), 8.05 (d, $J = 8.9$ Hz, 1H), 7.93 – 7.83 (m, 2H), 7.65 – 7.44 (m, 1H), 7.13 – 6.88 (m, 2H), 3.90 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 161.9, 160.9, 160.4, 150.9, 134.0, 130.8, 130.23, 128.4, 127.1, 126.8, 123.3, 114.0, 55.4; MS (ESI): 221.10 [M+H]$^\ddagger$.

2-(4-fluorophenyl)quinazoline (5e). yellow solid, 55% yield, mp. 121 – 123 °C. $^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 9.45 (s, 1H), 8.63 (dd, $J = 8.1$, 5.9 Hz, 2H), 8.07 (d, $J = 8.5$ Hz, 1H), 7.91 (t, $J = 7.9$ Hz, 2H), 7.62 (t, $J = 7.5$ Hz, 1H), 7.21 (t, $J = 8.6$ Hz, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 164.7 (d, $J_{C4'-F} = 250.4$ Hz, C4'), 160.5, 160.1, 150.7, 134.2 (d, $J_{C1'-F} = 2.9$ Hz, Cl'), 134.2, 130.7 (d, $J_{C2'-F} = 8.7$ Hz, C2'), 128.6, 127.3, 127.1, 123.5, 115.6 (d, $J_{C3'-F} = 21.6$ Hz, C3'); MS (ESI): 225.05 [M+H]$^\ddagger$.

2-(4-chlorophenyl)quinazoline (5f). white solid, 62% yield, mp. 123 – 124 °C. $^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 9.45 (s, 1H), 8.58 (d, $J = 8.6$ Hz, 2H), 8.08 (d, $J = 8.3$ Hz, 1H), 7.92 (t, $J = 7.7$ Hz, 2H), 7.63 (t, $J = 7.5$ Hz, 1H), 7.50 (d, $J = 8.6$ Hz, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 160.5, 160.0, 150.7, 136.8, 136.5, 134.2, 129.9, 128.8, 128.6, 127.4, 127.1, 123.6; MS (ESI): 241.05 [M+H]$^\ddagger$.

2-(naphthalen-1-yl)quinazoline (5g). yellow solid, 65% yield, mp. 115 – 117 °C. $^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 9.61 (s, 1H), 8.76 – 8.65 (m, 1H), 8.25 – 8.14 (m, 2H), 8.08 – 7.89 (m, 4H), 7.64 (dd, $J = 8.1$, 7.3 Hz, 1H), 7.60 – 7.49 (m, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 163.5, 160.4, 150.6, 136.3, 134.3, 134.2, 131.2, 130.4, 129.6, 128.7, 128.5, 127.7, 127.1, 126.9, 125.92, 125.89, 125.3, 123.1; MS (ESI): 257.05 [M+H]$^\ddagger$.

2-(pyridin-3-yl)quinazoline (5h). yellow solid, 35% yield, mp. 93 – 95 °C. $^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 9.81 (s, 1H), 9.46 (s, 1H), 8.86 (d, $J = 8.0$ Hz, 1H), 8.73 (d, $J = 4.6$ Hz, 1H), 8.09 (d, $J = 8.3$ Hz, 1H), 7.92 (t, $J = 7.7$ Hz, 2H), 7.64 (t, $J = 7.5$ Hz, 1H), 7.45 (dd, $J = 8.0$, 4.8 Hz, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 160.7, 159.2, 151.2, 150.6, 150.2, 135.8, 134.4, 133.6, 128.7, 127.8, 127.2, 123.8, 123.4; MS (ESI): 208.00 [M+H]$^\ddagger$.
2-(furan-2-yl)quinazoline (5i). yellow solid, 44% yield, mp. 130 – 133 °C. $^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 9.37 (s, 1H), 8.09 (d, $J = 9.0$ Hz, 1H), 8.01 – 7.83 (m, 2H), 7.69 (d, $J = 0.8$ Hz, 1H), 7.64 – 7.54 (m, 1H), 7.52 – 7.40 (m, 1H), 6.61 (dd, $J = 3.4$, 1.7 Hz, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 160.7, 154.1, 152.6, 150.5, 145.4, 134.5, 128.4, 127.3, 123.4, 114.1, 112.3; MS (ESI): 197.05 [M+H]$^+$. 

2-methylquinazoline (5j). yellow oil, 53% yield. $^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 9.29 (s, 1H), 7.92 (d, $J = 8.8$ Hz, 1H), 7.88 – 7.80 (m, 2H), 7.60 – 7.48 (m, 1H), 2.87 (s, 3 H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 164.5, 160.4, 150.4, 134.1, 127.7, 127.1, 127.0, 122.9, 26.4; MS (ESI): 145.00 [M+H]$^+$. 

3-phenyl-3,4-dihydro-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide (7a). white solid, 75% yield, mp. 129 – 132 °C. $^1$H NMR (300 MHz, DMSO-$d_6$) $\delta$ 7.87 (d, $J = 12.0$ Hz, 1H), 7.70 – 7.62 (m, 2H), 7.59 – 7.23 (m, 6H), 6.91 (d, $J = 8.3$ Hz, 1H), 6.76 (t, $J = 7.5$ Hz, 1H), 5.77 (d, $J = 12.1$ Hz, 1H); $^{13}$C NMR (100 MHz, DMSO-$d_6$) $\delta$ 143.9, 137.3, 132.8, 129.1, 128.5, 127.5, 123.7, 121.6, 116.7, 116.4, 68.4; MS (ESI): 261.05 [M+H]$^+$. 

3-(o-tolyl)-3,4-dihydro-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide (7b). white solid, 57% yield, mp. 179 – 181 °C. $^1$H NMR (300 MHz, DMSO-$d_6$) $\delta$ 7.78 (d, $J = 12.0$ Hz, 1H), 7.70 – 7.62 (m, 2H), 7.51 (d, $J = 7.9$ Hz, 1H), 7.44 – 7.15 (m, 5H), 6.93 (d, $J = 8.3$ Hz, 1H), 6.76 (t, $J = 7.5$ Hz, 1H), 5.95 (d, $J = 12.0$ Hz, 1H), 2.38 (s, 3 H); $^{13}$C NMR (100 MHz, DMSO-$d_6$) $\delta$ 144.2, 135.8, 135.1, 132.7, 130.3, 128.8, 126.6, 123.8, 121.7, 116.7, 116.5, 64.8, 18.4; MS (ESI): 274.95 [M+H]$^+$. HRMS (ESI) m/z calcd for C$_{14}$H$_{15}$N$_2$O$_2$S [M+H]$^+$ 275.0849, found 275.0853. 

3-(p-tolyl)-3,4-dihydro-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide (7c). white solid, 83% yield, mp. 150 – 153 °C. $^1$H NMR (300 MHz, DMSO-$d_6$) $\delta$ 7.81 (d, $J = 12.1$ Hz, 1H), 7.52 (t, $J = 7.3$ Hz, 3H), 7.38 – 7.20 (m, 4H), 6.89 (d, $J = 8.2$ Hz, 1H), 6.75 (t, $J = 7.5$ Hz, 1H), 5.72 (d, $J = 12.1$ Hz, 1H), 2.33
3-(4-methoxyphenyl)-3,4-dihydro-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide (7d). White solid, 58% yield, mp. 161 – 163 °C. 1H NMR (300 MHz, DMSO-d$_6$) $\delta$ 7.78 (d, $J = 12.1$ Hz, 1H), 7.57 (d, $J = 8.7$ Hz, 2H), 7.53 – 7.45 (m, 1H), 7.35 – 7.22 (m, 2H), 6.99 (d, $J = 8.7$ Hz, 2H), 6.88 (d, $J = 8.2$ Hz, 1H), 6.74 (t, $J = 7.3$ Hz, 1H), 5.71 (d, $J = 12.0$ Hz, 1H), 3.77 (s, 3H) ; 13C NMR (100 MHz, DMSO-d$_6$) $\delta$ 159.8, 143.9, 132.8, 129.5, 128.9, 123.7, 121.5, 116.6, 116.3, 113.8, 68.0, 55.2; MS (ESI): 290.95 [M+H]$^+$. 

3-(4-fluorophenyl)-3,4-dihydro-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide (7e). White solid, 39% yield, mp. 184 – 186 °C. 1H NMR (300 MHz, DMSO-d$_6$) $\delta$ 7.89 (d, $J = 12.0$ Hz, 1H), 7.71 (dd, $J = 8.6$, 5.6 Hz, 2H), 7.52 (d, $J = 7.4$ Hz, 1H), 7.45 – 7.16 (m, 4H), 6.89 (d, $J = 8.3$ Hz, 1H), 6.76 (t, $J = 7.5$ Hz, 1H), 5.79 (d, $J = 12.1$ Hz, 1H), 13C NMR (100 MHz, DMSO-d$_6$) $\delta$ 162.4 (d, $J_{C4'-F} = 245.2$ Hz, C4'), 143.8, 133.7 (d, $J_{C1'-F} = 3.0$ Hz, C1'), 132.9, 129.8 (d, $J_{C2'-F} = 8.5$ Hz, C2'), 123.7, 121.6, 116.8, 116.3, 115.3 (d, $J_{C3'-F} = 21.6$ Hz, C3'), 67.6; MS (ESI): 278.95 [M+H]$^+$. 

3-(4-chlorophenyl)-3,4-dihydro-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide (7f). White solid, 47% yield, mp. 199 – 210 °C. 1H NMR (300 MHz, DMSO-d$_6$) $\delta$ 7.92 (d, $J = 12.0$ Hz, 1H), 7.68 (d, $J = 8.5$ Hz, 2H), 7.59 – 7.45 (m, 3H), 7.38 (s, 1H), 7.35 – 7.25 (m, 1H), 6.89 (d, $J = 8.0$ Hz, 1H), 6.76 (t, $J = 7.2$ Hz, 1H), 5.80 (d, $J = 12.0$ Hz, 1H), 13C NMR (100 MHz, DMSO-d$_6$) $\delta$ 143.8, 136.2, 133.7, 132.9, 129.5, 128.5, 123.7, 121.7, 116.9, 116.4, 67.6; MS (ESI): 294.90 [M+H]$^+$. 

3-(2-bromophenyl)-3,4-dihydro-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide (7g). White solid, 51% yield, mp. 183 – 186 °C. 1H NMR (300 MHz, DMSO-d$_6$) $\delta$ 7.96 (d, $J = 12.0$ Hz, 1H), 7.87 (d, $J = 7.7$ Hz, 1H), 7.72 (d, $J = 7.9$ Hz, 1H), 7.52 (t, $J = 8.1$ Hz, 2H), 7.46 – 7.23 (m, 3H), 6.89 (d, $J = 8.3$ Hz, 1H), 6.78 (t, $J = 7.5$ Hz, 1H), 6.14 (d, $J = 12.0$ Hz, 1H), 13C NMR (100 MHz, DMSO-d$_6$) $\delta$ 143.8, 135.9, 132.9, 132.8, 131.1, 129.4, 128.1, 123.8, 122.8, 121.8, 117.0, 116.4, 67.4; MS (ESI): 338.85 [M+H]$^+$.
3-(2-iodophenyl)-3,4-dihydro-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide \((7h)\). white solid, 52% yield, mp. 209 – 211 °C. \(^1\)H NMR (300 MHz, DMSO-\(\text{d}_6\)) \(\delta\ 7.95 (d, J = 7.8 \text{ Hz}, 1H), 7.89 (d, J = 12.0 \text{ Hz}, 1H), 7.81 (d, J = 7.0 \text{ Hz}, 1H), 7.51 (t, J = 8.0 \text{ Hz}, 2H), 7.42 (s, 1H), 7.32 (t, J = 7.8 \text{ Hz}, 1H), 7.19 (t, J = 7.1 \text{ Hz}, 1H), 6.89 (d, J = 8.3 \text{ Hz}, 1H), 6.78 (t, J = 7.5 \text{ Hz}, 1H), 6.00 (d, J = 11.9 \text{ Hz}, 1H); \(^{13}\)C NMR (100 MHz, DMSO-\(\text{d}_6\)) \(\delta\ 143.8, 139.4, 138.9, 132.9, 131.2, 128.9, 128.6, 123.8, 121.8, 116.9, 116.4, 99.8, 72.4; MS (ESI): 386.80 \([\text{M+H}]^+\); HRMS (ESI) m/z calcd for \(\text{C}_{13}\text{H}_{12}\text{IN}_2\text{O}_2\text{S} \ [\text{M+H}]^+\) 386.9659, found 386.9649.

3-(naphthalen-1-yl)-3,4-dihydro-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide \((7i)\). white solid, 44% yield, mp. 208 – 210 °C. \(^1\)H NMR (300 MHz, DMSO-\(\text{d}_6\)) \(\delta\ 8.16 (d, J = 8.3 \text{ Hz}, 1H), 8.10 – 7.97 (m, 3H), 7.95 (d, J = 7.2 \text{ Hz}, 1H), 7.70 – 7.48 (m, 5H), 7.39 – 7.30 (m, 1H), 7.01 (d, J = 8.3 \text{ Hz}, 1H), 6.80 (t, J = 7.4 \text{ Hz}, 1H), 6.57 (d, J = 11.9 \text{ Hz}, 1H); \(^{13}\)C NMR (100 MHz, DMSO-\(\text{d}_6\)) \(\delta\ 144.2, 133.3, 132.9, 132.2, 130.0, 129.5, 128.7, 126.9, 126.1, 125.2, 124.7, 123.8, 121.8, 116.9, 116.8, 64.4; MS (ESI): 311.00 \([\text{M+H}]^+\); HRMS (ESI) m/z calcd for \(\text{C}_{17}\text{H}_{15}\text{N}_2\text{O}_2\text{S} \ [\text{M+H}]^+\) 311.0849, found 311.0843.

3-methyl-3,4-dihydro-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide \((7j)\). white solid, 24% yield, mp. 211 – 213 °C. \(^1\)H NMR (300 MHz, DMSO-\(\text{d}_6\)) \(\delta\ 7.43 (d, J = 9.1 \text{ Hz}, 2H), 7.32 – 7.20 (m, 1H), 7.08 (s, 1H), 6.75 (d, J = 8.3 \text{ Hz}, 1H), 6.68 (t, J = 7.5 \text{ Hz}, 1H), 4.80 (dq, J = 12.0, 6.0 \text{ Hz}, 1H), 1.40 (d, J = 6.1 Hz, 3H); \(^{13}\)C NMR (100 MHz, DMSO-\(\text{d}_6\)) \(\delta\ 143.8, 132.7, 123.6, 120.8, 116.1, 115.7, 61.8, 20.0; MS (ESI): 198.95 \([\text{M+H}]^+\).

3-heptyl-3,4-dihydro-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide \((7k)\). white solid, 29% yield, mp. 146 – 147 °C. \(^1\)H NMR (300 MHz, DMSO-\(\text{d}_6\)) \(\delta\ 7.42 (d, J = 7.9 \text{ Hz}, 1H), 7.33 (d, J = 11.8 \text{ Hz}, 1H), 7.29 – 7.19 (m, 1H), 6.97 (s, 1H), 6.78 (d, J = 8.3 \text{ Hz}, 1H), 6.67 (t, J = 7.5 \text{ Hz}, 1H), 4.75 – 4.47 (m, 1H), 1.79 – 1.64 (m, 2H), 1.44 (s, 2H), 1.34 – 1.21 (m, 8H), 0.91 – 0.82 (m, 3H); \(^{13}\)C NMR (100 MHz, DMSO-\(\text{d}_6\)) \(\delta\ 143.7, 132.6, 123.7, 121.2, 116.1, 115.8, 65.6, 33.4, 31.1, 28.6, 28.5, 24.1, 22.1, 13.9; MS (ESI):
283.00 [M+H]+; HRMS (ESI) m/z calcd for C_{14}H_{23}N_{2}O_{2}S [M+H]+ 283.1475, found 283.1470.

References
$^1$H- and $^{13}$C-NMR spectral data for products
Electronic Supplementary Material (ESI) for RSC Advances
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