

Supporting Information

KI/TBHP-promoted [3+2] cycloaddition of pyrrolo[1,2-a]quinoxaline and *N*-Arylsulfonylhydrazones

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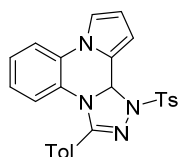
Experimental Section

Unless otherwise noted, all synthetic steps were performed under the air atmosphere using Schlenk tubes. The materials obtained from commercial sources were used without further purification. ^1H NMR and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra were recorded on a Bruker Advance III HD 400 MHz spectrometer in CDCl_3 or $\text{DMSO}-d_6$ solution. All chemical shifts were reported in ppm (δ) relative to the internal standard TMS (0 ppm). High-resolution mass spectra (HRMS) were acquired in electrospray ionization (ESI) mode using a TOF mass analyzer.

Characterization Data of Products

3-(p-tolyl)-1-tosyl-1,12b-dihydropyrrolo[1,2-a][1,2,4]triazolo[3,4-c]quinoxaline

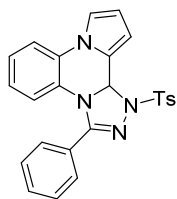
(3a)



Yield: 77%; Yellow solid; ^1H NMR (400 MHz, CDCl_3): δ 7.95 (d, $J = 8.3$ Hz, 2H), 7.41 (dd, $J = 8.2, 1.1$ Hz, 1H), 7.38 (d, $J = 8.1$ Hz, 2H), 7.22 (dd, $J = 2.6, 1.4$ Hz, 1H), 7.16 (td, $J = 8.1, 1.3$ Hz, 1H), 7.07 (d, $J = 7.9$ Hz, 2H), 6.93 (d, $J = 8.1$ Hz, 2H), 6.80 (td, $J = 8.0, 1.3$ Hz, 1H), 6.61 (dt, $J = 3.4, 1.2$ Hz, 1H), 6.54 (s, 1H), 6.42 (t, $J = 3.3$ Hz, 1H), 6.33 (dd, $J = 8.1, 1.2$ Hz, 1H), 2.47 (s, 3H), 2.32 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 156.80, 144.75, 141.12, 132.10, 130.02, 129.56, 129.00, 128.93, 126.96, 126.48, 124.29, 124.19, 123.70, 122.24, 115.64, 115.49, 111.69, 108.08, 73.01, 21.75, 21.50. HRMS (ESI): m/z calcd for $\text{C}_{26}\text{H}_{22}\text{N}_4\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$ 455.15299, found: 455.15246; IR (KBr): 2922, 1596, 1504, 1338, 1184, 1170, 760 cm^{-1} .

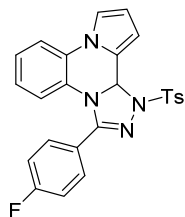
3-phenyl-1-tosyl-1,12b-dihydropyrrolo[1,2-a][1,2,4]triazolo[3,4-c]quinoxaline

(3b)



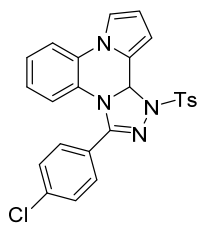
Yield: 69%; Yellow solid; ^1H NMR (400 MHz, CDCl_3): δ 7.96 (d, $J = 8.3$ Hz, 2H), 7.45 – 7.37 (m, 4H), 7.28 (t, $J = 7.0$ Hz, 2H), 7.24 (dd, $J = 2.7, 1.4$ Hz, 1H), 7.16 (td, $J = 8.1, 1.2$ Hz, 1H), 7.05 (d, $J = 7.2$ Hz, 2H), 6.79 (td, $J = 7.8, 1.1$ Hz, 1H), 6.63 (d, $J = 3.6$ Hz, 1H), 6.57 (s, 1H), 6.44 (t, $J = 3.3$ Hz, 1H), 6.30 (dd, $J = 8.1, 1.2$ Hz, 1H), 2.48 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 156.63, 144.82, 132.08, 130.81, 129.98, 129.60, 129.11, 128.96, 128.28, 126.90, 126.51, 125.27, 124.12, 124.06, 123.71, 115.66, 115.50, 111.74, 108.18, 73.01, 21.77. HRMS (ESI): m/z calcd for $\text{C}_{25}\text{H}_{20}\text{N}_4\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$ 441.1380, found: 441.1386; IR (KBr): 2924, 1594, 1504, 1348, 1176, 1164, 763 cm^{-1} .

3-(4-fluorophenyl)-1-tosyl-1,12b-dihydropyrrolo[1,2-a][1,2,4]triazolo[3,4-c]quinoxaline (3c)



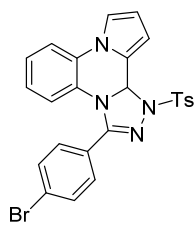
Yield: 80%; Green solid; ^1H NMR (400 MHz, CDCl_3): δ 7.95 (d, $J = 8.3$ Hz, 2H), 7.43 (dd, $J = 8.2, 1.2$ Hz, 1H), 7.39 (d, $J = 8.0$ Hz, 2H), 7.23 (dd, $J = 2.7, 1.5$ Hz, 1H), 7.19 (td, $J = 7.9, 1.3$ Hz, 1H), 7.07 – 7.02 (m, 2H), 7.00 – 6.93 (m, 2H), 6.82 (td, $J = 8.0, 1.3$ Hz, 1H), 6.61 (dt, $J = 3.5, 1.3$ Hz, 1H), 6.58 (s, 1H), 6.43 (t, $J = 3.36$ Hz, 1H), 6.31 (dd, $J = 8.1, 1.2$ Hz, 1H), 2.48 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 165.27, 162.76, 155.87, 144.92, 132.14, 131.39, 131.30, 130.12, 129.63, 128.89, 126.80, 124.18, 123.88, 123.79, 121.35, 121.32, 115.79, 115.73, 115.58, 115.51, 111.79, 108.24, 73.05, 21.77. HRMS (ESI): m/z calcd for $\text{C}_{25}\text{H}_{19}\text{FN}_4\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$ 459.1286, found: 459.1291.

3-(4-chlorophenyl)-1-tosyl-1,12b-dihydropyrrolo[1,2-a][1,2,4]triazolo[3,4-c]quinoxaline (3d)



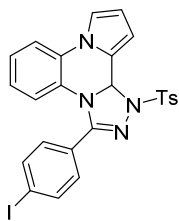
Yield: 74%; Yellow solid; ^1H NMR (400 MHz, CDCl_3): δ 7.94 (d, $J = 8.3$ Hz, 2H), 7.43 (dd, $J = 8.1, 1.0$ Hz, 1H), 7.39 (d, $J = 8.1$ Hz, 2H), 7.27 (d, $J = 1.9$ Hz, 1H), 7.25 (d, $J = 1.9$ Hz, 1H), 7.23 (dd, $J = 2.7, 1.4$ Hz, 1H), 7.19 (td, $J = 8.0, 1.3$ Hz, 1H), 7.00 (d, $J = 8.5$ Hz, 2H), 6.83 (td, $J = 8.0, 1.2$ Hz, 1H), 6.62 (d, $J = 3.5$ Hz, 1H), 6.58 (s, 1H), 6.44 (t, $J = 3.3$ Hz, 1H), 6.32 (dd, $J = 8.1, 1.1$ Hz, 1H), 2.48 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 155.69, 144.92, 137.15, 132.14, 130.49, 130.12, 129.63, 128.90, 128.67, 126.82, 126.78, 124.16, 123.82, 123.72, 115.81, 115.58, 111.82, 108.29, 73.08, 21.77. HRMS (ESI): m/z calcd for $\text{C}_{25}\text{H}_{19}\text{ClN}_4\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$ 475.0990, found: 475.0992; IR (KBr): 2929, 1597, 1506, 1400, 1338, 1171, 752 cm^{-1} .

3-(4-bromophenyl)-1-tosyl-1,12b-dihydropyrrolo[1,2-a][1,2,4]triazolo[3,4-c]quinoxaline (3e)



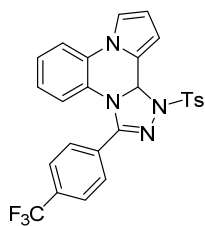
Yield: 71%; Yellow solid; ^1H NMR (400 MHz, CDCl_3): δ 7.94 (d, $J = 8.3$ Hz, 2H), 7.45 – 7.41 (m, 3H), 7.39 (d, $J = 8.2$ Hz, 2H), 7.23 (dd, $J = 2.6, 1.4$ Hz, 1H), 7.19 (td, $J = 8.2, 1.2$ Hz, 1H), 6.93 (d, $J = 8.5$ Hz, 2H), 6.84 (td, $J = 8.0, 1.2$ Hz, 1H), 6.62 (d, $J = 3.5$ Hz, 1H), 6.58 (s, 1H), 6.44 (t, $J = 3.3$ Hz, 1H), 6.33 (dd, $J = 8.1, 1.1$ Hz, 1H), 2.48 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 155.75, 144.93, 132.13, 131.62, 130.66, 130.11, 129.63, 128.90, 126.84, 126.76, 125.51, 124.19, 124.16, 123.84, 123.81, 115.82, 115.59, 111.82, 108.30, 73.09, 21.77. HRMS (ESI): m/z calcd for $\text{C}_{25}\text{H}_{19}\text{BrN}_4\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$ 519.0485, found: 519.0489, ($[\text{M} + 2]^+$, 521.0468); IR (KBr): 2924, 1597, 1506, 1352, 1338, 1171, 764 cm^{-1} .

3-(4-iodophenyl)-1-tosyl-1,12b-dihydropyrrolo[1,2-a][1,2,4]triazolo[3,4-c]quinoxaline (3f)



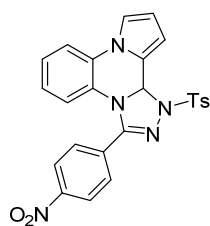
Yield: 72%; Yellow solid; ^1H NMR (400 MHz, CDCl_3): δ 7.94 (d, J = 8.2 Hz, 2H), 7.63 (d, J = 8.4 Hz, 2H), 7.43 (dd, J = 8.2, 0.8 Hz, 1H), 7.38 (d, J = 8.1 Hz, 2H), 7.23 (dd, J = 2.5, 1.3 Hz, 1H), 7.19 (td, J = 8.1, 1.2 Hz, 1H), 6.84 (td, J = 8.1, 1.1 Hz, 1H), 6.79 (d, J = 8.4 Hz, 2H), 6.61 (d, J = 3.5 Hz, 1H), 6.58 (s, 1H), 6.44 (t, J = 3.3 Hz, 1H), 6.33 (dd, J = 8.0, 1.0 Hz, 1H), 2.47 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 155.87, 144.92, 137.53, 132.12, 130.62, 130.10, 129.62, 128.90, 126.82, 126.76, 124.76, 124.17, 123.85, 123.82, 115.81, 115.58, 111.81, 108.29, 97.60, 73.10, 21.77. HRMS (ESI): m/z calcd for $\text{C}_{25}\text{H}_{19}\text{IN}_4\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$ 567.0346, found: 567.0349; IR (KBr): 2929, 1591, 1508, 1458, 1331, 1171, 755 cm^{-1} .

1-tosyl-3-(4-(trifluoromethyl)phenyl)-1,12b-dihydropyrrolo[1,2-a][1,2,4]triazolo[3,4-c]quinoxaline (3g)



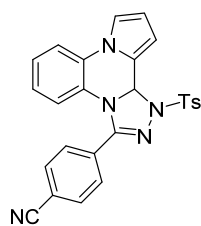
Yield: 70%; Yellow solid; ^1H NMR (400 MHz, CDCl_3): δ 7.95 (d, J = 8.2 Hz, 2H), 7.55 (d, J = 8.2 Hz, 2H), 7.43 (dd, J = 15.4, 8.0 Hz, 3H), 7.25 (d, J = 2.1 Hz, 1H), 7.20 (d, J = 8.1 Hz, 3H), 6.83 (t, J = 7.5 Hz, 1H), 6.63 (d, J = 1.2 Hz, 1H), 6.62 (s, 1H), 6.45 (t, J = 3.2 Hz, 1H), 6.30 (d, J = 7.6 Hz, 1H), 2.49 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 155.39, 145.04, 132.13, 130.13, 129.67, 129.66, 128.99, 128.91, 126.98, 126.68, 125.36, 125.32, 125.28, 125.25, 124.04, 123.89, 123.66, 115.89, 115.64, 111.87, 108.41, 73.18, 21.77. ^{19}F NMR (376 MHz, CDCl_3) δ -63.05. HRMS (ESI): m/z calcd for $\text{C}_{26}\text{H}_{19}\text{F}_3\text{N}_4\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$ 509.1254, found: 509.1260; IR (KBr): 2929, 1591, 1508, 1356, 1325, 1171, 730 cm^{-1} .

3-(4-nitrophenyl)-1-tosyl-1,12b-dihydropyrrolo[1,2-a][1,2,4]triazolo[3,4-c]quinoxaline (3h)



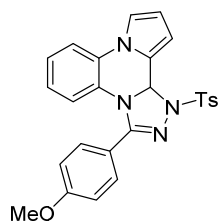
Yield: 69%; Green solid; ^1H NMR (400 MHz, CDCl_3): δ 8.15 (d, $J = 8.9$ Hz, 2H), 7.96 (d, $J = 8.2$ Hz, 2H), 7.46 (d, $J = 8.0$ Hz, 1H), 7.42 (d, $J = 8.1$ Hz, 2H), 7.28 (d, $J = 8.8$ Hz, 2H), 7.26 – 7.19 (m, 2H), 6.84 (t, $J = 7.6$ Hz, 1H), 6.65 (s, 1H), 6.64 (d, $J = 3.5$ Hz, 1H), 6.46 (t, $J = 3.3$ Hz, 1H), 6.30 (d, $J = 7.9$ Hz, 1H), 2.49 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 154.61, 149.10, 145.17, 132.13, 131.60, 131.14, 130.37, 130.20, 129.75, 128.88, 127.23, 126.57, 124.46, 123.94, 123.91, 123.48, 123.45, 116.05, 115.72, 111.95, 108.56, 73.26, 21.80. HRMS (ESI): m/z calcd for $\text{C}_{25}\text{H}_{19}\text{N}_5\text{O}_4\text{S}$ $[\text{M}+\text{H}]^+$ 486.1332, found: 486.1331; IR (KBr): 2922, 1597, 1512, 1423, 1371, 1348, 750 cm^{-1} .

4-(1-tosyl-1,12b-dihydropyrrolo[1,2-a][1,2,4]triazolo[3,4-c]quinoxalin-3-yl)benzotrinitile (3i)



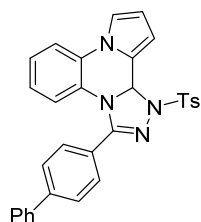
Yield: 70%; Yellow solid; ^1H NMR (400 MHz, CDCl_3): δ 7.94 (d, $J = 8.2$ Hz, 2H), 7.58 (d, $J = 8.5$ Hz, 2H), 7.45 (d, $J = 8.1$ Hz, 1H), 7.41 (d, $J = 8.0$ Hz, 2H), 7.25 (d, $J = 2.8$ Hz, 1H), 7.20 (d, $J = 8.3$ Hz, 3H), 6.84 (t, $J = 7.5$ Hz, 1H), 6.62 (s, 2H), 6.45 (t, $J = 3.2$ Hz, 1H), 6.29 (d, $J = 7.9$ Hz, 1H), 2.49 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 154.80, 145.12, 132.11, 132.05, 130.16, 129.89, 129.73, 128.87, 127.15, 126.61, 123.90, 123.49, 117.71, 116.00, 115.69, 114.75, 111.93, 108.51, 73.21, 21.79. HRMS (ESI): m/z calcd for $\text{C}_{26}\text{H}_{19}\text{N}_5\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$ 466.1332, found: 466.1331; IR (KBr): 2929, 2229, 1591, 1508, 1400, 1375, 1338, 1167, 758 cm^{-1} .

3-(4-methoxyphenyl)-1-tosyl-1,12b-dihydropyrrolo[1,2-a][1,2,4]triazolo[3,4-c]quinoxaline (3j)



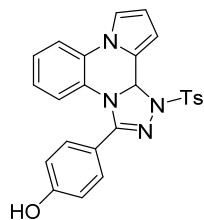
Yield: 72%; Yellow solid; ^1H NMR (400 MHz, CDCl_3): δ 7.95 (d, J = 8.3 Hz, 2H), 7.42 (dd, J = 8.1, 1.4 Hz, 1H), 7.38 (d, J = 8.0 Hz, 2H), 7.23 (dd, J = 3.1, 1.5 Hz, 1H), 7.18 (td, J = 7.8, 1.4 Hz, 1H), 7.00 (d, J = 8.8 Hz, 2H), 6.83 (td, J = 8.0, 1.3 Hz, 1H), 6.77 (d, J = 8.9 Hz, 2H), 6.61 (dt, J = 3.5, 1.2 Hz, 1H), 6.54 (s, 1H), 6.43 (t, J = 3.3 Hz, 1H), 6.36 (dd, J = 8.1, 1.2 Hz, 1H), 3.78 (s, 3H), 2.47 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 161.40, 156.54, 144.72, 132.15, 130.71, 130.11, 129.55, 128.92, 126.99, 126.51, 124.40, 124.25, 123.70, 117.22, 115.67, 115.48, 113.65, 111.71, 108.07, 73.02, 55.32, 21.76. HRMS (ESI): m/z calcd for $\text{C}_{26}\text{H}_{22}\text{N}_4\text{O}_3\text{S}$ $[\text{M}+\text{Na}]^+$ 493.1306, found: 493.1307; IR (KBr): 2929, 1577, 1524, 1406, 1346, 1169, 756 cm^{-1} .

3-([1,1'-biphenyl]-4-yl)-1-tosyl-1,12b-dihydropyrrolo[1,2-a][1,2,4]triazolo[3,4-c]quinoxaline (3k)



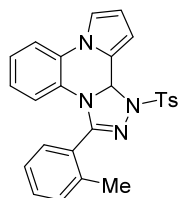
Yield: 57%; Yellow solid; ^1H NMR (400 MHz, CDCl_3): δ 7.98 (d, J = 8.3 Hz, 2H), 7.55 (d, J = 7.1 Hz, 2H), 7.50 (d, J = 8.4 Hz, 2H), 7.44 (dd, J = 6.9, 1.7 Hz, 2H), 7.41 (t, J = 6.2 Hz, 3H), 7.39 – 7.33 (m, 1H), 7.25 (dd, J = 3.1, 1.7 Hz, 1H), 7.18 (td, J = 7.8, 1.4 Hz, 1H), 7.14 (d, J = 8.4 Hz, 2H), 6.83 (td, J = 7.8, 1.3 Hz, 1H), 6.64 (dt, J = 3.5, 1.3 Hz, 1H), 6.59 (s, 1H), 6.45 (t, J = 3.2 Hz, 1H), 6.41 (dd, J = 8.1, 1.4 Hz, 1H), 2.48 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 156.44, 144.82, 143.57, 139.71, 132.16, 130.09, 129.61, 129.58, 128.96, 128.94, 128.08, 127.09, 126.95, 126.85, 126.61, 124.32, 124.15, 124.02, 123.78, 115.72, 115.54, 111.76, 108.19, 73.11, 21.78. HRMS (ESI): m/z calcd for $\text{C}_{31}\text{H}_{24}\text{N}_4\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$ 517.1693, found: 517.1692; IR (KBr): 2929, 1654, 1597, 1506, 1458, 1338, 1171, 768 cm^{-1} .

**4-(1-tosyl-1,12b-dihydropyrrolo[1,2-a][1,2,4]triazolo[3,4-c]quinoxalin-3-yl)pheno
l (3l)**



Yield: 52%; Yellow solid; ^1H NMR (400 MHz, CDCl_3): δ 7.91 (d, $J = 8.2$ Hz, 2H), 7.42 (dd, $J = 8.2, 1.3$ Hz, 1H), 7.36 (d, $J = 8.0$ Hz, 2H), 7.24 (dd, $J = 3.0, 1.5$ Hz, 1H), 7.19 (td, $J = 7.8, 1.4$ Hz, 1H), 6.83 (td, $J = 7.8, 1.3$ Hz, 1H), 6.77 (d, $J = 8.6$ Hz, 2H), 6.61 (d, $J = 8.7$ Hz, 2H), 6.59 (dt, $J = 3.5, 1.3$ Hz, 1H), 6.53 (s, 1H), 6.42 (t, $J = 3.2$ Hz, 1H), 6.32 (dd, $J = 8.1, 1.3$ Hz, 1H), 2.46 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 158.92, 158.31, 157.63, 148.65, 148.61, 145.09, 144.13, 135.29, 131.60, 130.59, 130.12, 129.68, 129.63, 129.07, 128.84, 127.90, 126.88, 126.66, 125.47, 124.54, 123.93, 123.88, 115.76, 115.73, 115.68, 115.65, 111.68, 107.99, 73.20, 21.76. HRMS (ESI): m/z calcd for $\text{C}_{25}\text{H}_{20}\text{N}_4\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$ 457.13264, found: 457.13244.

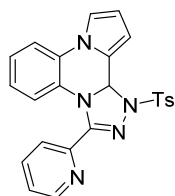
**3-(o-tolyl)-1-tosyl-1,12b-dihydropyrrolo[1,2-a][1,2,4]triazolo[3,4-c]quinoxaline
(3m)**



Yield: 35%; Green solid; ^1H NMR (400 MHz, CDCl_3): δ 7.96 (d, $J = 8.3$ Hz, 2H), 7.41 (d, $J = 8.1$ Hz, 2H), 7.38 (dd, $J = 8.2, 1.3$ Hz, 1H), 7.28 (td, $J = 7.6, 1.3$ Hz, 1H), 7.22 (dd, $J = 3.1, 1.5$ Hz, 1H), 7.13 (d, $J = 7.5$ Hz, 1H), 7.09 (dd, $J = 7.8, 1.1$ Hz, 1H), 7.06 (dd, $J = 4.5, 3.2$ Hz, 1H), 6.84 (dd, $J = 7.7, 1.3$ Hz, 1H), 6.68 (td, $J = 8.1, 1.3$ Hz, 1H), 6.66 (dd, $J = 3.4, 1.7$ Hz, 1H), 6.65 (s, 1H), 6.46 (t, $J = 3.2$ Hz, 1H), 6.12 (dd, $J = 8.1, 1.4$ Hz, 1H), 2.50 (s, 3H), 1.69 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 157.17, 144.82, 137.60, 132.44, 130.58, 130.18, 129.69, 129.45, 129.41, 129.15, 126.51, 126.10, 125.75, 125.20, 124.20, 123.91, 122.66, 115.39, 115.27, 111.83, 108.38, 72.09, 21.75, 18.39. HRMS (ESI): m/z calcd for $\text{C}_{26}\text{H}_{22}\text{N}_4\text{O}_2\text{S}$

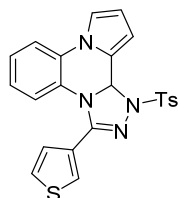
$[M+H]^+$ 455.1536, found: 455.1531; IR (KBr): 2924, 1655, 1591, 1506, 1363, 1336, 1171, 764 cm^{-1} .

3-(pyridin-2-yl)-1-tosyl-1,12b-dihydropyrrolo[1,2-a][1,2,4]triazolo[3,4-c]quinoxaline (3n)



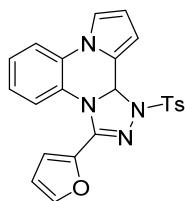
Yield: 59%; White solid; ^1H NMR (400 MHz, CDCl_3): δ 8.47 (d, $J = 3.7$ Hz, 1H), 7.91 (d, $J = 8.0$ Hz, 2H), 7.70 (t, $J = 7.5$ Hz, 1H), 7.61 (d, $J = 7.9$ Hz, 1H), 7.36 – 7.28 (m, 4H), 7.22 – 7.04 (m, 2H), 6.89 (dd, $J = 30.2, 6.0$ Hz, 2H), 6.60 (d, $J = 11.8$ Hz, 2H), 6.41 (s, 1H), 2.46 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 155.40, 148.79, 145.87, 144.79, 136.67, 132.01, 129.89, 129.66, 128.80, 126.83, 126.39, 125.67, 125.33, 125.23, 124.62, 123.42, 115.54, 115.40, 111.46, 108.03, 73.46, 21.76. HRMS (ESI): m/z calcd for $\text{C}_{24}\text{H}_{19}\text{N}_5\text{O}_2\text{S}$ $[M+H]^+$ 442.1332, found: 442.1335.

3-(thiophen-3-yl)-1-tosyl-1,12b-dihydropyrrolo[1,2-a][1,2,4]triazolo[3,4-c]quinoxaline (3o)



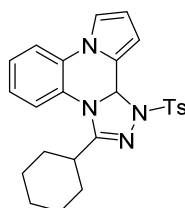
Yield: 51%; Yellow solid; ^1H NMR (400 MHz, CDCl_3): δ 7.93 (d, $J = 8.3$ Hz, 2H), 7.43 (dd, $J = 8.1, 1.2$ Hz, 1H), 7.35 (d, $J = 8.1$ Hz, 2H), 7.25 – 7.19 (m, 4H), 6.93 (dd, $J = 7.8, 1.2$ Hz, 1H), 6.90 (dd, $J = 4.9, 1.4$ Hz, 1H), 6.58 (dt, $J = 3.5, 1.2$ Hz, 1H), 6.57 (s, 1H), 6.54 (dd, $J = 8.0, 1.3$ Hz, 1H), 6.41 (t, $J = 3.2$ Hz, 1H), 2.46 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 153.36, 144.72, 132.27, 130.63, 129.50, 128.89, 128.81, 127.76, 127.20, 126.78, 125.87, 125.39, 125.05, 124.05, 123.70, 115.77, 115.55, 111.75, 108.22, 73.01, 21.74. HRMS (ESI): m/z calcd for $\text{C}_{23}\text{H}_{18}\text{N}_4\text{O}_2\text{S}_2$ $[M+H]^+$ 447.0944, found: 447.0948; IR (KBr): 2929, 1655, 1577, 1560, 1506, 1458, 1340, 1167, 758 cm^{-1} .

**3-(furan-2-yl)-1-tosyl-1,12b-dihydropyrrolo[1,2-a][1,2,4]triazolo[3,4-c]quinoxaline
e (3p)**



Yield: 63%; White solid; ^1H NMR (400 MHz, CDCl_3): δ 7.89 (d, J = 8.3 Hz, 2H), 7.42 – 7.38 (m, 2H), 7.31 (d, J = 8.0 Hz, 2H), 7.27 (td, J = 7.9, 1.4 Hz, 1H), 7.18 (d, J = 2.1 Hz, 1H), 7.02 (td, J = 7.8, 1.3 Hz, 1H), 6.85 (dd, J = 8.0, 1.4 Hz, 1H), 6.62 (dd, J = 3.5, 0.8 Hz, 1H), 6.55 (s, 1H), 6.55 – 6.53 (m, 1H), 6.38 – 6.34 (m, 2H), 2.44 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 149.94, 144.94, 144.73, 139.88, 132.19, 130.84, 129.68, 129.51, 128.70, 127.95, 127.63, 126.40, 125.96, 115.70, 115.69, 115.61, 111.58, 111.37, 108.22, 73.14, 21.73. HRMS (ESI): m/z calcd for $\text{C}_{23}\text{H}_{18}\text{N}_4\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$ 431.1172, found: 431.1175; IR (KBr): 2924, 1655, 1602, 1595, 1560, 1506, 1473, 1363, 1165, 768 cm^{-1} .

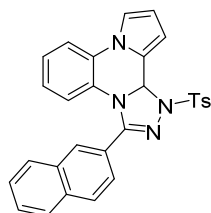
**3-cyclohexyl-1-tosyl-1,12b-dihydropyrrolo[1,2-a][1,2,4]triazolo[3,4-c]quinoxaline
(3q)**



Yield: 67%; White solid; ^1H NMR (400 MHz, CDCl_3): δ 7.84 (d, J = 8.3 Hz, 2H), 7.42 (dd, J = 8.1, 1.2 Hz, 1H), 7.32 (d, J = 8.0 Hz, 2H), 7.27 (td, J = 7.4, 1.4 Hz, 1H), 7.16 (dd, J = 3.1, 1.5 Hz, 1H), 7.08 (td, J = 7.7, 1.4 Hz, 1H), 6.84 (dd, J = 8.0, 1.4 Hz, 1H), 6.52 (dt, J = 3.5, 1.3 Hz, 1H), 6.43 (s, 1H), 6.38 (t, J = 3.3 Hz, 1H), 2.46 (s, 3H), 2.20 – 2.04 (m, 1H), 1.82 – 1.74 (m, 1H), 1.68 – 1.46 (m, 4H), 1.27 (dd, J = 8.4, 3.1 Hz, 2H), 1.15 – 1.21 (m, 2H), 0.99 – 0.86 (m, 1H). ^{13}C NMR (101 MHz, CDCl_3): δ 164.18, 144.37, 132.36, 130.55, 129.25, 128.90, 127.05, 126.57, 124.61, 124.23, 124.07, 115.80, 115.25, 111.71, 108.24, 72.00, 34.08, 31.07, 29.86, 25.86, 25.68, 25.51, 21.71. HRMS (ESI): m/z calcd for $\text{C}_{25}\text{H}_{26}\text{N}_4\text{O}_2\text{S}$ $[\text{M}+\text{Na}]^+$ 469.1669,

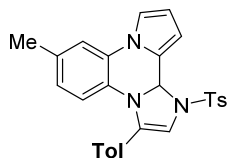
found: 469.1672; IR (KBr): 2929, 2854, 1655, 1601, 1597, 1504, 1473, 1361, 1167, 754 cm^{-1} .

3-(naphthalen-2-yl)-1-tosyl-1,12b-dihydropyrrolo[1,2-a][1,2,4]triazolo[3,4-c]quinoxaline (3r)



Yield: 39%; Yellow solid; ^1H NMR (400 MHz, CDCl_3): δ 8.01 (d, $J = 8.2$ Hz, 2H), 7.80 (d, $J = 8.0$ Hz, 1H), 7.72 (d, $J = 8.9$ Hz, 1H), 7.70 (d, $J = 7.4$ Hz, 1H), 7.60 (s, 1H), 7.53 (td, $J = 6.8, 1.0$ Hz, 1H), 7.49 (td, $J = 6.8, 1.0$ Hz, 1H), 7.43 (t, $J = 9.2$ Hz, 3H), 7.27 (dd, $J = 3.2, 1.6$ Hz, 1H), 7.16 (t, $J = 7.3$ Hz, 1H), 7.08 (dd, $J = 8.5, 1.7$ Hz, 1H), 6.73 (td, $J = 7.8, 1.3$ Hz, 1H), 6.65 (d, $J = 3.5$ Hz, 1H), 6.62 (s, 1H), 6.46 (t, $J = 3.3$ Hz, 1H), 6.34 (dd, $J = 8.1, 1.3$ Hz, 1H), 2.48 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 156.69, 144.85, 133.99, 132.26, 132.23, 130.08, 129.74, 129.63, 129.02, 128.43, 128.01, 127.80, 127.72, 126.90, 126.85, 126.59, 125.32, 124.24, 124.20, 123.76, 122.55, 115.71, 115.57, 111.78, 108.23, 99.99, 73.18, 21.78. HRMS (ESI): m/z calcd for $\text{C}_{29}\text{H}_{22}\text{N}_4\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$ 491.1536, found: 491.1541; IR (KBr): 2929, 1655, 1591, 1506, 1473, 1363, 1169, 752 cm^{-1} .

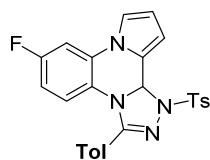
7-methyl-3-(p-tolyl)-1-tosyl-1,12b-dihydropyrrolo[1,2-a][1,2,4]triazolo[3,4-c]quinoxaline (3s)



Yield: 79%; Yellow solid; ^1H NMR (400 MHz, CDCl_3): δ 7.94 (d, $J = 8.3$ Hz, 2H), 7.37 (d, $J = 8.1$ Hz, 2H), 7.24 – 7.18 (m, 2H), 7.06 (d, $J = 8.0$ Hz, 2H), 6.93 (d, $J = 8.1$ Hz, 2H), 6.63 – 6.58 (m, 2H), 6.53 (s, 1H), 6.41 (t, $J = 3.3$ Hz, 1H), 6.22 (d, $J = 8.2$ Hz, 1H), 2.46 (s, 3H), 2.32 (d, $J = 2.7$ Hz, 6H). ^{13}C NMR (101 MHz, CDCl_3): δ 157.16, 144.66, 141.02, 136.74, 132.21, 129.86, 129.51, 129.01, 128.91, 128.87, 126.95, 124.42, 124.20, 122.32, 121.71, 116.12, 115.40, 111.53, 107.98,

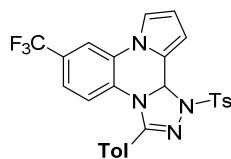
73.10, 21.74, 21.49, 21.29. HRMS (ESI): m/z calcd for $C_{27}H_{24}N_4O_2S$ $[M+H]^+$ 469.1693, found: 469.1693; IR (KBr): 2922, 1637, 1616, 1585, 1508, 1477, 1338, 1167, 733 cm^{-1} .

7-fluoro-3-(p-tolyl)-1-tosyl-1,12b-dihydropyrrolo[1,2-a][1,2,4]triazolo[3,4-c]quinoxaline (3t)



Yield: 52%; Yellow solid; 1H NMR (400 MHz, $CDCl_3$): δ 7.95 (d, $J = 8.2$ Hz, 2H), 7.39 (d, $J = 8.1$ Hz, 2H), 7.15 (dd, $J = 2.8, 1.4$ Hz, 1H), 7.12 (dd, $J = 9.1, 2.7$ Hz, 1H), 7.07 (d, $J = 8.0$ Hz, 2H), 6.90 (d, $J = 8.1$ Hz, 2H), 6.62 (d, $J = 3.5$ Hz, 1H), 6.56 (s, 1H), 6.52 (td, $J = 8.5, 2.7$ Hz, 1H), 6.45 (t, $J = 3.3$ Hz, 1H), 6.30 (dd, $J = 8.9, 5.3$ Hz, 1H), 2.47 (s, 3H), 2.33 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 161.93, 159.48, 157.20, 144.79, 141.24, 131.21, 131.10, 132.22, 129.56, 129.00, 128.97, 128.91, 126.83, 125.99, 125.90, 122.02, 120.33, 120.30, 115.63, 112.33, 110.62, 110.40, 108.70, 103.44, 103.17, 72.79, 21.76, 21.49. HRMS (ESI): m/z calcd for $C_{26}H_{21}FN_4O_2S$ $[M+H]^+$ 473.1442, found: 473.1445; IR (KBr): 3066, 2952, 2923, 1726, 1637, 1616, 1597, 1508, 1490, 1444, 1361, 1327, 1163, 756 cm^{-1} .

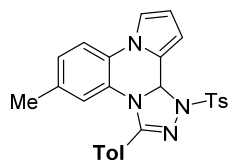
3-(p-tolyl)-1-tosyl-7-(trifluoromethyl)-1,12b-dihydropyrrolo[1,2-a][1,2,4]triazolo[3,4-c]quinoxaline (3u)



Yield: 65%; Yellow solid; 1H NMR (400 MHz, $CDCl_3$): δ 7.95 (d, $J = 8.3$ Hz, 2H), 7.63 (d, $J = 1.3$ Hz, 1H), 7.40 (d, $J = 8.2$ Hz, 2H), 7.21 (dd, $J = 8.1, 4.2$ Hz, 1H), 7.13 (d, $J = 8.0$ Hz, 2H), 7.04 (d, $J = 7.1$ Hz, 1H), 6.98 (d, $J = 8.1$ Hz, 2H), 6.67 (d, $J = 3.6$ Hz, 1H), 6.50 (t, $J = 3.2$ Hz, 1H), 6.48 (s, 1H), 6.42 (d, $J = 8.4$ Hz, 1H), 2.48 (s, 3H), 2.36 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 155.27, 145.00, 141.52, 131.73, 129.68, 129.25, 129.03, 128.88, 128.16, 127.83, 127.08, 126.81, 123.71, 121.91, 120.42, 120.39, 112.84, 112.80, 112.63, 108.94, 77.34, 21.76, 21.52. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.79. HRMS (ESI): m/z calcd for $C_{27}H_{21}F_3N_4O_2S$

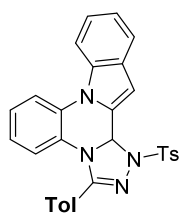
$[M+H]^+$ 523.1410, found: 523.1413; IR (KBr): 3060, 2924, 1726, 1655, 1616, 1597, 1514, 1444, 1361, 1328, 1163, 741 cm^{-1} .

6-methyl-3-(p-tolyl)-1-tosyl-1,12b-dihydropyrrolo[1,2-a][1,2,4]triazolo[3,4-c]quinoxaline (3v)



Yield: 82%; Yellow solid; ^1H NMR (400 MHz, CDCl_3): δ 7.95 (d, $J = 8.2$ Hz, 2H), 7.38 (d, $J = 8.1$ Hz, 2H), 7.29 (d, $J = 8.2$ Hz, 1H), 7.19 (dd, $J = 2.5, 1.4$ Hz, 1H), 7.07 (d, $J = 8.0$ Hz, 2H), 6.95 (d, $J = 8.1$ Hz, 3H), 6.59 (d, $J = 3.5$ Hz, 1H), 6.52 (s, 1H), 6.41 (t, $J = 3.2$ Hz, 1H), 6.13 (d, $J = 1.1$ Hz, 1H), 2.47 (s, 3H), 2.33 (s, 3H), 2.05 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 156.62, 144.67, 141.08, 133.61, 132.17, 129.56, 129.03, 128.91, 128.81, 127.72, 127.07, 126.76, 124.60, 123.98, 122.32, 115.36, 115.31, 111.33, 107.77, 73.11, 21.76, 21.50, 20.76. HRMS (ESI): m/z calcd for $\text{C}_{27}\text{H}_{24}\text{N}_4\text{O}_2\text{S}$ $[M+H]^+$ 469.1693, found: 469.1698; IR (KBr): 3032, 2922, 1720, 1654, 1616, 1595, 1516, 1473, 1363, 1338, 1169, 734 cm^{-1} .

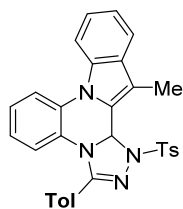
3-(p-tolyl)-1-tosyl-1,14b-dihydroindolo[1,2-a][1,2,4]triazolo[3,4-c]quinoxaline (3w)



Yield: 70(63)%; Yellow solid; ^1H NMR (400 MHz, CDCl_3): δ 8.00 – 7.94 (m, 3H), 7.87 (td, $J = 7.8, 1.8$ Hz, 1H), 7.72 (d, $J = 7.7$ Hz, 1H), 7.38 (d, $J = 8.0$ Hz, 2H), 7.35 – 7.28 (m, 2H), 7.24 (t, $J = 5.8$ Hz, 1H), 7.08 – 6.98 (m, 5H), 6.89 (td, $J = 7.8, 1.2$ Hz, 1H), 6.59 (d, $J = 1.2$ Hz, 1H), 6.44 (dd, $J = 8.0, 1.4$ Hz, 1H), 2.46 (s, 3H), 2.31 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 156.30, 148.77, 144.87, 141.37, 137.78, 135.00, 134.12, 132.08, 131.40, 129.81, 129.59, 128.96, 128.94, 128.93, 126.81, 124.83, 124.82, 124.16, 123.49, 123.40, 122.16, 121.88, 121.79, 121.63,

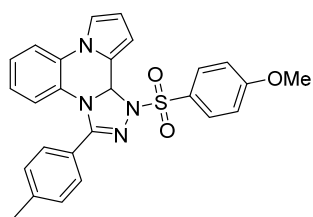
117.75, 111.44, 102.56, 73.26, 21.77, 21.50. HRMS (ESI): m/z calcd for $C_{30}H_{24}N_4O_2S$ $[M+H]^+$ 505.16892, found: 505.16855; .

14-methyl-3-(p-tolyl)-1-tosyl-1,14b-dihydroindolo[1,2-a][1,2,4]triazolo[3,4-c]quinoxaline (3x)



Yield: 72(65)%; Yellow solid; 1H NMR (400 MHz, $CDCl_3$): δ 7.98 (d, $J = 8.3$ Hz, 2H), 7.93 (t, $J = 8.0$ Hz, 2H), 7.67 (d, $J = 7.5$ Hz, 1H), 7.37 (d, $J = 8.1$ Hz, 2H), 7.36 – 7.29 (m, 2H), 7.25 (td, $J = 7.1$ Hz, 0.7Hz, 1H), 7.01 (d, $J = 8.0$ Hz, 2H), 6.93 (d, $J = 8.3$ Hz, 2H), 6.89 – 6.84 (m, 2H), 6.37 (dd, $J = 7.9, 1.5$ Hz, 1H), 2.69 (d, $J = 1.0$ Hz, 3H), 2.47 (s, 3H), 2.29 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 158.76, 144.77, 141.38, 133.47, 132.44, 132.27, 131.26, 129.39, 129.02, 128.95, 128.84, 128.30, 127.41, 125.71, 124.49, 123.70, 122.92, 121.77, 121.27, 119.81, 117.35, 112.67, 111.33, 74.41, 21.76, 21.48, 8.40. HRMS (ESI): m/z calcd for $C_{31}H_{26}N_4O_2S$ $[M+H]^+$ 519.18451, found: 519.18406.

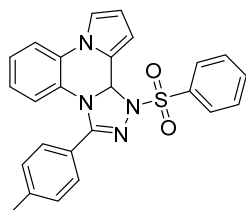
1-((4-methoxyphenyl)sulfonyl)-3-(p-tolyl)-1,12b-dihydropyrrolo[1,2-a][1,2,4]triazolo[3,4-c]quinoxaline (3y)



Yield: 72%; Yellow solid; 1H NMR (400 MHz, $CDCl_3$): δ 8.00 (d, $J = 9.0$ Hz, 2H), 7.41 (dd, $J = 8.1, 1.2$ Hz, 1H), 7.23 (dd, $J = 2.7, 1.5$ Hz, 1H), 7.16 (td, $J = 7.9, 1.3$ Hz, 1H), 7.06 (t, $J = 8.5$ Hz, 4H), 6.95 (d, $J = 8.2$ Hz, 2H), 6.81 (td, $J = 8.0, 1.3$ Hz, 1H), 6.61 (dt, $J = 3.5, 1.2$ Hz, 1H), 6.54 (s, 1H), 6.43 (t, $J = 3.4$ Hz, 1H), 6.36 (dd, $J = 8.1, 1.3$ Hz, 1H), 3.90 (s, 3H), 2.32 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 163.85, 156.79, 141.12, 131.09, 130.02, 129.00, 128.93, 126.99, 126.55, 126.45, 124.31, 124.22, 123.70, 122.26, 115.63, 115.47, 114.13, 111.70,

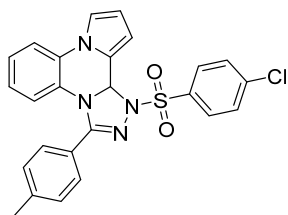
108.07, 73.02, 55.75, 21.50. HRMS (ESI): m/z calcd for $C_{26}H_{22}N_4O_3S$ $[M+H]^+$ 471.1485, found: 471.1487; IR (KBr): 3055, 2947, 2922, 1720, 1655, 1591, 1502, 1473, 1375, 1338, 1163, 752 cm^{-1} .

1-(phenylsulfonyl)-3-(p-tolyl)-1,12b-dihydropyrrolo[1,2-a][1,2,4]triazolo[3,4-c]quinoxaline (3z)



Yield: 68%; Yellow solid; 1H NMR (400 MHz, $CDCl_3$): δ 8.08 (dd, $J = 8.4, 1.2$ Hz, 2H), 7.69 (tt, $J = 7.4, 1.2$ Hz, 1H), 7.60 (t, $J = 7.6$ Hz, 2H), 7.41 (dd, $J = 8.1, 1.2$ Hz, 1H), 7.23 (dd, $J = 2.6, 1.5$ Hz, 1H), 7.17 (td, $J = 7.9, 1.4$ Hz, 1H), 7.06 (d, $J = 7.9$ Hz, 2H), 6.91 (d, $J = 8.2$ Hz, 2H), 6.80 (td, $J = 8.0, 1.3$ Hz, 1H), 6.62 (dt, $J = 3.5, 1.3$ Hz, 1H), 6.58 (s, 1H), 6.43 (t, $J = 3.4$ Hz, 1H), 6.30 (dd, $J = 8.1, 1.3$ Hz, 1H), 2.32 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 157.27, 141.17, 135.05, 133.77, 130.11, 128.98, 128.93, 128.90, 126.75, 126.64, 124.49, 124.11, 123.75, 122.09, 115.63, 115.56, 111.72, 108.13, 73.07, 21.50. HRMS (ESI): m/z calcd for $C_{25}H_{20}N_4O_2S$ $[M+H]^+$ 441.1380, found: 441.1385; IR (KBr): 2924, 1718, 1700, 1685, 1655, 1577, 1521, 1458, 1375, 1341, 1163, 746 cm^{-1} .

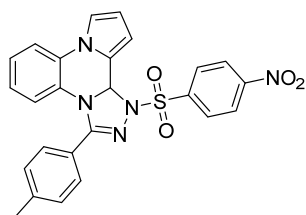
1-((4-chlorophenyl)sulfonyl)-3-(p-tolyl)-1,12b-dihydropyrrolo[1,2-a][1,2,4]triazolo[3,4-c]quinoxaline (4a)



Yield: 49%; Yellow solid; 1H NMR (400 MHz, $CDCl_3$): δ 8.01 (d, $J = 8.6$ Hz, 2H), 7.57 (d, $J = 8.6$ Hz, 2H), 7.42 (dd, $J = 8.1, 1.0$ Hz, 1H), 7.24 (dd, $J = 2.5, 1.4$ Hz, 1H), 7.18 (td, $J = 8.1, 1.3$ Hz, 1H), 7.08 (d, $J = 8.0$ Hz, 2H), 6.93 (d, $J = 8.1$ Hz, 2H), 6.83 (td, $J = 8.0, 1.2$ Hz, 1H), 6.60 (d, $J = 3.5$ Hz, 1H), 6.55 (s, 1H), 6.44 (t, $J = 3.3$ Hz, 1H), 6.39 (dd, $J = 8.1, 1.1$ Hz, 1H), 2.33 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 157.23, 141.35, 140.47, 133.70, 130.28, 130.05, 129.25, 129.03,

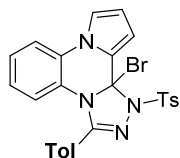
128.93, 126.71, 126.61, 124.47, 124.03, 123.83, 121.97, 115.67, 115.62, 111.75, 108.19, 72.99, 21.50. HRMS (ESI): m/z calcd for $C_{25}H_{19}ClN_4O_2S$ $[M+Na]^+$ 497.0809, found: 497.0813; IR (KBr): 3064, 2947, 1709, 1685, 1655, 1610, 1597, 1577, 1508, 1473, 1379, 1171, 725 cm^{-1} .

1-((4-nitrophenyl)sulfonyl)-3-(p-tolyl)-1,12b-dihydropyrrolo[1,2-a][1,2,4]triazolo[3,4-c]quinoxaline (4b)



Yield: 55%; Green solid; 1H NMR (400 MHz, $DMSO-d_6$): δ 8.49 (d, $J = 9.0$ Hz, 2H), 8.34 (d, $J = 9.0$ Hz, 2H), 7.78 (dd, $J = 8.2, 1.3$ Hz, 1H), 7.68 (dd, $J = 3.0, 1.5$ Hz, 1H), 7.27 (td, $J = 7.8, 1.4$ Hz, 1H), 7.12 (t, $J = 7.9$ Hz, 3H), 6.88 (td, $J = 7.8, 1.3$ Hz, 1H), 6.83 (d, $J = 8.2$ Hz, 1H), 6.42 (t, $J = 3.2$ Hz, 1H), 6.38 (d, $J = 3.4$ Hz, 1H), 6.36 (dd, $J = 8.0, 1.3$ Hz, 1H), 2.27 (s, 3H). ^{13}C NMR (101 MHz, $DMSO-d_6$): δ 159.63, 151.27, 141.61, 140.24, 130.84, 130.46, 129.49, 129.21, 127.83, 126.29, 125.55, 124.73, 124.59, 124.02, 121.86, 117.66, 116.55, 111.51, 107.45, 73.11, 21.38. HRMS (ESI): m/z calcd for $C_{25}H_{19}N_5O_4S$ $[M+H]^+$ 486.1231, found: 486.1236; IR (KBr): 2924, 1598, 1515, 1425, 1372, 1350, 754 cm^{-1} .

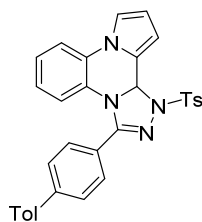
12b-bromo-3-(p-tolyl)-1-tosyl-1,12b-dihydropyrrolo[1,2-a][1,2,4]triazolo[3,4-c]quinoxaline (3aa)



Yield: 75%; Yellow solid; 1H NMR (400 MHz, $CDCl_3$): δ 8.28 (dd, $J = 8.4, 1.1$ Hz, 1H), 7.93 (d, $J = 8.3$ Hz, 2H), 7.37 (d, $J = 8.1$ Hz, 2H), 7.24 – 7.17 (m, 1H), 7.12 – 7.03 (m, 4H), 6.92 (td, $J = 7.9, 1.2$ Hz, 1H), 6.61 (dd, $J = 3.8, 1.0$ Hz, 1H), 6.46 (d, $J = 3.8$ Hz, 1H), 6.40 (dd, $J = 8.0, 1.3$ Hz, 1H), 6.37 (d, $J = 1.0$ Hz, 1H), 2.46 (s, 3H), 2.33 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 155.70, 144.83, 141.44, 131.98, 131.04, 130.10, 129.57, 129.01, 128.91, 125.95, 125.61, 124.96, 124.48, 121.85,

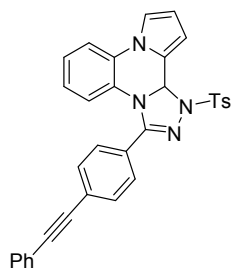
119.42, 116.19, 108.08, 98.27, 73.31, 21.76, 21.53. HRMS (ESI): m/z calcd for $C_{26}H_{21}BrN_4O_2S$ $[M+H]^+$ 533.0641, found: 533.0647 ($[M + 2]^+$, 535.0631); IR (KBr): 3033, 2922, 1720, 1649, 1610, 1585, 1502, 1458, 1390, 1169, 754 cm^{-1} .

3-(4'-methyl-[1,1'-biphenyl]-4-yl)-1-tosyl-1,12b-dihydropyrrolo[1,2-a][1,2,4]triazolo[3,4-c]quinoxaline (3fa)



Yield: 64%; Yellow solid; 1H NMR (400 MHz, $CDCl_3$): δ 7.97 (d, $J = 8.3$ Hz, 2H), 7.50 – 7.45 (m, 3H), 7.43 (dd, $J = 6.6, 1.5$ Hz, 2H), 7.40 (d, $J = 8.0$ Hz, 2H), 7.27 – 7.20 (m, 3H), 7.18 (td, $J = 8.0, 1.3$ Hz, 1H), 7.12 (d, $J = 8.5$ Hz, 2H), 6.82 (td, $J = 8.0, 1.3$ Hz, 1H), 6.63 (dt, $J = 3.5, 1.2$ Hz, 1H), 6.58 (s, 1H), 6.46 – 6.44 (m, 1H), 6.42 (dd, $J = 8.1, 1.2$ Hz, 1H), 2.48 (s, 3H), 2.38 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 156.47, 144.78, 143.49, 138.04, 136.81, 132.17, 130.09, 129.65, 129.60, 129.54, 128.96, 126.96, 126.90, 126.59, 126.57, 124.35, 124.19, 123.76, 123.67, 115.70, 115.52, 111.75, 108.18, 73.10, 21.78, 21.15. HRMS (ESI): m/z calcd for $C_{32}H_{26}N_4O_2S$ $[M+H]^+$ 531.1849, found: 531.1851; IR (KBr): 2924, 1701, 1637, 1608, 1577, 1540, 1508, 1473, 1375, 1338, 1169, 756 cm^{-1} .

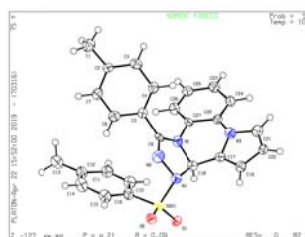
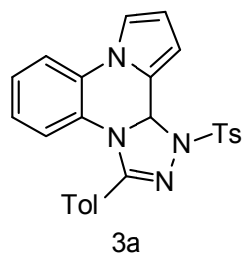
3-(4-(phenylethynyl)phenyl)-1-tosyl-1,12b-dihydropyrrolo[1,2-a][1,2,4]triazolo[3,4-c]quinoxaline (3fb)



Yield: 79%; Yellow solid; 1H NMR (400 MHz, $CDCl_3$): δ 7.96 (d, $J = 8.3$ Hz, 2H), 7.53 – 7.49 (m, 2H), 7.43 (d, $J = 8.3$ Hz, 3H), 7.40 (d, $J = 8.1$ Hz, 2H), 7.38 – 7.32 (m, 3H), 7.24 (dd, $J = 2.8, 1.4$ Hz, 1H), 7.19 (td, $J = 8.0, 1.3$ Hz, 1H), 7.05 (d, $J = 8.4$ Hz, 2H), 6.83 (td, $J = 7.9, 1.2$ Hz, 1H), 6.63 (dt, $J = 3.6, 1.3$ Hz, 1H), 6.58

(s, 1H), 6.45 (t, $J = 3.3$ Hz, 1H), 6.35 (dd, $J = 8.1, 1.2$ Hz, 1H), 2.48 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ 155.97, 144.88, 132.14, 131.68, 131.36, 130.07, 129.63, 129.12, 128.94, 128.78, 128.45, 126.86, 126.69, 126.01, 124.80, 124.17, 123.98, 123.79, 122.60, 115.77, 115.56, 111.79, 108.26, 91.77, 88.29, 73.10, 21.77. HRMS (ESI): m/z calcd for $\text{C}_{33}\text{H}_{24}\text{N}_4\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$ 541.1693, found: 541.1691; IR (KBr): 3055, 2929, 2214, 1608, 1597, 1577, 1506, 1458, 1363, 1336, 1171, 756 cm^{-1} .

Crystallographic data of 3a

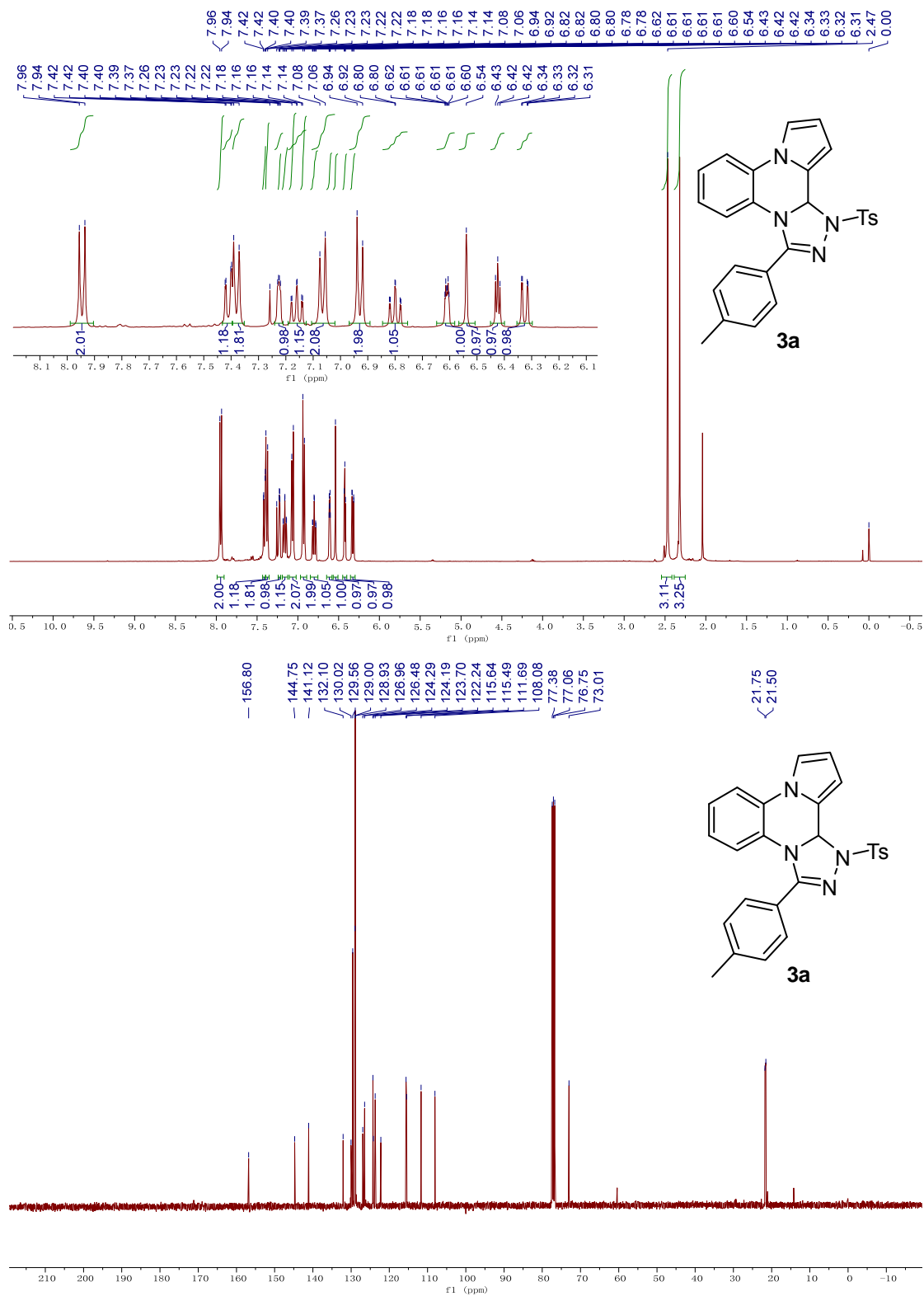


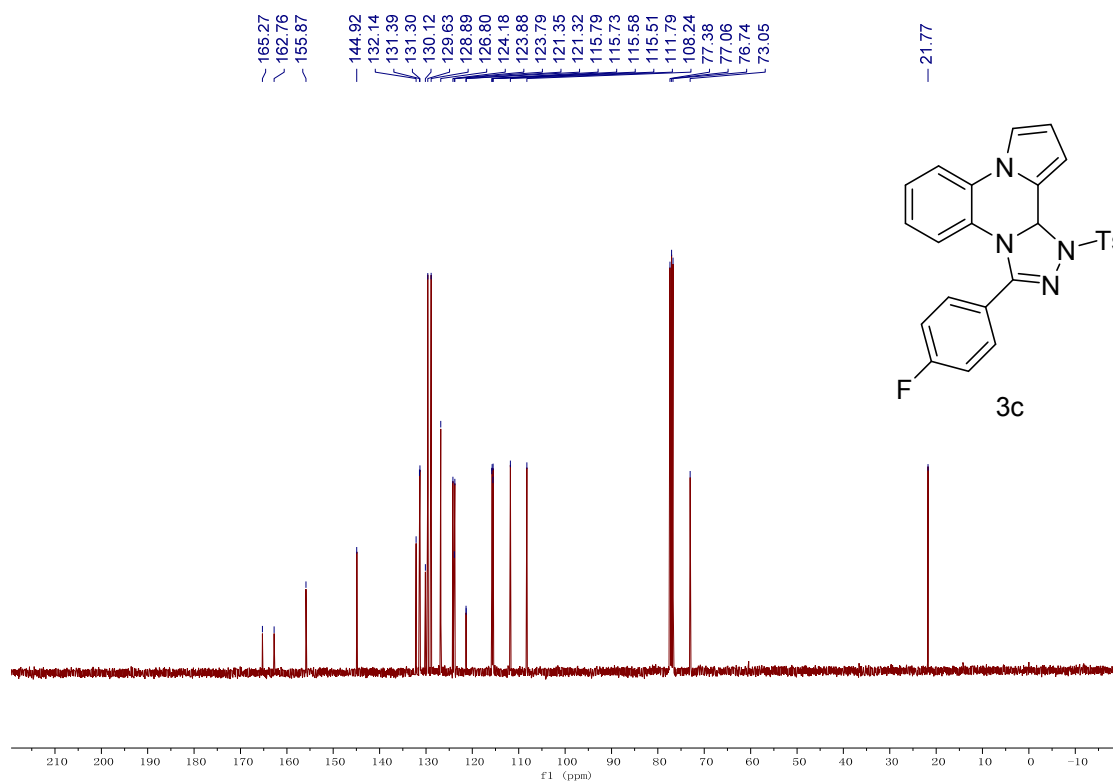
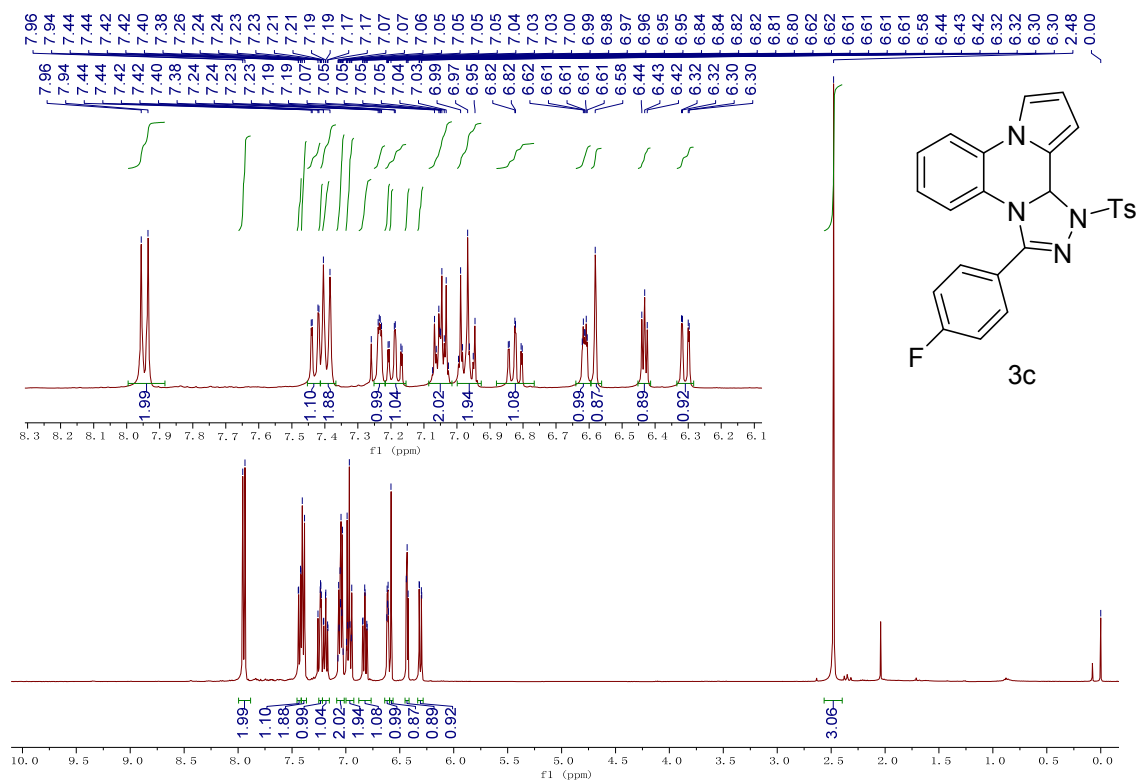
Structure of **3a**, CCDC: 1911560

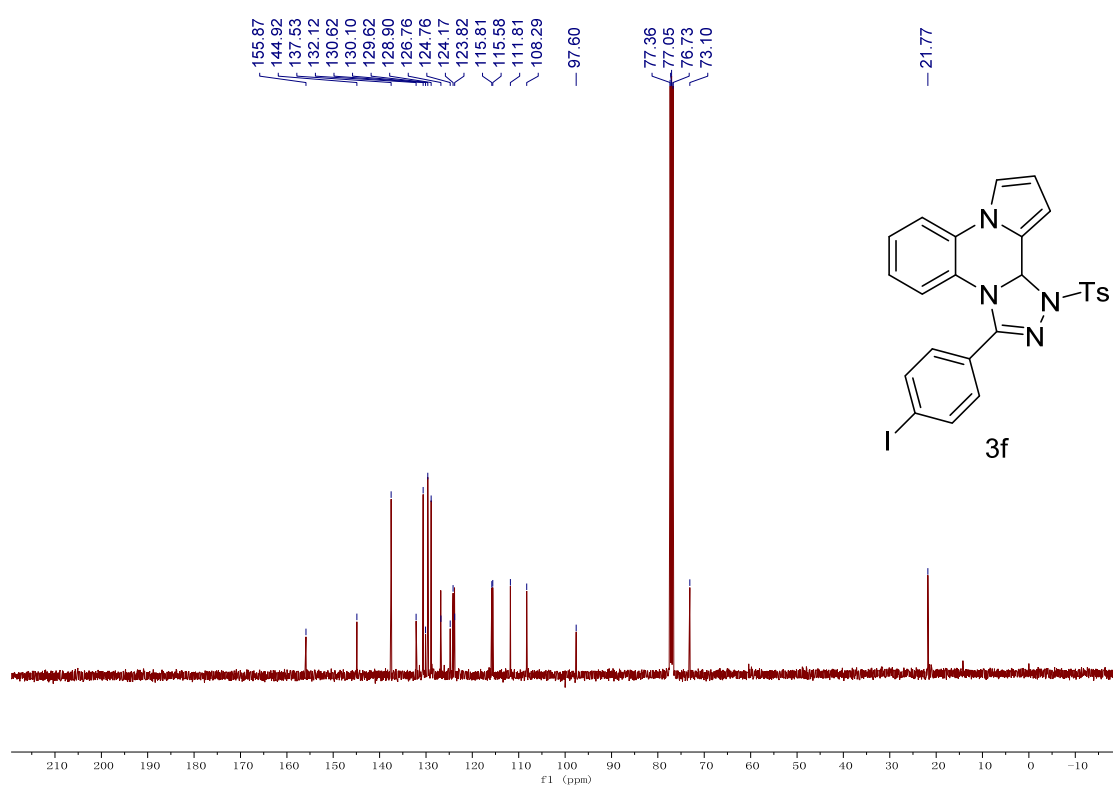
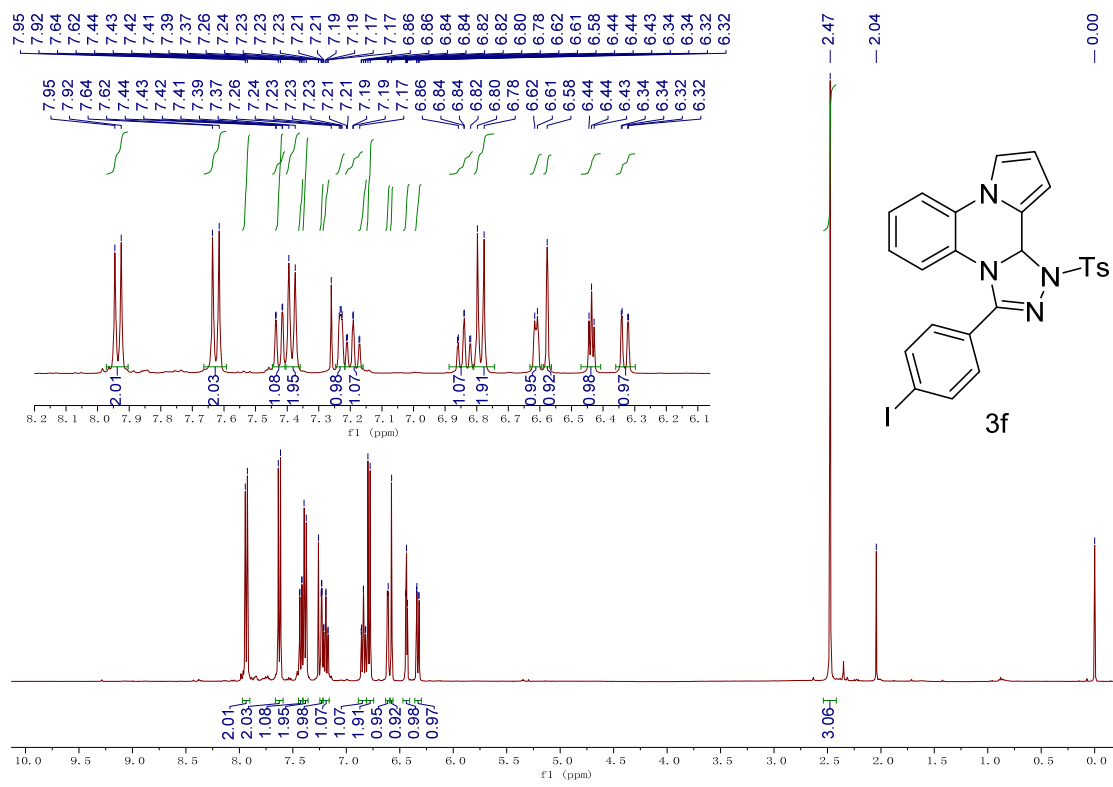
Table 1 Crystal data and structure refinement for **3a**.

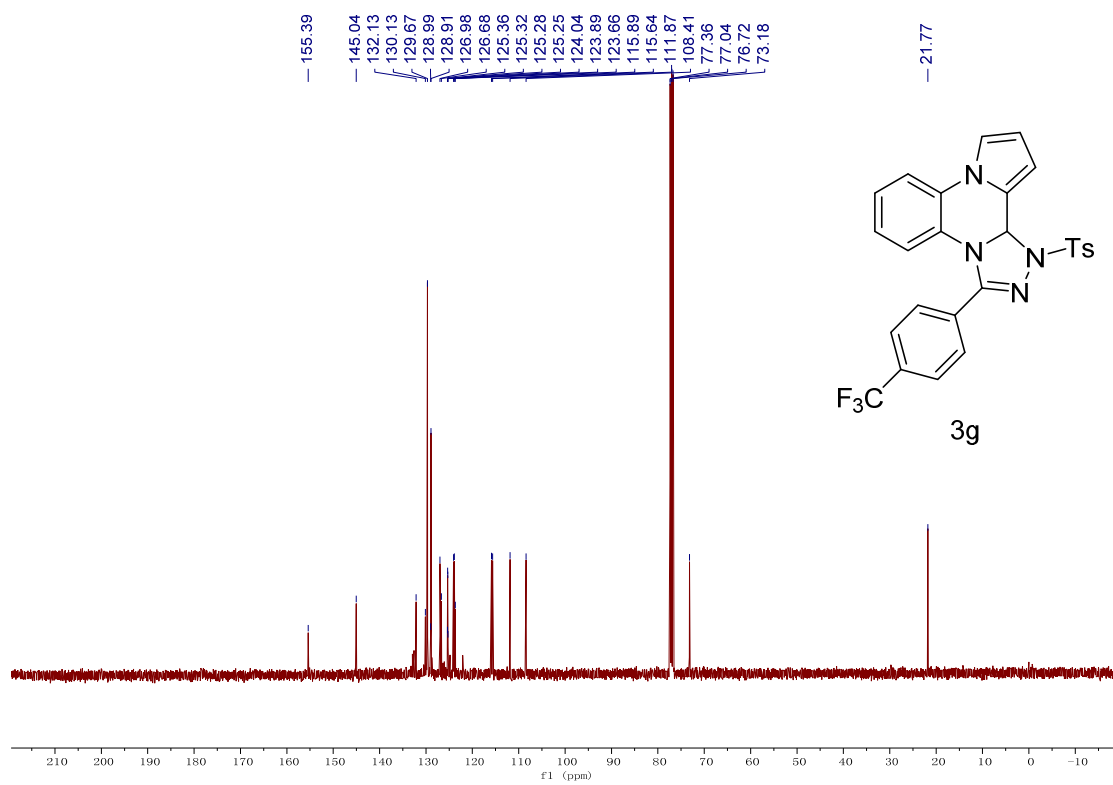
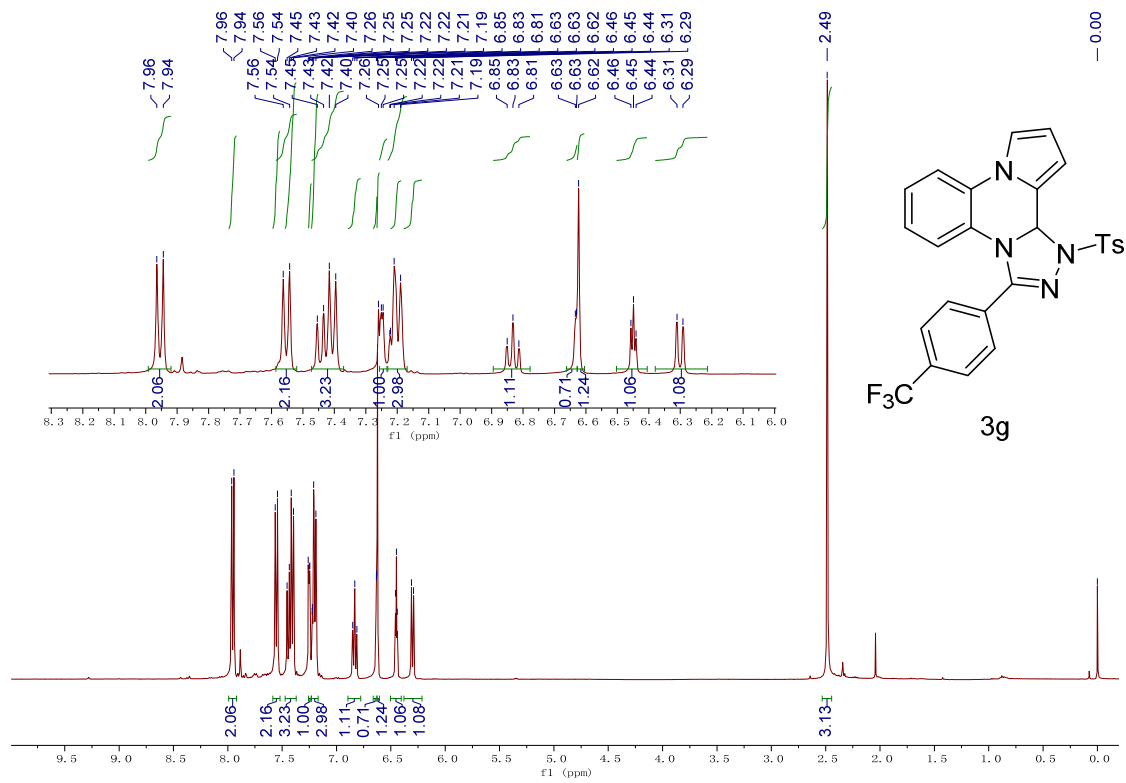
Identification code	3a
Empirical formula	C ₂₆ H ₂₂ N ₄ O ₂ S
Formula weight	454.53
Temperature/K	100.0
Crystal system	orthorhombic
Space group	Pca2 ₁
a/Å	11.5618(5)
b/Å	20.0595(10)
c/Å	20.7439(10)
α/°	90
β/°	90
γ/°	90
Volume/Å ³	4811.0(4)
Z	4
ρ _{calc} /cm ³	0.628
μ/mm ⁻¹	0.082
F(000)	952.0
Crystal size/mm ³	0.15 × 0.12 × 0.08
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	4.422 to 51
Index ranges	-13 ≤ h ≤ 14, -24 ≤ k ≤ 24, -25 ≤ l ≤ 25
Reflections collected	49632
Independent reflections	8922 [R _{int} = 0.1080, R _{sigma} = 0.0623]
Data/restraints/parameters	8922/605/301
Goodness-of-fit on F ²	1.096
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0924, wR ₂ = 0.2486
Final R indexes [all data]	R ₁ = 0.1026, wR ₂ = 0.2593
Largest diff. peak/hole / e Å ⁻³	0.44/-0.87
Flack parameter	0.6(2)

^1H , ^{13}C NMR Spectra for the Products









3g

