

Supporting Information for

One-Pot Synthesis of 1,4-Disubstituted 1,2,3-Triazoles from *in situ* Generated Azides

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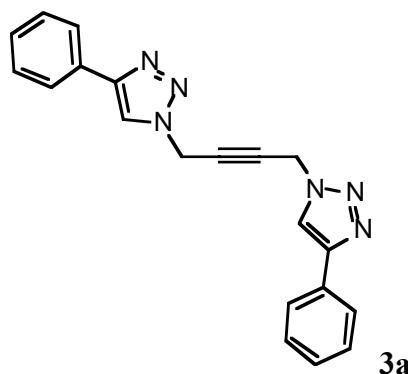
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The Scripps Research Institute, 10550 N. Torrey Pines Rd.,

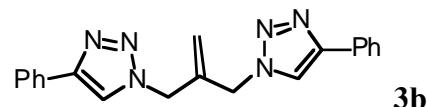
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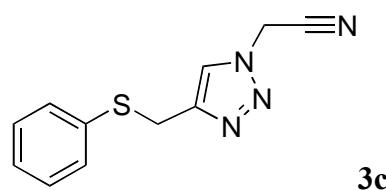
¹H and ¹³C NMR spectra were recorded on a Bruker AMX- 400, AMX-500 or AMX-600 spectrometers in CDCl₃ or d₆-DMSO with CHCl₃ (7.27 ppm for ¹H, 77 ppm for ¹³C) and DMSO (2.50 ppm for ¹H, 39.5 ppm for ¹³C) as standards. All melting points (mp) were taken on a Thomas Hoover Uni-melt melting point apparatus, and are uncorrected. Reagents and solvents were purchased from Aldrich, Acros or GFS and used without further purification.



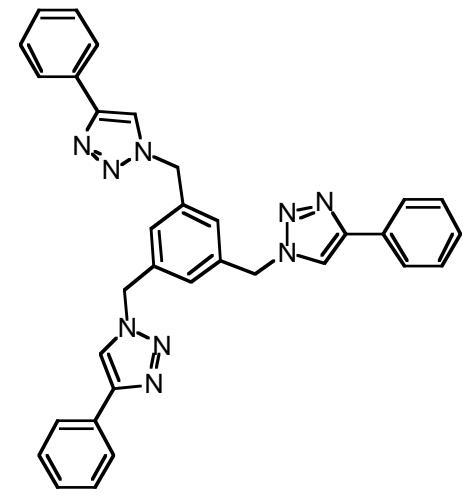
mp: 207-210 °C; EMS: m/z = 341.1 [M+H]⁺, calcd 341.1 [M+H]⁺. ¹H NMR (400MHz, *d*₆-DMSO) δ 8.68 (s, 2H), 7.86 (d, *J* = 8.2 Hz, 4H), 7.45 (t, *J* = 8.2 Hz, 4H), 7.33 (t, *J* = 7.0 Hz, 2H), 4.17 (s, 4H); ¹³C NMR (400MHz, *d*₆-DMSO) δ 146.7, 130.6, 129.0, 128.1, 125.3, 121.5, 79.4.



mp: 159-160 °C; EMS: m/z = 343.1 [M+H]⁺, calcd 343.2 [M+H]⁺. ¹H NMR (600MHz, *d*₆-DMSO) δ 8.54 (s, 2H), 7.85 (d, *J* = 8.3 Hz, 4H), 7.44 (t, *J* = 8.2 Hz, 4H), 7.33 (t, *J* = 7.4 Hz, 2H), 5.13 (s, 4H), 5.12 (s, 2H); ¹³C NMR (600MHz, *d*₆-DMSO) δ 146.5, 139.2, 130.6, 128.9, 127.9, 125.2, 121.9, 110.4, 51.8.

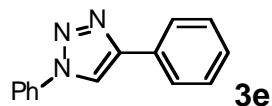


mp: 62-65 °C; EMS: m/z = 231.1 EMS: m/z = 231.1 [M+H]⁺, calcd 341.1 [M+H]⁺. ¹H NMR (400MHz, *d*₆-DMSO) δ 8.06 (s, 1H), 7.30 (m, 4H), 7.16 (t, *J* = 8.2 Hz, 1H), 5.67 (s, 2H), 4.27 (s, 2H); ¹³C NMR (400MHz, *d*₆-DMSO) δ 144.7, 135.2, 129.1, 128.2, 126.1, 124.1, 124.0, 114.9, 37.2, 26.7.

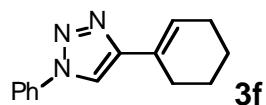


mp: 219-220 °C; EMS: m/z = 550.3 [M+H]⁺, calcd 550.2 [M+H]⁺. ¹H NMR (500MHz, *d*₆-DMSO) δ 8.60(s, 3H), 7.80 (d, *J* = 8.4 Hz, 6H), 7.41 (t, *J* = 7.3 Hz, 6H), 7.33 (m, 6H),

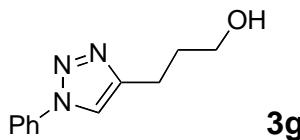
5.65 (s, 6H); ^{13}C NMR (400MHz, d_6 -DMSO) δ 146.7, 137.3, 130.6, 128.9, 127.9, 127.2, 125.2, 52.5.



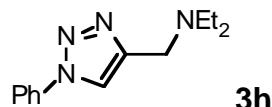
mp: 165-171 °C; EMS: m/z = 222.1 [M+H] $^+$, calcd 222.1 [M+H] $^+$. ^1H NMR (500MHz, CDCl_3) δ 8.33 (s, 1H), 7.97 (d, 2H), 7.82 (d, J = 8.1 Hz, 2H), 7.57 (t, J = 7.9 Hz, 2H), 7.49 (t, J = 3.3 Hz, 2H), 7.35-7.41 (m, 2H); ^{13}C NMR (500MHz, CDCl_3) δ 130.5, 129.6, 129.5, 129.2, 126.5, 121.3.



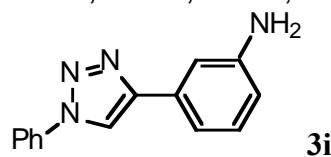
mp: 90-91 °C; EMS: m/z = 226.1 [M+H] $^+$, calcd 226.1 [M+H] $^+$. ^1H NMR (400MHz, d_6 -DMSO) δ 8.79 (s, 1H), 7.90 (d, J = 8.5 Hz, 2H), 7.56 (t, J = 7.6 Hz, 2H), 7.47 (t, J = 7.4 Hz, 1H), 6.53 (s, 1H), 2.40 (br s, 2H), 2.18 (br s, 2H), 1.72 (m, 2H), 1.63 (m, 2H); ^{13}C NMR (400MHz, d_6 -DMSO) δ 149.0, 136.7, 129.8, 128.4, 127.1, 124.3, 119.8, 117.9, 25.8, 24.7, 22.0, 21.8.



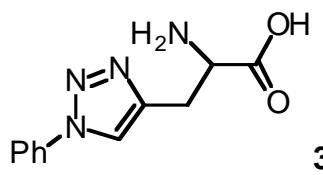
mp: 52 °C; EMS: m/z = 204.1 [M+H] $^+$, calcd 204.1 [M+H] $^+$. ^1H NMR (600MHz, CDCl_3) δ 7.80 (s, 1H), 7.68 (d, J = 7.9, 2H), 7.45 (t, J = 7.9, 2H), 7.39 (t, J = 7.4, 1H), 3.72 (t, J = 6.1, 2H), 2.90 (t, J = 7.5, 2H), 1.98 (q, J = 6.6, 2H); ^{13}C NMR (600MHz, CDCl_3) δ 148.2, 137.0, 129.6, 128.5, 120.3, 119.3, 61.3, 31.9, 21.8.



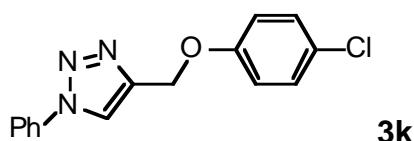
EMS: m/z = 231.1 [M+H] $^+$, calcd 231.2 [M+H] $^+$. ^1H NMR (500MHz, CDCl_3) δ 8.06 (s, 1H), 7.75 (d, J = 8.0 Hz, 2H), 7.54 (t, J = 5.3 Hz, 2H), 7.44 (t, J = 7.4 Hz, 1H), 3.94 (s, 2H), 2.68 (q, J = 7.0 Hz, 4H), 1.16 (t, J = 7.0 Hz, 6H); ^{13}C NMR (400MHz, CDCl_3) δ 130.1, 129.0, 121.6, 120.8, 48.0, 47.1, 11.8.



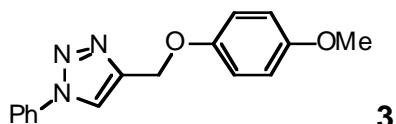
mp: 121-124 °C; EMS: m/z = 237.1 [M+H]⁺, calcd 237.1 [M+H]⁺. ¹H NMR (400MHz, *d*₆-DMSO) δ 9.15 (s, 1H), 7.97 (d, *J* = 7.6 Hz, 2H), 7.64 (t, *J* = 7.6 Hz, 2H), 7.48-7.53 (m, 1H), 7.21 (t, *J* = 1.9 Hz, 1H), 7.12 (t, *J* = 7.9 Hz, 1H), 7.04 (dt, *J* = 7.7 Hz, 1H), 6.56 (ddd, *J* = 7.9, 2.4, 0.9 Hz, 1H), 5.23 (s, 2H); ¹³C NMR (400MHz, *d*₆-DMSO) δ 149.2, 148.1, 136.7, 130.7, 129.9, 129.5, 128.6, 120.0, 119.2, 114.0, 113.3, 110.6.



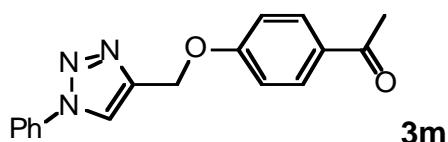
EMS: m/z = 233.1 [M+H]⁺, calcd 233.1 [M+H]⁺. ¹H NMR (400MHz, *d*₆-DMSO) δ 9.31 (s, 1H), 8.00 (s, 1H), 7.59 (m, 2H), 6.95 (s, 2H), 6.50 (s, 2H), 6.43 (s, 1H), 4.97 (br s, 2H), 2.95 (m, 1H); ¹³C NMR (600MHz, *d*₆-DMSO) δ 128.9, 115.6, 113.9, 40.4.



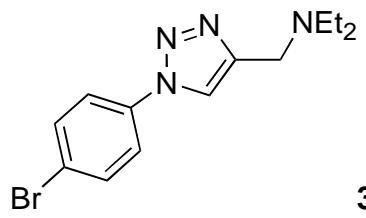
mp: 105-107 °C; EMS: m/z = 286.0 [M+H]⁺, calcd 286.1 [M+H]⁺. ¹H NMR (400MHz, *d*₆-DMSO) δ 8.97 (s, 1H), 7.90 (d, *J* = 7.9 Hz, 2H), 7.60 (t, *J* = 8.0 Hz, 2H), 7.49 (t, *J* = 8.0 Hz, 1H), 7.33 (d, *J* = 7.6 Hz, 2H), 7.11 (d, *J* = 8.8 Hz, 2H), 5.24 (s, 2H); ¹³C NMR (400MHz, *d*₆-DMSO) δ 156.9, 143.6, 136.6, 130.0, 129.4, 128.9, 124.8, 123.1, 120.2, 116.6, 61.3.



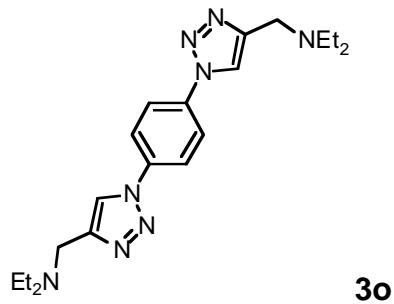
mp: 97-99 °C; EMS: m/z = 282.1 [M+H]⁺, calcd 282.1 [M+H]⁺. ¹H NMR (500MHz, *d*₆-DMSO) δ 8.12 (s, 1H), 7.75 (d, *J* = 8.0 Hz, 2H), 7.54 (t, *J* = 7.7 Hz, 2H), 7.46 (t, *J* = 7.4 Hz, 1H), 6.98 (d, *J* = 8.8 Hz, 2H), 6.86 (d, *J* = 8.5 Hz, 2H), 5.26 (s, 2H), 3.79 (s, 3H).



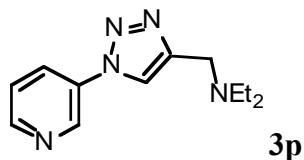
mp: 144-145 °C; EMS: m/z = 294.1 [M+H]⁺, calcd 294.1 [M+H]⁺. ¹H NMR (400MHz, *d*₆-DMSO) δ 8.97 (s, 1H), 7.93 (d, *J* = 8.5 Hz, 2H), 7.89 (d, *J* = 7.6 Hz, 2H), 7.58 (t, *J* = 7.6 Hz, 2H), 7.48 (t, *J* = 7.0 Hz, 1H), 7.17 (d, *J* = 8.5 Hz, 2H), 5.33 (s, 2H), 2.50 (s, 3H); ¹³C NMR (400MHz, *d*₆-DMSO) δ 196.4, 161.8, 143.4, 136.5, 130.5, 130.2, 129.9, 128.8, 123.1, 120.2, 114.6, 61.3, 26.5.



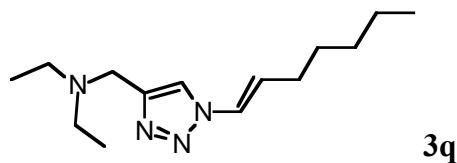
EMS: $m/z = 309.1$ [M+H]⁺, calcd 309.1 [M+H]⁺. ¹H NMR (400MHz, CDCl₃) δ 8.05 (s, 1H), 7.65 (s, 4H), 3.92 (s, 2H), 2.66 (q, 4H), 1.15 (t, 6H); ¹³C NMR (400MHz, CDCl₃) δ 136.0, 132.8, 122.2, 121.8, 121.0, 47.6, 46.7, 11.4.



mp: 135-138 °C; EMS: $m/z = 383.5$ [M+H]⁺, calcd 383.5 [M+H]⁺. ¹H NMR (500MHz, CDCl₃) δ 8.25 (s, 1H), 8.17 (s, 1H), 7.95 (s, 4H), 4.00 (s, 2H), 3.97 (s, 2H), 2.72 (q, $J = 7.0$ Hz, 8H), 1.19 (t, $J = 7.0$ Hz, 12H); ¹³C NMR (500MHz, CDCl₃) δ 137.5, 122.9, 122.2, 115.4, 48.3, 47.4, 47.3, 12.1, 11.8.

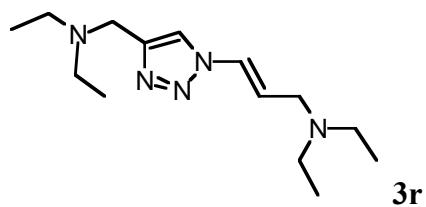


EMS: $m/z = 232.1$ [M+H]⁺, calcd 232.2 [M+H]⁺. ¹H NMR (400MHz, CDCl₃) δ 9.02 (s, 1H), 8.70 (d, $J = 4.0$ Hz, 1H), 8.15 (dt, $J = 8.2, 1.4$ Hz, 1H), 8.08 (s, 1H), 7.50 (dd, $J = 8.4, 4.8$ Hz, 1H), 3.92 (s, 2H), 2.66 (q, $J = 7.2$ Hz, 4H), 1.15 (t, $J = 7.0$ Hz, 6H); ¹³C NMR (400MHz, d₆-DMSO) δ 149.4, 145.3, 141.1, 133.4, 127.6, 124.6, 122.0, 46.6, 46.1, 11.9.



EMS: $m/z = 251.2$ [M+H]⁺, calcd 251.2 [M+H]⁺. ¹H NMR (500MHz, CDCl₃) δ 7.67 (s, 1H), 7.09 (d, $J = 14.3$ Hz, 1H), 6.19 (dt, $J = 14.3, 7.0$ Hz, 1H), 3.80 (s, 2H), 2.56 (q, $J = 6.9$ Hz, 4H), 2.21 (m, 2H), 1.50 (m, 2H); 1.33 (m, 4H), 1.09 (t, $J = 6.9$ Hz, 6H), 0.9 (m,

3H); ^{13}C NMR (500MHz, CDCl_3) δ 124.2, 123.1, 119.5, 47.6, 46.8, 31.2, 29.6, 28.6, 22.4, 14.0, 11.8.



EMS: $m/z = 266.2$ [M+H] $^+$, calcd 266.2 [M+H] $^+$. ^1H NMR (500MHz, CDCl_3) δ 7.71 (s, 1H), 7.28 (d, $J = 6.6$ Hz, 1H), 6.21 (dt, $J = 14.7, 6.6$ Hz, 1H), 3.81 (s, 2H), 3.26 (d, $J = 6.6$ Hz, 2H), 2.58 (m, 8H), 1.08 (m, 12H); ^{13}C NMR (400MHz, d_6 -DMSO) δ 143.5, 125.9, 121.3, 118.8, 50.8, 46.0, 45.9, 45.8, 11.5, 11.3.