Supporting Information
for

$N^1$-Selective alkenylation of 1-sulfonyl-1,2,3-triazoles with alkyne via gold catalysis

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1. General information

All reactions were performed using Schlenk tubes, septa, and syringes without protection of nitrogen. THF, toluene and DCM, DCE were freshly distilled over sodium/benzophenone and calcium hydride, respectively. Commercial reagents were used as supplied or were purified by standard techniques where necessary. Column chromatography was performed using Qingdao Haiyang Chemical Co., Ltd silica gel (200–300 mesh) with the appropriate solvent system, as determined by TLC analysis (Qingdao Haiyang Chemical Co., Ltd, silica gel F254) using UV light and KMnO₄ stain to visualize the reaction components. Melting points were determined using a WRS-1B digital melting point instrument. IR spectra were recorded on a Nicoletisso FTIR spectrometer using KBr disks. Unless otherwise noted, nuclear magnetic resonance spectra were recorded at room temperature on an Agilent 400 MHz spectrometer using CDCl₃ as the solvent and TMS as the internal reference. Chemical shifts for ¹³C NMR spectra were recorded in parts per million relative to tetramethylsilane using the central peak of deuterochloroform (77.0 ppm) as the internal standard. HRMS was performed using a Bruker Daltonics Bio TOF mass spectrometer.

1-Sulfonyl-1,2,3-trizoles 1a-1j were prepared according to the published methods.¹ Alkyne were obtained commercially and used without further purification.

**General procedure for N¹-Selective gold-catalyzed alkenylation of 4-phenyl-1-sulfonyl-1,2,3-trizole 1a with phenylacetylene 2a.**

To a Schlenk tube charged with nitrogen was added IPrAuCl/AgOTf (5 mol%) in dry DCE (3 mL). After three minutes, 4-phenyl-1-sulfonyl-1,2,3-trizole 1a (0.1 mmol), phenylacetylene 2a (0.5 mmol) and H₂O (0.2 mmol) were added to the reaction. Then the reaction mixture was stirred at 80 °C for 12 h until complete consumption of starting material as monitored by TLC. Concentration of the reaction mixture in vacuo followed by purification through flash chromatography on silica gel column (hexane/EtOAc = 30/1) afforded 3a (22.8 mg, 92% yield) as yellow oily liquid.
2. Spectral Data

4-phenyl-1-(1-phenylvinyl)-1H-1,2,3-triazole (3a)

Yellow oily liquid; yield, 92% (22.8 mg); IR (neat) 3038, 2934, 1496, 1459, 756 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.84 (d, \(J = 7.6\) Hz, 2H), 7.79 (s, 1H), 7.43 – 7.21 (m, 8H), 5.85 (s, 1H), 5.54 (s, 1H); \(^13\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 147.48, 142.86, 134.51, 130.09, 129.83, 128.80, 128.79, 128.27, 127.26, 125.71, 119.78, 109.37; HRMS (ESI) calcd for C\(_{16}\)H\(_{14}\)N\(_3\)\(^+\) [M+H]\(^+\) 248.1182; found, 248.1182.

4-phenyl-1-(1-(p-tolyl)vinyl)-1H-1,2,3-triazole (3b)

Yellow oily liquid; yield, 88% (23.0 mg); IR (neat) 3038, 2937, 1499, 1457, 756 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.84 (d, \(J = 7.2\) Hz, 2H), 7.80 (s, 1H), 7.41 (t, \(J = 7.5\) Hz, 2H), 7.33 (t, \(J = 7.4\) Hz, 1H), 7.24 (q, \(J = 8.0\) Hz, 4H), 5.80 (s, 1H), 5.50 (s, 1H), 2.39 (s, 3H); \(^13\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 147.39, 142.85, 140.04, 131.69, 130.12, 129.47, 128.78, 128.25, 127.18, 125.71, 119.80, 108.58, 21.24; HRMS (ESI) calcd for C\(_{17}\)H\(_{16}\)N\(_3\)\(^+\) [M+H]\(^+\) 262.1339; found, 262.1339.

4-phenyl-1-(1-(4-propylphenyl)vinyl)-1H-1,2,3-triazole (3c)

Yellow oily liquid; yield, 86% (24.9 mg); IR (neat) 3038, 2937, 1496, 1460, 762 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.85 (d, \(J = 7.1\) Hz, 2H), 7.81 (s, 1H), 7.42 (t, \(J = 7.5\) Hz, 2H), 7.33 (t, \(J = 7.4\) Hz, 1H), 7.28 (d, \(J = 8.2\) Hz, 2H), 7.22 (d, \(J = 8.2\) Hz, 2H), 5.80 (s, 1H), 5.51 (s, 1H), 2.65 – 2.60 (m, 2H), 1.71 – 1.62 (m, 2H), 0.97 (t, \(J = 7.3\) Hz, 3H); \(^13\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 147.42, 144.82, 142.92, 131.92, 130.18, 128.88, 128.78, 128.24, 127.16, 125.74, 119.84, 108.64, 37.72, 24.32, 13.77. HRMS (ESI) calcd for C\(_{19}\)H\(_{20}\)N\(_3\)\(^+\) [M+H]\(^+\) 290.1652; found, 290.1652.
1-(1-(4-(tert-butyl)phenyl)vinyl)-4-phenyl-1H-1,2,3-triazole (3d)

Yellow oily liquid; yield, 88% (26.7 mg); IR (neat) 3041, 2937, 1502, 1457, 756 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.85 (d, \(J = 7.6\) Hz, 2H), 7.81 (s, 1H), 7.45 – 7.40 (m, 4H), 7.35 – 7.30 (m, 3H), 5.82 (s, 1H), 5.52 (s, 1H), 1.35 (s, 9H); \(^13\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 153.22, 147.48, 142.86, 131.68, 130.24, 128.81, 128.26, 127.04, 125.79, 125.78, 119.86, 108.69, 34.78, 31.18; HRMS (ESI) calcd for C\(_{20}\)H\(_{22}\)N\(_3\) \([\text{M+H}]^+\) 304.1808; found, 304.1807.

1-(1-(4-methoxyphenyl)vinyl)-4-phenyl-1H-1,2,3-triazole (3e)

Yellow oily liquid; yield, 78% (21.6 mg); IR (neat) 3035, 2931, 1499, 1457, 759 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 8.01 (s, 1H), 7.85 (d, \(J = 7.2\) Hz, 2H), 7.46 – 7.36 (m, 5H), 6.94 (d, \(J = 8.8\) Hz, 2H), 5.87 (s, 1H), 5.33 (s, 1H), 3.85 (s, 3H); \(^13\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 160.40, 148.56, 145.75, 132.32, 129.92, 129.63, 128.88, 128.80, 127.20, 126.18, 113.71, 110.00, 105.98, 55.34; HRMS (ESI) calcd for C\(_{17}\)H\(_{16}\)N\(_3\)O \([\text{M+H}]^+\) 278.1288; found, 278.1288.

1-(1-(4-fluorophenyl)vinyl)-4-phenyl-1H-1,2,3-triazole (3f)

Yellow oily liquid; yield, 63% (16.7 mg); IR (neat) 3035, 2937, 1499, 1457, 758 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.85 (d, \(J = 7.3\) Hz, 2H), 7.81 (s, 1H), 7.43 (t, \(J = 7.5\) Hz, 2H), 7.39 – 7.33 (m, 3H), 7.12 (t, \(J = 8.6\) Hz, 2H), 5.82 (s, 1H), 5.52 (s, 1H); \(^13\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 163.55 (d, \(J = 249.2\) Hz), 147.63, 142.02, 129.94 (d, \(J = 4.8\) Hz), 129.32 (d, \(J = 8.4\) Hz), 128.86, 128.42, 127.94, 125.78, 119.69, 115.95 (d, \(J = 21.8\) Hz), 109.28; HRMS (ESI) calcd for C\(_{16}\)H\(_{13}\)FN\(_3\) \([\text{M+H}]^+\) 266.1088; found, 266.1089.
1-(1-(4-chlorophenyl)vinyl)-4-phenyl-1H-1,2,3-triazole (3g)

White solid; M p, 109.7 – 111.6 ºC; yield, 75% (21.1 mg); IR (neat) 3038, 2934, 1496, 1454, 762 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.85 (d, J = 7.7 Hz, 2H), 7.81 (s, 1H), 7.45 – 7.39 (m, 4H), 7.37 – 7.31 (m, 3H), 5.84 (s, 1H), 5.56 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 147.73, 142.01, 135.97, 133.01, 129.98, 129.10, 128.87, 128.63, 128.43, 125.78, 119.66, 109.78; HRMS (ESI) calcd for C₁₆H₁₃ClN₃⁺ [M+H]⁺ 282.0793; found, 282.0793.

1-(1-(4-bromophenyl)vinyl)-4-phenyl-1H-1,2,3-triazole (3h)

Yellow oily liquid; yield, 81% (26.3 mg); IR (neat) 3038, 2935, 1496, 1460, 762 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.85 (d, J = 7.1 Hz, 2H), 7.81 (s, 1H), 7.57 (d, J = 8.5 Hz, 2H), 7.44 (t, J = 7.4 Hz, 2H), 7.36 (t, J = 7.4 Hz, 1H), 7.25 (d, J = 6.4 Hz, 2H), 5.86 (s, 1H), 5.57 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 147.77, 142.09, 133.49, 132.09, 129.98, 129.10, 128.87, 128.43, 125.78, 119.64, 109.99, 109.84; HRMS (ESI) calcd for C₁₆H₁₃BrN₃⁺ [M+H]⁺ 326.0287; found, 326.0287.

1-(1-(3-fluorophenyl)vinyl)-4-phenyl-1H-1,2,3-triazole (3i)

Yellow oily liquid; yield, 25% (6.7 mg); IR (neat) 3035, 2934, 1501, 758, 702 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.86 (d, J = 7.3 Hz, 2H), 7.82 (s, 1H), 7.44 (t, J = 7.5 Hz, 2H), 7.40 – 7.34 (m, 2H), 7.19 – 7.07 (m, 3H), 5.88 (s, 1H), 5.61 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 162.76 (d, J = 274.3 Hz), 147.65, 141.80, 130.53 (d, J = 8.3 Hz), 128.88, 128.45, 125.82, 123.02 (d, J = 3.1 Hz), 119.72, 116.92 (d, J = 21.1 Hz), 114.44 (d, J = 23.1 Hz), 110.48; HRMS (ESI) calcd for C₁₆H₁₃FN₃⁺ [M+H]⁺ 266.1088; found, 266.1088.

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1-(hex-1-en-2-yl)-4-phenyl-1H-1,2,3-triazole (3j)
White solid; M p, 78.8 – 79.9 °C; yield, 64% (24.9 mg); IR (neat) 3038, 2934, 1499, 1459, 702 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.97 (s, 1H), 7.87 (d, J = 7.4 Hz, 2H), 7.44 (t, J = 7.5 Hz, 2H), 7.35 (t, J = 7.4 Hz, 1H), 5.47 (s, 1H), 5.01 (s, 1H), 2.79 (t, J = 7.6 Hz, 2H), 1.62 – 1.54 (m, 2H), 1.47 – 1.38 (m, 2H), 0.94 (t, J = 7.3 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 147.48, 143.87, 130.24, 128.85, 128.31, 125.79, 117.28, 109.99, 104.00, 32.58, 29.16, 22.12, 13.79; HRMS (ESI) calcd for C₁₄H₁₈N₃⁺ [M+H]⁺ 228.1495; found, 228.1498.

1-(1-cyclopentylvinyl)-4-phenyl-1H-1,2,3-triazole (3k)
White solid; M p, 56.9 – 57.8 °C; yield, 80% (19.2 mg); IR (neat) 3041, 2934, 1608, 1499, 756 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.97 (s, 1H), 7.87 (d, J = 7.2 Hz, 2H), 7.43 (t, J = 7.5 Hz, 2H), 7.34 (t, J = 7.4 Hz, 1H), 5.44 (s, 1H), 5.07 (s, 1H), 3.38 – 3.28 (m, 1H), 2.06 – 2.02 (m, 2H), 1.80 – 1.73 (m, 2H), 1.72 – 1.63 (m, 2H), 1.61 – 1.51 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 147.48, 143.87, 130.24, 128.85, 128.31, 125.79, 117.28, 109.99, 104.00, 32.58, 29.16, 22.12, 13.79; HRMS (ESI) calcd for C₁₅H₁₈N₃⁺ [M+H]⁺ 240.1495; found, 240.1493.

1-(1-cyclopropylvinyl)-4-phenyl-1H-1,2,3-triazole (3l)
Yellow oily liquid; yield, 64% (13.5 mg); IR (neat) 3041, 2934, 1605, 1501, 1457, 761 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.07 (s, 1H), 7.81 (d, J = 6.8 Hz, 2H), 7.38 (t, J = 7.2 Hz, 2H), 7.28 (t, J = 7.3 Hz, 1H), 5.67 (s, 1H), 4.89 (s, 1H), 1.86 – 1.79 (m, 1H), 0.95 – 0.90 (m, 2H), 0.73 – 0.70 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 130.32, 128.82, 128.22, 125.72, 117.32, 109.97, 102.91, 13.39, 6.44; HRMS (ESI) calcd for C₁₃H₁₄N₃⁺ [M+H]⁺ 212.1182; found, 212.1182.
Yellow oily liquid; yield, 58% (14.7 mg); IR (neat) 3061, 2974, 2381, 1429, 768 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.81 (d, \(J = 7.7\) Hz, 2H), 7.47 (s, 1H), 7.37 (t, \(J = 7.5\) Hz, 2H), 7.27 (t, \(J = 7.3\) Hz, 1H), 5.54 (t, \(J = 7.4\) Hz, 1H), 2.46 (t, \(J = 7.3\) Hz, 2H), 1.89 (q, \(J = 7.2\) Hz, 2H), 1.38 – 1.30 (m, 4H), 0.87 – 0.83 (m, 3H), 0.83 – 0.79 (m, 3H). \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 146.85, 136.00, 130.46, 128.82, 128.12, 127.31, 125.66, 120.21, 109.97, 38.10, 29.16, 22.49, 20.12, 13.68, 13.26.

Yellow oily liquid; yield, 67% (17.5 mg); IR (neat) 3041, 2934, 1501, 1457, 759 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.75 (d, \(J = 3.3\) Hz, 2H), 7.72 (s, 1H), 7.47 – 7.34 (m, 5H), 7.22 (d, \(J = 7.6\) Hz, 2H), 5.84 (s, 1H), 5.53 (s, 1H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 147.60, 142.94, 138.15, 134.60, 129.81, 129.48, 128.79, 127.30, 125.65, 119.43, 109.26, 21.24; HRMS (ESI) calcd for C\(_{17}\)H\(_{16}\)N\(_3\) \([M+H]^+\) 262.1339; found, 262.1339.

Yellow oily liquid; yield, 84% (24.4 mg); IR (neat) 3035, 2934, 1496, 1457, 703 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.80 – 7.77 (m, 2H), 7.76 (s, 1H), 7.44 – 7.42 (m, 3H), 7.39 – 7.37 (m, 2H), 5.88 (s, 1H), 5.56 (s, 1H), 2.61 (t, \(J = 7.5\) Hz, 2H), 1.71 – 1.61 (m, 2H), 0.95 (t, \(J = 7.3\) Hz, 3H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 143.25, 142.94, 134.53, 129.92, 129.00, 128.88, 127.84, 127.36, 125.78, 119.60, 110.00, 109.55, 37.81, 24.44, 13.76; HRMS (ESI) calcd for C\(_{19}\)H\(_{20}\)N\(_3\) \([M+H]^+\) 290.1652; found, 290.1652.
4-(4-(tert-butyl)phenyl)-1-(1-phenylvinyl)-1H-1,2,3-triazole (4d)
Yellow oily liquid; yield, 75% (23.1 mg); IR (neat) 3038, 2937, 1499, 1454, 758, 700 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.79 – 7.77 (m, 3H), 7.51 – 7.31 (m, 7H), 5.85 (s, 1H), 5.54 (s, 1H), 1.34 (s, 9H); ¹³C NMR (100 MHz, CDCl₃) δ 151.43, 147.53, 142.93, 134.63, 129.82, 128.80, 127.30, 125.73, 125.50, 119.50, 109.29, 34.63, 31.23; HRMS (ESI) calcd for C₂₀H₂₂N₃⁺ [M+H]⁺ 304.1808; found, 304.1807.

4-(4-methoxyphenyl)-1-(1-phenylvinyl)-1H-1,2,3-triazole (4e)
Yellow oily liquid; yield, 47% (13.3 mg); IR (neat) 3038, 2932, 1628, 1499, 756 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.78 (d, J = 8.8 Hz, 2H), 7.72 (s, 1H), 7.49 – 7.40 (m, 3H), 7.39 – 7.37 (m, 2H), 6.96 (d, J = 7.8 Hz, 2H), 5.86 (s, 1H), 5.55 (s, 1H), 3.85 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 159.82, 142.98, 134.58, 129.91, 128.87, 127.38, 127.20, 122.58, 119.06, 114.30, 110.01, 109.45, 55.33; HRMS (ESI) calcd for C₁₇H₁₆N₃O⁺ [M+H]⁺ 278.1288; found, 278.1287.

4-(4-fluorophenyl)-1-(1-phenylvinyl)-1H-1,2,3-triazole (4f)
Yellow oily liquid; yield, 64% (17.1 mg); IR (neat) 3035, 2934, 1499, 1457, 761 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.86 – 7.78 (m, 2H), 7.76 (s, 1H), 7.48 – 7.39 (m, 3H), 7.38 – 7.36 (m, 2H), 7.11 (t, J = 8.6 Hz, 2H), 5.85 (s, 1H), 5.55 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 162.69 (d, J = 246.1 Hz), 146.67, 142.88, 134.49, 129.89, 128.84, 127.50 (d, J = 8.2 Hz), 127.29, 126.38 (d, J = 3.3 Hz), 119.55, 115.81 (d, J = 21.6 Hz), 109.44; HRMS (ESI) calcd for C₁₀H₁₃FN₃⁺ [M+H]⁺ 266.1088; found, 266.1088.
4-(4-chlorophenyl)-1-(1-phenylvinyl)-1H-1,2,3-triazole (4g)

Yellow oily liquid; yield, 70% (20.0 mg); IR (neat) 3041, 2937, 1496, 1460, 705 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.81 – 7.78 (m, 2H), 7.77 (s, 1H), 7.48 – 7.32 (m, 7H), 5.86 (s, 1H), 5.56 (s, 1H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 146.47, 142.86, 134.44, 134.09, 129.95, 129.04, 128.88, 127.31, 127.02, 119.87, 109.57; HRMS (ESI) calcd for C\(_{16}\)H\(_{13}\)ClN\(_3\) \([M+H]^+\) 282.0793; found, 282.0792.

4-(2-fluorophenyl)-1-(1-phenylvinyl)-1H-1,2,3-triazole (4h)

Yellow oily liquid; yield, 62% (16.5 mg); IR (neat) 3035, 2931, 1496, 1457, 758 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 8.37 (td, \(J = 7.6, 1.8\) Hz, 1H), 7.99 (d, \(J = 3.6\) Hz, 1H), 7.44 – 7.40 (m, 3H), 7.39 – 7.36 (m, 2H), 7.34 – 7.27 (m, 2H), 7.15 – 7.11 (m, 1H), 5.86 (s, 1H), 5.59 (s, 1H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 159.17 (d, \(J = 246.8\) Hz), 142.97, 134.47, 129.89, 129.50 (d, \(J = 8.5\) Hz), 128.83, 127.92 (d, \(J = 3.5\) Hz), 127.24, 124.62 (d, \(J = 3.3\) Hz), 122.92 (d, \(J = 12.8\) Hz), 115.65 (d, \(J = 21.5\) Hz), 109.64; HRMS (ESI) calcd for C\(_{16}\)H\(_{13}\)FN\(_3\) \([M+H]^+\) 266.1088; found, 266.1084.

4-(3-fluorophenyl)-1-(1-phenylvinyl)-1H-1,2,3-triazole (4i)

Yellow oily liquid; yield, 58% (15.5 mg); IR (neat) 3035, 2931, 1496, 1457, 758 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.81 (s, 1H), 7.59 (t, \(J = 10.2\) Hz, 2H), 7.45 – 7.41 (m, 3H), 7.38 (s, 3H), 7.03 (t, \(J = 8.4\) Hz, 1H), 5.87 (s, 1H), 5.57 (s, 1H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 163.12 (d, \(J = 244.5\) Hz), 142.85, 134.46, 132.32 (d, \(J = 8.5\) Hz), 130.43 (d, \(J = 8.5\) Hz), 129.97, 128.90, 127.32, 121.37 (d, \(J = 3.0\) Hz), 120.17, 115.14 (d, \(J = 21.1\) Hz), 112.73 (d, \(J = 22.9\) Hz), 109.98, 109.60; HRMS (ESI) calcd for C\(_{16}\)H\(_{13}\)FN\(_3\) \([M+H]^+\) 266.1088; found, 266.1088.
1-(1-phenylvinyl)-4-(thiophen-3-yl)-1H-1,2,3-triazole (4j)

Yellow oily liquid; yield, 84% (21.3 mg); IR (neat) 3038, 2934, 1501, 1460, 759 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.72 (s, 1H), 7.70 (s, 1H), 7.46 – 7.41 (m, 4H), 7.39 – 7.36 (m, 3H), 5.85 (s, 1H), 5.55 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 143.74, 142.87, 134.56, 131.37, 129.87, 128.83, 127.30, 126.39, 125.74, 121.42, 119.57, 109.42; HRMS (ESI) calcd for C₁₄H₁₂N₃S⁺ [M+H]⁺ 254.0746; found, 254.0747.

3. References

4. Deuterium-Labeling Experiment Result

The incorporation of deuterium at the f1 = 5.53 ppm of 3a is (1-0.25)/1*100% = 75%.
5. $^1$H and $^{13}$C NMR Spectra