Supporting Information

Synthesis of Allene Triazole through Iron Catalyzed Regioselective Addition to Propargyl Alcohols

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II. Compounds CharacterizationIII. ORTEP Drawing of the Crystal Structure	\$3-\$25 \$26-\$30

I. General Methods and Materials

All of the reactions dealing with air and/or moisture-sensitive reactions were carried out under an atmosphere of nitrogen using oven/flame-dried glassware and standard syringe/septa techniques. Unless otherwise noted, all commercial reagents and solvents were obtained from the commercial provider and used without further purification. ¹H NMR and ¹³C NMR spectra were recorded on Varian 600 MHz spectrometers. Chemical shifts were reported relative to internal tetramethylsilane (δ 0.00 ppm) or CDCl₃ (δ 7.26 ppm) for ¹H and CDCl₃ (δ 77.0 ppm) for ¹³C. Melting points were measured on a Mel-Temp 1001D apparatus and uncorrected. Infrared (IR) spectra were obtained on a FT-IR spectrometer.Flash column chromatography was performed on 230-430 mesh silica gel. Analytical thin layer chromatography was performed with precoated glass baked plates (250µ) and visualized by fluorescence and by charring after treatment with *p*-anisaldehyde or potassium permanganate stain. HRMS were recorded on LTQ-FTUHRA spectrometer. UV-visible spectra were obtained on a Shimadzu UV-2550.

Propargylic alcohols **3** were synthesized according to the literatures as below: Yan, W.; Wang, Q.; Chen, Y.; Petersen, J.; Shi, X. *Org. Lett.* **2010**, *12*, 3308-3311.

Representative procedure for propargylation of 4 with triazoles



A solution of triazole (1.3 mmol) with catalyst iron(III) chloride (0.1 mmol) in 1,2dichlorethane(DCE) (5 ml) was stirred at 60 °C for one hour, then propargyl alcohol **3** (1.0 mmol) was added. The reaction mixture was quenched with 10 ml distilled water and then extracted with EtOAc (3 x 10 mL) after 5 hours. The combined organic phases were washed with water and brine, dried with anhydrous MgSO₄, and filtered. The filtrate was concentrated under reduced pressure and the residue was purified by flash chromatography on silica gel (hexanes/ethyl acetate, V/V, 20/1) to produce the desired product.

II. Compounds Characterization



1-(1-(trimethylsilyl)-3,3-diphenylpropa-1,2-dienyl)-1*H*-benzo[*d*][1,2,3]triazole (4a) was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as white solid. Isolated yield 84%; m. p. 127-129 °C; R*f* (hexanes/ethyl acetate, V/V, 10/1) = 0.49; UV absorption: 232(0.182), 263(0.134), 295(0.126); IR (neat), 2957, 1598, 1489, 1447, 1285, 1245, 1062, 936, 833, 767, 694; ¹H-NMR (600 MHz, CDCl₃) δ 8.09 (d, *J* = 7.8 Hz, 1H), 7.82 (d, *J* = 7.8 Hz, 1H), 7.50-7.47 (m, 4H), 7.43-7.38 (m, 5H), 7.37-7.32 (m, 3H), 0.50 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 200.4 (C), 146.2 (C), 135.8 (C), 132.5 (C), 128.7 (CH), 128.4 (CH), 128.1 (CH), 127.9 (CH), 124.3 (CH), 118.0 (CH), 115.3 (C), 111.9 (CH), 108.8 (C), -0.5 (CH₃); HRMS Calculated for C₂₄H₂₄N₃Si [M+H]⁺: 382.1734, Found: 382.1735.



1-(1,1-diphenylhepta-1,2-dien-3-yl)-1*H***-benzo[***d***][1,2,3]triazole (4b) was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 74%; R***f* **(hexanes/ethyl acetate, V/V, 10/1) = 0.45; UV absorption: 233(0.160), 259(0.129), 295(0.100); IR (neat), 2935, 1603, 1485, 1447, 1281, 1244, 1056, 957, 785, 744, 691; ¹H-NMR (600 MHz, CDCl₃) \delta 8.08 (d,** *J* **= 7.8 Hz, 1H), 7.54 (d,** *J* **= 7.8 Hz, 1H), 7.46-7.43 (m, 4H), 7.42-7.30 (m, 8H), 3.22 (t,** *J* **= 7.8 Hz, 2H), 1.75 (quin,** *J* **= 7.8 Hz, 2H), 1.47 (sex,** *J* **= 7.8 Hz, 2H), 0.93 (t,** *J* **= 7.8 Hz, 3H); ¹³C-NMR (150 MHz, CDCl₃) \delta 197.0 (C), 146.3 (C), 135.9 (C), 132.1 (C), 128.7 (CH), 128.6 (CH), 128.4 (CH), 127.9 (CH), 124.3 (CH), 120.0 (CH), 119.8 (C), 113.5 (C), 111.6 (CH), 31.2 (CH₂), 29.2 (CH₂), 22.3 (CH₂), 13.8 (CH₃); HRMS Calculated for C₂₅H₂₄N₃ [M+H]⁺: 366.1965, Found: 366.1964.**



1-(1-(trimethylsilyl)-3-phenyl-3*p***-tolylpropa-1,2-dienyl)-1***H***-benzo**[*d*][1,2,3]triazole (4c) was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 80%; R*f* (hexanes/ethyl acetate, V/V, 10/1) = 0.51; UV absorption: 234(0.301), 263(0.209), 299(0.195); IR (neat), 2930, 1600, 1485, 1449, 1281, 1246, 1068, 935, 838, 764, 693; ¹H-NMR (600 MHz, CDCl₃) δ 8.07 (d, *J* = 7.8 Hz, 1H), 7.79 (d, *J* = 7.8 Hz, 1H), 7.44 (d, *J* = 7.8 Hz, 2H), 7.40-7.36 (m, 4H), 7.35-7.32 (m, 3H), 7.20 (d, *J* = 7.8 Hz, 2H), 2.38 (s, 3H), 0.46 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 200.4 (C), 146.2 (C), 138.0 (C), 136.0 (C), 132.8 (C), 132.5 (C), 129.5 (CH), 128.7 (CH), 128.5 (CH), 128.4 (CH), 128.0 (CH), 127.8 (CH), 124.3 (CH), 120.0 (CH), 115.2 (C), 112.0 (CH), 108.7 (C), 21.2 (CH₃), -0.5 (CH₃); HRMS Calculated for C₂₅H₂₆N₃Si [M+H]⁺: 396.1887, Found: 396.1883.



1-(1-cyclopropyl-3,3-diphenylpropa-1,2-dienyl)-1*H*-benzo[*d*][1,2,3]triazole (4d) was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as white solid. Isolated yield 82%; m. p. 107-109 °C; R*f* (hexanes/ethyl acetate, V/V, 10/1) = 0.48; UV absorption: 229(0.205), 260(0.146), 295(0.102); IR (neat), 3008, 1598, 1490, 1449, 1278, 1161, 1078, 977, 853, 747, 692; ¹H-NMR (600 MHz, CDCl₃) δ 8.09-8.07 (m, 1H), 7.54-7.51 (m, 1H), 7.41-7.32 (m, 12H), 2.51-2.45 (m, 1H), 1.13-1.09 (m, 2H), 0.85-0.81 (m, 2H); ¹³C-NMR (150 MHz, CDCl₃) δ 196.4 (C), 146.4 (C), 135.7 (C), 132.0 (C), 128.7 (CH), 128.6 (CH), 128.5 (CH), 127.9 (CH), 124.3 (CH), 120.9 (C), 120.0 (CH), 116.6 (C), 111.4 (CH), 11.8 (CH), 7.7 (CH₂); HRMS Calculated for $C_{24}H_{20}N_3$ [M+H]⁺: 350.1652, Found: 350.1653.



1-(4,4-dimethyl-1,1-diphenylpenta-1,2-dien-3-yl)-1*H*-benzo[*d*][1,2,3]triazole (4e) was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 91%; m. p. 81-83 °C; R*f* (hexanes/ethyl acetate, V/V, 10/1) = 0.47; UV absorption: 236(0.193), 265(0.215); IR (neat), 2972, 1589, 1490, 1451, 1274, 1231, 1062, 947, 810, 766, 694; ¹H-NMR (600 MHz, CDCl₃) δ 8.06-8.02 (m, 1H), 7.39-7.33 (m, 10H), 7.31-7.28 (m, 2H), 7.18-7.16 (m, 1H), 1.38 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 200.6 (C), 145.0 (C), 135.2 (C), 134.3 (C), 128.6 (CH), 128.5 (CH), 128.3 (CH), 127.5 (CH), 123.8 (CH), 119.7 (CH), 119.1 (C), 117.2 (C), 110.6 (CH), 37.2 (C), 29.1 (CH₃); HRMS Calculated for C₂₅H₂₄N₃ [M+H]⁺: 366.1965, Found: 366.1966.



1-(4-methyl-1,1-diphenylpenta-1,2,4-trien-3-yl)-1*H*-benzo[*d*][1,2,3]triazole (4f) was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 86%; R*f* (hexanes/ethyl acetate, V/V, 10/1) = 0.52; UV absorption: 235(0.165), 265(0.096), 297(0.062); IR (neat), 3057, 1597, 1490, 1448, 1278, 1160, 1065, 1002, 908, 743, 695; ¹H-NMR (600 MHz, CDCl₃) δ 8.08 (d, *J* = 7.8 Hz, 1H), 7.45-7.34 (m, 12H), 7.29 (d, *J* = 7.8 Hz, 1H), 5.17 (s, 1H), 4.66 (s, 1H), 2.15 (s, 3H); ¹³C-NMR (150 MHz, CDCl₃) δ 204.6 (C), 145.4 (C), 136.0 (C), 134.6 (C), 133.7 (C), 128.9 (CH), 128.8 (CH), 128.7 (CH), 127.7 (CH), 124.0 (CH), 120.0 (CH), 118.7 (C), 115.4 (CH), 113.4 (C), 110.4 (CH₂), 20.5 (CH₃); HRMS Calculated for C₂₄H₂₀N₃ [M+H]⁺: 350.1651, Found: 350.1650.



1-(3-(2-(4-methoxybenzyloxy)phenyl)-1-(trimethylsilyl)-3-phenylpropa-1,2-dienyl)-1H-benzo[*d*][**1,2,3]triazole (4h)** was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 90%; R*f* (hexanes/ethyl acetate, V/V, 6/1) = 0.58; UV absorption: 231(0.186), 263(0.145), 299(0.128); IR (neat), 2976, 1583, 1493, 1450, 1286, 1240, 1063, 938, 831, 757, 692; ¹H-NMR (600 MHz, CDCl₃) δ 8.05 (d, *J* = 8.4 Hz, 1H), 7.98 (d, *J* = 8.4 Hz, 1H), 7.42-7.31 (m, 7H), 7.24 (t, *J* = 8.4 Hz, 1H), 7.07-7.03 (m, 2H), 6.85 (d, *J* = 8.4 Hz, 2H), 6.81 (s, 1H), 6.69 (d, *J* = 8.4 Hz, 2H), 4.93 (q, *J* = 11.4 Hz, 2H), 3.78 (s, 3H), 0.5(s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 200.0 (C), 159.0 (C), 156.1 (C), 145.9 (C), 136.4 (C), 132.4 (C), 130.8 (C), 129.5 (C), 128.6 (CH), 128.5 (CH), 128.4 (CH), 127.5 (CH), 127.4 (CH), 127.0 (CH), 125.0 (CH), 124.1 (CH), 121.0 (CH), 119.4 (CH), 113.5 (CH), 112.8 (CH), 112.3 (CH), 111.8 (C), 108.4 (C), 69.5 (CH₂), 55.2 (CH₃), -0.4 (CH₃); HRMS Calculated for $C_{32}H_{32}N_3O_2Si [M+H]^+$: 517.2179, Found: 517.5180.



1-(3-(2-methoxyphenyl)-1-(trimethylsilyl)-3-phenylpropa-1,2-dienyl)-1H-

benzo[*d*][1,2,3]triazole (4h) was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as white solid. Isolated yield 90%; m. p. 131-133 °C; R*f* (hexanes/ethyl acetate, V/V, 6/1) = 0.60; UV absorption: 230(0.200), 264(0.210), 295(0.173); IR (neat), 2957, 1599, 1490, 1453, 1286, 1245, 1066, 939, 829, 740, 691; ¹H-NMR (600 MHz, CDCl₃) δ 8.15 (d, *J* = 7.8 Hz, 1H), 8.06 (d, *J* = 7.8 Hz, 1H), 7.42-7.32 (m, 8H), 7.28 (t, *J* = 7.8 Hz, 1H), 7.03 (t, *J* = 7.8 Hz, 1H), 6.98 (d, *J* = 7.8 Hz, 1H), 3.71 (s, 3H), 0.51(s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 200.0 (C), 157.1 (C), 146.1 (C), 136.0 (C), 132.5 (C), 130.8 (CH), 129.5 (CH), 128.5 (CH), 127.5 (CH), 127.4 (CH), 127.0 (CH), 124.5 (CH), 124.2 (CH), 120.8 (CH), 119.6 (CH), 112.7 (C), 111.3 (C), 111.2 (CH), 108.3 (C), 55.1 (CH₃), - 0.4 (CH₃); HRMS Calculated for C₂₅H₂₆N₃OSi [M+H]⁺: 412.1840, Found: 412.1841.



1-(3-(4-methoxyphenyl)-1-(trimethylsilyl)-3-phenylpropa-1,2-dienyl)-1H-

benzo[*d*][1,2,3]triazole (4i) was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 91%; R*f* (hexanes/ethyl acetate, V/V, 6/1) = 0.64; UV absorption: 231(0.197), 262(0.184), 296(0.155); IR (neat), 2963, 1603, 1498, 1466, 1270, 1235, 1055, 930, 821, 747, 695; ¹H-NMR (600 MHz, CDCl₃) δ 8.08 (d, *J* = 7.2 Hz, 1H), 7.80 (d, *J* = 7.2 Hz, 1H), 7.47 (d, *J* = 9.0 Hz, 2H), 7.41-7.32 (m, 7H), 6.94 (d, *J* = 9.0 Hz, 2H), 3.84 (s, 3H), 0.47 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 200.6 (C), 159.8 (C), 146.4 (C), 136.3 (C), 132.7 (C), 129.9 (CH), 129.0 (CH), 128.7 (CH), 128.3 (CH), 128.1 (CH), 124.6 (CH), 120.2 (CH), 115.3 (C), 114.5 (CH), 112.2 (CH), 108.9 (C), 55.6 (CH₃), -0.22 (CH₃); HRMS Calculated for C₂₅H₂₆N₃OSi [M+H]⁺: 412.1838, Found: 412.1840.



4-(3-(1*H*-benzo[*d*][1,2,3]triazol-1-yl)-3-(trimethylsilyl)-1-phenylpropa-1,2-

dienyl)phenol (4j) was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 80%; R*f* (hexanes/ethyl acetate, V/V, 4/1) = 0.44; UV absorption: 233(0.217), 257(0.166), 271(0.187), 300(0.134); IR (neat), 3363, 2988, 1620, 1476, 1433, 1271, 1212, 1055, 938, 811, 745, 698; ¹H-NMR (600 MHz, CDCl₃) δ 8.06 (d, *J* = 7.2 Hz, 1H), 7.80 (d, *J* = 7.2 Hz, 1H), 7.45 (d, *J* = 7.2 Hz, 2H), 7.41-7.37 (m, 4H), 7.36-7.30 (m, 3H), 6.95 (d, *J* = 7.2 Hz, 2H), 0.45 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 200.5 (C), 156.4 (C), 145.7 (C), 136.0 (C), 132.5 (C), 129.8 (CH), 128.7 (CH), 128.5 (CH), 128.0 (CH), 127.3 (CH), 124.7 (CH), 119.6 (CH), 115.9 (CH), 115.3 (C), 112.2 (CH), 108.6 (C), -0.51 (CH₃); HRMS Calculated for C₂₄H₂₄N₃OSi [M+H]⁺: 398.1681, Found: 398.1682.



4-(3-(1*H***-benzo[***d***][1,2,3]triazol-1-yl)-4,4-dimethyl-1-phenylpenta-1,2-dienyl)phenol (4k) was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 83%; R***f* **(hexanes/ethyl acetate, V/V, 4/1) = 0.43; UV absorption: 231(0.233), 270(0.209), 298(0.174); IR (neat), 3345, 2995, 1605, 1455, 1445, 1287, 1225, 1043, 936, 814, 748, 695; ¹H-NMR (600 MHz, CDCl₃) \delta 8.06-8.03 (m, 1H), 7.40-7.35 (m, 5H), 7.33-7.30 (m, 2H), 7.24 (d,** *J* **= 8.4 Hz, 2H), 7.20-7.17 (m, 1H), 6.93 (d,** *J* **= 8.4 Hz, 2H), 1.36 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) \delta 200.4 (C), 156.5 (C), 144.5 (C), 135.5 (C), 134.4 (C), 132.9 (CH), 130.0 (CH), 128.7 (CH), 128.6 (CH), 128.3 (CH), 128.2 (CH), 127.7 (CH), 124.1 (CH), 119.4 (CH), 115.7 (CH), 115.3 (C), 110.8 (C), 37.2 (C), 29.2 (CH₃); HRMS Calculated for C₂₅H₂₄N₃O [M+H]⁺: 382.1912, Found: 382.1910.**



1-(4,4-dimethyl-1-phenyl-1-(thiophen-2-yl)penta-1,2-dien-3-yl)-1H-

benzo[*d*][1,2,3]triazole (4I) was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 95%; R*f* (hexanes/ethyl acetate, V/V, 6/1) = 0.46; UV absorption: 236(0.189), 260(0.237), 289(0.125); IR (neat), 2988, 1621, 1490, 1454, 1268, 1221, 1034, 951, 830, 745, 688; ¹H-NMR (600 MHz, CDCl₃) δ 8.09 (d, *J* = 8.4 Hz, 1H), 7.86 (d, *J* = 8.4 Hz, 1H), 7.57 (d, *J* = 7.2 Hz, 2H), 7.45-7.36 (m, 5H), 7.34 (dd, *J* = 5.4 Hz, 1.2 Hz, 1H), 7.12 (dd, *J* = 3.6 Hz, 1.2 Hz, 1H), 7.08 (dd, *J* = 5.4 Hz, 3.6 Hz, 1H), 0.50 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 199.9 (C), 146.2 (C), 139.4 (C), 135.5 (C), 132.4 (C), 128.8 (CH), 128.4 (CH), 128.2 (CH), 128.0 (CH), 127.8 (CH), 127.0 (CH), 126.4 (CH), 124.4 (CH), 120.0 (CH), 111.9 (CH), 110.5 (C), 109.0 (C), -0.57 (CH₃); HRMS Calculated for C₂₃H₂₂N₃S [M+H]⁺: 372.1528, Found: 372.1527.



N-2-4m

2-(1-(trimethylsilyl)-3,3-diphenylpropa-1,2-dienyl)-4*-p*-tolyl-2*H*-1,2,3-triazole (N-2-**4m**) was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 60%; R*f* (hexanes/ethyl acetate, V/V, 10/1) = 0.62; UV absorption: 237(0.202), 264(0.153), 299(0.135); IR (neat), 2923, 1633, 1487, 1446, 1281, 1243, 1039, 931, 827, 779, 692; ¹H-NMR (600 MHz, CDCl₃) δ 8.01 (s, 1H), 7.77 (d, *J* = 7.8 Hz, 2H), 7.45-7.40 (m, 8H), 7.39-7.36 (m, 2H), 7.24 (d, *J* = 7.8 Hz, 2H), 2.39 (s, 3H), 0.47 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 201.3 (C), 147.6 (C), 138.0 (C), 135.2 (C), 129.4 (CH), 128.7 (CH), 128.4 (CH), 128.3 (CH), 127.5 (C), 125.6 (CH), 117.0 (CH), 116.1 (C), 109.3 (C), 21.2 (CH₃), -0.62 (CH₃); HRMS Calculated for C₂₇H₂₈N₃Si [M+H]⁺: 422.2046, Found: 422.2044.



1-(1-(trimethylsilyl)-3,3-diphenylpropa-1,2-dienyl)-4*p***-tolyl-1***H***-1,2,3-triazole** (N-1-**4m**) was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid.

Isolated yield 12%; R*f* (hexanes/ethyl acetate, V/V, 10/1) = 0.29; UV absorption: 236(0.179), 265(0.144), 297(0.114); IR (neat), 2928, 1635, 1469, 1433, 1287, 1222, 1032, 930, 816, 770, 694; ¹H-NMR (600 MHz, CDCl₃) δ 7.63 (s, 1H), 7.30-7.27 (m, 6H), 7.07 (d, *J* = 7.8 Hz, 2H), 7.05-7.03 (m, 4H), 6.73 (d, *J* = 7.8 Hz, 2H), 2.14 (s, 3H), 0.32 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 203.8 (C), 138.8 (C), 137.8 (C), 135.0 (C), 133.3 (C), 128.9 (CH), 128.7 (CH), 128.5 (CH), 128.3 (CH), 127.8 (CH), 124.3 (CH), 114.2 (C), 107.3 (C), 21.2 (CH₃), -0.66 (CH₃); HRMS Calculated for C₂₇H₂₈N₃Si [M+H]⁺: 422.2046, Found: 422.2045.



2-(3-(trimethylsilyl)-1,1-diphenylprop-2-ynyl)-4*p***-tolyl-2***H***-1,2,3-triazole** (N-2-4m') was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 13%; R*f* (hexanes/ethyl acetate, V/V, 10/1) = 0.48; UV absorption: 244(0.408), 255(0.418); IR (neat), 3108, 2960, 1490, 1456, 1354, 1296, 1071, 974, 833, 764, 734, 687; ¹H-NMR (600 MHz, CDCl₃) δ 7.91 (s, 1H), 7.68 (d, *J* = 7.8 Hz, 2H), 7.36-7.33 (m, 6H), 7.32-7.29 (m, 4H), 7.21 (d, *J* = 7.8 Hz, 2H), 2.37 (s, 3H), 0.28 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 148.0 (C), 141.2 (C), 138.3 (C), 131.2 (CH), 129.4 (CH), 128.3 (CH), 128.2 (CH), 128.1 (CH), 127.5 (C), 126.0 (CH), 104.4 (C), 94.2 (C), 73.8 (C), 21.3 (CH₃), -0.28 (CH₃); HRMS Calculated for C₂₇H₂₈N₃Si [M+H]⁺: 422.2046, Found: 422.2047.



1-(3-(trimethylsilyl)-1,1-diphenylprop-2-ynyl)-4*p***-tolyl-2***H***-1,2,3-triazole** (N-1-4m') was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 5%; Rf (hexanes/ethyl acetate, V/V, 10/1) = 0.24; UV absorption:

243(0.314), 253(0.298); IR (neat), 3083, 2936, 1490, 1456, 1425, 1156, 1073, 976, 833, 751, 730, 686; ¹H-NMR (600 MHz, CDCl₃) δ 7.97 (s, 1H), 7.73 (d, *J* = 7.8 Hz, 2H), 7.37-7.35 (m, 6H), 7.32-7.29 (m, 4H), 7.22 (d, *J* = 7.8 Hz, 2H), 2.38 (s, 3H), 0.29 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 146.8 (C), 140.6 (C), 137.9 (C), 129.4 (CH), 128.7 (CH), 128.4 (CH), 128.0 (CH), 127.7 (C), 125.6 (CH), 120.2 (CH), 104.1 (C), 94.9 (C), 70.0 (C), 21.2 (CH₃), -0.37 (CH₃); HRMS Calculated for C₂₇H₂₈N₃Si [M+H]⁺: 422.2046, Found: 422.2049.



N-2-4n

4-(4-methoxyphenyl)-2-(1-(trimethylsilyl)-3-phenyl-3-*p***-tolylpropa-1,2-dienyl)-2***H***-1,2,3-triazole (N-2-4n)** was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. R*f* (hexanes/ethyl acetate, V/V, 6/1) = 0.66; Isolated yield 70%; UV absorption: 244(0.223), 271(0.189), 298(0.154); IR (neat), 2987, 1621, 1503, 1454, 1268, 1237, 1067, 941, 832, 754, 687; ¹H-NMR (600 MHz, CDCl₃) δ 7.92 (s, 1H), 7.77 (d, *J* = 9.0 Hz, 2H), 7.39 (d, *J* = 9.0 Hz, 4H), 7.28 (d, *J* = 7.8 Hz, 2H), 7.21 (d, *J* = 7.8 Hz, 2H), 6.94 (d, *J* = 9.0 Hz, 2H), 3.84 (s, 3H), 2.39 (s, 3H), 0.42 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 201.3 (C), 159.7 (C), 147.4 (C), 138.3 (C), 135.4 (C), 132.2 (C), 129.5 (CH), 128.7 (CH), 128.4 (CH), 128.3 (CH), 128.2 (CH), 127.1 (CH), 123.1 (C), 116.6 (CH), 116.0 (C), 114.2 (CH), 109.2 (C), 55.3 (CH₃), 21.2 (CH₃), -0.59 (CH₃); HRMS Calculated for C₂₈H₃₀N₃OSi [M+H]⁺: 452.2153, Found: 452.2156.



4-(4-methoxyphenyl)-1-(1-(trimethylsilyl)-3-phenyl-3-p-tolylpropa-1,2-dienyl)-1H-

1,2,3-triazole (N-1-4n) was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 14%; R*f* (hexanes/ethyl acetate, V/V, 6/1) = 0.30; UV absorption: 244(0.165), 273(0.132), 299(0.103); IR (neat), 2960, 1611, 1494, 1469, 1284, 1232, 1049, 938, 819, 732, 691; ¹H-NMR (600 MHz, CDCl₃) δ 7.62 (s, 1H), 7.36-7.33 (m, 2H), 7.20-7.14 (m, 3H), 7.10 (d, *J* = 9.0 Hz, 4H), 7.07-7.05 (m, 2H), 6.46 (d, *J* = 7.8 Hz, 2H), 3.64 (s, 3H), 2.36 (s, 3H), 0.31 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 204.0 (C), 160.2 (C), 142.9 (C), 137.9 (C), 135.4 (C), 132.3 (C), 130.5 (CH), 129.3 (CH), 128.8 (CH), 128.5 (CH), 128.3 (CH), 128.2 (CH), 128.0 (C), 127.9 (CH), 120.0 (C), 113.9

(CH), 107.4 (C), 55.2 (CH₃), 21.3 (CH₃), -0.45 (CH₃); HRMS Calculated for $C_{28}H_{30}N_3OSi [M+H]^+$: 452.2153, Found: 452.2150.



4-(4-methoxyphenyl)-2-(3-(trimethylsilyl)-1-phenyl-1-*p***-tolylprop-2-ynyl)-2***H***-1,2,3triazole (N-2-4n') was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 10%;** *Rf* **(hexanes/ethyl acetate, V/V, 6/1) = 0.51; UV absorption: 256(0.413), 269(0.424); IR (neat), 3096, 2943, 1482, 1423, 1368, 1299, 1065, 975, 830, 751, 724, 689; ¹H-NMR (600 MHz, CDCl₃) \delta 7.83 (s, 1H), 7.70 (d,** *J* **= 8.4 Hz, 2H), 7.32-7.29 (m, 2H), 7.25-7.23 (m, 2H), 7.18 (d,** *J* **= 8.4 Hz, 2H), 7.12 (t,** *J* **= 8.4 Hz, 3H), 6.91 (t,** *J* **= 8.4 Hz, 2H), 3.81 (s, 3H), 2.34 (s, 3H), 0.26 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) \delta 159.8 (C), 147.7 (C), 141.5 (C), 138.3 (C), 137.4 (C), 130.8 (CH), 128.8 (CH), 128.2 (CH), 128.1 (CH), 128.0 (CH), 127.9 (CH), 127.4 (CH), 123.1 (C), 114.1 (CH), 104.6 (C), 93.9 (C), 73.5 (C), 55.2 (CH₃), 21.1 (CH₃), -0.26 (CH₃); HRMS Calculated for C₂₈H₃₀N₃OSi [M+H]⁺: 452.2153, Found: 452.2150.**





4-(4-methoxyphenyl)-1-(3-(trimethylsilyl)-1-phenyl-1-*p***-tolylprop-2-ynyl)-1***H***-1,2,3triazole (N-1-4n') was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 4%; R***f* **(hexanes/ethyl acetate, V/V, 6/1) = 0.33; UV absorption: 256(0.335), 266(0.356); IR (neat), 3090, 2955, 1498, 1453, 1434, 1149, 1068, 956, 837, 750, 721, 680; ¹H-NMR (600 MHz, CDCl₃) \delta 7.90 (s, 1H), 7.75 (d,** *J* **= 9.0 Hz, 2H), 7.36-7.34 (m, 3H), 7.29-7.25 (m, 2H), 7.19 (d,** *J* **= 8.4 Hz, 2H), 7.15 (d,** *J* **= 8.4 Hz, 2H), 6.94 (d,** *J* **= 9.0 Hz, 2H), 3.84 (s, 3H), 2.36 (s, 3H), 0.27 (s, 9H); ¹³C-NMR (150** MHz, CDCl₃) δ 159.6 (C), 146.6 (C), 140.8 (C), 138.6 (C), 137.6 (C), 129.0 (CH), 128.6 (CH), 128.4 (CH), 128.0 (CH), 127.9 (CH), 127.0 (CH), 123.4 (C), 119.7 (CH), 114.2 (CH), 104.3 (C), 94.6 (C), 69.8 (C), 55.3 (CH₃), 21.1 (CH₃), -0.35 (CH₃); HRMS Calculated for C₂₈H₃₀N₃OSi [M+H]⁺: 452.2153, Found: 452.2151.



4-(4-chlorophenyl)-2-(1-(trimethylsilyl)-3-phenyl-3-p-tolylpropa-1,2-dienyl)-2H-

1,2,3-triazole (N-2-40) was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 57%; R*f* (hexanes/ethyl acetate, V/V, 10/1) = 0.57; UV absorption: 238(0.329), 269(0.254), 301(0.216); IR (neat), 2937, 1623, 1477, 1450, 1276, 1235, 1063, 932, 818, 745, 696; ¹H-NMR (600 MHz, CDCl₃) δ 7.99 (s, 1H), 7.78 (d, *J* = 8.4 Hz, 2H), 7.40-7.38 (m, 5H), 7.37-7.35 (m, 2H), 7.28 (d, *J* = 7.8 Hz, 2H), 7.21 (d, *J* = 7.8 Hz, 2H), 2.39 (s, 3H), 0.43 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 201.3 (C), 146.5 (C), 138.4 (C), 135.3 (C), 134.0 (C), 132.1 (C), 129.5 (CH), 129.0 (CH), 128.9 (CH), 128.8 (CH), 128.4 (CH), 128.3 (CH), 128.2 (C), 127.0 (CH), 117.5 (CH), 116.2 (C), 109.2 (C), 21.2 (CH₃), -0.62 (CH₃); HRMS Calculated for C₂₇H₂₇ClN₃Si [M+H]⁺: 456.1655, Found: 456.1652.



4-(4-chlorophenyl)-1-(1-(trimethylsilyl)-3-phenyl-3*-p***-tolylpropa-1,2-dienyl)-1***H***-1,2,3-triazole (N-1-40)** was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 15%; R*f* (hexanes/ethyl acetate, V/V, 10/1) = 0.29; UV absorption: 242(0.308), 261(0.249), 300(0.233); IR (neat), 2946, 1589, 1480, 1441, 1292, 1231, 1063, 939, 825, 756, 694; ¹H-NMR (600 MHz, CDCl₃) δ 7.65 (s, 1H), 7.32-7.28 (m, 3H), 7.11 (d, *J* = 8.4 Hz, 2H), 7.07 (d, *J* = 8.4 Hz, 2H), 7.05-7.02 (m, 2H), 6.92 (d, *J* = 8.4 Hz, 2H), 6.85 (d, *J* = 8.4 Hz, 2H), 2.38 (s, 3H), 0.34 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 204.0 (C), 138.0 (C), 136.6 (C), 135.0 (C), 134.8 (C), 133.5 (C), 131.6 (C), 129.9 (CH), 129.2 (CH), 128.5 (CH), 128.4 (CH), 128.3 (CH), 128.2 (CH), 128.0 (CH), 125.8 (CH), 114.5 (C), 107.2 (C), 21.2 (CH₃), -0.67 (CH₃); HRMS Calculated for C₂₇H₂₇ClN₃Si [M+H]⁺: 456.1655, Found: 456.1654.



4-(4-chlorophenyl)-2-(3-(trimethylsilyl)-1-phenyl-1-p-tolylprop-2-ynyl)-2H-1,2,3-

triazole (N-2-4o') was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 19%; R*f* (hexanes/ethyl acetate, V/V, 10/1) = 0.47; UV absorption: 250(0.378), 265(0.345); IR (neat), 3100, 2947, 1498, 1434, 1367, 1292, 1049, 967, 854, 788, 730, 691; ¹H-NMR (600 MHz, CDCl₃) δ 7.90 (s, 1H), 7.71 (d, *J* = 8.4 Hz, 2H), 7.36 (d, *J* = 8.4 Hz, 2H), 7.35-7.33 (m, 3H), 7.27-7.24 (m, 2H), 7.18 (d, *J* = 8.4 Hz, 2H), 7.15 (t, *J* = 8.4 Hz, 2H), 2.36 (s, 3H), 0.27 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 146.9 (C), 141.3 (C), 138.3 (C), 138.1 (C), 134.2 (C), 131.2 (CH), 128.9 (CH), 128.8 (CH), 128.3 (CH), 128.1 (CH), 128.0 (CH), 127.4 (CH), 104.4 (C), 94.2 (C), 73.8 (C), 21.1 (CH₃), -0.28 (CH₃); HRMS Calculated for C₂₇H₂₇ClN₃Si [M+H]⁺: 456.1655, Found: 456.1654.



4-(4-chlorophenyl)-1-(3-(trimethylsilyl)-1-phenyl-1-*p***-tolylprop-2-ynyl)-2***H***-1,2,3triazole (N-1-4o') was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 5%; R***f* **(hexanes/ethyl acetate, V/V, 10/1) = 0.26; UV absorption: 248(0.268), 263(0.247); IR (neat), 3054, 2921, 1495, 1458, 1421, 1150, 1054, 971, 827, 749, 720, 688; ¹H-NMR (600 MHz, CDCl₃) \delta 7.95 (s, 1H), 7.75 (d,** *J* **= 8.4 Hz, 2H), 7.38-7.33 (m, 5H), 7.28-7.25 (m, 2H), 7.18 (d,** *J* **= 9.0 Hz, 2H), 7.15 (d,** *J* **= 9.0 Hz, 2H), 2.35 (s, 3H), 0.27 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) \delta 145.9 (C), 140.8 (C), 139.0 (C), 137.7 (C), 134.0 (C), 129.4 (CH), 129.2 (CH), 128.9 (CH), 128.6 (CH), 128.2 (CH), 128.1 (CH), 127.2 (CH), 120.8 (CH), 104.3 (C), 95.1 (C), 70.3 (C), 21.3 (CH₃), -0.13 (CH₃); HRMS Calculated for C₂₇H₂₇ClN₃Si [M+H]⁺: 456.1655, Found: 456.1655.**



N-2-4p

4-(4-fluorophenyl)-2-(1-(trimethylsilyl)-3-phenyl-3-p-tolylpropa-1,2-dienyl)-2H-

1,2,3-triazole (N-2-4p) was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 62%; R*f* (hexanes/ethyl acetate, V/V, 10/1) = 0.55; UV absorption: 257(0.405), 263(0.353), 311(0.252); IR (neat), 2966, 1586, 1493, 1444, 1282, 1234, 1039, 933, 854, 756, 682; ¹H-NMR (600 MHz, CDCl₃) δ 7.97 (s, 1H), 7.84-7.81 (m, 2H), 7.42-7.40 (m, 4H), 7.38-7.35 (m, 1H), 7.30 (d, *J* = 7.8 Hz, 2H), 7.22 (d, *J* = 7.8 Hz, 2H), 7.11 (t, *J* = 7.8 Hz, 2H), 2.40 (s, 3H), 0.44 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 201.3 (C), 163.5 (C), 161.9 (C), 146.6 (C), 138.4 (C), 135.3 (C), 132.1 (C), 129.5 (CH), 128.7 (CH), 128.4 (CH), 128.3 (CH), 128.2 (CH), 127.5 (CH), 127.4 (CH), 126.7 (C), 126.6 (C), 117.2 (CH), 116.1 (C), 115.8 (CH), 115.7 (CH), 109.2 (C), 21.2 (CH₃), -0.63 (CH₃); HRMS Calculated for C₂₇H₂₇FN₃Si [M+H]⁺: 440.1951, Found: 440.1950.



4-(4-fluorophenyl)-1-(1-(trimethylsilyl)-3-phenyl-3-p-tolylpropa-1,2-dienyl)-1H-

1,2,3-triazole (N-1-4p) was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 14%; R*f* (hexanes/ethyl acetate, V/V, 10/1) = 0.25; UV absorption: 253(0.333), 261(0.279), 313(0.223); IR (neat), 2987, 1618, 1464, 1426, 1289, 1235, 1052, 946, 823, 745, 688; ¹H-NMR (600 MHz, CDCl₃) δ 7.64 (s, 1H), 7.31-7.28 (m, 3H), 7.14-7.11 (m, 2H), 7.10 (d, *J* = 7.8 Hz, 2H), 7.06-7.03 (m, 2H), 6.94 (d, *J* = 7.8 Hz, 2H), 6.59 (t, *J* = 7.8 Hz, 2H), 2.37 (s, 3H), 0.32 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 203.8 (C), 163.7 (C), 163.0 (C), 162.0 (C), 138.0 (C), 136.8 (C), 134.9 (C), 133.5 (CH), 131.7 (CH), 130.8 (C), 130.7 (C), 129.2 (CH), 128.4 (CH), 128.4 (CH), 128.3 (CH), 128.0 (CH), 123.3 (CH), 115.4 (CH), 115.3 (CH), 114.4 (C), 107.2 (C), 21.2 (CH₃), -0.67 (CH₃); HRMS Calculated for C₂₇H₂₇FN₃Si [M+H]⁺: 440.1951, Found: 440.1954.



4-(4-fluorophenyl)-2-(3-(trimethylsilyl)-1-phenyl-1-p-tolylprop-2-ynyl)-2H-1,2,3-

triazole (N-2-4p') was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 15%; R*f* (hexanes/ethyl acetate, V/V, 10/1) = 0.45; UV absorption: 271(0.513), 285(0.446); IR (neat), 3118, 2937, 1476, 1424, 1375, 1299, 1055, 963, 850, 781, 727, 690; ¹H-NMR (600 MHz, CDCl₃) δ 7.87 (s, 1H), 7.77-7.74 (m, 2H), 7.35-7.32 (m, 3H), 7.28-7.24 (m, 2H), 7.19 (d, *J* = 8.4 Hz, 2H), 7.15 (d, *J* = 8.4 Hz, 2H), 7.08 (t, *J* = 8.4 Hz, 2H), 2.36 (s, 3H), 0.27 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 163.7 (C), 162.0 (C), 147.0 (C), 141.4 (C), 138.3 (C), 138.2 (C), 131.0 (CH), 128.9 (CH), 128.3 (CH), 128.2 (CH), 128.1 (CH), 128.0 (CH), 127.9 (CH), 127.8 (CH), 126.7 (C), 126.6 (C), 115.8 (CH), 115.6 (CH), 104.4 (C), 94.1 (C), 73.7 (C), 21.1 (CH₃), -0.27 (CH₃); HRMS Calculated for C₂₇H₂₇FN₃Si [M+H]⁺: 440.1951, Found: 440.1948.



4-(4-fluorophenyl)-1-(3-(trimethylsilyl)-1-phenyl-1-p-tolylprop-2-ynyl)-2H-1,2,3-

triazole (N-1-4p') was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 4%; R*f* (hexanes/ethyl acetate, V/V, 10/1) = 0.28; UV absorption: 270(0.436), 283(0.389); IR (neat), 3089, 2931, 1488, 1433, 1363, 1281, 1042, 965, 864, 774, 735, 695; ¹H-NMR (600 MHz, CDCl₃) δ 7.94 (s, 1H), 7.81-7.78 (m, 2H), 7.36-7.34 (m, 3H), 7.29-7.27 (m, 2H), 7.18 (d, *J* = 8.4 Hz, 2H), 7.16 (d, *J* = 8.4 Hz, 2H), 7.10 (t, *J* = 8.4 Hz, 2H), 2.36 (s, 3H), 0.28 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 163.5 (C), 161.8 (C), 145.9 (C), 140.6 (C), 138.7 (C), 137.5 (C), 129.1 (CH), 128.7 (CH), 128.4 (CH), 128.0 (CH), 127.9 (CH), 127.5 (CH), 127.4 (CH), 125.9 (C), 125.8 (C), 120.3 (CH), 115.8 (CH), 115.7 (CH), 104.1 (C), 94.8 (C), 70.0 (C), 21.0 (CH₃), -0.36 (CH₃); HRMS Calculated for C₂₇H₂₇FN₃Si [M+H]⁺: 440.1951, Found: 440.1953.



N-2-4q

2-(4,4-dimethyl-1,1-diphenylpenta-1,2-dien-3-yl)-4*p***-tolyl-2***H***-1,2,3-triazole (N-2-4q)** was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 65%; R*f* (hexanes/ethyl acetate, V/V, 10/1) = 0.60; UV absorption: 240(0.214), 258(0.182), 294(0.195); IR (neat), 2956, 1588, 1497, 1441, 1264, 1245, 1072, 958, 815, 760, 675; ¹H-NMR (600 MHz, CDCl₃) δ 7.77 (s, 1H), 7.74 (d, *J* = 7.8 Hz, 2H), 7.44-7.39 (m, 8H), 7.38-7.34 (m, 2H), 7.22 (d, *J* = 7.8Hz, 2H), 2.37 (s, 3H), 1.39 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 199.4 (C), 146.8 (C), 138.0 (C), 135.2 (C), 129.4 (CH), 128.7 (CH), 128.5 (CH), 128.4 (CH), 127.6 (C), 125.6 (CH), 121.0 (C), 120.6 (CH), 117.6 (C), 36.3 (C), 29.1 (CH₃), 21.3 (CH₃); HRMS Calculated for C₂₈H₂₈N₃ [M+H]⁺: 406.2280, Found: 406.2280.



N-1-4q

1-(4,4-dimethyl-1,1-diphenylpenta-1,2-dien-3-yl)-4*p***-tolyl-2***H***-1,2,3-triazole (N-1-4q)** was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 11%; R*f* (hexanes/ethyl acetate, V/V, 10/1) = 0.28; UV absorption: 243(0.253), 259(0.298), 297(0.203); IR (neat), 2934, 1576, 1501, 1433, 1237, 1216, 1066, 939, 811, 773, 683; ¹H-NMR (600 MHz, CDCl₃) δ 7.69 (s, 1H), 7.40-7.33 (m, 10H), 7.02 (d, *J* = 7.8 Hz, 2H), 6.84 (d, *J* = 7.8 Hz, 2H), 2.29 (s, 3H), 1.11 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 202.6 (C), 163.0 (C), 138.9 (C), 134.7 (C), 132.1 (CH), 129.1 (CH), 128.9 (CH), 128.7 (CH), 128.6 (CH), 128.3 (CH), 124.2 (C), 119.1 (C), 117.1 (C), 37.1 (C), 29.1 (CH₃), 21.3 (CH₃); HRMS Calculated for C₂₈H₂₈N₃ [M+H]⁺: 406.2280, Found: 406.2285.



2-(4,4-dimethyl-1,1-diphenylpent-2-ynyl)-4-*p***-tolyl-2***H***-1,2,3-triazole** (N-2-4q') was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 15%; R*f* (hexanes/ethyl acetate, V/V, 10/1) = 0.45; UV absorption: 240(0.267), 253(0.305); IR (neat), 3123, 2956, 1500, 1431, 1362, 1280, 1040, 968, 842, 781, 733, 701; ¹H-NMR (600 MHz, CDCl₃) δ 7.88 (s, 1H), 7.67 (d, *J* = 7.8 Hz, 2H), 7.35-7.31 (m, 6H), 7.30-7.27 (m, 4H), 7.20 (d, *J* = 7.8 Hz, 2H), 2.37 (s, 3H), 1.35 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 147.7 (C), 142.1 (C), 138.1 (C), 131.0 (CH), 129.4 (CH), 128.1 (CH), 128.1 (CH), 128.0 (CH), 127.7 (C), 126.0 (CH), 97.7 (C), 79.0 (C), 73.4 (C), 30.6 (CH₃), 27.8 (C), 21.3 (CH₃); HRMS Calculated for C₂₈H₂₈N₃ [M+H]⁺: 406.2280, Found: 406.2284.



N-1-4q'

1-(4,4-dimethyl-1,1-diphenylpent-2-ynyl)-4-*p***-tolyl-2***H***-1,2,3-triazole** (N-1-4q') was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 4%; R*f* (hexanes/ethyl acetate, V/V, 10/1) = 0.25; UV absorption: 242(0.253), 254(0.236); IR (neat), 3076, 2927, 1463, 1448, 1354, 1290, 1033, 985, 855, 793, 721, 698; ¹H-NMR (600 MHz, CDCl₃) δ 7.96 (s, 1H), 7.71 (d, *J* = 7.8 Hz, 2H), 7.36-7.33 (m, 6H), 7.31-7.27 (m, 4H), 7.21 (d, *J* = 7.8 Hz, 2H), 2.37 (s, 3H), 1.35 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 163.0 (C), 146.7 (C), 141.3 (C), 137.9 (C), 129.4 (CH), 128.5 (CH), 128.3 (CH), 128.0 (CH), 125.6 (CH), 120.2 (CH), 98.3 (C), 78.9 (C), 69.7 (C), 30.6 (CH₃), 27.9 (C), 21.3 (CH₃); HRMS Calculated for C₂₈H₂₈N₃ [M+H]⁺: 406.2280, Found: 406.2279.



N-2-4r

2-(4-methyl-1,1-diphenylpenta-1,2,4-trien-3-yl)-4-*p***-tolyl-2***H***-1,2,3-triazole** (N-2-4r) was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 70%; R*f* (hexanes/ethyl acetate, V/V, 10/1) = 0.64; UV absorption: 231(0.405), 263(0.353), 311(0.252); IR (neat), 3033, 1586, 1495, 1438, 1266, 1153, 1071, 992, 903, 734, 694; ¹H-NMR (600 MHz, CDCl₃) δ 7.86 (s, 1H), 7.74 (d, *J* = 8.4 Hz, 2H), 7.47-7.45 (m, 4H), 7.43-7.35 (m, 6H), 7.23 (d, *J* = 8.4 Hz, 2H), 5.21 (s, 1H), 4.88 (s, 1H), 2.38 (s, 3H), 2.09 (s, 3H); ¹³C-NMR (150 MHz, CDCl₃) δ 203.5 (C), 147.3 (C), 138.1 (C), 136.2 (C), 134.6 (C), 129.5 (CH), 128.9 (CH), 128.7 (CH), 128.7 (CH), 127.5 (C), 125.7 (CH), 120.8 (CH), 119.0 (C), 115.4 (CH₂), 114.8 (C), 21.3 (CH₃), 20.7 (CH₃); HRMS Calculated for C₂₇H₂₄N₃ [M+H]⁺: 390.1960, Found: 390.1962.



2-(4-methyl-1,1-diphenylpent-4-en-2-ynyl)-4-*p***-tolyl-2***H***-1,2,3-triazole (N-2-4r') was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 10%; R***f* **(hexanes/ethyl acetate, V/V, 10/1) = 0.50; UV absorption: 248(0.231), 259(0.210); IR (neat), 3110, 2930, 1471, 1423, 1373, 1297, 1053, 960, 838, 779, 718, 679; ¹H-NMR (600 MHz, CDCl₃) \delta 7.91 (s, 1H), 7.67 (d,** *J* **= 7.8 Hz, 2H), 7.36-7.33 (m, 6H), 7.31-7.28 (m, 4H), 7.20 (d,** *J* **= 7.8 Hz, 2H), 5.48 (s, 1H), 5.35 (quin,** *J* **= 1.8 Hz, 1H), 2.37 (s, 3H), 2.01 (s, 3H); ¹³C-NMR (150 MHz, CDCl₃) \delta 148.0 (C), 141.5 (C), 138.4 (C), 131.2 (CH), 129.4 (CH), 128.3 (CH), 128.2 (CH), 128.1 (CH), 127.5 (C), 126.1 (C), 126.0 (CH), 123.1 (CH₂), 90.2 (C), 88.0 (C), 73.8 (C), 23.2 (CH₃), 21.3 (CH₃); HRMS Calculated for C₂₇H₂₄N₃ [M+H]⁺: 390.1960, Found: 390.1962.**



Mixture of 1-(4-methyl-1,1-diphenylpenta-1,2,4-trien-3-yl)-4-p-tolyl-2H-1,2,3triazole (N-2-4r) and 1-(4-methyl-1,1-diphenylpent-4-en-2-ynyl)-4-p-tolyl-2H-1,2,3triazole (N-1-4r') couldn't separated by flash chromatography with different developing solvent systems which were Hexane-EtOAc (v/v: 20/1) and Hexane-ethylene chloride (v/v: 5/1) as yellow liquid. Rf (hexanes/ethyl acetate, V/V, 10/1) = 0.29; Isolated yield 11%; UV absorption: 233(0.333), 245(0.200), 261(0.257), 313(0.163); IR (neat), 3066, 2935, 1589, 1477, 1448, 1350, 1284, 1165, 1049, 997, 913, 857 732, 688; ¹H-NMR (600 MHz, CDCl₃) & 7.88 (s, 1.00H), 7.57-7.54 (m, 3.47H), 7.38-7.34 (m, 3.88H), 7.33-7.28 (m, 7.77H), 7.25-7.23 (m, 4.18H), 7.19 (d, J = 7.8 Hz, 2.20H), 7.01 (d, J = 7.8 Hz, 2.10H), 2.41 (s, 2.62H), 2.34 (s, 3.00H), 2.01 (s, 3.03H); ¹³C-NMR (150 MHz, CDCl₃) δ 205.3 (C), 163.0 (C), 143.2 (C), 139.2 (C), 138.8 (C), 137.0 (C), 134.0 (C), 131.7 (C), 129.4 (CH), 128.9 (CH), 128.6 (CH), 128.5 (CH), 128.5 (CH), 128.3 (CH), 127.9 (CH), 126.0 (CH), 123.7 (CH₂), 118.8 (C), 115.0 (CH₂), 113.9 (C), 92.4 (C), 85.8 (C), 74.5 (C), 32.7 (CH₃), 21.3 (CH₃), 20.2 (CH₃); HRMS Calculated for C₂₇H₂₄N₃ [M+H]⁺: 390.1960, Found: 390.1962.



N-2-4s

2-(1-cyclopropyl-3,3-diphenylpropa-1,2-dienyl)-4-*p*-tolyl-2*H*-1,2,3-triazole (N-2-4s) was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 87%; R*f* (hexanes/ethyl acetate, V/V, 10/1) = 0.61; UV absorption: 226(0.242), 257(0.166), 299(0.129); IR (neat), 2962, 1583, 1480, 1423, 1262, 1151, 1067, 956, 862, 742, 690; ¹H-NMR (600 MHz, CDCl₃) δ 7.97 (s, 1H), 7.74 (d, *J* = 7.8 Hz, 2H), 7.42-7.36 (m, 10H), 7.23 (d, *J* = 7.8 Hz, 2H), 2.38 (s, 3H), 2.29-2.24 (m, 1H), 1.11-1.07 (m, 2H), 0.83-0.79 (m, 2H); ¹³C-NMR (150 MHz, CDCl₃) δ 196.7 (C), 147.8 (C), 138.1 (C), 135.4 (C), 129.5 (CH), 128.7 (CH), 128.6 (CH), 128.6 (CH), 127.6 (C), 125.7 (CH), 121.2 (C), 117.4 (CH), 116.6 (C), 21.3 (CH₃), 10.8 (CH), 7.5 (CH₂); HRMS Calculated for C₂₇H₂₄N₃ [M+H]⁺: 390.1960, Found: 390.1963.



1-(1-cyclopropyl-3,3-diphenylpropa-1,2-dienyl)-4-*p*-tolyl-1*H*-1,2,3-triazole (N-1-4s) was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 9%; R*f* (hexanes/ethyl acetate, V/V, 10/1) = 0.30; UV absorption: 229(0.199), 258(0.113), 298(0.098); IR (neat), 3001, 1597, 1474, 1444, 1273, 1175, 1073, 976, 849, 737, 694; ¹H-NMR (600 MHz, CDCl₃) δ 7.69 (s, 1H), 7.32-7.27 (m, 6H), 7.17-7.13 (m, 6H), 6.88 (d, *J* = 7.8 Hz, 2H), 2.25 (s, 3H), 1.94-1.88 (m, 1H), 0.91-0.86 (m, 2H), 0.69-0.65 (m, 2H); ¹³C-NMR (150 MHz, CDCl₃) δ 200.6 (C), 138.9 (C), 137.8 (C), 134.8 (C), 132.8 (CH), 129.2 (CH), 128.8 (CH), 128.4 (CH), 128.3 (CH), 128.2 (CH), 123.9 (C), 119.1 (C), 114.1 (C), 21.3 (CH₃), 13.3 (CH), 7.3 (CH₂); HRMS Calculated for C₂₇H₂₄N₃ [M+H]⁺: 390.1960, Found: 390.1959.



1-(1,5-bis(trimethylsilyl)-3-phenylpenta-1,2-dien-4-ynyl)-1*H***-benzo**[*d*][1,2,3]triazole (4t) was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 76%; R*f* (hexanes/ethyl acetate, V/V, 10/1) = 0.46; UV absorption: 234(0.093), 250(0.077), 296(0.054); IR (neat), 3057, 2950, 1587, 1476, 1418, 1256, 1160, 1079, 987, 813, 710, 685; ¹H-NMR (600 MHz, CDCl₃) δ 8.07 (d, *J* = 8.4 Hz, 1H), 7.79 (d, *J* = 8.4 Hz, 1H), 7.64 (d, *J* = 8.4 Hz, 2H), 7.44 (t, *J* = 8.4 Hz, 1H), 7.39 (t, *J* = 8.4 Hz, 1H), 7.32 (t, *J* = 8.4 Hz, 1H), 0.48 (s, 9H), 0.29 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 205.8 (C), 146.0 (C), 132.8 (C), 132.4 (C), 128.8 (CH), 128.4 (CH), 128.2 (CH), 126.3 (CH), 124.6 (CH), 119.9 (CH), 111.8 (CH), 110.2 (C), 102.1 (C), 99.1 (C), 96.9 (C), -0.10 (CH₃), -0.63 (CH₃); HRMS Calculated for C₂₃H₂₈N₃Si₂ [M+H]⁺: 402.1820, Found: 402.1819.



1-(3-(1-benzyl-1H-1,2,3-triazol-4-yl)-1-(trimethylsilyl)-3-phenylpropa-1,2-dienyl)-

1*H***-benzo[***d***][1,2,3]triazole (4u) was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as white solid. R***f* **(hexanes/ethyl acetate, V/V, 2/1) = 0.45; UV absorption: 233(0.081), 253(0.06), 295(0.071); IR (neat), 3150, 3030, 2951, 1448, 1286, 1241, 1108, 1048, 938, 835, 766, 697; Isolated yield 58%; m. p. 155-157 °C; ¹H-NMR (600 MHz, CDCl₃) \delta 8.05 (d,** *J* **= 7.2 Hz, 1H), 7.87 (d,** *J* **= 7.2 Hz, 1H), 7.59-7.56 (m, 2H), 7.48 (s, 1H), 7.41-7.29 (m, 10H), 5.57 (s, 2H), 0.44 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) \delta 200.9 (C), 146.1 (C), 143.6 (C), 134.4 (C), 134.3 (C), 132.6 (C), 129.2 (CH), 128.9 (CH), 128.4 (CH), 128.1 (CH), 128.0 (CH), 127.8 (CH), 124.4 (CH), 122.4 (CH), 119.9 (CH), 112.1 (CH), 109.4 (C), 106.0 (C), 54.4 (CH₂), -0.55 (CH₃); HRMS Calculated for C₂₇H₂₇N₆Si [M+H]⁺: 463.2056, Found: 46.04059.**



1-(1-(trimethylsilyl)-3-(4-nitrophenyl)-3-phenylpropa-1,2-dienyl)-1H-

benzo[*d*][1,2,3]triazole (4v) was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 71%; R*f* (hexanes/ethyl acetate, V/V, 6/1) = 0.48; UV absorption: 231(0.078), 256(0.059), 299(0.041); IR (neat), 2967, 1634, 1523, 1438, 1299, 1235, 1157, 1045, 933, 847, 722; ¹H-NMR (600 MHz, CDCl₃) δ 8.24 (d, *J* = 8.4 Hz, 2H), 8.10 (d, *J* = 7.2 Hz, 1H), 7.70 (d, *J* = 7.2 Hz, 1H), 7.61 (d, *J* = 8.4 Hz, 2H), 7.46-7.38 (m, 7H), 0.48 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 200.9 (C), 147.4 (C), 146.3 (C), 143.0 (C), 134.6 (C), 132.4 (C), 129.2 (CH), 129.0 (CH), 128.7 (CH), 128.3 (CH), 128.2 (CH), 124.6 (CH), 124.1 (CH), 120.3 (CH), 114.0 (C), 111.4 (CH), 109.7 (C), -0.45 (CH₃); HRMS Calculated for C₂₄H₂₃N₄O₂Si [M+H]⁺: 427.1593, Found: 427.1590.



1-(3-(4-fluorophenyl)-1-(trimethylsilyl)-3-phenylpropa-1,2-dienyl)-1H-

benzo[*d*][1,2,3]triazole (4w) was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as white solid. Isolated yield 88%; m. p. 114-116 °C; R*f* (hexanes/ethyl acetate, V/V, 10/1) = 0.46; UV absorption: 234(0.203), 262(0.160), 300(0.141); IR (neat), 2955, 1603, 1504, 1447, 1285, 1248, 1155, 1066, 936, 833, 744, 692; ¹H-NMR (600 MHz, CDCl₃) δ 8.08 (d, *J* = 7.2 Hz, 1H), 7.77 (d, *J* = 7.2 Hz, 1H), 7.46-7.34 (m, 9H), 7.12-7.06 (m, 2H), 0.47 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 200.2 (C), 163.4 (C), 161.7 (C), 146.2 (C), 135.7 (C), 132.4 (C), 131.82 (C), 131.80 (C), 130.1 (CH), 130.0 (CH), 128.8 (CH), 128.3 (CH), 128.2 (CH), 128.0 (CH), 124.4 (CH), 120.0 (CH), 115.9 (CH), 115.7 (CH), 114.5 (C), 111.8 (C), 109.0 (CH), -0.49 (CH₃); HRMS Calculated for C₂₄H₂₃FN₃Si [M+H]⁺: 400.1655, Found: 400.1658.



1-(3-(4-chlorophenyl)-1-(trimethylsilyl)-3-phenylpropa-1,2-dienyl)-1H-

benzo[*d*][1,2,3]triazole (4x) was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as white solid. Isolated yield 72%; m. p. 139-141 °C; R*f* (hexanes/ethyl acetate, V/V, 10/1) = 0.47; UV absorption: 238(0.229), 264(0.167), 299(0.156); IR (neat), 2957, 1485, 1448, 1285, 1248, 1156, 1069, 937, 876, 831, 743, 692; ¹H-NMR (600 MHz, CDCl₃) δ 8.09 (d, *J* = 7.8 Hz, 1H), 7.76 (d, *J* = 7.8 Hz, 1H), 7.46-7.35 (m, 11H), 0.49 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 200.2 (C), 146.2 (C), 135.4 (C), 134.4 (C), 134.0 (C), 132.4 (C), 129.6 (CH), 129.0 (CH), 128.9 (CH), 128.3 (CH), 128.2 (CH), 128.0 (CH), 124.4 (CH), 120.0 (CH), 114.4 (C), 111.7 (CH), 109.1 (C), -0.49 (CH₃); HRMS Calculated for C₂₄H₂₃ClN₃Si [M+H]⁺: 416.1344, Found: 416.1346.



1-(3,3-bis(4-fluorophenyl)-1-(trimethylsilyl)propa-1,2-dienyl)-1H-

benzo[*d*][1,2,3]triazole (4y) was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as white solid. Isolated yield 84%; m. p. 118-120 °C; R*f* (hexanes/ethyl acetate, V/V, 10/1) = 0.43; UV absorption: 235(0.175), 261(0.151), 299(0.127); IR (neat), 2964, 1602, 1504, 1450, 1282, 1223, 1157, 1069, 937, 836, 752; ¹H-NMR (600 MHz, CDCl₃) δ 8.08 (d, *J* = 7.8 Hz, 1H), 7.75 (d, *J* = 7.8 Hz, 1H), 7.45-7.40 (m, 5H), 7.38 (t, *J* = 7.8 Hz, 1H), 7.13-7.08 (m, 4H), 0.48 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 200.0 (C), 163.4 (C), 161.7 (C), 146.2 (C), 132.4 (C), 131.7 (C), 131.6 (C), 130.0 (CH), 129.9 (CH), 128.0 (CH), 124.4 (CH), 120.1 (CH), 116.0 (CH), 115.8 (CH), 113.6 (C), 111.6 (CH), 109.1 (C), -0.53 (CH₃); HRMS Calculated for C₂₄H₂₂F₂N₃Si [M+H]⁺: 418.1546, Found: 418.1550.



N-2-4z

2-(3-(4-chlorophenyl)-1-(trimethylsilyl)-3-phenylpropa-1,2-dienyl)-4-p-tolyl-2H-

1,2,3-triazole (N-2-4z) was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 59%; R*f* (hexanes/ethyl acetate, V/V, 10/1) = 0.60; UV absorption: 243(0.318), 270(0.267), 295(0.116); IR (neat), 2917, 1613, 1457, 1443, 1278, 1233, 1073, 929, 816, 738, 699; ¹H-NMR (600 MHz, CDCl₃) δ 7.94 (s, 1H), 7.74 (d, *J* = 8.4 Hz, 2H), 7.41 (d, *J* = 7.8 Hz, 2H), 7.39-7.36 (m, 5H), 7.34 (d, *J* = 7.8 Hz, 2H), 7.22 (d, *J* = 8.4 Hz, 2H), 2.16 (s, 3H), 0.43 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 201.2 (C), 147.7 (C), 138.2 (C), 134.8 (C), 134.3 (C), 133.8 (C), 129.6 (CH), 129.5 (CH), 129.0 (CH), 128.9 (CH), 128.5 (CH), 128.3 (CH), 127.4 (CH), 125.7 (CH), 117.0 (C), 115.2 (CH), 109.7 (C), 21.3 (CH₃), -0.60 (CH₃); HRMS Calculated for C₂₇H₂₇ClN₃Si [M+H]⁺: 456.1655, Found: 456.1652.



N-1-4z

1-(3-(4-chlorophenyl)-1-(trimethylsilyl)-3-phenylpropa-1,2-dienyl)-4-p-tolyl-2H-

1,2,3-triazole (N-1-4z) was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 15%; R*f* (hexanes/ethyl acetate, V/V, 10/1) = 0.33; UV absorption: 244(0.295), 264(0.244), 299(0.138); IR (neat), 2936, 1588, 1477, 1422, 1278, 1213, 1034, 932, 843, 771, 687; ¹H-NMR (600 MHz, CDCl₃) δ 7.63 (s, 1H), 7.30-7.28 (m, 3H), 7.24 (d, *J* = 8.4 Hz, 2H), 7.05 (d, *J* = 7.8 Hz, 2H), 7.03-7.01 (m, 2H), 6.96 (d, *J* = 8.4 Hz, 2H), 6.76 (d, *J* = 7.8 Hz, 2H), 2.16 (s, 3H), 0.32 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 203.6 (C), 138.9 (C), 137.8 (C), 134.6 (C), 133.7 (C), 133.6 (C), 133.4 (C), 129.6 (CH), 129.0 (CH), 128.7 (CH), 128.5 (CH), 128.4 (CH), 128.3 (CH), 128.0 (CH), 124.3 (C), 113.2 (CH), 107.6 (C), 21.2 (CH₃), -0.68 (CH₃); HRMS Calculated for C₂₇H₂₇ClN₃Si [M+H]⁺: 456.1655, Found: 456.1659.



2-(1-(4-chlorophenyl)-3-(trimethylsilyl)-1-phenylprop-2-ynyl)-4-p-tolyl-2H-1,2,3-

triazole (N-2-4z') was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 15%; R*f* (hexanes/ethyl acetate, V/V, 10/1) = 0.49; UV absorption: 256(0.408), 271(0.393); IR (neat), 3077, 2934, 1483, 1446, 1343, 1297, 1041, 961, 852, 777, 739, 695; ¹H-NMR (600 MHz, CDCl₃) δ 7.91 (s, 1H), 7.67 (d, *J* = 7.8 Hz, 2H), 7.37-7.34 (m, 3H), 7.33-7.31 (m, 2H), 7.29-7.26 (m, 4H), 7.21 (d, *J* = 7.8 Hz, 2H), 2.38 (s, 3H), 0.29 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 148.1 (C), 140.9 (C), 139.8 (C), 138.5 (C), 134.4 (C), 131.3 (CH), 129.8 (CH), 129.4 (CH), 128.5 (CH), 128.3 (CH), 128.2 (CH), 127.9 (CH), 127.4 (C), 126.0 (CH), 103.8 (C), 94.8 (C), 73.2 (C), 21.3 (CH₃), -0.32 (CH₃); HRMS Calculated for C₂₇H₂₇ClN₃Si [M+H]⁺: 456.1655, Found: 456.1652.



1-(1-(4-chlorophenyl)-3-(trimethylsilyl)-1-phenylprop-2-ynyl)-4-p-tolyl-2H-1,2,3-

triazole (N-1-4z') was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as yellow liquid. Isolated yield 4%; R*f* (hexanes/ethyl acetate, V/V, 10/1) = 0.30; UV absorption: 255(0.358), 273(0.367); IR (neat), 3089, 2928, 1487, 1455, 1433, 1148, 1052, 989, 820, 734, 709, 679; ¹H-NMR (600 MHz, CDCl₃) δ 8.01 (s, 1H), 7.73 (d, *J* = 7.8 Hz, 2H), 7.39-7.35 (m, 3H), 7.33 (d, *J* = 8.4 Hz, 2H), 7.29-7.27 (m, 2H), 7.25 (d, *J* = 8.4 Hz, 2H), 7.23 (d, *J* = 7.8 Hz, 2H), 2.38 (s, 3H), 0.29 (s, 9H); ¹³C-NMR (150 MHz, CDCl₃) δ 147.0 (C), 140.2 (C), 139.1 (C), 138.0 (C), 134.8 (C), 129.6 (CH), 129.5 (CH), 128.9 (CH), 128.5 (CH), 127.8 (CH), 127.6 (C), 125.6 (CH), 120.1 (CH), 103.5 (C), 95.6 (C), 69.5 (C), 21.3 (CH₃), -0.41 (CH₃); HRMS Calculated for C₂₇H₂₇ClN₃Si [M+H]⁺: 456.1655, Found: 456.1650.



1-(3-(2-methoxyphenyl)-3-phenylpropa-1,2-dienyl)-1*H*-benzo[*d*][1,2,3]triazole (7a) was purified by flash chromatography (Hexane-EtOAc, v/v 20/1) as white solid. Isolated yield 98%; m. p. 173-175 °C; R*f* (hexanes/ethyl acetate, V/V, 6/1) = 0.42; UV absorption: 235(0.327), 299(0.206); IR (neat), 3056, 1596, 1491, 1443, 1278, 1172, 1061, 741, 694; ¹H-NMR (600 MHz, CDCl₃) δ 8.26 (s, 1H), 8.07 (d, *J* = 8.4 Hz, 1H), 8.00 (d, *J* = 8.4 Hz, 1H), 7.44-7.27 (m, 9H), 7.01 (t, *J* = 7.8 Hz, 1H), 6.96 (d, *J* = 8.4 Hz, 1H), 3.68 (s, 3H); ¹³C-NMR (150 MHz, CDCl₃) δ 196.6 (C), 157.0 (C), 146.6 (C), 135.3 (C), 131.4 (C), 130.9 (CH), 130.0 (CH), 128.5 (CH), 128.4 (CH), 127.9 (CH), 127.6 (CH), 124.5 (CH), 124.1 (CH), 120.8 (CH), 119.9 (CH), 117.8 (C), 111.9 (CH), 111.3 (C), 99.4 (CH), 55.3 (CH₃); HRMS Calculated for C₂₂H₁₈N₃O [M+H]⁺: 340.1458, Found: 340.1455.

III. ORTEP Drawing of the Crystal Structure



Figure 1. Perspective view of the molecular structure of **4a** (C₂₄H₂₃N₃Si) with the atom labeling scheme. The thermal ellipsoids are scaled to enclose 30% probability. CCDC number: 851290.



Figure 2. Perspective view of the molecular structure of **4g** (C₂₅H₂₅N₃SiO) with the atom labeling scheme. The thermal ellipsoids are scaled to enclose 30% probability. CCDC number: 851291.



Figure 3. Perspective view of the molecular structure of 4u (C₂₇H₂₆N₆Si) with the atom labeling scheme. The thermal ellipsoids are scaled to enclose 30% probability. CCDC number: 851293.



Figure 4. Perspective view of the molecular structure of 4y ($C_{24}H_{21}F_2N_3Si$) with the atom labeling scheme. The thermal ellipsoids are scaled to enclose 30% probability. CCDC number: 851294.



Figure 5. Perspective view of the molecular structure of 7a (C₂₂H₁₇N₃O) with the atom labeling scheme. The thermal ellipsoids are scaled to enclose 30% probability. CCDC number: 851292.

VII. NMR Spectra Data











-






¹H 600 MHz NMR 4d





¹³C 150 MHz NMR 4d





¹H 600 MHz NMR 4e





¹³C 150 MHz NMR 4e





¹H 600 MHz NMR 4f



--N N







¹³C 150 MHz NMR 4g







¹³C 150 MHz NMR 4h





















¹³C 150 MHz NMR 4I















¹³C 150 MHz NMR N-2-4m'







¹³C 150 MHz NMR N-1-4m'













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F



























t-Bu

Ρh

N^N













¹H 600 MHz NMR N-2-4r'





















TMS N^N N

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¹³C 150 MHz NMR 4w







¹³C 150 MHz NMR 4x









¹³C 150 MHz NMR 4y























Η

N