Supporting Information

Simple Synthesis of 1-Substituted-4-vinyl-1,2,3-triazoles Based on Polystyrene-supported Sulfonyl Chloride

Zhe Wang,^{1,2} Shou-Ri Sheng,^{1,2} Mei-Hong Wei¹ and Xiao-Ling Liu¹

¹ National Research Center for Carbohydrate Synthesis, Jiangxi Normal University, Nanchang, 330022, P. R. China

² Key Laboratory of Functional Small Organic Molecule, Ministry of Education, Jiangxi Normal University, Nanchang, 330022, P. R. China

1. Characterization data of the products.

1-Benzyl-4-vinyl-1*H*-1,2,3-triazole (4a): White solid, mp 36–38 °C (lit.^[1] 36–39°C); ¹H NMR (400 MHz, CDCl₃): δ = 7.45 (s, 1 H), 7.44–7.38 (m, 3 H), 7.30–7.27 (m, 2 H), 6.65 (dd, *J* = 17.8, 11.2 Hz, 1 H), 5.85 (d, *J* = 17.8 Hz, 1 H), 5.49 (s, 2 H), 5.30 (d, *J* = 11.2 Hz, 1 H); ¹³C NMR (100 MHz, CDCl₃): δ = 146.8, 134.8, 129.3, 128.8, 128.2, 125.8, 120.3, 116.1, 54.2.

1-(4-Methoxybenzyl)-4-vinyl-1*H*-1,2,3-triazole (4b): White solid, mp 45–47 °C (lit.^[2] 46–38 °C); ¹H NMR (400 MHz, CDCl₃): δ = 7.42 (s, 1 H), 7.25 (d, *J* = 8.0 Hz, 2 H), 6.95 (d, *J* = 8.0 Hz, 2 H), 6.66 (dd, *J* = 17.8, 10.8 Hz, 1 H), 5.84 (d, *J* = 17.8 Hz, 1 H), 5.47 (s, 2 H), 5.30 (d, *J* = 10.8 Hz, 1 H), 3.84 (s, 3 H); ¹³C NMR (100 MHz, CDCl₃): δ = 160.3, 146.7, 129.9, 126.7, 128.7, 120.3, 116.1, 114.8, 55.8, 53.8.

1-(4-Bromobenzyl)-4-vinyl-1*H*-1,2,3-triazole (4c): White solid, mp 134–136 °C (lit.^[3] 135–137°C); ¹H NMR (400 MHz, CDCl₃): δ = 7.52 (s, 1 H), 7.70 (d, *J* = 6.8 Hz, 2 H), 7.45 (d, *J* = 6.8 Hz, 2 H), 6.68 (dd, *J* = 18.2, 10.6 Hz, 1 H), 5.82 (d, *J* = 18.2 Hz, 1 H),

5.23 (s, 2 H), 5.35 (d, $J = 10.6$ Hz, 1 H); ^{13}C NMR (100 MHz, CDCl_3): $\delta = 147.0, 134.6, 132.4, 129.8, 129.0, 123.1, 120.5, 116.3, 53.5$.

1-(*n*-Butyl)-4-vinyl-1*H*-1,2,3-triazole (4d): Colorless oil (lit.^[2]); ^1H NMR (400 MHz, CDCl_3): $\delta = 7.48$ (s, 1 H), 6.56 (dd, $J = 17.8, 11.2$ Hz, 1 H), 5.85 (d, $J = 17.8$ Hz, 1 H), 5.18 (d, $J = 11.2$ Hz, 1 H), 4.20 (t, $J = 7.2$ Hz, 2 H), 1.75–1.71 (m, 2 H), 1.25–1.20 (m, 2 H), 0.82 (t, $J = 7.2$ Hz, 3 H); ^{13}C NMR (100 MHz, CDCl_3): $\delta = 146.2, 125.6, 120.6, 115.8, 49.7, 32.3, 19.8, 13.3$.

2-(4-Vinyl-1,2,3-triazol-1-yl)ethanol (4e): Colorless oil (lit.^[2]); ^1H NMR (400 MHz, CDCl_3): $\delta = 7.63$ (s, 1 H), 6.61 (dd, $J = 19.2, 11.2$ Hz, 1 H), 5.82 (d, $J = 19.0$ Hz, 1 H), 5.32 (d, $J = 11.2$ Hz, 1 H), 4.63 (t, $J = 9.8$ Hz, 2 H), 4.08 (t, $J = 9.8$ Hz, 2 H), 2.73 (s, 1 H); ^{13}C NMR (100 MHz, CDCl_3): $\delta = 145.8, 125.2, 121.8, 116.1, 60.9, 52.7$.

Methyl 3-(4-vinyl-1,2,3-triazol-1-yl)propanoate (4f): Colorless oil (lit.^[2]); ^1H NMR (400 MHz, CDCl_3): $\delta = 7.60$ (s, 1 H), 6.64 (dd, $J = 19.0, 11.4$ Hz, 1 H), 5.84 (d, $J = 19.0$ Hz, 1 H), 5.32 (d, $J = 11.4$ Hz, 1 H), 4.60 (t, $J = 12.8$ Hz, 2 H), 3.69 (s, 3 H), 2.95 (t, $J = 12.8$ Hz, 2 H); ^{13}C NMR (100 MHz, CDCl_3): $\delta = 171.2, 146.7, 125.9, 121.5, 116.3, 52.5, 45.8, 34.7$.

1-Phenyl-4-vinyl-1*H*-1,2,3-triazole (4g): White solid, mp 41–42 °C (lit.^[4] 40–42°C); ^1H NMR (400 MHz, CDCl_3): $\delta = 7.94$ (s, 1 H), 7.73 (d, $J = 7.4$ Hz, 2 H), 7.55 (t, $J = 15.5$ Hz, 2 H), 7.44 (t, $J = 8.1$ Hz, 1 H), 6.80 (dd, $J = 18.8, 11.2$ Hz, 1 H), 6.00 (d, $J = 18.8$ Hz, 1 H), 5.42 (d, $J = 11.2$ Hz, 1 H); ^{13}C NMR (100 MHz, CDCl_3): $\delta = 148.7, 129.8, 128.7, 125.8, 125.3, 120.5, 118.5, 116.7$.

1-(4-Methoxyphenyl)-4-vinyl-1*H*-1,2,3-triazole (4h): White solid, mp 65–67 °C; ^1H NMR (400 MHz, CDCl_3): $\delta = 7.65$ (s, 1 H), 7.55 (d, $J = 8.8$ Hz, 2 H), 6.94 (d, $J = 8.8$

Hz, 2 H), 6.71 (dd, $J = 18.4, 11.2$ Hz, 1 H), 5.94 (d, $J = 18.4$ Hz, 1 H), 5.43 (d, $J = 11.2$ Hz, 1 H), 3.79 (s, 3 H); ^{13}C NMR (100 MHz, CDCl_3): $\delta = 159.7, 148.5, 130.2, 129.7, 125.7, 121.7, 116.7, 114.4, 55.6$; IR (KBr): $\nu = 3070, 2927, 2860, 1640, 1545, 1495, 1457, 1378, 1220, 996, 910, 825, 721\text{ cm}^{-1}$; Anal. Calcd for $\text{C}_{11}\text{H}_{11}\text{N}_3\text{O}$: C 65.66, H 5.51, N 20.88; found: C 65.53 H, 5.62, N 20.98.

1-(3-Methylphenyl)-4-vinyl-1*H*-1,2,3-triazole (4i): Yellow oil; ^1H NMR (400 MHz, CDCl_3): $\delta = 7.70$ (s, 1 H), 7.57 (s, 1 H), 7.44 (d, $J = 8.4$ Hz, 1 H), 7.34 (d, $J = 7.6$ Hz, 1 H), 7.21 (d, $J = 7.2$ Hz, 1 H), 6.73 (dd, $J = 18.4, 10.8$ Hz, 1 H), 5.93 (d, $J = 18.4$ Hz, 1 H), 5.44 (d, $J = 10.8$ Hz, 1 H), 2.40 (s, 3 H); ^{13}C NMR (100 MHz, CDCl_3): $\delta = 148.8, 139.8, 136.8, 130.6, 129.5, 128.9, 126.0, 121.5, 117.7, 116.8, 20.8$; IR (film): $\nu = 3112, 3068, 2925, 2872, 1638, 1551, 1496, 1437, 1378, 1222, 995, 866, 695\text{ cm}^{-1}$; Calcd for $\text{C}_{11}\text{H}_{11}\text{N}_3$: C 71.33, H 5.99, N 22.69; found: C 71.22, H 6.12, N 22.80.

1-(2-Methylphenyl)-4-vinyl-1*H*-1,2,3-triazole (4j): Yellow oil; ^1H NMR (400 MHz, CDCl_3): $\delta = 7.70$ (s, 1 H), 7.44–7.31 (m, 3 H), 7.21 (d, $J = 8.0$ Hz, 1 H), 6.86 (dd, $J = 18.4, 10.8$ Hz, 1 H), 5.93 (d, $J = 18.4$ Hz, 1 H), 5.48 (d, $J = 10.8$ Hz, 1 H), 2.33 (s, 3 H); ^{13}C NMR (100 MHz, CDCl_3): $\delta = 148.4, 136.8, 132.9, 131.2, 130.1, 129.5, 125.9, 125.3, 121.7, 116.8, 20.9$; IR (film): $\nu = 3115, 3085, 2925, 2872, 1640, 1551, 1496, 1455, 1375, 1222, 995, 866, 695\text{ cm}^{-1}$; Calcd for $\text{C}_{11}\text{H}_{11}\text{N}_3$: C 71.33, H 5.99, N 22.69; found: C 71.20, H 6.10, N 22.81.

1-(2-Chlorophenyl)-4-vinyl-1*H*-1,2,3-triazole (4k): Yellow oil; ^1H NMR (400 MHz, CDCl_3): $\delta = 7.77$ (s, 1 H), 7.73 (d, $J = 6.8$ Hz, 1 H), 7.49–7.42 (m, 2 H), 7.34 (t, $J = 7.0$ Hz, 1 H), 6.77 (dd, $J = 18.4, 11.2$ Hz, 1 H), 5.95 (d, $J = 18.4$ Hz, 1 H), 5.49 (d, $J = 11.2$ Hz, 1 H); ^{13}C NMR (100 MHz, CDCl_3): $\delta = 149.0, 133.4, 131.7, 130.9, 130.6, 129.8,$

128.2, 127.5, 125.9, 116.2; IR (film): ν = 3120, 3095, 2927, 2875, 1642, 1550, 1495, 1440, 1225, 999, 906, 817, 698 cm^{-1} ; Calcd for $\text{C}_{10}\text{H}_8\text{N}_3\text{Cl}$: C 58.41, H 3.92, N 20.43; found: C 58.30, H 4.03, N 20.31.

1-(4-Bromophenyl)-4-vinyl-1*H*-1,2,3-triazole (4l): Pale yellow solid, mp 140–142 °C (lit.^[3] 141–143 °C); ^1H NMR (400 MHz, CDCl_3): δ = 7.84 (s, 1 H), 7.70 (d, J = 8.8 Hz, 2 H), 7.51 (d, J = 8.8 Hz, 2 H), 6.80 (dd, J = 18.8, 11.6 Hz, 1 H), 6.02 (dd, J = 18.8, 1.2 Hz, 1 H), 5.51 (dd, J = 11.6, 1.2 Hz, 1 H); ^{13}C NMR (100 MHz, CDCl_3): δ = 148.8, 138.7, 134.2, 130.1, 129.8, 126.1, 120.3, 116.8.

1-(4-Nitrophenyl)-4-vinyl-1*H*-1,2,3-triazole (4m): Pale yellow solid, mp 177–179 °C; ^1H NMR (400 MHz, CDCl_3): δ = 8.42 (d, J = 8.8 Hz, 2 H), 7.99 (d, J = 8.8 Hz, 2 H), 7.69 (s, 1 H), 6.79 (dd, J = 18.0, 11.2 Hz, 1 H), 6.02 (d, J = 17.6 Hz, 1 H), 5.51 (d, J = 11.2 Hz, 1 H); ^{13}C NMR (100 MHz, CDCl_3): δ = 151.3, 149.1, 141.2, 130.1, 126.4, 125.7, 120.5, 117.0; IR (KBr): ν = 3121, 1637, 1606, 1529, 1496, 1455, 1350, 1239, 1073, 993, 919, 775, 730 cm^{-1} ; Calcd for $\text{C}_{10}\text{H}_8\text{N}_4\text{O}_2$: C 55.55, H 3.73, N 25.91; found: C 55.43, H 3.84, N 25.99.

2. References

- (1) Reddy, M. N.; Swamy, K. C. K. *Eur. J. Org. Chem.* **2012**, 2013–2022.
- (2) Takizawa, K.; Nulwala, H.; Thibault, R. J.; Lowenhielm, P.; Yoshinaga, K.; Wooley, K. L.; Hawker, C. J. *J. Polym. Sci., Part A: Polym. Chem.* **2008**, *46*, 2897–2912.
- (3) Cardoen, H.; Toppet, S.; Smets, G.; L'abbé, G. *J. Heterocycl. Chem.* **1972**, *9*, 971–972.
- (4) Thibault, R. J.; Takizawa, K.; Lowenhielm, P.; Helms, B.; Mynar, J. L.; Fréchet, J. M. J.; Hawker, C. J. *J. Am. Chem. Soc.* **2006**, *128*, 12084–12085.

3. Copies of ^1H NMR and ^{13}C NMR spectra of new compounds, IR for resin 1, resin 2 and representative resin 3a.

Current Data Parameters
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EXPNO 93
PROCNO 1

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FIDRES 0.126314 Hz
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RG 114
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D1 1.00000000 sec
MCHST 0.00000000 sec
MCWK 0.01500000 sec

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P1 13.00 usec
PL1 -2.00 dB
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F2 - Processing parameters
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SSB 0
LB 0.30 Hz
GB 9
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Current Data Parameters
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PROCNO 1

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DE 6.00 usec
TE 296.1 K
D1 2.00000000 sec
d11 0.03000000 sec
MCHST 0.00000000 sec
MCWK 0.01500000 sec

===== CHANNEL f1 =====
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PL1 -2.00 dB
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===== CHANNEL f2 =====
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PL2 120.00 dB
PL12 12.00 dB
PL13 12.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127090 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

IR for the resin 1

IR for the resin 2

IR for the resin 3a