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Palladium-triethylborane Triggered direct and regioselective conversion of allylic alcohols to allyl phenyl sulfones

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General: The chemicals were purchased from Aldrich and used as supplied: Pd(OAc)₂, PPh₃ and triethylborane (1.0 M solution in THF) were used without further purification. *N,N*-Dimethyl formamide was distilled over calcium hydride. Silicagel (60-120 mesh) was obtained from Acme's, India. The products were eluted using Hexane and Ethylacetate in the ratio of 9:1.

¹H NMR spectra were recorded as solutions in CDCl₃ at room temperature on a Varian Gemini spectrometer at 200 MHz and mass spectra were recorded on Finnigan MAT 1020B or micro mass VG 70-70H spectrometer operating at 70 eV using direct inlet system.

Physical data of the products are as follows:

{[2*E*]-3-Phenylprop-2-enyl)sulfonyl} benzene (1a): ¹H NMR (200 MHz, CDCl₃): δ 7.90 (d, 2H, *J* = 8.0 Hz), 7.70-7.40 (m, 3H), 7.40-7.10 (m, 5H), 6.30 (d, 1H, *J* = 16.0 Hz), 6.20-5.95 (m, 1H), 3.90 (d, 2H, *J* = 8.2 Hz).

¹³C NMR (75 MHz, CDCl₃): δ 139.50, 138.87, 136.17, 134.10, 129.4, 129.00, 128.80, 126.91, 126.02, 115.50, 60.88.

EIMS (*m/z*): (*M*⁺) 259, 136, 117, 81, 69.

HRMS (EI) for C₉H₉ calculated (*M*⁺) 117.070425 Found 117.070533.

(2E)-3-(4-Methylphenyl)prop-2-enyl phenyl sulfone (2a): ^1H NMR (200 MHz, CDCl_3): δ 7.85 (d, 2H, $J = 6.2$ Hz), 7.73-7.38 (m, 3H), 7.30-6.90 (m, 4H), 6.26 (d, 1H, $J = 15.6$ Hz), 6.14-5.90 (m, 1H), 3.95-3.40 (d, 2H, $J = 6.2$ Hz), 2.35 (s, 3H).

^{13}C NMR (50 MHz, CDCl_3): δ 139.0, 138.5, 133.6, 133.0, 129.3, 129.0, 128.5, 126.5, 125.4, 114.0, 60.5, 21.1.

EIMS (m/z): (M^+) 272, 149, 131, 105, 89, 77.

HRMS (EI) for $\text{C}_{10}\text{H}_{11}$ calculated (M^+) 131.086075 Found 131.086067.

(2E)-3-(4-Methoxyphenyl)prop-2-enyl phenyl sulfone (3a): ^1H NMR (200 MHz, CDCl_3): δ 8.01 (d, 2H, $J = 6.3$ Hz), 7.75-7.50 (m, 3H), 7.45 (d, 2H, $J = 6.3$ Hz), 6.95 (d, 2H, $J = 6.3$ Hz), 6.40 (d, 1H, $J = 6.3$ Hz), 6.20-5.90 (m, 1H), 4.10-3.80 (m, 5H).

^{13}C NMR (50 MHz, CDCl_3): δ 160.0, 145.2, 138.7, 133.6, 129.0, 128.7, 128.5, 127.9, 114.2, 112.8, 126.5, 60.6.

EIMS (m/z): (M^+) 288, 259, 207, 147, 141, 91, 55.

HRMS (EI) for $\text{C}_{10}\text{H}_{11}\text{O}$ calculated (M^+) 147.080990 Found 147.081262.

(2E)-3-(4-Bromophenyl) prop-2-enyl phenyl sulfone (4a): ^1H NMR (200 MHz, CDCl_3): δ 7.90 (d, 2H, $J = 6.2$ Hz), 7.72-7.40 (m, 3H), 7.40-7.00 (m, 4H), 6.30 (d, 1H, $J = 12.5$ Hz), 6.15-5.91 (m, 1H), 3.85 (d, 2H, $J = 8.0$ Hz).

^{13}C NMR (50 MHz, CDCl_3): δ 144.9, 139.0, 133.6, 133.3, 129.0, 126.5, 128.5, 128.1, 126.6, 114.1, 60.57.

EIMS (m/z): (M^+) 337, 281, 195, 141, 73, 57.

HRMS (EI) for $\text{C}_9\text{H}_8\text{Br}$ calculated (M^+) 195.980936 Found 195.980600.

(2E)-3-(4-Fluorophenyl)prop-2-enyl phenyl sulfone (5a): ^1H NMR (200 MHz, CDCl_3): δ 7.85 (d, 2H, $J = 6.8$ Hz), 7.70-7.41 (m, 3H), 7.41-7.12 (m, 2H), 7.10-6.91 (m, 2H), 6.32 (d, 1H, $J = 13.7$ Hz), 6.15-5.90 (m, 1H), 3.92 (d, 2H, $J = 6.8$ Hz).

^{13}C NMR (50 MHz, CDCl_3): δ 160.2, 137.6, 136.8, 132.7, 128.1, 127.4, 127.2, 114.8, 114.5, 113.9, 59.4.

EIMS (m/z): (M^+) 276, 259, 159, 141, 135, 109, 81, 57.

HRMS (EI) for $\text{C}_9\text{H}_8\text{F}$ calculated (M^+) 135.061004 Found 135.061200

((1E,3E)-5-[[1E,3Z)-1-Vinylpenta-1,3-diethyl]sulfonyl]penta-1,3-dienyl)benzene (6a): ^1H NMR (200 MHz, CDCl_3): δ 7.86 (d, 2H, $J = 7.5$ Hz), 7.66-7.50 (m, 3H), 7.36-7.17 (m, 5H), 6.75-6.64 (m, 1H), 6.45 (d, 1H, $J = 15.8$ Hz), 6.21-6.09 (m, 1H), 5.75-5.59 (m, 1H), 3.83 (d, 2H, $J = 7.5$ Hz).

^{13}C NMR (50 MHz, CDCl_3): δ 139.4, 136.5, 134.8, 133.7, 129.0, 128.6, 128.4, 128.1, 127.1, 126.5, 125.9, 118.2, 60.4.

EIMS (m/z): (M^+) 284, 257, 143, 141, 111, 71, 57.

HRMS (EI) for $\text{C}_{11}\text{H}_{11}$ calculated (M^+) 143.086075 Found 143.085820.

[(2E)-Oct-2-enylsulfonyl]benzene (7a): ^1H NMR (200 MHz, CDCl_3): δ 7.84 (d, 2H, $J = 6.8$ Hz), 7.61 (d, 1H, $J = 6.8$ Hz), 7.52 (t, 2H, $J = 7.5$ Hz), 5.54-5.32 (m, 2H), 3.69 (d, 2H, $J = 6.0$ Hz), 2.04-1.94 (m, 2H), 1.41-1.12 (m, 6H), 0.87 (t, 3H, $J = 6.0$ Hz).

^{13}C NMR (50 MHz, CDCl_3): δ 141.7, 138.6, 133.5, 128.9, 128.5, 115.9, 60.2, 32.4, 31.1, 28.3, 22.3, 15.2.

EIMS (m/z): (M^+) 252, 175, 111, 71, 57.

HRMS (EI) for C_8H_{15} calculated (M^+) 111.117376 Found 111.117000.

[(2*E*)-5,9-Dimethyldeca-2,8-dienyl]sulfonylbenzene (8a): ¹H NMR (200 MHz, CDCl₃): δ 7.84 (d, 2H, *J* = 7.0 Hz), 7.61 (t, 1H, *J* = 7.0 Hz), 7.52 (t, 2H, *J* = 7.8 Hz), 5.53-5.32 (m, 2H), 5.0 (t, 1H, *J* = 6.2 Hz), 3.70 (d, 2H, *J* = 7.0 Hz), 2.06-1.79 (m, 3H), 1.67 (s, 3H), 1.58 (s, 3H), 1.47-1.17 (m, 4H), 0.76 (d, 3H, *J* = 6.2 Hz).

¹³C NMR (50 MHz, CDCl₃): δ 140.0, 133.3, 128.9, 128.7, 126.5, 124.7, 123.7, 117.5, 60.3, 40.1, 36.6, 25.9, 25.6, 19.4, 17.8.

EIMS (*m/z*): (*M*⁺) 306, 279, 165, 141, 109, 81.

HRMS (EI) for C₁₂H₂₁ calculated (*M*⁺) 165.164326 Found 165.163900.

2,2-Dimethyl-5-[(1*E*)-3-(phenylsulfonyl)prop-1-enyl]-6-benzyloxytetrahydrofuro[2,3-*d*][1,3]dioxole (9a): ¹H NMR (200 MHz, CDCl₃): δ 7.84-7.81 (m, 2H), 7.64-7.44 (m, 3H), 7.36-7.19 (m, 5H), 5.82-5.73 (m, 3H), 4.60-4.40 (m, 4H), 3.79-3.76 (m, 3H), 1.48-1.24 (m, 6H).

¹³C NMR (50 MHz, CDCl₃): δ 134.4, 133.7, 129.0, 128.4, 128.3, 127.9, 127.5, 120.6, 119.5, 104.8, 84.5, 83.9, 83.4, 82.8, 73.9, 72.1, 59.2, 26.7.

FABMS (*m/z*): (*M*⁺) 430, 445, 367, 355, 289, 141, 57.

HRMS (FABMS) for C₁₇H₂₁O₄ calculated (*M*⁺) 289.143984 Found 289.143500.

4-(3-Benzenesulfonylpropenyl)-2,2-dimethylloxazolidine-3-carboxylic acid *tert*-butyl ester (10a): ¹H NMR (200 MHz, CDCl₃): δ 7.86 (d, 2H, *J* = 7.4 Hz), 7.62 (t, 1H, *J* = 6.7 Hz), 7.54 (t, 2H, *J* = 7.4 Hz), 5.68-5.54 (m, 1H), 5.41 (dd, 1H, *J*_{1,2} = 7.4, *J*_{1,3} = 15.6 Hz), 4.36-4.20 (m, 1H), 3.96-3.88 (m, 1H), 3.76-3.66 (m, 2H), 3.48 (d, 1H, *J* = 8.9 Hz), 1.48-1.24 (m, 15H).

¹³C NMR (50 MHz, CDCl₃): δ 151.8, 139.5, 138.3, 133.6, 129.0, 128.5, 117.9, 80.2, 67.5, 65.7, 59.4, 28.4, 27.1, 15.2.

FABMS (*m/z*): (*M*⁺) 381, 321, 240, 141, 57.

HRMS (FABMS) for $C_{13}H_{22}NO_3$ calculated (M+) 240.159969 Found 240.159400.

{[(2E)-5-Phenylpent-2-enyl] sulfonyl} benzene (11a): 1H NMR (200 MHz, $CDCl_3$): δ 7.86 (d, 2H, $J = 7.5$ Hz), 7.70-7.50 (m, 3H), 7.35-7.15 (m, 3H), 7.10 (d, 2H, $J = 7.5$ Hz), 5.66-5.35 (m, 2H), 3.75 (d, 2H, $J = 7.5$ Hz), 2.60 (t, 2H, $J_{1,2} = 7.1$, $J_{1,3} = 15.05$ Hz), 2.40-2.27 (q, 2H).

^{13}C NMR (50 MHz, $CDCl_3$): δ 140.9, 140.4, 133.4, 128.8, 128.3, 128.2, 125.8, 116.5, 59.9, 55.0, 34.9, 34.0, 29.5.

EIMS (m/z): (M⁺) 286, 257, 145, 141.

HRMS (EI) for $C_{11}H_{13}$ calculated (M+) 145.101875 Found 145.101526.