Supporting Information

$B(C_6F_5)_3$-Catalyzed Allylation of Secondary Benzylic Acetates with Allylsilanes

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NMR spectra were recorded on Bruker Avance DPX-400 (400 MHz) and DRX-500 (500 MHz) instruments. IR spectra were recorded on Genesis II FT-IR Mattson spectrometer. High-resolution mass spectra were recorded on CONCEPT/EXTREL mass spectrometer. GC/MS analyses were performed on a Hewlett Packard Model 6890 GC interfaced to a Hewlett Packard Model 5973 mass selective detector (15 m x 0.25 mm capillary column, HP-5MS). The same GC system with FID (30 m x 0.25 mm capillary column, HP-5) was used for capillary GLC analyses.

All manipulations were conducted under an argon atmosphere using a combination of glovebox and standard Schlenk techniques. Anhydrous ether, dichloromethane and pyridine were purchased from Aldrich. $B(C_6F_5)_3$ is commercially available, but for our purpose it was prepared according to the known procedure.[1] Acetates **3i-m** were prepared by acylation of commercially available secondary benzylic alcohols (Acros Organic, Aldrich) with acetic anhydride in pyridine.[2] Diacetate **3n** and alcohol **1c** were prepared according to the known procedures.[3, 4] Syntheses of functionally substituted substrates

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(2) Greene, T. W.; Wuts, P. G. *Protective Groups in Organic Synthesis*, 3rd ed.; Wiley: New York, 1999.

(3) Nukada, T.; Borces, A.; Whitfield D. M. *J. Org. Chem.* **1999**, *64*, 9030.

(4) Okumura, K.; Shimazaki, T.; Aoki, Y.; Yamashita, H.; Tanaka, E.; Banba, S.; Yazawa, K.; Kibayashi, K.; Banno, H. *J. Med. Chem.* **1998**, *41*, 4036.

6a-e and their analytical data are provided below. All other starting materials, solvents and reagents were purchased from Acros Organics or Aldrich.

Products **2a**[5], **2b**[6], **4a,b**[7] and **4e,f**[8] are known compounds, and their analytical data were in agreement with the literature data. The spectral data for new compounds **2c**, **4d,g,h, 7a-c** are provided below, as well as for known compounds **4e, 6a, 6c, 6e**, for which spectral data presented in literature are incomplete. (+) and (-) represent positive and negative intensities of signals in ^{13}C DEPT-135 experiment.

4-(Tetrahydropyranyloxy)-1-phenylbutanol-1.

To a stirred solution of phenylmagnesium bromide (60 mmol) in dry ether (200 mL) at 0ºC 4-(tetrahydropyranyloxy)-1-phenyl-butanal[9] (48 mmol) was added dropwise. The reaction mixture was stirred for 2 h, then it was quenched (saturated aqueous NH_4Cl) and extracted (ether). Combined etheral phases were washed (water and brine), dried (Na_2SO_4) and concentrated. Residual oil was purified by column chromatography on Silica gel, eluent hexane-EtOAc (2:1) to obtain the title compound as yellowish oil. Yield 8.41 g (33.6 mmol, 76%).

^{1}H NMR ($CDCl_3$, 500.13 MHz) δ 7.38-7.33 (m, 4H), 7.28 (t, 1H), 4.72 (t, J = 6.3 Hz, 1H), 4.60 (t, J = 3.2 Hz, 1H), 3.85 (m, 1H), 3.79 (m, 1H), 3.52 (m, 1H), 3.42 (m, 1H), 2.94 (br. s, 1H), 1.93-1.82 (m, 3H), 1.80-1.67 (m, 3H), 1.63-1.49 (m, 4H); ^{13}C NMR ($CDCl_3$, 125.76 MHz)[10] δ 145.3, 128.8 (+), 127.7 (+), 126.2 (+), 99.3 & 99.2 (+), 74.6 & 74.5 (+), 68.0 & 67.9 (-), 62.7 & 62.6 (-), 36.93 & 36.91 (-), 31.0 (-), 26.7 & 26.6 (-), 25.8 (-), 19.93 & 19.89 (-).

4-(Tetrahydropyranyloxy)-1-phenylbutyl-1-acetate.

4-(Tetrahydropyranyloxy)-1-phenylbutanol-1 (8.4 g, 33.6 mmol) was stirred in dry dichloromethane (100 mL) with dry pyridine (5 mL) and DMAP (0.1 g). Acetic anhydride (4.5 mL) was added. The reaction mixture was stirred overnight, quenched (diluted HCl) and extracted (dichloromethane). Combined organic phases were washed (diluted HCl, aqueous $NaHCO_3$, and brine), dried (Na_2SO_4) and concentrated. Preparative

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(10) Certain lines in ^{13}C NMR spectrum are split due to presence of two diastereomers.

column chromatography of the residue on Silica gel (eluent hexane-EtOAc, 3:1) gave 9.65 g (33 mmol, 98%) of acetate.
^{1}H NMR ($CDCl_3$, 400.13 MHz) δ 7.34-7.32 (m, 4H), 7.32-7.25 (m, 1H), 5.77 (t, J = 7.0 Hz), 4.56-4.53 (m, 1H), 3.85-3.80 (m, 1H), 3.77-3.70 (m, 1H), 3.51-3.45 (m, 1H), 3.41-3.34 (m, 1H), 2.07 (s, 3H), 2.00-1.45 (m, 10H); ^{13}C NMR ($CDCl_3$, 100.61 MHz) δ 170.3, 140.6, 128.4 (+), 127.9 (+), 126.5 (+), 98.8 (+), 75.9 (+), 67.0 (-), 62.3 (-), 33.1 (-), 30.7 (-), 25.8 (-), 25.4 (-), 21.3 (-), 19.6 (+); FT-IR (film, cm^{-1}) 2944, 2870, 1738, 1495, 1453, 1371, 1234, 1222, 1076, 1034, 788, 762, 700.

6d: 4-(Tetrahydropyranyloxy)-1-phenylbutyl-1-acetate (7.3 g, 25 mmol) was stirred in a mixture of glacial AcOH (200 mL), THF (100 mL), and water (50 mL) at 45ºC for 40 h, until TLC showed no starting material left. The mixture was poured into ice-cold water (700 mL) and extracted with ether. Combined etheral layers were neutralized by washing with semisaturated Na_2CO_3, washed (brine), dried ($MgSO_4$) and concentrated. The residue was purified by preparative column chromatography on Silica gel (eluent hexane-EtOAc, 3:1 → 1:1). Yield 3.09 g (14.8 mmol, 59%).
^{1}H NMR ($CDCl_3$, 400.13 MHz) δ 7.34-7.30 (m, 4H), 7.29-7.26 (m, 1H), 5.74 (dd, J = 7.5 Hz, 6.4 Hz, 1H), 3.59 (t, J = 6.5 Hz, 2H), 2.15 (br. s, 1H), 2.06 (s, 3H), 1.96 (m, 1H), 1.86 (m, 1H), 1.56 (m, 1H), 1.49 (m, 1H); ^{13}C NMR ($CDCl_3$, 100.61 MHz) δ 170.6, 140.4, 128.5 (+), 127.0 (+), 126.5 (+), 75.9 (+), 62.2 (-), 32.6 (-), 28.5 (-), 21.3 (+); 1H-13C HMBC showed signal fp_1 = 170.6, fp_2 = 5.74 ppm; FT-IR (film, cm^{-1}) 3438 br, 2945, 2871, 1736, 1454, 1373, 1241, 1026, 961, 763, 701.

6a: 4-Hydroxy-1-phenylbutyl-1-acetate (**6d**) (500 mg, 2.4 mmol) was stirred in dry dichloromethane (10 mL) and dry pyridine (1.5 mL) was added, followed by addition of acetic anhydride (1 mL). The reaction mixture was stirred overnight, quenched (diluted HCl) and extracted (ether). Combined organic layers were washed (diluted aqueous Na_2CO_3, brine), dried ($MgSO_4$) and concentrated. The residue was purified by preparative column chromatography on Silica gel (eluent hexane-EtOAc 4:1) to obtain 521 mg (2.08 mmol, 87%) of diacetate **6a** (identical to reported in literature[11]).
^{1}H NMR ($CDCl_3$, 400.13 MHz) δ 7.35-7.26 (m, 5H), 5.75 (dd, J = 7.7 Hz, 6.0 Hz, 1H), 4.05 (t, J = 6.8 Hz, 2H), 2.07 (s, 3H), 2.03 (s, 3H), 1.94 (m, 1H), 1.85 (m, 1H), 1.68 (m, 1H), 1.60 (m, 1H); ^{13}C NMR ($CDCl_3$, 100.61 MHz) δ 171.1, 170.3, 140.3, 128.5 (+), 128.0 (+), 126.4 (+), 75.5 (+), 64.0 (-), 32.8 (-), 24.8 (-), 21.2 (+), 20.9 (+).

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6b: 4-Hydroxy-1-phenylbutyl-1-acetate (**6d**) (1.0 g, 4.8 mmol) was added to a stirred solution of CBr_4 (5.1 mmol) and PPh_3 (11 mmol) in dry dichloromethane (35 mL) at 0ºC. The reaction mixture was allowed to warm to room temperature and stirred overnight, then diluted with ether and filtered through sintered funnel. Filtrate was concentrated and the residue was purified by preparative column chromatography on Silica gel (eluent hexane-CH_2Cl_2-EtOAc 10:2:1). Yield 970 mg (3.58 mmol, 75%).
^{1}H NMR ($CDCl_3$, 500.13 MHz) δ 7.38-7.30 (m, 5H), 5.80 (dd, J = 7.6 Hz, 5.7 Hz, 1H), 3.42 (t, J = 6.5 Hz, 2H), 2.11 (s, 3H), 2.07 (m, 1H), 2.01-1.90 (m, 2H), 1.85 (m, 1H); ^{13}C NMR ($CDCl_3$, 125.76 MHz) δ 170.7, 140.5, 129.0 (+), 128.5 (+), 126.8 (+), 75.5 (+), 35.3 (-), 33.5 (-), 29.1 (-), 21.67 (+); GC/MS m/z 270 (M^+, <3%), 228 (M^+-CH_2CO, 25%), 107 (100%)

6e: To a stirred suspension of sodium cyanide (700 mg) in dry DMF (20 mL) a solution of 4-bromo-1-phenylbutyl-1-acetate (**6b**) (800 mg) in DMF (2 mL) was added dropwise. The reaction mixture was stirred at room temperature for 1.5 h, quenched (water) and extracted (EtOAc). Combined organic layers were washed (brine), dried ($MgSO_4$) and concentrated. The residue was purified by preparative column chromatography on Silica gel (eluent hexane-EtOAc 3:1) to obtain 598 mg (2.75 mmol, 87%) of nitrile **6e** (identical to reported in literature[12]).
^{1}H NMR ($CDCl_3$, 400.13 MHz) δ 7.38-7.26 (m, 5H), 5.76 (dd, J = 7.6 Hz, 5.9 Hz, 1H), 2.35 (t, J = 7.2 Hz, 2H), 2.09 (s, 3H), 2.07 (m, 1H), 1.94 (m, 1H), 1.74-1.56 (m, 2H); ^{13}C NMR ($CDCl_3$, 100.61 MHz) δ 170.2, 139.7, 128.7 (+), 128.2 (+), 126.3 (+), 119.2, 74.8 (+), 35.2 (-), 21.6 (-), 21.2 (+), 16.9 (-); FT-IR (film, cm^{-1}) 3063, 3032, 2944, 2873, 2245, 1747, 1494, 1454, 1428, 1372, 1247, 1232, 1046, 1023, 954, 908, 762, 701; GC/MS m/z 175 (M^+-CH_2CO, 15%), 117 (100%).

6c: Solution of 4-benzyloxy-butanal[13] (278 mg, 1.56 mmol) in dry ether (2 mL) was added dropwise to a stirred solution of phenylmagnesium bromide (3 mmol) in dry ether (10 mL) at 0ºC. The reaction mixture was allowed to warm to room temperature and stirred for 4 h, quenched (saturated aqueous NH_4Cl) and extracted (ether). Combined etheral phases were washed (brine), dried ($MgSO_4$) and concentrated. Purification of the residue by short column chromatography on Silica gel (eluent hexane-EtOAc 4:1) gave 4-benzyloxy-1-phenylbutanol-1 (identical to reported in literature[14]). This alcohol was then

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dissolved in dry dichloromethane (10 mL), and a solution of DMAP (5 mg) in dry pyridine (1.5 mL) was added, followed by addition of acetic anhydride (1 mL). The reaction mixture was stirred for 5 h, quenched (diluted HCl) and extracted (dichloromethane). Combined organic phases were washed (diluted HCl, diluted Na_2CO_3, brine), dried ($MgSO_4$), and concentrated. Purification of the residue by preparative column chromatography on Silica gel (eluent hexane-EtOAc 10:1) gave 326 mg (1.09 mmol, 70% for 2 steps) of desired acetate **6c** (identical to reported in literature[14]).
^{1}H NMR ($CDCl_3$, 400.13 MHz) δ 7.38-7.26 (m, 10H), 5.78 (dd, J = 7.5 Hz, 6.3 Hz, 1H), 4.92 (s, 2H), 3.48 (t, J = 6.4 Hz, 2H), 2.08 (s, 3H), 2.00 (m, 1H), 1.93 (m, 1H), 1.67 (m, 1H), 1.60 (m, 1H); ^{13}C NMR ($CDCl_3$, 100.61 MHz) δ 170.4, 140.6, 138.4, 128.5 (+), 128.4 (+), 127.9 (+), 127.7 (+), 127.6 (+), 126.5 (+), 75.8 (+), 72.9 (-), 69.8 (-), 33.1 (-), 25.9 (-), 21.3 (+); GC/MS m/z 255 (M-CH_3CO, 1%), 91 (100%).

Pocedure for allylation of benzylic substrates
The preparation of **4a** is representative. To a stirred solution of $B(C_6F_5)_3$ (26 mg, 5 mol%) in anhydrous CH_2Cl_2 (1 mL) **3f** (1 mmol, 164 mg) was added, followed by addition of allyltrimethylsilane (1.5 mmol, 240 μL). The mixture was stirred at room temperature and the reaction course was monitored by capillary GLC analysis. After the reaction was complete (12 h for **4a**), the mixture was filtered through a short column (Silica gel) and concentrated. Purification by column chromatography (Silica gel, hexane as an eluent) gave 133 mg of **4a** (91%).

2c: ^{1}H NMR ($CDCl_3$, 500.13 MHz) δ 7.02 (d, J = 8.4 Hz, 1H), 6.76 (d, J = 2.6 Hz, 1H), 6.72 (dd, J = 8.4 Hz, 2.6 Hz, 1H), 4.86 (br. s, 1H), 4.76 (br. s, 1H), 3.82 (s, 3H), 2.96 (ps.-sextet, J = 5.1 Hz, 1H), 2.73 (m, 2H), 2.45 (dd, J = 13.9 Hz, 4.4 Hz, 1H), 2.28 (dd, J = 13.9 Hz, 10.7 Hz, 1H), 1.84 (br. s, 3H), 1.88-1.68 (m, 4H); ^{13}C NMR ($CDCl_3$, 125.76 MHz) δ 157.9, 144.7, 142.7, 130.3 (+), 129.7, 114.0 (+), 112.7 (_), 112.0 (+), 55.7 (+), 46.2 (-)35.8 (+), 29.3 (-), 27.0 (-), 22.5 (+), 19.9 (-);FT-IR (film, cm^{-1}) 3070, 2931, 2858, 2839, 1645, 1609, 1577, 1499, 1453, 1312, 1254, 1156, 1121, 1042, 889, 857, 802, 732; GC/MS m/z 216 (M^+, 8%), 161 (M^+-methallyl, 100%).

4d: ^{1}H NMR ($CDCl_3$, 400.13 MHz) δ 7.31 (t, 2H), 7.21 (m, 3H), 4.70 (s, 1H), 4.62 (s, 1H), 2.67 (m, 1H), 2.42-2.30 (m, 2H), 1.74 (m, 1H), 1.69 (s, 3H), 1.54 (m, 1H), 0.80 (t, J = 7.4 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100.61 MHz) δ 145.4, 144.1, 128.2 (+), 127.7 (+), 125.9 (+), 112.0 (-), 45.7 (+), 45.2 (-), 29.1 (-), 22.4 (+), 12.1 (+); FT-IR (film, cm^{-1}) 3070, 3026, 2963, 2926, 2874, 1646, 1601, 1493, 1450, 1375, 887, 754, 699, 547;

GC/MS m/z 174 (M^+, 5%), 91 ($C_7H_7^+$, 100%); HRMS calcd for $C_{13}H_{18}$ 174.1409, found 174.1411.

4e: ^{1}H NMR ($CDCl_3$, 400.13 MHz) δ 7.14 (d, J = 8.6 Hz, 2H), 6.87 (d, J = 8.6 Hz, 2H), 5.73 (m, 1H), 5.01 (m, J = 17.5 Hz, 1H), 4.98 (m, J = 10.5 Hz, 1H), 3.81 (s, 3H), 2.77 (ps.-sextet, J = 7.0 Hz, 1H), 2.41-2.25 (m, 2H), 1.25 (d, J = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100.61 MHz) δ 157.8, 139.2, 137.3 (+), 127.8 (+), 115.8 (-), 113.7 (+), 55.2 (+), 43.0 (-), 38.9 (+), 21.7 (+).GC/MS m/z 176 (M^+, 5%), 135 (M-Allyl, 100%).

4g: ^{1}H NMR ($CDCl_3$, 500.13 MHz) δ 7.18 (dd, J_{HH} = 8.5 Hz, $^4J_{HF}$ = 5.6 Hz, 2H), 7.01 (ps-t, J_{HH} = 8.5 Hz, $^3J_{HF}$ = 8.5 Hz, 2H), 5.73 (m, 1H), 5.03 (m, 1H), 5.00 (m, 1H), 2.82 (ps-sexstet, J = 7.0 Hz, 1H), 2.35 (m, 2H), 1.28 (d, J = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125.76 MHz) δ 161.6 (d, $^1J_{CF}$ = 243 Hz), 143.0, 137.3 (+), 128.7 (+)(d, $^3J_{CF}$ = 7.7 Hz), 116.5 (-), 115.4 (+)(d, $^2J_{CF}$ = 21.0 Hz), 43.2 (-), 39.5 (+), 22.1 (+); ^{19}F NMR ($CDCl_3$, 470.59 MHz) δ -119.20; FT-IR (film, cm^{-1}) 3075, 2963, 2924, 1640, 1603, 1509, 1455, 1375, 1226, 1158, 993, 914, 831, 541; GC/MS m/z 164 (M^+, <3%), 123 (M-Allyl, 100%); HRMS calcd for $C_{11}H_{13}F$ 164.1001, found 164.1005.

4h: ^{1}H NMR ($CDCl_3$, 500.13 MHz) δ 7.32 (d, J = 8.1 Hz, 2H), 7.23 (d, J = 8.1 Hz, 2H), 5.73 (m, 1H), 5.11 (s, 2H), 5.03 (m, J = 15.6 Hz, 1H), 4.99 (m, J = 10.1 Hz, 1H), 2.83 (ps-sextet, J = 7.0 Hz, 1H), 2.41 (m, 1H), 2.33 (m, 1H), 2.13 (s, 3H), 1.28 (d, J = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125.76 MHz) δ 171.4, 147.7, 137.4 (+), 133.9, 128.9 (+), 127.6 (+), 116.5 (-), 66.7 (-), 43.0 (-), 39.9 (+), 21.9 (+), 21.5 (+); FT-IR (film, cm^{-1}) 2961, 2925, 1746, 1639, 1513, 1452, 1378, 1225, 1025, 914, 818; GC/MS m/z 218 (M^+, 5%), 177 (M-Allyl, 100%); HRMS calcd for $C_{14}H_{18}O_2$ 218.1307, found 218.1311.

7a: ^{1}H NMR ($CDCl_3$, 400.13 MHz) δ 7.30 (t, 2H), 7.20 (t, 1H), 7.15 (d, 2H), 5.66 (m, 1H), 4.97 (m, J = 17.4 Hz, 1H), 4.94 (m, J = 11.1 Hz, 1H), 3.99 (t, J = 6.6 Hz, 2H), 2.61 (m, 1H), 2.37 (t, J = 7.1 Hz, 2H), 2.02 (s, 3H), 1.75 (m, 1H), 1.61 (m, 1H), 1.48 (m, 2H); ^{13}C NMR ($CDCl_3$, 100.61 MHz) δ 171.2, 144.6, 136.8 (+), 128.4 (+), 127.6 (+), 126.2 (+), 116.1 (-), 64.5 (-), 45.5 (+), 41.3 (-), 32.0 (-), 26.6 (-), 21.0 (+); FT-IR (film, cm^{-1}) 3076, 3063, 3026, 3000, 2972, 2921, 2858, 1741, 1639, 1492, 1451, 1386, 1364, 1241, 1232, 1039, 995, 913, 760, 701; GC/MS m/z 232 (M^+, <1%), 191 (M-Allyl, 8%), 131 (100%); HRMS calcd for $C_{15}H_{20}O_2$ 232.1463, found 232.1466.

7b: ^{1}H NMR ($CDCl_3$, 500.13 MHz) δ 7.33 (t, 2H), 7.23 (t, 1H), 7.18 (d, 2H), 5.69 (m, 1H), 5.01 (m, J = 16.9 Hz, 1H), 4.97 (m, J = 10.2 Hz, 1H), 3.36 (t, J = 6.6 Hz, 2H), 2.65

(m, 1H), 2.40 (ps-t, J = 7.1 Hz, 2H), 1.90 (m, 1H), 1.78-1.66 (m, 3H); ^{13}C NMR ($CDCl_3$, 125.76 MHz) δ 144.9, 137.1 (+), 128.9 (+), 128.0 (+), 126.7 (+), 116.6 (-), 45.7 (+), 41.8 (-), 34.7 (-), 34.4 (-), 31.1 (-); FT-IR (film, cm^{-1}) 3076, 3062, 3025, 3001, 2922, 2854, 1639, 1601, 1492, 1450, 1284, 1259, 1240, 993, 913, 759, 670, 644; GC/MS m/z 252 (M^+, <1%), 211 (M-Allyl, 23%), 91 ($C_7H_7^+$, 100%); HRMS calcd for $C_{13}H_{17}{}^{79}Br$ 252.0514, found 252.0515.

7c: ^{1}H NMR ($CDCl_3$, 400.13 MHz) δ 7.36-7.25 (m, 7H), 7.21-7.13 (m, 3H), 5.65 (m, 1H), 4.97 (d, J = 17.0 Hz, 1H), 4.92 (d, J = 10.6 Hz, 1H), 4.46 (s, 2H), 3.41 (ps-t, J = 6.3 Hz, 2H), 2.60 (m, 1H), 2.38 (ps-t, J = 7.1 Hz, 2H), 1.82 (m, 1H), 1.61 (m, 1H), 1.49 9m, 2H); ^{13}C NMR ($CDCl_3$, 100.61 MHz) δ 145.0, 138.6, 137.1 (+), 128.34 (+), 128.28 (+), 127.7 (+), 127.6 (+), 127.5 (+), 126.1 (+), 115.9 (-), 72.8 (-), 70.3 (-), 45.7 (+), 41.4 (-), 32.4 (-), 27.7 (-); FT-IR (film, cm^{-1}) 3062, 3026, 3002, 2974, 2934, 2918, 2854, 2790, 1639, 1601, 1493, 1451, 1361, 1204, 1103, 1027, 994, 911, 786, 758, 734, 699.