

# Supplementary Material (ESI) for Chemical Communications  
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**Supporting Information**

**for**

**Phosphazene base-promoted functionalization of aryltrimethylsilanes**

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### General comment

<sup>1</sup>H-NMR spectra were recorded on a JEOL AL-400 using tetramethylsilane as an internal standard. Chemical shifts are expressed in  $\delta$ (ppm) values, and coupling constants are expressed in Hertz (Hz). The following abbreviations are used: s = singlet, d = doublet, m = multiplet, t = triplet, brs = broad singlet, dd = double-doublet, dt = double-triplet and ddd = double-doublet-doublet. Mass spectra were recorded on JEOL JMS-DX303 or JEOL JMS-AX500 spectrometer. IR spectra were measured with SensIR ATR FT-IR. All the reactions dealing with air or moisture sensitive compounds were carried out in a dry reaction vessel under argon atmosphere unless otherwise noted. Flash column chromatography was carried out using Kanto Chemical Silica gel 60N (70-230 mesh). Dry THF, dry dimethylformamide (DMF) and diethylzinc 1.0 M solution in *n*-hexane were purchased from Kanto Chemical Company and used as supplied. *tert*-Butyl P4 base 1.0 M solution in *n*-hexane was purchased from Fulka Chemie and used as supplied.

### General Procedure for Table 1 and Table 2

Under Ar atmosphere, to a mixture of an aryltrimethylsilane (0.3 mmol), an aldehyde (0.45 mmol), dry DMF (1 ml), *t*-Bu-P4 base (0.06 mmol) was added at  $-40\text{ }^{\circ}\text{C}$  and the mixture was stirred for the time listed in tables. After the reaction, aq.  $\text{NH}_4\text{Cl}$  was added to the mixture and extracted with AcOEt. The organic layer was dried over  $\text{MgSO}_4$  and the solvent was removed under reduced pressure. TBAF (1M THF solution, 0.3 ml) was added to the residue and the mixture was stirred at room temperature for 1 h. After the reaction, aq.  $\text{NH}_4\text{Cl}$  was added to the mixture and extracted with AcOEt. The organic layer was dried over  $\text{MgSO}_4$  and the solvent was removed under reduced pressure. The residue was purified by  $\text{SiO}_2$  column chromatography.

### Spectral Data

#### 2,2-Dimethyl-1-naphthalen-1-ylpropan-1-ol (2a)

<sup>1</sup>H-NMR (400MHz,  $\text{CDCl}_3$ ) $\delta$ (ppm): 0.99 (9H, s), 5.41 (1H, s), 7.4-7.55 (3H, m), 7.68 (1H, d,  $J=7.1$  Hz), 7.77 (1H, d,  $J=8.1$  Hz), 7.8-7.9 (1H, m), 8.14 (1H, d,  $J=7.6$  Hz); IR(neat): 3328, 3058, 1598, 1509, 1493, 1451, 1395, 1164, 1052, 1034, 1003, 778, 699; LRMS (EI)  $m/z$  214( $\text{M}^+$ ); HRMS calcd for  $\text{C}_{15}\text{H}_{18}\text{O}$  214.1357, found 214.1362.

#### Naphthalen-1-ylphenylmethanol (2b)

<sup>1</sup>H-NMR (400MHz,  $\text{CDCl}_3$ ) $\delta$ (ppm): 2.34 (1H, s), 6.53 (1H, s), 7.26 (1H, t,  $J=7.1$  Hz), 7.32 (2H, s), 7.35-7.55 (5H, s), 7.62 (1H, d,  $J=7.1$  Hz), 7.80 (1H, d,  $J=8.1$  Hz), 7.83-7.9 (1H, m), 8.03 (1H, d,  $J=7.1$  Hz); IR(neat): 3442, 2952, 1725, 1596, 1511, 1478, 1465, 1393, 1362, 1235, 1212, 1164, 1061; LRMS (EI)  $m/z$  234( $\text{M}^+$ ); HRMS calcd for  $\text{C}_{17}\text{H}_{14}\text{O}$  234.1044, found 234.1024.

**(4-Methoxyphenyl)naphthalen-1-ylmethanol (2c)**

<sup>1</sup>H-NMR (500MHz, CDCl<sub>3</sub>)δ(ppm): 2.31 (1H, s), 3.76 (3H, s), 6.48 (1H, s), 6.84 (2H, d, *J*= 8.5 Hz), 7.30 (2H, d, *J*= 8.5 Hz), 7.35-7.55 (3H, m), 7.68 (1H, d, *J*= 7.1 Hz), 7.80 (1H, d, *J*= 8.3 Hz), 7.83-7.88 (1H, m), 7.98 (1H, d, *J*= 8.3 Hz); IR(neat): 3431, 1609, 1509, 1246, 1173, 1032; LRMS (EI) *m/z* 264(M<sup>+</sup>); HRMS calcd for C<sub>18</sub>H<sub>16</sub>O<sub>2</sub> 264.1150, found 264.1143.

**(2-Methoxyphenyl)naphthalen-1-ylmethanol (2d)**

<sup>1</sup>H-NMR (400MHz, CDCl<sub>3</sub>)δ(ppm): 3.06 (1H, s), 3.93 (3H, s), 6.75-6.9 (2H, m), 6.9-7.0 (2H, m), 7.2-7.3 (1H, m), 7.35-7.55 (3H, m), 7.66 (1H, dd, *J*=7.1 Hz, *J*=1.0 Hz), 7.75-7.9 (2H, m), 7.99 (1H, d, *J*= 7.1 Hz); IR(neat): 3186, 3037, 1600, 1488, 1459, 1432, 1301, 1237, 1038, 787, 756; LRMS (EI) *m/z* 264(M<sup>+</sup>); HRMS calcd for C<sub>18</sub>H<sub>16</sub>O<sub>2</sub> 264.1150, found 264.1122.

**2,2-Dimethyl-2-naphthalen-1-ylpropan-1-ol (4a)**

<sup>1</sup>H-NMR (400MHz, CDCl<sub>3</sub>)δ(ppm): 0.97 (9H, s), 1.99 (1H, s), 4.56 (1H, s), 7.4-7.5 (2H, m), 7.7-7.85 (4H, m); IR(neat): 3450, 2952, 2867, 1725, 1602, 1507, 1478, 1362, 1237, 1169, 1123, 1048, 1007; LRMS (EI) *m/z* 214 (M<sup>+</sup>); HRMS calcd for C<sub>15</sub>H<sub>18</sub>O 214.1358, found 214.1350.

**1-(4-Fluorophenyl)-2,2-dimethylpropan-1-ol (4b)**

<sup>1</sup>H-NMR (400MHz, CDCl<sub>3</sub>)δ(ppm): 0.90 (9H, s), ?, ?, 6.99 (2H, dd, *J*=8.8 Hz, *J*= 8.8 Hz), 7.27 (2H, dd, *J*= 8.8 Hz, *J*= 5.6 Hz); IR(neat): 3498, 2956, 1727, 1603, 1509, 1374, 1239, 1221, 1158, 1046, 1009, 837, 758; LRMS (EI) *m/z* 182 (M<sup>+</sup>); HRMS calcd for C<sub>11</sub>H<sub>15</sub>FO 182.1107, found 182.1107.

**1-(4-Bromophenyl)-2,2-dimethylpropan-1-ol (4c)**

<sup>1</sup>H-NMR (400MHz, CDCl<sub>3</sub>)δ(ppm): 0.90 (9H, s), 1.86 (1H, s), 4.36 (1H, s), 7.18 (2H, d, *J*=8.0 Hz), 7.43 (2H, d, *J*= 8.0 Hz); IR(neat): 3651, 3303, 2952, 2929, 2902, 2867, 1609, 1590, 1478, 1403, 1364, 1071, 1046, 1007; LRMS (EI) *m/z* 242 (M<sup>+</sup>); HRMS calcd for C<sub>11</sub>H<sub>15</sub>BrO 242.0306, found 242.0312.

**1-[4-Trifluoromethylphenyl]-2,2-dimethylpropan-1-ol (4d)**

<sup>1</sup>H-NMR (400MHz, CDCl<sub>3</sub>)δ(ppm): 0.92 (9H, s), 1.96 (1H, s), 4.45 (1H, s), 7.43 (2H, d, *J*=8.0 Hz), 7.57 (2H, d, *J*= 8.0 Hz); IR(neat): 3440, 2958, 2873, 1324, 1162, 1123, 1067, 1007; LRMS (EI) *m/z* 232 (M<sup>+</sup>); HRMS calcd for C<sub>12</sub>H<sub>15</sub>F<sub>3</sub>O 232.1075, found 232.1078.

**1-[2-Trifluoromethylphenyl]-2,2-dimethylpropan-1-ol (4e)**

<sup>1</sup>H-NMR (400MHz, CDCl<sub>3</sub>)δ(ppm): 0.97 (9H, s), 1.99 (1H, s), 4.90 (1H, s), 7.36 (1H, t, *J*=7.6 Hz), 7.53 (1H, t, *J*= 7.7 Hz), 7.62 (1H, d, *J*= 7.8 Hz), 7.77 (1H, d, *J*= 8.1 Hz); IR(neat): 3448, 2958, 1727,

1306, 1262, 1156, 1119, 1034, 1003; LRMS (EI)  $m/z$  232 ( $M^+$ ); HRMS calcd for  $C_{12}H_{15}F_3O$  232.1075, found 232.1099.

**Methyl 4-(1-hydroxy-2,2-dimethylpropyl)benzoate (4f)**

$^1H$ -NMR (400MHz,  $CDCl_3$ ) $\delta$ (ppm): 0.92 (9H, s), 3.90 (3H, s), 4.44 (1H, s), 7.37 (2H, d,  $J=8.3$  Hz), 7.96 (2H, d,  $J=8.3$  Hz); IR(neat): 3483, 2954, 2869, 1706, 1611, 1436, 1277, 1177, 1106, 1054, 1011, 862, 745, 706; LRMS (EI)  $m/z$  222 ( $M^+$ ); HRMS calcd for  $C_{13}H_{18}O_3$  222.1256, found 222.1272.

**2,2-Dimethyl-1-(2-pyridyl)propan-1-ol (4g)**

$^1H$ -NMR (400MHz,  $CDCl_3$ ) $\delta$ (ppm): 0.92 (9H, s), 4.35 (1H, s), 7.15-7.25 (2H, m), 7.62 (1H, dt,  $J=7.6$  Hz,  $J=1.6$  Hz), 8.55 (1H, dd,  $J=5.2$  Hz,  $J=1.8$  Hz); IR(neat): 3228, 2948, 1594, 1476, 1434, 1389, 1102, 1067, 1019, 1003; LRMS (EI)  $m/z$  108 ( $M^+-C_4H_9$ ); HRMS calcd for  $C_6H_6NO$  108.0449, found 108.0453.

**2,2-Dimethyl-1-(3-pyridyl)propan-1-ol (4h)**

$^1H$ -NMR (400MHz,  $CDCl_3$ ) $\delta$ (ppm): 0.93 (9H, s), 2.21 (1H, s), 4.43 (1H, s), 7.2-7.3 (1H, m), 7.68 (1H, dd,  $J=7.3$  Hz,  $J=1.8$  Hz), 8.45-8.55 (2H, m); IR(neat): 3228, 2964, 2931, 2867, 1578, 1472, 1422, 1362, 1308, 1235, 1173, 1065, 1028, 1011, 816, 758, 716; LRMS (EI)  $m/z$  165 ( $M^+$ ); HRMS calcd for  $C_{10}H_{15}NO$  165.1154, found 165.1129.

**2,2-Dimethyl-1-(2-thienyl)propan-1-ol (4i)**

$^1H$ -NMR (400MHz,  $CDCl_3$ ) $\delta$ (ppm): 0.98 (9H, s), 2.03 (1H, s), 4.66 (1H, s), 6.9-7.0 (2H, m), 7.23 (1H, dd,  $J=5.0$  Hz,  $J=1.3$  Hz); IR(neat): 3448, 2954, 2869, 1478, 1364, 1233, 1183, 1040, 1003; LRMS (EI)  $m/z$  170 ( $M^+$ ); HRMS calcd for  $C_9H_{14}OS$  170.0765, found 170.0756.

**3-Phenylphthalide (6)**

$^1H$ -NMR (400MHz,  $CDCl_3$ ) $\delta$ (ppm): 6.41 (1H, s), 7.26-7.30 (2H, m), 7.37 (1H, d,  $J=7.6$ ), 7.36-7.40 (3H, m), 7.56 (1H, t,  $J=7.6$  Hz), 7.65 (1H, dt,  $J=7.6$  Hz, 1.2 Hz), 7.97 (1H, t,  $J=7.6$  Hz); IR(neat): 3064, 3033, 1744, 1600, 1465, 1335, 1285, 1210, 1183, 1098, 1067, 1013, 965; LRMS (EI)  $m/z$  210 ( $M^+$ ); HRMS calcd for  $C_{14}H_{10}O_2$  210.0680, found 210.0692.

**4,4-Dimethyl-2-phenylpent-1-en-3-ol (8a)**

$^1H$ -NMR (400MHz,  $CDCl_3$ ) $\delta$ (ppm): 0.82 (9H, s), 4.48 (1H, s), 5.35-5.4 (2H, m), 7.2-7.35 (3H, m), 7.35-7.4 (2H, m); IR(neat): 3465, 2954, 2904, 2869, 1478, 1364, 1108, 1050, 1007, 911, 776, 697; LRMS (EI)  $m/z$  190 ( $M^+$ ); HRMS calcd for  $C_{13}H_{18}O$  190.1358, found 190.1347.

**1-(2-Methoxyphenyl)-2-phenylprop-2-en-1-ol (8b)**

<sup>1</sup>H-NMR (400MHz, CDCl<sub>3</sub>)δ(ppm): 2.69 (1H, s), 3.84 (3H, s), 5.40 (1H, dd, *J*=1.5 Hz, *J*= 1.2 Hz), 5.52 (1H, dd, *J*= 1.2 Hz, *J*= 1.0 Hz), 6.03 (1H, s), 6.8-7.0 (2H, m), 7.15-7.45 (7H, m); IR(neat): 3400, 2937, 2836, 1600, 1490, 1463, 1437, 1287, 1239, 1021, 907; LRMS (EI) *m/z* 240 (M<sup>+</sup>); HRMS calcd for C<sub>16</sub>H<sub>16</sub>O<sub>2</sub> 240.1150, found 240.1129.

**1-(4-Methoxyphenyl)-2-phenylprop-2-en-1-ol (8c)**

<sup>1</sup>H-NMR (500MHz, CDCl<sub>3</sub>)δ(ppm): 1.99 (1H, s), 3.77 (3H, s), 5.48-5.52 (2H, m), 5.65 (1H, s), 6.84 (2H, d, *J*= 8.7 Hz), 7.2-7.35 (7H, m); IR(neat): 3413, 3056, 3006, 2933, 2836, 1609, 1509, 1441, 1302, 1246, 1171, 1023, 909, 830, 778, 754, 702; LRMS (EI) *m/z* 240 (M<sup>+</sup>); HRMS calcd for C<sub>16</sub>H<sub>16</sub>O<sub>2</sub> 240.1150, found 240.1135.