SUPPORTING INFORMATION

Palladium Complexes of 1,3,5,7-Tetramethyl-2,4,8-Trioxa-6-Phenyl-6-Phospha-adamantane: Synthesis, Crystal Structure and Use in the Suzuki and Sonogashira Reactions and the α -Arylation of Ketones

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EXPERIMENTAL

General: Toluene was distilled under argon from sodium. ¹H spectra were recorded at either 300 or 200 MHz while ¹³C NMR spectra were recorded at either 75 or 50 MHz with chloroform-d as the solvent and internal reference unless otherwise noted. Ions for low resolution mass spectra (MS) and high resolution mass spectra (HRMS) were generated using electron impact (EI).

2-Phenyltoluene (Table 1, entry 3). As per the general procedure described in the paper for Suzuki coupling, Pd(PA-Ph)₂.dba (14 mg, 0.015 mmol), K₃PO₄ (255 mg, 1.2 mmol), phenylboronic acid (73 mg, 0.60 mmol) and 2-chlorotoluene (63 mg, 0.50 mmol) in toluene (1.5 mL) were used. The reaction was heated at 60 °C and was complete after 20 h. Work-up and column chromatography (hexane) yielded 72 mg (88%) of the title compound as a colourless oil: The physical and spectral properties of 2-phenyltoluene match those previously reported.¹

1-Mesitylnaphthalene (Table 1, entry 4). As per the general procedure described in the paper for Suzuki coupling, Pd(PA-Ph)₂.dba (28 mg, 0.03 mmol), K₃PO₄ (509 mg, 2.4 mmol), 1-naphthaleneboronic acid (142 mg, 1.20 mmol) and 2-bromomesitylene (0.153 mL, 1.00 mmol) in toluene (3 mL) were used. The reaction was stirred at room temperature and was complete after 40 h. Work-up and column chromatography (5% EtOAc in hexane) yielded 245 mg (85%) of the title compound as a colourless oil: ¹H NMR: (CDCl₃, 200 MHz): δ 7.99-7.90 (m, 2H), 7.64-7.32 (m, 5H), 7.09 (s, 2H), 2.47 (s, 3H), 1.97 (s, 6H); ¹³C NMR: (CDCl₃, 50 MHz): δ 138.9, 2 x 136.9, 133.8, 132.0, 129.1, 128.3, 2 x 128.1, 127.2, 127.0, 126.8, 126.1, 2 x 125.8, 125.6, 21.2, 2 x 20.4; MS[EI⁺]: *m/z* (RI%): 246 (100), 231 (75), 215 (46), 202 (12) ; HRMS: for C₁₉H₁₈: calculated 246.1409, observed 246.1409.

4-(Phenylethynyl)acetophenone (Table 2, entry 2). As per the general procedure described in the paper for Sonogashira cross-coupling, Pd(PA-Ph)₂.dba (14 mg, 0.015 mmol), 4-iodoacetophenone (246 mg, 1.00 mmol), phenylacetylene (0.165 mL, 1.50 mmol), CuI (4 mg, 0.02 mmol), (*i*-Pr)₂NEt (0.210 mL, 1.20 mmol), and acetonitrile (2 mL). After 1 hour at room temperature, workup and column chromatography (20% EtOAc in hexane) yielded 204 mg (93%) of the title compound as a pale yellow solid. Compound showed: ¹H NMR: (CDCl₃, 300 MHz): δ 7.95 (d, *J* = 8.2 Hz, 2H), 7.62 (d, *J* = 8.3 Hz, 2H), 7.59-7.56 (m, 2H), 7.40-7.35 (m, 3H); 2.62 (s, 3H); ¹³C NMR: (CDCl₃, 75 MHz): δ 197.3, 136.2, 2 x 131.8, 2 x 131.7, 128.9, 2 x 128.5, 2 x 128.3, 128.2, 122.7, 92.8, 88.70, 26.7; MS[EI⁺]: *m/z*

(RI%): 220 (72), 205 (100), 176 (38), 151 (17); HRMS: for C₁₆H₁₂O: calculated 220.0888, observed 220.0891.

4-(Phenylethynyl)aniline (Table 2, entry 3). As per the general procedure described in the paper for Sonogashira cross-coupling, Pd(PA-Ph)₂.dba (14 mg, 0.015 mmol), 4-iodoaniline (218 mg, 0.997 mmol), phenylacetylene (0.165 mL, 1.50 mmol), CuI (4 mg, 0.020 mmol), (*i*-Pr)₂NEt (0.210 mL, 1.20 mmol), and acetonitrile (1 mL). After 1 hour at room temperature, workup and column chromatography (20% EtOAc in hexane) yielded 176 mg (91%) of the title compound as a yellow solid. The compound showed: ¹H NMR: (CDCl₃, 200 MHz): δ 7.60-7.50 (m, 2H), 7.43-7.30 (m, 5H), 6.63 (d, *J* = 8.2 Hz, 2H), 3.81 (s, broad, 2H); ¹³C NMR: (CDCl₃, 50 MHz): δ 146.7, 2 x 132.9, 2 x 131.3, 2 x 128.3, 127.7, 123.9, 2 x 114.8, 112.5, 90.2 87.4; MS[EI⁺]: *m/z* (RI%): 193 (100), 165 (12.6); HRMS: for C₁₄H₁₁N: calculated 193.0891, observed 193.0885.

2-(Phenylethynyl)toluene (Table 2, entry 4). As per the general procedure described in the paper for Sonogashira cross-coupling, Pd(PA-Ph)₂.dba (14 mg, 0.015 mmol), 2-iodotoluene (0.125 mL, 0.982 mmol), phenylacetylene (0.165 mL, 1.50 mmol), CuI (4 mg, 0.020 mmol), (*i*-Pr)₂NEt (0.210 mL, 1.20 mmol), and acetonitrile (1 mL). After 1 hour at room temperature, workup and column chromatography (hexane) yielded 173 mg (93%) of the title compound as a colourless liquid. The compound showed: ¹H NMR: (CDCl₃, 300 MHz): δ 7.66-7.59 (m, 3H), 7.42-7.40 (m, 3H), 7.33-7.31 (m, 2H), 7.28-7.26 (m, 1H), 2.62 (s, 3H); ¹³C NMR: (CDCl₃, 50 MHz): δ 140.2, 131.9, 2 x 131.6, 129.5, 3 x 128.4, 128.2, 125.7, 123.6, 123.1, 93.4, 88.4, 20.8; MS[EI⁺]: *m/z* (RI%): 192 (100), 191 (83), 165 (18), 115 (12); HRMS: for C₁₅H₁₂: calculated 192.0939, observed 192.0944.

4-(Phenylethynyl)anisole (Table 2, entry 5). As per the general procedure described in the paper for Sonogashira cross-coupling, Pd(PA-Ph)₂.dba (14 mg, 0.015 mmol), 4-iodoanisole (234 mg, 1.00 mmol), phenylacetylene (0.165 mL, 1.50 mmol), CuI (4 mg, 0.020 mmol), (*i*-Pr)₂NEt (0.210 mL, 1.20

mmol) [or Cs₂CO₃ (391 mg, 1.2 mmol)], and acetonitrile (1 mL). After 1 hour at room temperature, workup and column chromatography (1% EtOAc in hexane) yielded 196 mg (94%) of the title compound as a pale yellow solid. The compound showed: mp 56-58 °C; ¹H NMR: (CDCl₃, 300 MHz): δ 7.61-7.53 (m, 4H), 7.40-7.36 (m, 3H), 6.94 (d, *J* = 8.7 Hz, 2H), 3.85 (s, 3H); ¹³C NMR: (CDCl₃, 75 MHz): δ 159.6, 2 x 133.1, 2 x 131.5, 2 x 128.2, 128.0, 123.6, 115.4, 2 x 114.0, 89.5, 88.1, 55.4; IR (KBr, cm⁻¹) 2217 (C≡C); MS[EI⁺]: *m/z* (RI%): 208 (100), 193 (28), 165 (16); HRMS: for C₁₅H₁₂O: calculated 208.0888, observed 208.0886.

4-(4-Methoxyphenyl)-2-methylbut-3-yn-2-ol (Table 2, entry 6). As per the general procedure described in the paper for Sonogashira cross-coupling, Pd(PA-Ph)₂.dba (14 mg, 0.015 mmol), 4-iodoanisole (234 mg, 1.00 mmol), 2-methyl-3-butyn-2-ol (0.150 mL, 1.50 mmol), CuI (4 mg, 0.020 mmol), (*i*-Pr)₂NEt (0.210 mL, 1.20 mmol), and acetonitrile (1 mL). After 1 hour at room temperature, workup and column chromatography (20% EtOAc in hexane) yielded 175mg (92%) of the title compound as a yellow liquid. The compound showed: ¹H NMR: (CDCl₃, 300 MHz): δ 7.36 (d, *J* = 8.8 Hz, 2H), 6.83 (d, *J* = 8.8 Hz, 2H), 3.80 (s, 3H), 3.40 (s, broad, 1H), 1.62 (s, 6H); ¹³C NMR: (CDCl₃, 75 MHz): δ 159.5, 2 x 133.1, 114.9, 2 x 113.9, 92.5, 82.0, 65.6, 55.3, 2 x 31.6; IR (thin film, cm⁻¹) 3386 (OH), 2228 (C≡C); MS[EI⁺]: *m/z* (RI%): 190 (52), 175 (100); HRMS: for C₁₂H₁₄O₂: calculated 190.0994, observed 190.0992.

4-(Phenylethynyl)toluene (Table 3, entry 1). As per the general procedure described in the paper for Sonogashira cross-coupling, Pd(PA-Ph)₂.dba (20.7 mg, 0.022 mmol), 4-bromotoluene (0.125 mL, 1.00 mmol), phenylacetylene (0.165 mL, 1.50 mmol), Cs₂CO₃ (476 mg, 1.46 mmol) and acetonitrile (1 mL). After 6 h at 50 °C, work-up and column chromatography (hexane) yielded 178 mg (95%) of the title compound as a white solid. Spectral data were the same as listed for Table 2, entry 1.

4-(Phenylethynyl)acetophenone (Table 3, entry 2). Following As per the general procedure described in the paper for Sonogashira cross-coupling, Pd(PA-Ph)₂.dba (20.7 mg, 0.022 mmol), 4'-bromoacetophenone (198.5 mg, 0.997 mmol), phenylacetylene (0.165 mL, 1.50 mmol), Cs₂CO₃ (476 mg, 1.46 mmol) and acetonitrile (1 mL). After 3 hours at 50°C, work-up and column chromatography (10% EtOAc in hexane) yielded 196 mg (91%) of the title compound as a pale yellow solid. Spectral data were the same as listed for Table 2, entry 2

4-(4-Acetylphenyl)-2-methylbut-3-yn-2-ol (Table 3, entry 3). As per the general procedure described in the paper for Sonogashira cross-coupling, Pd(PA-Ph)₂.dba (34.5 mg, 0.037 mmol), 4'-bromoacetophenone (200 mg, 1.00 mmol), 2-methyl-3-butyn-2-ol (0.200 mL, 2.06 mmol), Cs₂CO₃ (391 mg, 1.20 mmol) and acetonitrile (1 mL). After 3 hours at 50°C, work-up and column chromatography (10% EtOAc in hexane) yielded 183 mg (90%) of the title compound as a pale yellow liquid. The compound showed: ¹H NMR: (CDCl₃, 200 MHz): δ 7.87 (d, *J* = 8.3 Hz, 2H), 7.47 (d, *J* = 8.3 Hz, 2H), 2.58 (s, 3H), 2.35 (s, broad, 1H), 1.62 (s, 6H); ¹³C NMR: (CDCl₃, 75 MHz): δ 197.8, 135.9, 2 x 131.6, 2 x 128.1, 127.8, 97.5, 81.1, 65.3, 2 x 31.2, 26.5; MS[EI⁺]: *m/z* (RI%): 202 (23), 187 (100); HRMS: for C₁₃H₁₄O₂: calculated 202.0994, observed 202.0997.

2-(Phenylethynyl)toluene (Table 3, entry 4). As per the general procedure described in the paper for Sonogashira cross-coupling, Pd(PA-Ph)₂.dba (20.7 mg, 0.022 mmol), 2-bromotoluene (0.120 mL, 0.998 mmol), phenylacetylene (0.165 mL, 1.50 mmol), Cs₂CO₃ (488 mg, 1.50 mmol) and acetonitrile (1 mL). After 6 hours at 50°C, workup and column chromatography (hexane) yielded 179 mg (93%) of the title compound as a colourless liquid. Spectral data were the same as listed for Table 2, entry 4.

4-(Phenylethynyl)-*N,N*-dimethylaniline (Table 3, entry 5). As per the general procedure described in the paper for Sonogashira cross-coupling, Pd(PA-Ph)₂.dba (20.7 mg, 0.022 mmol), 4-bromo-*N,N*-dimethylaniline (174.6 mg, 0.873 mmol), phenylacetylene (0.165 mL, 1.50 mmol), Cs₂CO₃ (488 mg,

1.50 mmol) and acetonitrile (1 mL). After 8 hours at 50°C, workup and column chromatography (2% EtOAc in hexane) yielded 176 mg (91%) of the title compound as a pale yellow solid. The compound showed: ¹H NMR: (CDCl₃, 300 MHz): δ 7.54 (dd, *J* = 6.9 & 1.4 Hz, 2H), 7.45 (dd, *J* = 6.9 & 1.8 Hz, 2H), 7.36-7.32 (m, 3H), 7.69 (d, *J* = 8.8 Hz, 2H), 3.02 (s, 6H); ¹³C NMR: (CDCl₃, 75 MHz): δ 150.2, 2 x 132.8, 2 x 131.4, 2 x 128.3, 127.5, 124.2, 2 x 111.9, 110.1, 90.7, 87.4, 2 x 40.3; IR (thin film, cm⁻¹) 2205 (C≡C); MS[EI⁺]: *m/z* (RI%): 221 (100), 220 (45), 110 (21); HRMS: for C₁₆H₁₅N: calculated 221.1204, observed 221.1210.

4-(Phenylethynyl)anisole (Table 3, entry 6). As per the general procedure described in the paper for Sonogashira cross-coupling, Pd(PA-Ph)₂.dba (20.7 mg, 0.022 mmol), 4-bromoanisole (0.125 mL, 1.00 mmol), phenylacetylene (0.165 mL, 1.50 mmol), Cs₂CO₃ (488 mg, 1.50 mmol) and acetonitrile (1 mL). After 24 hours at 60°C, workup and column chromatography (hexane) yielded 188 mg (90%) of the title compound as a pale yellow solid. Spectral data were the same as listed for Table 2, entry 5.

4-(4-Methoxyphenyl)-2-methylbut-3-yn-2-ol (Table 3, entry 7). As per the general procedure described in the paper for Sonogashira cross-coupling, Pd(PA-Ph)₂.dba (34.6 mg, 0.037 mmol), 4-bromoanisole (0.125 mL, 1.00 mmol), 2-methyl-3-buten-2-ol (0.195 mL, 2.00 mmol), Cs₂CO₃ (391 mg, 1.20 mmol) and acetonitrile (1 mL). After 1 h at 50°C, work-up and column chromatography (10% EtOAc in hexane) yielded 175 mg (92%) of the title compound as a yellow liquid. Spectral data were the same as listed for Table 2, entry 6.

1-(Phenylethynyl)-2,4,6-trimethylbenzene, (Table 3, entry 8). As per the general procedure described in the paper for Sonogashira cross-coupling, Pd(PA-Ph)₂.dba (20.7 mg, 0.022 mmol), 2-bromomesitylene (195 mg, 0.980 mmol), phenylacetylene (0.165 mL, 1.50 mmol), Cs₂CO₃ (488 mg, 1.50 mmol) and acetonitrile (1 mL). After 12 hours at 60°C, work-up and column chromatography (hexane) afforded 201 mg (93%) of the title compound as a colourless liquid. The compound showed:

^1H NMR: (CDCl_3 , 200 MHz): δ 7.62-7.57 (m, 2H), 7.36-7.32 (m, 3H), 6.89 (s, 2H), 2.47 (s, 6H), 2.30 (s, 3H); ^{13}C NMR: (CDCl_3 , 75 MHz): δ 2 x 140.1, 137.8, 2 x 131.4, 2 x 128.4, 127.9, 2 x 127.7, 124.1, 120.0, 97.1, 87.5, 21.4, 2 x 21.0; MS[EI $^+$]: m/z (RI%): 220 (100), 205 (41); HRMS: for $\text{C}_{17}\text{H}_{16}$: calculated 220.1252, observed 220.1252.

2-(4-Methylphenyl)-1-phenylpropa-1-none (Table 4, entry 2). As per the general procedure described in the paper for ketone arylations, $(\text{PA-Ph})_2\text{Pd.dba}$ (2, 13.4 mg, 0.015 mmol), NaO^tBu (192 mg, 2.00 mmol), 4-bromotoluene (0.108 mL, 1.00 mmol), propiophenone (0.146 mL, 1.10 mmol) and toluene/THF (1.5 mL: 0.5 mL) were used. After 24 h at 40 $^\circ\text{C}$, work-up and column chromatography (5% EtOAc in hexane) gave 208 mg (96%) of the title compound as a pale yellow liquid. The compound showed: ^1H NMR: (CDCl_3 , 300 MHz): δ 8.03 (dd, $J = 7.4$ & 1.5 Hz, 2H), 7.50 (dd, $J = 7.5$, 1H), 7.41 (dd, $J = 7.8$, 2H), 7.27 (d, $J = 8.1$ Hz, 2H), 7.16 (d, $J = 8.0$ Hz, 2H), 4.74 (q, $J = 6.8$, 1H), 2.33 (s, 3H), 1.61 (d, $J = 6.9$ Hz, 3H); ^{13}C NMR: (CDCl_3 , 75 MHz): δ 200.3, 138.4, 136.4, 136.4, 132.6, 2 x 129.6, 2 x 128.7, 2 x 128.4, 2 x 127.6, 47.4, 20.9, 19.5; MS[EI $^+$]: m/z (RI%): 224 (6), 119 (54), 105 (100); HRMS: for $\text{C}_{16}\text{H}_{16}\text{O}$: calculated 224.1201, observed 224.1199.

2-(2-Methylphenyl)-1-phenylpropan-1-one (Table 4, entry 3). As per the general procedure described in the paper for ketone arylations, $(\text{PA-Ph})_2\text{Pd.dba}$ (2, 14.0 mg, 0.015 mmol), NaO^tBu (192 mg, 2.00 mmol), 2-bromotoluene (0.120 mL, 1.00 mmol), propiophenone (0.146 mL, 1.10 mmol) and toluene/THF (1.5 mL: 0.5 mL) were used. After 16 h at 40 $^\circ\text{C}$, work-up and column chromatography (5% EtOAc in hexane) gave 206 mg (95%) of the title compound as a pale yellow liquid. The compound showed: ^1H NMR: (CDCl_3 , 300 MHz): δ 7.71 (dd, $J = 7.4$ & 1.1 Hz, 2H), 7.29 (br.dd, $J = 7.3$ Hz, 1H), 7.19 (br.dd, $J = 7.8$ Hz, 2H), 7.07 (d, $J = 6.5$ Hz, 1H), 6.98-6.92 (m, 3H), 4.63 (q, $J = 6.8$ Hz, 1H), 2.36 (s, 3H), 1.35 (d, $J = 6.8$ Hz, 3H); ^{13}C NMR: (CDCl_3 , 75 MHz): δ 201.1, 140.2, 136.6, 134.6, 132.7, 131.1, 4 x 128.6, 127.0, 126.9, 126.8, 44.6, 19.7, 18.1; MS[EI $^+$]: m/z (RI%): 224 (14), 119 (24), 105 (105); HRMS: for $\text{C}_{16}\text{H}_{16}\text{O}$: calculated 224.1201, observed 224.1201.

2-(4-Methoxyphenyl)-1-phenylpropan-1-one (Table 4, entry 4). As per the general procedure described in the paper for ketone arylations, (PA-Ph)₂Pd.dbu (2, 14.0 mg, 0.015 mmol), NaO^tBu (144 mg, 1.50 mmol), 4-bromoanisole (0.125 mL, 1.00 mmol), propiophenone (0.150 mL, 1.13 mmol) and toluene (2 mL) were used. After 21 h at 40 °C, work-up and column chromatography (10% EtOAc in hexane) gave 230 mg (96%) of the title compound as a pale yellow liquid. The compound showed: ¹H NMR: (CDCl₃, 300 MHz): δ 7.83 (dd, *J* = 7.7 & 1.2 Hz, 2H), 7.30 (br.dd, *J* = 7.4 Hz, 1H), 7.21 (br.dd, *J* = 7.8 Hz, 2H), 7.08 (dd, *J* = 8.7 & 2.8 Hz, 2H), 6.70 (dd, *J* = 8.7 & 2.8 Hz, 2H), 4.53 (q, *J* = 6.8 Hz, 1H), 3.56 (s, 3H), 1.38 (d, *J* = 6.8 Hz, 3H); ¹³C NMR: (CDCl₃, 75 MHz): δ 200.4, 158.4, 136.4, 133.4, 132.6, 4 x 128.7, 2 x 128.4, 2 x 114.3, 55.0, 46.8, 19.5; MS[EI⁺]: *m/z* (RI%): 240 (5.6), 135 (100); HRMS: for C₁₆H₁₆O₂: calculated 240.1150, observed 240.1159.

2-(4-*N,N*-Dimethylaminophenyl)-1-phenylpropan-1-one (Table 4, entry 5). As per the general procedure described in the paper for ketone arylations, (PA-Ph)₂Pd.dbu (2, 14.0 mg, 0.015 mmol), NaO^tBu (192 mg, 2.00 mmol), 4-bromo-*N,N*-dimethylaniline (200 mg, 1.00 mmol), propiophenone (0.150 mL 1.13 mmol) and toluene/THF (1.5 mL: 0.5 mL) were used. After 20 h at 40 °C, work-up and column chromatography (10% EtOAc in hexane) gave 240 mg (95%) of the title compound as a pale yellow solid. The compound showed: ¹H NMR: (CDCl₃, 300 MHz): δ 7.84 (dd, *J* = 7.7 & 1.4 Hz, 2H), 7.28 (br.dd, *J* = 7.4 Hz, 1H), 7.20 (br.dd, *J* = 7.7 Hz, 2H), 7.02 (dd, *J* = 6.7 & 2.0 Hz, 2H), 6.51 (dd, *J* = 6.7 & 2.0 Hz, 2H), 4.47 (q, *J* = 6.8 Hz, 1H), 2.72 (s, 6H), 1.38 (d, *J* = 6.8 Hz, 3H); ¹³C NMR: (CDCl₃, 75 MHz): δ 200.6, 149.3, 136.6, 132.4, 128.9, 2 x 128.7, 4 x 128.3, 2 x 112.9, 46.8, 2 x 40.4, 19.4; MS[EI⁺]: *m/z* (RI%): 253 (7), 148 (100); HRMS: for C₁₇H₁₉NO: calculated 253.1467, observed 253.1468.

2-(4-*N,N*-Dimethylaminophenyl)-2-methyl-1-phenylpropan-1-one (Table 4, entry 6). As per the general procedure described in the paper for ketone arylations, (PA-Ph)₂Pd.dbu (2, 14.0 mg, 0.015

mmol), NaO^tBu (192 mg, 2.00 mmol), 4-bromo-*N,N*-dimethylaniline (200 mg, 1.00 mmol), isobutyrophenone (0.169 mL, 1.12 mmol) and toluene/THF (1.5 mL: 0.5 mL) were used. After 22 h at 70 °C, work-up and column chromatography (10% EtOAc in hexane) gave 232 mg (93%) of the title compound as a pale yellow oil. The compound showed: ¹H NMR: (CDCl₃, 300 MHz): δ 7.56 (d, *J* = 7.2 Hz, 2H), 7.37 (br.dd, *J* = 7.0 Hz, 1H), 7.27-7.21 (m, 4H), 6.77 (d, *J* = 8.8 Hz, 2H), 2.97 (s, 6H), 1.60 (s, 6H); ¹³C NMR: (CDCl₃, 75 MHz): δ 204.5, 149.3, 136.8, 132.6, 131.4, 2 x 129.6, 2 x 127.9, 2 x 126.5, 2 x 113.0, 50.4, 2 x 40.9, 2 x 28.2; MS[EI⁺]: *m/z* (RI%): 267 (3), 162 (100); HRMS: for C₁₈H₂₁NO: calculated 267.1623, observed 267.1627.

2-(2,4-Dimethoxyphenyl)-1-phenylpropan-1-one (Table 4, entry 7). As per the general procedure described in the paper for ketone arylations, (PA-Ph)₂Pd.dbu (2, 14.0 mg, 0.015 mmol), NaO^tBu (144 mg, 1.50 mmol), 1-bromo-2,4-dimethoxybenzene (217 mg, 1.00 mmol), propiophenone (0.150 mL, 1.13 mmol) and toluene (3 mL) were used. After 24 h at 40 °C, work-up and column chromatography (10% EtOAc in hexane) gave 217 mg (80%) of the title compound as a pale yellow liquid. The compound showed: ¹H NMR: (CDCl₃, 200 MHz): δ 7.94 (dd, *J* = 7.7 & 1.3 Hz, 2H), 7.45 – 7.30 (m, 3H), 7.00 (d, *J* = 8.4 Hz, 2H), 6.45 – 6.35 (m, 2H), 5.00 (q, *J* = 6.8 Hz, 1H), 3.85 (s, 3H), 3.71 (s, 3H), 1.42 (d, 3H); ¹³C NMR: (CDCl₃, 75 MHz): δ 201.5, 159.7, 156.7, 136.5, 132.9, 3 x 128.5, 2 x 128.3, 122.5, 104.6, 98.8, 55.5, 55.2, 39.7, 17.8; MS[EI⁺]: *m/z* (RI%): 270 (3), 165 (100); HRMS: for C₁₇H₁₈O₃: calculated 270.1256, observed 270.1260.

2-(2,4,6-Trimethylphenyl)-1-phenylpropan-1-one (Table 4, entry 8). As per the general procedure described in the paper for ketone arylations, (PA-Ph)₂Pd.dbu (2, 14.0 mg, 0.015 mmol), NaO^tBu (144 mg, 1.50 mmol), 2-bromomesitylene (199.1 mg, 1.00 mmol), propiophenone (0.150 mL, 1.13 mmol) and toluene (3 mL) were used. After 24 h at 40 °C, work-up and column chromatography (5% EtOAc in hexane) gave 219 mg (87%) of the title compound as a pale yellow liquid. The compound showed: ¹H NMR: (CDCl₃, 300 MHz): δ 7.77 (d, *J* = 7.8 Hz, 2H), 7.43 (br.dd, *J* = 7.5 Hz,

1H), 7.31 (br.dd, $J = 7.7$ Hz, 2H), 6.83 (s, 2H), 4.54 (q, $J = 6.8$ Hz, 1H), 2.30 (s, 3H), 2.24 (s, 6H), 1.53 (d, $J = 6.8$ Hz, 3H); ^{13}C NMR: (CDCl_3 , 75 MHz): δ 202.5, 2 x 136.9, 136.1 2 x 135.4, 132.4, 2 x 130.3, 4 x 128.2, 45.8, 20.8, 2 x 20.5, 15.1; MS[EI^+]: m/z (RI%): 252 (16), 147 (100), 105 (27); HRMS: for $\text{C}_{18}\text{H}_{20}\text{O}$: calculated 252.1514, observed 252.1517.

1,2-Diphenylpropan-1-one (Table 4, entry 9). As per the general procedure described in the paper for ketone arylations, $(\text{PA-Ph})_2\text{Pd.dba}$ (2, 20.7 mg, 0.022 mmol), NaO^tBu (192 mg, 2.00 mmol), chlorobenzene (0.125 mL, 1.00 mmol), propiophenone (0.150 mL 1.13 mmol) and toluene/THF (1.5 mL: 0.5 mL) were used. After 20 h at 70 °C, work-up and column chromatography (5% EtOAc in hexane) gave 158 mg (75%) of the title compound as a pale yellow liquid. Spectral data were the same as those listed for Table 4, entry 1.

2-(4-Methylphenyl)-1-phenylpropan-1-one (Table 4, entry 10). As per the general procedure described in the paper for ketone arylations, $(\text{PA-Ph})_2\text{Pd.dba}$ (2, 20.7 mg, 0.022 mmol), NaO^tBu (192 mg, 2.00 mmol), 4-chlorotoluene (127 mg, 1.00 mmol), propiophenone (152 mg 1.13 mmol) and toluene/THF (1.5 mL: 0.5 mL) were used. After 21 h at 70 °C, work-up and column chromatography (5% EtOAc in hexane) gave 175 mg (78%) of the title compound as a pale yellow liquid. Spectral data were the same as those listed for Table 4, entry 2.

References:

1. Littke, A. F.; Dai, C.; Fu, G. C. *J. Am. Chem. Soc.* **2000**, *122*, 4020

Pd(PA-Ph)₂dba

Compound **2**

Pd(PA-Ph)₂O₂

Compound **3**

Current Data Parameters
 NAME GA-3-63
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20040525
 Time 15.35
 INSTRUM av200
 PROBHD 5 mm QNP 1H/1
 PULPROG zg30
 TD 16384
 SOLVENT MeOH
 NS 4
 DS 2
 SWH 2604.167 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 1625.5
 DW 192.000 usec
 DE 15.50 usec
 TE 300.0 K
 D1 2.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 6.35 usec
 PL1 6.00 dB
 SF01 200.1311696 MHz

F2 - Processing parameters
 SI 16384
 SF 200.1300094 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 0.00 cm
 F1P 8.968 ppm
 F1 1794.80 Hz
 F2P 1.756 ppm
 F2 351.53 Hz
 PPMCM 0.32780 ppm/cm
 HZCM 65.60332 Hz/cm

Suzuki reaction of 4-iodoacetophenone and naphthylboronic acid

Table 1, Entry 1

Table 1, Entry 2

naphthyl acetophenone

Current Data Parameters
 NAME GA-3-70
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20040525
 Time 15.40
 INSTRUM av200
 PROBHD 5 mm QNP 1H/1
 PULPROG zg30
 TD 16384
 SOLVENT MeOH
 NS 4
 DS 2
 SWH 2604.167 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 406.4
 DW 192.000 usec
 DE 15.50 usec
 TE 300.0 K
 D1 2.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 6.35 usec
 PL1 6.00 dB
 SF01 200.1311696 MHz

F2 - Processing parameters
 SI 16384
 SF 200.1300094 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 0.00 cm
 F1P 8.897 ppm
 F1 1780.54 Hz
 F2P 1.628 ppm
 F2 325.86 Hz
 PPMCM 0.33039 ppm/cm
 HZCM 66.12193 Hz/cm

Suzuki reaction of 2-chlorotoluene and phenylboronic acid

Table1, Entry 3

Table 1. Entry 4

mesityl bromide and naphthylboronic acid

Current Data Parameters
 NAME GA-3-71
 EXPNO 1
 PROCNO 1

Table 2, Entry 1

Sonogashira reaction with 4-iodotoluene and phenylacetylene

F2 - Acquisition Parameters
 Date_ 20040525
 Time 11.53
 INSTRUM av200
 PROBHD 5 mm QNP 1H/1
 PULPROG zg30
 TD 16384
 SOLVENT MeOH
 NS 8
 DS 2
 SWH 2604.167 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 456.1
 DW 192.000 usec
 DE 15.50 usec
 TE 300.0 K
 D1 2.0000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 6.35 usec
 PL1 6.00 dB
 SFO1 200.1311696 MHz

F2 - Processing parameters
 SI 16384
 SF 200.1300094 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 0.00 cm
 F1P 8.042 ppm
 F1 1609.40 Hz
 F2P 1.001 ppm
 F2 200.35 Hz
 PPMCM 0.32003 ppm/cm
 HZCM 64.04751 Hz/cm

Current Data Parameters
 NAME GA-3-73
 EXPNO 1
 PROCNO 1

Table 2, Entry 2

Sonogashira rxn with 4-iodoacetophenone and phenylacetylene

F2 - Acquisition Parameters
 Date_ 20040520
 Time 16.28
 INSTRUM av200
 PROBHD 5 mm QNP 1H/1
 PULPROG zg30
 TD 16384
 SOLVENT MeOH
 NS 4
 DS 2
 SWH 2604.167 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 812.7
 DW 192.000 usec
 DE 15.50 usec
 TE 300.0 K
 D1 2.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 6.35 usec
 PL1 6.00 dB
 SFO1 200.1311696 MHz

F2 - Processing parameters
 SI 16384
 SF 200.1300094 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 0.00 cm
 F1P 8.408 ppm
 F1 1682.74 Hz
 F2P 1.743 ppm
 F2 348.76 Hz
 PPMCM 0.30298 ppm/cm
 HZCM 60.63568 Hz/cm

Current Data Parameters
 NAME GA-3-74
 EXPNO 1
 PROCNO 1

Table 2, Entry 3

Sonogashira coupling of 4-iodoaniline and phenylacetylene

F2 - Acquisition Parameters
 Date_ 20040526
 Time 20.50
 INSTRUM av200
 PROBHD 5 mm QNP 1H/1
 PULPROG zg30
 TD 16384
 SOLVENT CDCl3
 NS 4
 DS 2
 SWH 2604.167 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 2048
 DW 192.000 usec
 DE 15.50 usec
 TE 300.0 K
 D1 2.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 6.35 usec
 PL1 6.00 dB
 SF01 200.1311696 MHz

F2 - Processing parameters
 SI 16384
 SF 200.1300094 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 0.00 cm
 F1P 8.142 ppm
 F1 1629.36 Hz
 F2P 0.688 ppm
 F2 137.60 Hz
 PPMCM 0.33882 ppm/cm
 HZCM 67.80738 Hz/cm

Current Data Parameters
 NAME GA-3-72
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20040528
 Time 13.26
 INSTRUM av200
 PROBHD 5 mm QNP 1H/1
 PULPROG zg30
 TD 16384
 SOLVENT MeOH
 NS 4
 DS 2
 SWH 2604.167 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 256
 DW 192.000 usec
 DE 15.50 usec
 TE 300.0 K
 D1 2.0000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 6.35 usec
 PL1 6.00 dB
 SFO1 200.1311696 MHz

F2 - Processing parameters
 SI 16384
 SF 200.130094 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 0.00 cm
 F1P 8.495 ppm
 F1 1700.05 Hz
 F2P 0.978 ppm
 F2 195.71 Hz
 PPMCM 0.34167 ppm/cm
 HZCM 68.37875 Hz/cm

Sonogashira coupling of 2-iodotoluene and phenylacetylene

Table 2, Entry 4

Current Data Parameters
 NAME GA-3-70
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20040526
 Time 11.48
 INSTRUM av200
 PROBHD 5 mm QNP 1H/1
 PULPROG zg30
 TD 16384
 SOLVENT MeOH
 NS 4
 DS 2
 SWH 2604.167 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 1824.6
 DW 192.000 usec
 DE 15.50 usec
 TE 300.0 K
 D1 2.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 6.35 usec
 PL1 6.00 dB
 SFO1 200.1311696 MHz

F2 - Processing parameters
 SI 16384
 SF 200.1300094 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 0.00 cm
 F1P 8.555 ppm
 F1 1712.08 Hz
 F2P 1.856 ppm
 F2 371.49 Hz
 PPMCM 0.30448 ppm/cm
 HZCM 60.93589 Hz/cm

Sonogashira coupling of 4-iodoanisole and phenylacetylene

Table 2, Entry 5

Current Data Parameters
 NAME GA-3-75
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20040526
 Time 20.16
 INSTRUM av200
 PROBHD 5 mm QNP 1H/1
 PULPROG zg30
 TD 16384
 SOLVENT MeOH
 NS 4
 DS 2
 SWH 2604.167 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 645.1
 DW 192.000 usec
 DE 15.50 usec
 TE 300.0 K
 D1 2.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 6.35 usec
 PL1 6.00 dB
 SFO1 200.1311696 MHz

F2 - Processing parameters
 SI 16384
 SF 200.1300094 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 0.00 cm
 F1P 7.928 ppm
 F1 1586.58 Hz
 F2P 0.773 ppm
 F2 154.72 Hz
 PPMCM 0.32521 ppm/cm
 HZCM 65.08472 Hz/cm

Sonogashira reaction of 4-iodoanisole and 2-methyl-3-butyn-2-ol

Table 2, Entry 6

Current Data Parameters
 NAME GA-3-77
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20040526
 Time 11.54
 INSTRUM av200
 PROBHD 5 mm QNP 1H/1
 PULPROG zg30
 TD 16384
 SOLVENT MeOH
 NS 4
 DS 2
 SWH 2604.167 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 1290.2
 DW 192.000 usec
 DE 15.50 usec
 TE 300.0 K
 D1 2.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 6.35 usec
 PL1 6.00 dB
 SFO1 200.1311696 MHz

F2 - Processing parameters
 SI 16384
 SF 200.1300094 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 0.00 cm
 FIIP 8.199 ppm
 F1 1640.77 Hz
 F2P 1.756 ppm
 F2 351.53 Hz
 PPMCM 0.29282 ppm/cm
 HZCM 58.60217 Hz/cm

Sonogashira coupling of 4-bromotoluene and phenylacetylene

Table 3, Entry 1

Table 3, Entry 2

Sonogashira reaction of 4-bromoacetophenone and phenylacetylene

Current Data Parameters

NAME GA-3-78
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20040525
Time 12.09
INSTRUM av200
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 16384
SOLVENT MeOH
NS 8
DS 2
SWH 2604.167 Hz
FIDRES 0.158946 Hz
AQ 3.1457779 sec
RG 456.1
DN 192.000 usec
DE 15.50 usec
TE 300.0 K
D1 2.00000000 sec

===== CHANNEL f1 =====

NUC1 1H
P1 6.35 usec
PL1 6.00 dB
SFO1 200.1311696 MHz

F2 - Processing parameters

SI 16384
SF 200.1300094 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 22.00 cm
CY 0.00 cm
F1P 8.498 ppm
F1 1700.67 Hz
F2P 1.813 ppm
F2 362.94 Hz
PPMCM 0.30383 ppm/cm
HZCM 60.80624 Hz/cm

Current Data Parameters
 NAME GA-3-67B
 EXPNO 1
 PROCNO 1

Sonogashira reaction of 4-bromoacetophenone and 2-methyl-3-butyn-2-ol

F2 - Acquisition Parameters
 Date_ 20040526
 Time 20.22
 INSTRUM av200
 PROBHD 5 mm QNP 1H/1
 PULPROG zg30
 TD 16384
 SOLVENT MeOH
 NS 4
 DS 2
 SWH 2604.167 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 574.7
 DW 192.000 usec
 DE 15.50 usec
 TE 300.0 K
 D1 2.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 6.35 usec
 PL1 6.00 dB
 SFO1 200.1311696 MHz

F2 - Processing parameters
 SI 16384
 SF 200.1300094 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 0.00 cm
 F1P 8.441 ppm
 F1 1689.26 Hz
 F2P 0.930 ppm
 F2 186.09 Hz
 PPMCM 0.34141 ppm/cm
 HZCM 68.32599 Hz/cm

ppm
 7.891
 7.849
 7.487
 7.445

2.611
 2.580

1.619

Sonogashira coupling of 2-bromotoluene and phenylacetylene

Current Data Parameters
 NAME GA-3-80
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20040526
 Time 16.26
 INSTRUM av200
 PROBHD 5 mm QNP 1H/1
 PULPROG zg30
 TD 16384
 SOLVENT CDCl3
 NS 4
 DS 2
 SWH 2604.167 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 1149.4
 DW 192.000 usec
 DE 15.50 usec
 TE 300.0 K
 D1 2.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 6.35 usec
 PL1 6.00 dB
 SFO1 200.1311696 MHz

F2 - Processing parameters
 SI 16384
 SF 200.1300094 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 0.00 cm
 F1P 8.757 ppm
 F1 1752.58 Hz
 F2P 1.741 ppm
 F2 348.47 Hz
 PPMCM 0.31891 ppm/cm
 HZCM 63.82314 Hz/cm

Sonogashira coupling of 4-bromo-N,N-dimethoxyaniline and phenylacetylene

Table 3, Entry 5

Current Data Parameters
 NAME GA-3-81
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20040526
 Time 11.40
 INSTRUM av200
 PROBHD 5 mm QNP 1H/1
 PULPROG zg30
 TD 16384
 SOLVENT MeOH
 NS 4
 DS 2
 SWH 2604.167 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 2580.3
 DW 192.000 usec
 DE 15.50 usec
 TE 300.0 K
 D1 2.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 6.35 usec
 PL1 6.00 dB
 SF01 200.1311696 MHz

F2 - Processing parameters
 SI 16384
 SF 200.1300094 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 0.00 cm
 F1P 8.538 ppm
 F1 1708.76 Hz
 F2P 1.903 ppm
 F2 380.79 Hz
 PPMCM 0.30162 ppm/cm
 HZCM 60.36247 Hz/cm

Sonogashira coupling of 4-bromoanisole and phenylacetylene

Table 3, Entry 6

Sonogashira coupling of 4-bromoanisole and 2-methyl-3-butyn-2-ol

Table 3, Entry 7

Current Data Parameters
 NAME GA-3-83
 EXPNO 1
 PROCNO 1

Table 3, Entry 8

Sonogashira reaction of 2-bromomesitylene and phenylacetylene

F2 - Acquisition Parameters
 Date_ 20040525
 Time 12.18
 INSTRUM av200
 PROBHD 5 mm QNP 1H/1
 PULPROG zg30
 TD 16384
 SOLVENT MeOH
 NS 8
 DS 2
 SWH 2604.167 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 2298.8
 DW 192.000 usec
 DE 15.50 usec
 TE 300.0 K
 D1 2.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 6.35 usec
 PL1 6.00 dB
 SFO1 200.1311696 MHz

F2 - Processing parameters
 SI 16384
 SF 200.1300094 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 0.00 cm
 F1P 8.056 ppm
 F1 1612.25 Hz
 F2P 1.671 ppm
 F2 334.41 Hz
 PPMCM 0.29023 ppm/cm
 HZCM 58.08357 Hz/cm

Table 4, Entry 1

Table 4. Entry 2

Table 4, Entry 3

Table 4, Entry 4

Table 4, Entry 5

Table 4, Entry 6

Current Data Parameters
 NAME GA-4-60
 EXPNO 1
 PROCNO 1

Ketone arylation with bromo-2,4-dimethoxybenzene and propiophenone

F2 - Acquisition Parameters
 Date_ 20040526
 Time 16.20
 INSTRUM av200
 PROBHD 5 mm QNP 1H/1
 PULPROG zg30
 TD 16384
 SOLVENT CDCl3
 NS 4
 DS 2
 SWH 2604.167 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 724.1
 DW 192.000 usec
 DE 15.50 usec
 TE 300.0 K
 D1 2.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 6.35 usec
 PL1 6.00 dB
 SF01 200.1311696 MHz

F2 - Processing parameters
 SI 16384
 SF 200.130094 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 0.00 cm
 F1P 8.583 ppm
 F1 1717.79 Hz
 F2P 0.274 ppm
 F2 54.88 Hz
 PPMCM 0.37769 ppm/cm
 HZCM 75.58643 Hz/cm

Table 4, Entry 8

Table 4, Entry 9

chlorobenzene and propiophenone

Table 4, Entry 10

4-chlorotoluene and propiophenone

File # 1 : GA3

Number of Scans: 16

Comment: 4-bromo-N,N-dimethylaniline and phenylacetylene, thin film

View Mode: Overlay

5/27/04 2:50 PM Res=8cm-1

File # 1 : GA1

Number of Scans: 16

Comment: Sonogashira reaction with 4-bromoanisole and phenylacetylene, KBr dis

View Mode: Overlay

5/27/04 1:32 PM Res=8cm⁻¹

File # 1 : GA

Number of Scans: 16

Comment:

View Mode: Overlay

5/27/04 1:03 PM Res=8cm-1