TsOH-Catalyzed Dehydroxylative Cross-Coupling of Alcohols with

Phenols: Rapid Access to Propofol Derivatives

Yuqiu Liang,^a Chengxiu, Liu, ^a Youchun Li, ^{*b} Lu Ouyang ^{*a}

^a School of Pharmacy, Gannan Medical University, Ganzhou 341000, Jiangxi Province, P. R. China. oyl3074@163.com

^b The Affiliated Ganzhou Hospital, Jiangxi Medical College, Nanchang University, Ganzhou 341000, Jiangxi Province, P. R. China.liyouchun2007@163.com

Supporting Information

Table of Contents

A. General Methods	S2
B. Procedure for dehydroxylative coupling of alcohols and phenols	S2
C. Procedure for dehydroxylative coupling of alcohols and aryl ethers	S2
D. Procedure for gram-scale experiment	
E. Control experiments	S3
F.	Analytical
DataS5	
G. References	S23
H. NMR Spectra	S25

A. General Methods

Unless otherwise stated, all reactions were magnetically stirred and conducted under air and applied dried Schlenk tubes under confined conditions. All solvents and reagents were used as received from commercial suppliers unless otherwise indicated. Column chromatography was carried out using silica gel (100-400 mesh) and detected at 254 nm. All ¹H NMR, ¹³C NMR, ¹⁹F NMR spectra for compound characterization were recorded on a Bruker AVANCE-NEO 400 WB spectrometer in a suitable deuterated solvent unless specified otherwise. Chemical shifts were given in parts per million (ppm, δ), referenced to the solvent peak of CDCl₃, defined at δ = 7.26 (¹H NMR), defined at δ = 77.16 (¹³C NMR). Coupling constants were quoted in Hz (J). ¹H NMR spectroscopy splitting patterns were designated as singlet (s), doublet (d), triplet (t), and quartet (q). HRMS was performed on a high-resolution mass spectrometer (LCMS-IT-TOF). Melt points were measured with WRR melting point apparatus.

B. Procedure for dehydroxylative coupling of alcohols with phenols



In the Schlenk tube, **1** (0.5 mmol), **2** (1.0 equiv., 0.5 mmol), TsOH (20 mol %, 0.1 mmol), TFEA (1.5 mL) were added. The mixture was stirred at room temperature for 1 h under confined conditions. After the reaction was completed, the mixture was diluted with EtOAc (5.0 mL) carefully quenched with 5.0 mL of saturated NaHCO₃ solution. To determine the separation yield of product, the mixture was extracted with EtOAc (10.0 mL \times 3 times), the organic layers were combined, washed with saturated NaCl. and dried with anhydrous MgSO₄. After removal of the EtOAc under vacuum, the crude product was purified by column chromatography on silica gel with hexanes or petroleum ether/ethyl acetate (5:1 to 200:1) to give the desired products.

C. Procedure for dehydroxylative coupling of alcohols with aryl ethers



In the Schlenk tube, **4** (0.5 mmol), **2** (1.0 equiv., 0.5 mmol), TsOH (20 mol %, 0.1 mmol), TFEA (1.5 mL) were added. The mixture was stirred at room temperature for 1 h under confined conditions. After the reaction was completed, the mixture was diluted with EtOAc (5.0 mL) carefully quenched with 5.0 mL of saturated NaHCO₃ solution. To determine the separation yield of product, the mixture was extracted with EtOAc (10.0 mL \times 3 times), the organic layers were combined, washed with saturated NaCl. and dried with anhydrous MgSO₄. After removal of the EtOAc under vacuum, the crude product was purified by column chromatography on silica gel with hexanes or petroleum ether/ethyl acetate (5:1 to 200:1) to give the desired products.

D. Procedure for gram-scale experiment



In the Schlenk tube were added **1a** (10.0 mmol), **2a** (1.0 equiv., 10 mmol), TsOH (20 mol%), TFEA (30.0 mL). The mixture was stirred at room temperature for 1 h under confined conditions. After the reaction was completed, the mixture was diluted with EtOAc (50.0 mL) carefully quenched with 50.0 mL of saturated NaHCO₃ solution. To determine the separation yield of product, the mixture was extracted with EtOAc (50.0 mL \times 3 times), the organic layers were combined and washed with saturated NaCl and dried with anhydrous MgSO₄. After removal of the EtOAc under vacuum, the crude product was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (50:1) to give the desired product.

E. Control experiments.

The chiral alcohol $2\mathbf{k}$ was employed in this catalytic system to access detailed mechanistic process. As anticipated, only racemic product $3\mathbf{a}\mathbf{k}$ was produced using (*R*)-(-)-1-phenylethanol ($2\mathbf{k}$) to react with propofol $1\mathbf{a}$, which evidenced the formation of benzyl carbocationic intermediate (Scheme S1).



Scheme S1 Chiral alcohol employed in this deoxygenative cross-coupling.



Racemic product of 1-phenylethanol (2k)

Chiral product of (3ak')

F. Analytical Data

4-benzhydryl-2,6-diisopropylphenol (3aa)¹: Prepared in 98% yield (168.1 mg) as a white solid; m.p.102-104 °C. $R_f = 0.49$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.23 (t, J = 7.4 Hz, 4H), 7.13 (dd, J = 17.8, 7.2 Hz, 6H),

6.80 (s, 2H), 5.47 (s, 1H), 4.66 (s, 1H), 3.12-3.02 (m, 2H), 1.15 (d, J = 7.0 Hz, 12H). ¹³C NMR (100 MHz, CDCl₃) δ 148.3, 144.6, 135.5, 133.3, 129.3, 128.1, 126.0, 124.5, 56.6, 27.2, 22.7.

2,6-diisopropyl-4-(phenyl(*p***-tolyl)methyl)phenol (3ab)**: Prepared in 92% yield (164.8 mg) as a white solid; m.p.114-117 °C. $R_f = 0.53$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.23 (t, J = 7.4 Hz, 2H), 7.16 (d, J = 7.4 Hz, 1H), 7.12-7.08 (m, 2H), 7.06 (d, J = 7.9 Hz, 2H), 6.99 (d, J = 7.9 Hz, 2H), 6.80 (s, 2H), 5.43 (s, 1H), 4.66 (s, 1H), 3.12-3.02 (m, 2H), 2.29 (s, 3H), 1.16 (dd, J = 6.9, 1.7 Hz, 12H). ¹³C NMR (100 MHz, CDCl₃) δ 148.3, 144.9, 141.6, 135.7, 135.4, 133.2, 129.3, 129.2, 128.8, 128.1, 125.9, 124.5, 56.2, 27.3, 22.7, 21.0. HRMS-ESI (m/z): [M+H]⁺ Calcd for C₂₆H₃₀O 357.2224; Found 357.2222.

2,6-diisopropyl-4-((4-methoxyphenyl)(phenyl)methyl)phenol (3ac)²: Prepared in 86% yield (160.9 mg) as a colourless oil. $R_f = 0.49$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.25 (t, J = 7.4 Hz, 2H), 7.18 (d, J = 7.3 Hz, 1H), 7.13-7.07 (m, 2H), 7.05-6.99 (m, 2H), 6.85-6.74 (m, 4H), 5.42 (s, 1H), 4.70 (s, 1H), 3.77 (s, 3H), 3.14-3.04 (m, 2H), 1.17 (d, J = 6.9 Hz, 12H). ¹³C NMR (100 MHz, CDCl₃) δ 157.8, 148.3, 145.0, 136.9, 135.8, 133.2, 130.2, 129.3, 128.1, 125.9, 124.5, 113.5, 55.8, 55.2, 27.3, 22.7 (d, J = 1.7 Hz).

4-benzhydryl-2,6-diisopropylphenol (3ad)³: Prepared in 96% yield (179.2 mg) as a colourless oil. $R_f = 0.55$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.32-7.23 (m, 8H), 7.06 (s, 2H), 5.64 (s, 1H), 4.92 (s, 1H), 3.37-3.27 (m, 2H), 2.52 (s, 6H), 1.41 (d, J = 7.0 Hz, 12H). ¹³C NMR (100 MHz, CDCl₃) δ 148.2, 141.9, 135.9, 135.3, 133.2, 129.1, 128.8, 124.5, 55.9, 27.3, 22.7, 20.9.

4-(di-*p***-tolylmethyl)-2,6-diisopropylphenol (3ae)**: Prepared in 84% yield (168.9 mg) as a white solid; m.p.107-109 °C. $R_f = 0.33$ (petroleum ether/ethyl acetate = 5/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.01 (d, J = 8.7 Hz, 4H), 6.83-6.76 (m, 6H), 5.37 (s, 1H), 4.72 (s, 1H), 3.76 (s, 6H), 3.14-3.04 (m, 2H), 1.17 (d, J = 6.9 Hz, 12H). ¹³C NMR (100 MHz, CDCl₃) δ 157.7, 148.2, 137.2, 136.1, 133.2, 130.1, 124.4, 113.4, 55.1, 27.3, 22.7. HRMS-ESI (m/z): [M+H]⁺ Calcd for C₂₇H₃₂O₃ 403.2279; Found 403.2277.

4-(di(naphthalen-1-yl)methyl)-2,6-diisopropylphenol (3af): Prepared in 82% yield (181.5 mg) as a white solid;m.p.198-200 °C. $R_f = 0.44$ (petroleum ether/ethyl acetate

= 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.98 (d, *J* = 8.5 Hz, 2H), 7.84 (d, *J* = 8.1 Hz, 2H), 7.72 (d, *J* = 8.2 Hz, 2H), 7.46-7.38 (m, 2H), 7.32 (dt, *J* = 19.3, 8.1 Hz, 4H), 6.93 (d, *J* = 7.2 Hz, 2H), 6.86 (s, 1H), 6.82 (s, 2H), 4.67 (s, 1H), 3.10-3.00 (m, 2H), 1.11 (d, *J* = 6.9 Hz, 12H). ¹³C NMR (100 MHz, CDCl₃) δ 148.4, 140.5, 134.8, 133.9, 133.4, 131.8, 128.7, 127.5, 127.1, 126.1, 125.3, 125.3, 124.9, 124.2, 49.2, 27.3, 22.6. HRMS-ESI (m/z): [M+H]⁺ Calcd for C₃₃H₃₂O 443.2380; Found 443.2379.

4-(9*H***-fluoren-9-yl)-2,6-diisopropylphenol (3ag)**: Prepared in 60% yield (103.4 mg) as a colourless oil. $R_f = 0.42$ (petroleum ether/ethyl acetate = 50/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.79 (dd, J = 7.6, 1.2 Hz, 2H), 7.39-7.32 (m, 4H), 7.27-7.23 (m, 2H), 6.78 (s, 2H), 4.99 (s, 1H), 4.68 (s, 1H), 3.14-3.04 (m, 2H), 1.19 (d, J = 6.9 Hz, 12H). ¹³C NMR (100 MHz, CDCl₃) δ 148.9, 148.1, 140.8, 133.7, 133.0, 127.1, 127.0, 125.2, 123.3, 119.7, 54.3, 27.3, 22.7. HRMS-ESI (m/z): [M+H]⁺ Calcd for C₂₅H₂₆O 341.1911; Found 341.1909.

2,6-diisopropyl-4-(9-phenyl-9*H***-fluoren-9-yl)phenol (3ah)**: Prepared in 95% yield (198.1 mg) as a white solid; m.p.157-159°C. $R_f = 0.38$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.72 (d, J = 7.5 Hz, 2H), 7.39 (d, J = 7.6 Hz, 2H), 7.28 (t, J = 6.8 Hz, 2H), 7.21 (t, J = 7.5 Hz, 2H), 7.17-7.09 (m, 5H), 6.90 (s, 2H), 3.07-2.97 (m, 2H), 1.09 (d, J = 7.0 Hz, 12H). ¹³C NMR (100 MHz, CDCl₃) δ 151.8, 148.6, 146.6, 140.0, 137.2, 132.9, 128.0, 127.9, 127.5, 127.2, 126.3, 126.0,

123.6, 120.0, 65.3, 27.3, 22.6. HRMS-ESI (m/z): $[M+H]^+$ Calcd for $C_{31}H_{30}O$ 417.2224; Found 417.2223.

ethene-1,1-diyldibenzene (3ai)⁴: Prepared in 47% yield (42.0 mg) as a colourless oil. $R_f = 0.44$ (petroleum ether/ethyl acetate = 50/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.32 (td, J = 5.9, 5.3, 3.0 Hz, 10H), 5.45 (s, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 150.0, 141.4, 128.2, 128.1, 127.7, 114.3.

4,4'-(ethene-1,1-diyl)bis(chlorobenzene) (**3aj**)⁵: Prepared in 86% yield (106.4 mg) as a colourless oil. $R_f = 0.44$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.34-7.16 (m, 8H), 5.43 (s, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 147.8, 139.4, 133.8, 129.4, 128.4, 115.1.

2,6-diisopropyl-4-(1-phenylethyl)phenol (3ak): Prepared in 70% yield (98.4 mg) as a colourless oil. $R_f = 0.44$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.29-7.19 (m, 4H), 7.18-7.10 (m, 1H), 6.90 (s, 2H), 4.65 (s, 1H), 4.08 (q, *J* = 7.2 Hz, 1H), 3.15-3.06 (m, 2H), 1.61 (d, *J* = 7.2 Hz, 3H), 1.23 (d, *J* = 7.9 Hz, 12H). ¹³C NMR (100 MHz, CDCl₃) δ 148.2, 147.0, 138.0, 133.3, 128.2, 127.5, 125.7, 122.6, 44.6, 27.3, 22.7 (d, *J* = 1.4 Hz), 22.3. HRMS-ESI (m/z): [M+H]⁺ Calcd for C₂₀H₂₆O 281.1911; Found 281.1908.

2,6-diisopropyl-4-(1-(*o***-tolyl)ethyl)phenol (3al)**: Prepared in 94% yield (139.6 mg) as a colourless oil. $R_f = 0.48$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.25-7.21 (m, 1H), 7.16 (td, J = 7.6, 7.0, 2.3 Hz, 1H), 7.13-7.06 (m, 2H), 6.84 (s, 2H), 4.62 (s, 1H), 4.25 (q, J = 7.2 Hz, 1H), 3.14-3.04 (m, 2H), 2.27 (s, 3H), 1.58 (d, J = 7.2 Hz, 3H), 1.21 (dd, J = 6.9, 1.8 Hz, 12H). ¹³C NMR (100 MHz, CDCl₃) δ 148.0, 144.7, 137.8, 135.8, 133.2, 130.2, 126.5, 125.9, 125.7, 122.7, 40.6, 27.3, 22.7 (d, J = 1.4 Hz), 22.2, 19.7. HRMS-ESI (m/z): [M+H]⁺ Calcd for C₂₁H₂₈O 295.2067; Found 295.2065.

2,6-diisopropyl-4-(1-(*p***-tolyl)ethyl)phenol (3am)**: Prepared in 94% yield (139.3 mg) as a colourless oil. $R_f = 0.48$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.08 (q, J = 8.2 Hz, 4H), 6.90 (s, 2H), 4.63 (s, 1H), 4.04 (q, J = 7.2 Hz, 1H), 3.14-3.05 (m, 2H), 2.29 (s, 3H), 1.59 (d, J = 7.2 Hz, 3H), 1.23 (d, J = 7.0 Hz, 12H). ¹³C NMR (100 MHz, CDCl₃) δ 148.1, 144.1, 138.2, 135.1, 133.3, 128.9, 127.3, 122.6, 44.2, 27.3, 22.7, 22.4, 20.9. HRMS-ESI (m/z): [M+H]⁺ Calcd for C₂₁H₂₈O 295.2067; Found 295.2063.

2,6-diisopropyl-4-(1-(4-methoxyphenyl)ethyl)phenol (3an)⁶: Prepared in 81% yield (125.6 mg) as a colourless oil. $R_f = 0.32$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.13 (d, J = 8.7 Hz, 2H), 6.89 (s, 2H), 6.81 (d, J = 8.7 Hz, 2H), 4.68 (s, 1H), 4.03 (q, J = 7.2 Hz, 1H), 3.76 (s, 3H), 3.16-3.06 (m, 2H), 1.58 (d, J = 7.3 Hz, 3H), 1.22 (d, J = 6.9 Hz, 12H). ¹³C NMR (100 MHz, CDCl₃) δ 157.6, 148.1, 139.2, 138.4, 133.3, 128.3, 122.5, 113.6, 55.2, 43.7, 27.3, 22.7(d, J = 1.8 Hz), 22.5.

4-(1-(4-hydroxyphenyl)ethyl)-2,6-diisopropylphenol (3ao): Prepared in 72% yield (107.2 mg) as a white solid; m.p.89-91 °C. $R_f = 0.27$ (petroleum ether/ethyl acetate = 3/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.06 (d, J = 8.2 Hz, 2H), 6.88 (s, 2H), 6.72 (d, J = 8.3 Hz, 2H), 5.35 (s, 1H), 4.75 (s, 1H), 4.01 (q, J = 7.2 Hz, 1H), 3.16-3.06 (m, 2H), 1.57 (d, J = 7.2 Hz, 3H), 1.21 (d, J = 6.9 Hz, 12H). ¹³C NMR (100 MHz, CDCl₃) δ 153.4, 148.0, 139.3, 138.5, 133.4, 128.6, 122.5, 115.0, 43.7, 27.3, 22.7(d, J = 1.6 Hz), 22.5. HRMS-ESI (m/z): [M+H]⁺ Calcd for C₂₀H₂₆O₂ 297.1860; Found 297.1857.

4-(1-(4-chlorophenyl)ethyl)-2,6-diisopropylphenol (3ap): Prepared in 79% yield (125.6 mg) as a colourless oil. $R_f = 0.44$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.22 (d, J = 8.5 Hz, 2H), 7.13 (d, J = 8.4 Hz, 2H), 6.86 (s, 2H), 4.67 (s, 1H), 4.05 (q, J = 7.2 Hz, 1H), 3.16-3.06 (m, 2H), 1.58 (d, J = 7.2 Hz, 3H), 1.23 (d, J = 6.9 Hz, 12H). ¹³C NMR (100 MHz, CDCl₃) δ 148.3, 145.6, 137.5, 133.5, 131.4, 128.9, 128.3, 122.5, 44.0, 27.3, 22.7(d, J = 2.0 Hz), 22.2. HRMS-ESI (m/z): [M+H]⁺ Calcd for C₂₀H₂₅ClO 315.1521; Found 315.1522.

4-(1-(4-fluorophenyl)ethyl)-2,6-diisopropylphenol (3aq): Prepared in 94% yield (140.8 mg) as a colourless oil. $R_f = 0.46$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.16 (dd, J = 8.5, 5.5 Hz, 2H), 6.94 (t, J = 8.7 Hz, 2H), 6.87 (s, 2H), 4.68 (s, 1H), 4.06 (q, J = 7.2 Hz, 1H), 3.16-3.06 (m, 2H), 1.59 (d, J = 7.2 Hz, 3H), 1.23 (d, J = 6.9 Hz, 12H). ¹³C NMR (100 MHz, CDCl₃) δ 161.1 (d, J = 243.4 Hz), 148.2, 142.7 (d, J = 3.2 Hz), 137.9, 133.4, 128.8 (d, J = 7.7 Hz), 122.5, 114.9 (d,

J = 21.0 Hz), 43.8, 27.3, 22.7 (d, J = 1.8 Hz), 22.4. ¹⁹F NMR (377 MHz, CDCl₃) δ - 117.8. HRMS-ESI (m/z): [M+H]⁺ Calcd for C₂₀H₂₅FO 299.1817; Found 299.1815.

2,6-diisopropyl-4-(1-(naphthalen-2-yl)ethyl)phenol (3ar): Prepared in 95% yield (158.2 mg) as a white solid; m.p.112-114 °C. $R_f = 0.44$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 8.14 (dd, J = 7.6, 2.0 Hz, 1H), 7.82 (dd, J = 7.7, 1.8 Hz, 1H), 7.69 (d, J = 8.1 Hz, 1H), 7.47-7.37 (m, 3H), 7.35-7.30 (m, 1H), 6.95 (s, 2H), 4.88 (q, J = 7.1 Hz, 1H), 4.64 (s, 1H), 3.13-3.03 (m, 2H), 1.73 (d, J = 7.1 Hz, 3H), 1.19 (t, J = 7.0 Hz, 12H). ¹³C NMR (100 MHz, CDCl₃) δ 148.1, 142.7, 137.9, 133.9, 133.3, 131.6, 128.7, 126.6, 125.7, 125.5, 125.2, 124.2, 123.8, 122.8, 40.0, 27.3, 22.7 (d, J = 6.2 Hz). HRMS-ESI (m/z): [M+H]⁺ Calcd for C₂₄H₂₈O 331.2067; Found 331.2068.

2,6-diisopropyl-4-(1-(6-methoxynaphthalen-2-yl)ethyl)phenol (3as): Prepared in 84% yield (151.7 mg) as a colourless oil. $R_f = 0.36$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.70-7.58 (m, 3H), 7.29 (dd, J = 8.5, 1.9 Hz, 1H), 7.14-7.06 (m, 2H), 6.94 (s, 2H), 4.67 (s, 1H), 4.20 (q, J = 7.2 Hz, 1H), 3.87 (s, 3H), 3.14-3.04 (m, 2H), 1.68 (d, J = 7.2 Hz, 3H), 1.22 (d, J = 6.9 Hz, 12H). ¹³C NMR (100 MHz, CDCl₃) δ 157.2, 148.2, 142.2, 138.1, 133.3, 133.0, 129.2, 128.9, 127.3, 126.6, 125.0, 122.7, 118.5, 105.6, 55.2, 44.4, 27.3, 22.7(d, J = 2.7 Hz), 22.3. HRMS-ESI (m/z): [M+H]⁺ Calcd for C₂₅H₃₀O₂ 361.2173; Found 361.2172.

2,6-diisopropyl-4-(1-(6-methoxynaphthalen-2-yl)ethyl)phenol (3at): Prepared in 87% yield (128.1 mg) as a colourless oil. $R_f = 0.44$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.28-7.21 (m, 4H), 7.18-7.11 (m, 1H), 6.91 (s, 2H), 4.63 (s, 1H), 3.71 (t, J = 7.8 Hz, 1H), 3.15-3.10 (m, 2H), 2.07-1.99 (m, 2H), 1.23 (dd, J = 6.9, 1.5 Hz, 12H), 0.88 (t, J = 7.3 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 148.1, 145.7, 137.0, 133.2, 128.2, 127.8, 125.7, 122.8, 53.1, 29.1, 27.3, 22.7, 12.9. HRMS-ESI (m/z): [M+H]⁺ Calcd for C₂₁H₂₈O 295.2067; Found 295.2066.

2,6-diisopropyl-4-(2-methyl-1-phenylpropyl)phenol (3au): Prepared in 83% yield (128.5 mg) as a colourless oil. $R_f = 0.44$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.29-7.21 (m, 4H), 7.11 (t, J = 7.0 Hz, 1H), 6.94 (s, 2H), 4.59 (s, 1H), 3.31 (d, J = 10.7 Hz, 1H), 3.14-3.04 (m, 2H), 2.42 (dq, J = 17.3, 6.5 Hz, 1H), 1.23 (dd, J = 6.9, 2.3 Hz, 12H), 0.85 (dd, J = 8.8, 6.5 Hz, 6H). ¹³C NMR (100 MHz, CDCl₃) δ 148.0, 145.6, 136.7, 133.2, 128.3, 127.9, 125.6, 122.9, 60.6, 32.2, 27.2, 22.8 (d, J = 6.9 Hz), 21.9 (d, J = 3.6 Hz). HRMS-ESI (m/z): [M+H]⁺ Calcd for C₂₂H₃₀O 309.2224; Found 309.2223.

2,6-diisopropyl-4-(2-methyl-1-phenylpropyl)phenol (3av): Prepared in 87% yield (134.5 mg) as a colourless oil. $R_f = 0.44$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.29-7.22 (m, 4H), 7.16 (td, J = 6.1, 5.5, 2.7 Hz, 1H), 6.94 (s, 2H), 4.65 (s, 1H), 3.18-3.06 (m, 3H), 1.22 (d, J = 7.0 Hz, 12H), 0.69-0.57 (m, 2H), 0.34-0.22 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 148.2, 145.7, 136.9, 133.1, 128.1, 128.1, 125.8, 123.2, 55.3, 27.3, 22.7 (d, J = 3.1 Hz), 17.0, 5.3 (d, J = 14.0 Hz). HRMS-ESI (m/z): [M+H]⁺ Calcd for C₂₂H₂₈O 307.2067; Found 307.2066.

2,6-diisopropyl-4-(2-phenylpropan-2-yl)phenol (3aw): Prepared in 97% yield (143.3 mg) as a colourless oil. $R_f = 0.49$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.23 (d, J = 1.6 Hz, 4H), 7.16-7.10 (m, 1H), 6.91 (d, J = 1.6 Hz, 2H), 4.66 (s, 1H), 3.16-3.06 (m, 2H), 1.67 (s, 6H), 1.20 (d, J = 6.9 Hz, 12H). ¹³C NMR (100 MHz, CDCl₃) δ 151.1, 147.7, 142.3, 132.7, 127.8, 126.7, 125.3, 121.9, 42.6, 31.0, 27.4, 22.7. HRMS-ESI (m/z): [M+H]⁺ Calcd for C₂₁H₂₈O 295.2067; Found 295.2065.

4-(1,3-diphenylallyl)-2,6-diisopropylphenol (3ax): Prepared in 68% yield (124.9 mg) as a colourless oil. $R_f = 0.44$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.36 (d, J = 7.4 Hz, 2H), 7.32-7.16 (m, 8H), 6.92 (s, 2H), 6.66 (dd, J = 15.8, 7.6 Hz, 1H), 6.34 (d, J = 15.8 Hz, 1H), 4.82 (d, J = 7.6 Hz, 1H), 3.16-3.06 (m, 2H), 1.22 (d, J = 6.9 Hz, 12H). ¹³C NMR (100 MHz, CDCl₃) δ 148.5, 144.0, 137.5, 135.1, 133.6, 133.3, 130.8, 128.5, 128.4, 128.3, 127.1, 126.3, 126.2, 123.7, 54.0, 27.3, 22.7. HRMS-ESI (m/z): [M+H]⁺ Calcd for C₂₇H₃₀O 369.2224; Found 369.2223.

2,6-diisopropyl-4-(2-methyl-4-phenylbut-3-yn-2-yl)phenol (3ay): Prepared in 76% yield (122.1 mg) as a colourless oil. $R_f = 0.44$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.47-7.42 (m, 2H), 7.35-7.26 (m, 5H), 4.72 (s,

1H), 3.22-3.11 (m, 2H), 1.66 (s, 6H), 1.30 (d, J = 6.9 Hz, 12H). ¹³C NMR (100 MHz, CDCl₃) δ 148.4, 138.8, 133.1, 131.5, 128.2, 127.5, 124.1, 120.7, 97.2, 36.2, 31.9, 27.5, 22.8. HRMS-ESI (m/z): [M+H]⁺ Calcd for C₂₃H₂₈O 319.2067; Found 319.2066.

4-benzhydryl-2-methylphenol (3ba): Prepared in 80% yield (109.0 mg) as a colourless oil. $R_f = 0.32$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.28-7.22 (m, 4H), 7.20-7.14 (m, 2H), 7.11-7.07 (m, 4H), 6.87 (d, J = 2.3 Hz, 1H), 6.76 (dd, J = 8.2, 2.3 Hz, 1H), 6.60 (d, J = 8.2 Hz, 1H), 5.44 (s, 1H), 4.85 (s, 1H), 2.14 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 152.1, 144.2, 136.1, 132.0, 129.3, 128.2, 127.9, 126.1, 123.6, 114.6, 56.0, 15.8. HRMS-ESI (m/z): [M+H]⁺ Calcd for C₂₀H₁₈O 273.1285; Found 273.1284.

4-benzhydryl-2-ethylphenol (3ca): Prepared in 87% yield (125.9 mg) as a colourless oil. $R_f = 0.30$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.25 (dd, J = 8.1, 6.5 Hz, 4H), 7.19 (d, J = 7.3 Hz, 2H), 7.13-7.06 (m, 4H), 6.90 (d, J = 2.3 Hz, 1H), 6.75 (dd, J = 8.2, 2.3 Hz, 1H), 6.60 (d, J = 8.2 Hz, 1H), 5.46 (s, 1H), 4.82 (s, 1H), 2.54 (q, J = 7.6 Hz, 2H), 1.14 (t, J = 7.6 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 151.7, 144.3, 136.1, 130.4, 129.7, 129.3, 128.2, 127.7, 126.1, 114.8, 56.0, 23.0, 14.0. HRMS-ESI (m/z): [M+H]⁺ Calcd for C₂₁H₂₀O 287.1441; Found 287.1440.

4-benzhydryl-2-isopropylphenol (3da): Prepared in 71% yield (106.8 mg) as a colourless oil. $R_f = 0.29$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.30-7.22 (m, 4H), 7.21-7.16 (m, 2H), 7.13-7.06 (m, 4H), 6.97 (d, J = 2.3 Hz, 1H), 6.73 (dd, J = 8.2, 2.3 Hz, 1H), 6.59 (d, J = 8.2 Hz, 1H), 5.48 (s, 1H), 4.75 (s, 1H), 3.19-3.09 (m, 1H), 1.16 (d, J = 6.9 Hz, 6H). ¹³C NMR (100 MHz, CDCl₃) δ 151.1, 144.4, 136.1, 134.1, 129.3, 128.2, 127.6, 127.4, 126.1, 114.9, 56.2, 27.1, 22.5. HRMS-ESI (m/z): [M+H]⁺ Calcd for C₂₂H₂₂O 301.1598; Found 301.1597.

4-benzhydryl-2-(*tert*-butyl)phenol (3ea)⁷: Prepared in 81% yield (128.4 mg) as a colourless oil. $R_f = 0.30$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.24 (t, J = 7.4 Hz, 4H), 7.20-7.13 (m, 2H), 7.10 (d, J = 7.0 Hz, 4H), 7.04 (d, J = 2.3 Hz, 1H), 6.72 (dd, J = 8.1, 2.2 Hz, 1H), 6.46 (d, J = 8.1 Hz, 1H), 5.46 (s, 1H), 1.32 (s, 9H). ¹³C NMR (100 MHz, CDCl₃) δ 152.5, 144.5, 135.7, 135.5, 129.3, 128.3, 128.2, 127.6, 126.1, 116.2, 56.3, 34.5, 29.5.

4-benzhydryl-2-methylphenol (3fa): Prepared in 73% yield (108.4 mg) as a colourless oil. $R_f = 0.29$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.29-7.21 (m, 4H), 7.17 (t, J = 7.3 Hz, 2H), 7.09 (dd, J = 7.2, 1.8 Hz, 4H), 6.87 (d, J = 2.3 Hz, 1H), 6.81 (dd, J = 8.2, 2.3 Hz, 1H), 6.68 (d, J = 8.2 Hz, 1H), 5.95 (ddt, J = 16.7, 10.2, 6.3 Hz, 1H), 5.46 (s, 1H), 5.14-5.05 (m, 2H), 5.02 (s, 1H), 3.31 (d, J = 6.4 Hz, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 152.5, 144.2, 136.4, 136.2, 131.4, 129.3, 128.7, 128.2, 126.1, 125.0, 116.4, 115.6, 56.0. HRMS-ESI (m/z): [M+H]⁺ Calcd for C₂₂H₂₀O 299.1441; Found 299.1440.

4-benzhydryl-2,6-dimethylphenol (3ga)⁸: Prepared in 95% yield (136.2 mg) as a white solid; m.p.124-126 °C. $R_f = 0.48$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.23 (t, J = 7.4 Hz, 4H), 7.17-7.12 (m, 2H), 7.12-7.07 (m, 4H), 6.70 (s, 2H), 5.40 (s, 1H), 4.60 (s, 1H), 2.11 (s, 6H). ¹³C NMR (100 MHz, CDCl₃) δ 150.5, 144.3, 135.4, 129.4, 129.3, 128.1, 126.0, 122.8, 56.0, 15.9.

4-benzhydryl-2-ethyl-6-methylphenol (3ha): Prepared in 93% yield (141.1 mg) as a white solid; m.p.148-150 °C. $R_f = 0.52$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.26 (dd, J = 8.1, 6.7 Hz, 4H), 7.22-7.16 (m, 2H), 7.11 (dd, J = 7.0, 1.8 Hz, 4H), 6.81-6.65 (m, 2H), 5.43 (s, 1H), 4.53 (s, 1H), 2.55 (q, J = 7.6 Hz, 2H), 2.16 (s, 3H), 1.16 (t, J = 7.5 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 150.1, 144.4, 135.6, 129.3, 128.2, 128.0, 126.1, 122.7, 56.2, 23.2, 16.0, 14.1. HRMS-ESI (m/z): [M+H]⁺ Calcd for C₂₂H₂₂O 301.1598; Found 301.1597.

2-allyl-4-benzhydryl-6-methylphenol (3ia): Prepared in 89% yield (140.1 mg) as a colourless oil. $R_f = 0.44$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.24 (t, J = 7.5 Hz, 4H), 7.17 (d, J = 7.3 Hz, 2H), 7.10 (d, J = 6.8 Hz, 4H), 6.73 (dd, J = 23.1, 2.3 Hz, 2H), 5.93 (ddt, J = 16.6, 10.0, 6.3 Hz, 1H), 5.42 (s, 1H), 5.18-5.06 (m, 2H), 4.91 (s, 1H), 3.29 (d, J = 6.4 Hz, 2H), 2.13 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 151.0, 144.3, 136.5, 135.6, 130.2, 129.3, 129.0, 128.2, 126.1,

124.1, 124.0, 116.5, 56.0, 35.7, 16.0. HRMS-ESI (m/z): [M+H]⁺ Calcd for C₂₃H₂₂O 313.1598; Found 313.1599.

4-benzhydryl-2,6-di*tert***-butylphenol (3ja)**⁹: Prepared in 96% yield (178.2 mg) as a white solid; m.p.141-143 °C. $R_f = 0.51$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.24 (dd, J = 8.3, 6.8 Hz, 4H), 7.18-7.09 (m, 6H), 6.91 (s, 2H), 5.45 (s, 1H), 5.06 (s, 1H), 1.35 (s, 18H).¹³C NMR (100 MHz, CDCl₃) δ 152.1, 144.8, 135.4, 134.1, 129.4, 128.1, 126.0, 56.8, 34.3, 30.3.

((4-methoxyphenyl)methylene)dibenzene (5aa)¹⁰: Prepared in 59% yield (80.6 mg) as a colourless oil. $R_f = 0.44$ (petroleum ether/ethyl acetate = 50/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.28-7.24 (m, 4H), 7.21-7.18 (m, 2H), 7.10 (dd, J = 7.0, 1.8 Hz, 4H), 7.04-6.99 (m, 2H), 6.84-6.77 (m, 2H), 5.49 (s, 1H), 3.75 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 157.9, 144.2, 136.0, 130.3, 129.3, 128.2, 126.2, 113.6, 55.9, 55.1.

((4-ethoxyphenyl)methylene)dibenzene (5ab)¹¹: Prepared in 72% yield (103.6 mg) as a colourless oil. $R_f = 0.48$ (petroleum ether/ethyl acetate = 50/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.25 (dd, J = 8.2, 6.6 Hz, 4H), 7.20-7.15 (m, 2H), 7.13-7.04 (m, 4H), 7.04-6.96 (m, 2H), 6.84-6.76 (m, 2H), 5.48 (s, 1H), 3.97 (q, J = 7.0 Hz, 2H), 1.37 (t, J

= 7.0 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 157.3, 144.2, 135.9, 130.3, 129.3, 128.2, 126.1, 114.1, 63.3, 56.0, 14.8.

((4-isopropoxyphenyl)methylene)dibenzene (5ac)¹²: Prepared in 76% yield (114.2 mg) as a colourless oil. $R_f = 0.49$ (petroleum ether/ethyl acetate = 50/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.26 (dd, J = 8.2, 6.7 Hz, 4H), 7.19 (d, J = 7.3 Hz, 2H), 7.13-7.06 (m, 4H), 6.99 (d, J = 8.6 Hz, 2H), 6.79 (d, J = 8.6 Hz, 2H), 5.48 (s, 1H), 4.53-4.44 (m, 1H), 1.30 (d, J = 6.1 Hz, 6H). ¹³C NMR (100 MHz, CDCl₃) δ 156.3, 144.3, 135.8, 130.3, 129.4, 128.2, 126.1, 115.5, 69.7, 56.0, 22.1.

((4-(allyloxy)phenyl)methylene)dibenzene (5ad): Prepared in 85% yield (127.5 mg) as a colourless oil. $R_f = 0.41$ (petroleum ether/ethyl acetate = 50/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.26 (dd, J = 8.1, 6.5 Hz, 4H), 7.19 (dd, J = 7.6, 1.7 Hz, 2H), 7.12-7.08 (m, 4H), 7.03-6.98 (m, 2H), 6.84-6.79 (m, 2H), 6.03 (ddd, J = 22.6, 10.6, 5.3 Hz, 1H), 5.49 (s, 1H), 5.38 (dd, J = 17.3, 1.6 Hz, 1H), 5.25 (dd, J = 10.5, 1.4 Hz, 1H), 4.48 (dt, J = 5.4, 1.6 Hz, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 157.0, 144.2, 136.2, 133.3, 130.3, 129.3, 128.2, 126.2, 117.6, 114.4, 68.7, 55.9. HRMS-ESI (m/z): [M+H]⁺ Calcd for C₂₂H₂₀O 299.1441; Found 299.1437.

((3-chloro-4-methoxyphenyl)methylene)dibenzene (5ae)¹²: Prepared in 52% yield (80.0 mg) as a colourless oil. $R_f = 0.44$ (petroleum ether/ethyl acetate = 50/1, v/v). ¹H

NMR (400 MHz, CDCl₃) δ 7.31-7.26 (m, 4H), 7.24-7.19 (m, 2H), 7.14-7.07 (m, 5H), 6.95 (dd, J = 8.5, 2.2 Hz, 1H), 6.83 (dd, J = 8.5, 1.0 Hz, 1H), 5.47 (s, 1H), 3.86 (d, J = 1.0 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 153.4, 143.5, 137.1, 131.0, 129.3, 128.5, 128.4, 126.4, 122.1, 111.7, 56.1, 55.7.

((4-methoxy-3-methylphenyl)methylene)dibenzene (5af)¹³: Prepared in 92% yield (132.0 mg) as a colourless oil. $R_f = 0.44$ (petroleum ether/ethyl acetate = 50/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.47 (t, J = 7.4 Hz, 4H), 7.37 (dd, J = 23.6, 7.3 Hz, 6H), 7.15 (s, 1H), 7.09 (d, J = 8.3 Hz, 1H), 6.92 (d, J = 8.3 Hz, 1H), 5.69 (s, 1H), 3.96 (s, 3H), 2.39 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 156.1, 144.3, 135.5, 131.7, 129.3, 128.2, 127.5, 126.3, 126.1, 109.5, 56.0, 55.1, 16.3.

((4-methoxy-3,5-dimethylphenyl)methylene)dibenzene (5ag)¹⁴: Prepared in 86% yield (130.5 mg) as a colourless oil. $R_f = 0.44$ (petroleum ether/ethyl acetate = 50/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.24 (dd, J = 8.2, 6.7 Hz, 4H), 7.17 (d, J = 7.4 Hz, 2H), 7.13-7.08 (m, 4H), 6.74 (s, 2H), 5.42 (s, 1H), 3.66 (s, 3H), 2.19 (s, 6H). ¹³C NMR (100 MHz, CDCl₃) δ 155.3, 144.1, 138.9, 130.4, 129.7, 129.3, 128.2, 126.1, 59.5, 56.2, 16.1.

4-allyl-5-benzhydryl-2-methoxyphenol (5ah): Prepared in 90% yield (148.2 mg) as a colourless oil. $R_f = 0.32$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.23 (dd, J = 8.2, 6.6 Hz, 4H), 7.17 (d, J = 7.3 Hz, 2H), 7.08-6.98 (m, 4H), 6.66 (s, 1H), 6.47 (s, 1H), 5.90 (ddt, J = 16.4, 10.1, 6.1 Hz, 1H), 5.66 (s, 1H), 5.43 (s, 1H), 5.08-4.97 (m, 2H), 3.81 (s, 3H), 3.22 (d, J = 6.1 Hz, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 144.8, 143.7, 143.5, 137.5, 135.1, 129.4, 129.4, 128.2, 126.1, 116.4, 115.5, 112.4, 55.8, 52.0, 36.9. HRMS-ESI (m/z): [M+H]⁺ Calcd for C₂₃H₂₂O₂ 329.1547; Found 329.1548.

5-benzhydryl-2,3-dihydrobenzofuran (5ai): Prepared in 82% yield (181.5 mg) as a colourless oil. $R_f = 0.44$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.24 (dd, J = 8.1, 6.7 Hz, 4H), 7.19-7.14 (m, 2H), 7.10 (dd, J = 7.1, 1.8 Hz, 4H), 6.91 (d, J = 1.8 Hz, 1H), 6.82 (dd, J = 8.3, 2.0 Hz, 1H), 6.67 (d, J = 8.2 Hz, 1H), 5.46 (s, 1H), 4.47 (t, J = 8.7 Hz, 2H), 3.06 (t, J = 8.7 Hz, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 158.5, 144.3, 136.0, 129.3, 129.0, 128.2, 126.9, 126.1, 125.8, 108.8, 71.1, 56.2, 29.7. HRMS-ESI (m/z): [M+H]⁺ Calcd for C₂₁H₁₈O 286.1358; Found 286.1356.

(4-benzhydryl-2-methylphenyl)(methyl)sulfane (5aj)¹⁵: Prepared in 90% yield (130.2 mg) as a colourless oil. $R_f = 0.44$ (petroleum ether/ethyl acetate = 10/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.29-7.25 (m, 4H), 7.19 (dd, J = 15.8, 7.9 Hz, 4H), 7.11-7.08 (m, 4H), 7.03 (d, J = 8.3 Hz, 2H), 5.50 (s, 1H), 2.43 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 143.7, 140.9, 136.1, 129.9, 129.3, 128.3, 126.6, 126.3, 56.2, 15.9.

N,N-dimethyl-4-(phenyl(p-tolyl)methyl)aniline (5bk)¹⁶: Prepared in 45% yield (67.7 mg) as a colourless oil. $R_f = 0.47$ (petroleum ether/ethyl acetate = 50/1, v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.33 (t, *J* = 7.2 Hz, 2H), 7.25 (d, *J* = 7.2 Hz, 1H), 7.17 (dd, *J* = 17.2, 7.5 Hz, 4H), 7.10-7.01 (m, 4H), 6.75 (d, *J* = 8.8 Hz, 2H), 5.50 (s, 1H), 2.97 (s, 6H), 2.38 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 148.8, 144.8, 141.6, 135.5, 130.0, 129.3, 129.2, 128.9, 128.2, 128.1, 125.9, 112.6, 55.5, 40.8, 21.0.

G. References

 Bai, Y.; Lin, Z.; Ye, Z.; Dong, D.; Wang, J.; Chen, L.; Xie, F.; Li, Y.; Dixneuf, P.
H.; Zhang, M. Ruthenium-catalyzed regioselective hydrohalogenation of alkynes mediated by trimethylsilyl triflate. *Organic Letters* 2022, *24* (43), 7988-7992.

Burmester, A.; HB, S., Alkylierung von 2-t-Butylphenol mit Diarylcarbinolen.
1981.

3. Luo, R.; Liang, Y.; Wang, S.; Liao, J.; Ouyang, L. Iridium-catalyzed selective para-C-alkylation of anilines/phenols with aryl alkynes. *Journal of Catalysis* **2023**, *428*, 115184.

4. Mejri, E.; Higashida, K.; Kondo, Y.; Nawachi, A.; Morimoto, H.; Ohshima, T.; Sawamura, M.; Shimizu, Y. Visible-Light-Induced Aminochlorination of Alkenes. *Organic Letters* **2023**, *25* (24), 4581-4585.

5. Nath, N. K.; Nilapwar, S.; Nangia, A. Chiral and racemic tetramorphs of 2, 6-di-tbutylditolylfuchsone. *Crystal Growth & Design* **2012**, *12* (3), 1613-1625.

6. Singh, S.; Mahato, R.; Sharma, P.; Yadav, N.; Vodnala, N.; Kumar Hazra, C. Development of Transition-Metal-Free Lewis Acid-Initiated Double Arylation of Aldehyde: A Facile Approach Towards the Total Synthesis of Anti-Breast-Cancer Agent. *Chemistry–A European Journal* **2022**, *28* (14), e202104545.

7. Xiong, B.; Si, L.; Zhu, L.; Wu, R.; Liu, Y.; Xu, W.; Zhang, F.; Tang, K. W.; Wong, W. Y. Room-Temperature ZnBr₂-Catalyzed Regioselective, 6-Hydroarylation of Electron-Rich Arenes to para-Quinone Methides: Synthesis of Unsymmetrical Triarylmethanes. *Chemistry–An Asian Journal* **2023**, *18* (3), e202201156.

8. Yu, J.; Chen, S.; Liu, K.; Yuan, L.; Mei, L.; Chai, Z.; Shi, W. Uranyl-catalyzed hydrosilylation of para-quinone methides: access to diarylmethane derivatives. *Organic & Biomolecular Chemistry* **2021**, *19* (7), 1575-1579.

9. Zhang, Y.; Hou, J.; Yang, H.; Wang, S.; Yuan, K. Electrochemically enhanced deoxygenative cross-coupling of aryl ketones with heteroarenes through in situ generated benzyl carbocations. *Organic & Biomolecular Chemistry* **2023**, *21* (1), 80-84.

10. Li, H.; Li, W.; Liu, W.; An Efficient and General Iron-Catalyzed C-C Bond Activation with 1, 3-Dicarbonyl Units as a Leaving Groups. *Angewandte Chemie International Edition*, **2011**, *13*(50): 2975-2978.

11. Collection of Czechoslovak Chemical Communications, 1976, 41, 2919 – 2927

12. Li, Z.; Li ,B.; J, Lu X Y, et al. Cross Dehydrogenative Arylation (CDA) of a Benzylic C-H Bond with Arenes by Iron Catalysis. *Angewandte Chemie International Edition*, **2009**, *48*(21): 3817-3820.

13. Courant, T.; Lombard, M.; Boyarskaya, D. V. Tritylium assisted iodine catalysis for the synthesis of unsymmetrical triarylmethanes. *Organic & Biomolecular Chemistry*, **2020**, *18*(33): 6502-6508.

14. Lielpetere, A.; Jirgensons, A. Friedel–Crafts Alkylation with Carbenium Ions Generated by Electrochemical Oxidation of Stannylmethyl Ethers. *European Journal of Organic Chemistry*, **2020**, *2020*(29): 4510-4516.

15. Liu, C. R.; Li, M. B.; Yang, C. F. Selective Benzylic and Allylic Alkylation of Protic Nucleophiles with Sulfonamides through Double Lewis Acid Catalyzed Cleavage of sp3 Carbon–Nitrogen Bonds. *Chemistry–A European Journal*, **2009**, *15*(3): 793-797.

16. Ouyang, L.; Liang, Y.; Wang, S.; Liao, J.; Luo, R. Access of arylmethanes via iridium-catalyzed deoxygenative cross-coupling of aryl ketones with anilines/phenols. *Journal of Catalysis*, **2024**, *433*, 115492.

H. NMR Spectra

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 f1 (ppm)

0 -10

10

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 f1 (ppm)

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 f1 (ppm)

¹H NMR (400 MHz, CDCl₃) spectrum of 3ai

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 f1 (ppm)

210 200 150 150 170 160 150 140 130 120 110 100 50 50 70 60 50 40 30 20 10 0 -10 f1 (ppm)

¹⁹F NMR (377 MHz, CDCl₃) spectrum of 3aq

20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -2 f1 (ppm)

S51

¹H NMR (400 MHz, CDCl₃) spectrum of 3fa

¹H NMR (400 MHz, CDCl₃) spectrum of 3ia

¹³C NMR (100 MHz, CDCl₃) spectrum of 3ia

¹H NMR (400 MHz, CDCl₃) spectrum of 5ad

¹³C NMR (100 MHz, CDCl₃) spectrum of 5ad

- 157.00	144.17 156.18 133.32 133.32 133.33 133.32 133.33 133.33 126.18 128.23 126.18 126.18 126.18	77.32 CDCI3 77.00 CDCI3 76.68 CDCI3 - 68.73	55.94
1		-68	- 55

¹H NMR (400 MHz, CDCl₃) spectrum of 5ae

¹H NMR (400 MHz, CDCl₃) spectrum of 5ah

¹³C NMR (100 MHz, CDCl₃) spectrum of 5ah

	CC CC		
4 8 0 - 0 4 0 0 4 6 0 9	888		
44.8 43.5 33.1 33.1 22 29.4 28.2 28.2 28.2 28.2 28.2 28.2 28.2 28	7.32 7.00 6.68	5.83	6.87
	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	v v 	ñ

![](_page_66_Figure_5.jpeg)

### ¹H NMR (400 MHz, CDCl₃) spectrum of 5ai

![](_page_67_Figure_1.jpeg)

## ¹³C NMR (100 MHz, CDCl₃) spectrum of 5ai

![](_page_67_Figure_3.jpeg)

![](_page_67_Figure_4.jpeg)

![](_page_68_Figure_0.jpeg)

![](_page_69_Figure_0.jpeg)

¹³C NMR (100 MHz, CDCl₃) spectrum of 5bk

![](_page_69_Figure_2.jpeg)