Supporting Information

Replacing Pd(OAc)$_2$ with supported palladium nanoparticles in ortho-directed CDC reaction of alkylbenzenes

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1. Figures S1–S2

**Figure S1.** XRD patterns of catalysts with different loadings

**Figure S2.** TEM images of catalysts: (a) 1 wt% Pd/γ-Al₂O₃ and (b) 5 wt% Pd/γ-Al₂O₃. (c, d) PdNPs size distributions of 1 wt% Pd/γ-Al₂O₃ and 5 wt% Pd/γ-Al₂O₃, respectively.
2. GC-MS Analysis of Reaction of 1a with 2a and 1a with 2e
The GC spectra of reaction solution of 1a with 2a:

- RT: 0.00 - 21.03
- TLC MS:

01_150515
093237
The GC spectra of reaction solution of 1a with 2e:

[Image of GC spectra showing peaks at specific RT and time.

RT: 0.00 - 21.02

Relative Abundance

Time (min)

0 2 4 6 8 10 12 14 16 18 20

0 10 20 30 40 50 60 70 80 90 100

[Diagram of molecular structures with labels COOH and CH2OH.

NL: 6.00E9
TIC: MS
02_15051500250

m/z 50 100 150 200 250 300 350 400

Relative Abundance

0 10 20 30 40 50 60 70 80 90 100

[Diagram of molecular spectrum with labels COOH and CH2OH.

NL: 3.15E8
T: m/z Full scan [50.00-400.00]
3. Characterization Data for the Products

phenyl(2-(pyridin-2-yl)phenyl)methanone 3aa.\(^1\) Conversion: 83\% (GC). \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta\) 8.39 (d, \(J = 4.0\) Hz, 1H), 7.78 (d, \(J = 7.7\) Hz, 1H), 7.67 (d, \(J = 7.5\) Hz, 2H), 7.63 – 7.57 (m, 2H), 7.57 – 7.49 (m, 3H), 7.41 – 7.35 (m, \(J = 7.4\) Hz, 1H), 7.30 – 7.24 (m, \(J = 7.7\) Hz, 2H), 7.09 – 6.99 (m, 1H).

(2-(pyridin-2-yl)phenyl)(p-tolyl)methanone 3ab.\(^1\) Yield: 80\% (43.7 mg). \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta\) 8.40 (d, \(J = 4.5\) Hz, 1H), 7.77 (d, \(J = 7.7\) Hz, 1H), 7.63 – 7.54 (m, 4H), 7.52 – 7.47 (m, 3H), 7.08 (d, \(J = 8.0\) Hz, 2H), 7.03 (dd, \(J = 7.1, 5.4\) Hz, 1H), 2.32 (s, 3H).

(2-(pyridin-2-yl)phenyl)(o-tolyl)methanone 3ac.\(^1\) Yield: 64\% (35.0 mg). \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta\) 8.43 (d, \(J = 4.6\) Hz, 1H), 7.67 – 7.50 (m, 5H), 7.41 (d, \(J = 7.8\) Hz,
1H), 7.16 (d, J = 7.4 Hz, 2H), 7.08 (d, J = 7.6 Hz, 1H), 7.05 – 6.98 (m, 1H), 6.97 – 6.90 (m, 1H), 2.57 (s, 3H).

(2-(pyridin-2-yl) phenyl) (m-tolyl) methanone 3ad.² Yield: 76% (41.5 mg). ¹H NMR (500 MHz, CDCl₃) δ 8.40 (d, J = 4.4 Hz, 1H), 7.77 (d, J = 7.7 Hz, 1H), 7.63 – 7.57 (m, 2H), 7.55 – 7.44 (m, 5H), 7.23 – 7.18 (m, 1H), 7.16 (t, J = 7.6 Hz, 1H), 7.08 – 7.02 (m, 1H), 2.29 (s, 3H).

(4-methoxyphenyl)(2-(pyridin-2-yl)phenyl)methanone 3ae.¹ Yield: 81% (46.9 mg). ¹H NMR (500 MHz, CDCl₃) δ 8.44 (d, J = 3.8 Hz, 1H), 7.77 (d, J = 7.9 Hz, 1H), 7.68 (d, J = 8.8 Hz, 2H), 7.62 – 7.56 (m, 1H), 7.51 (d, J = 4.0 Hz, 2H), 7.48 (d, J = 7.8 Hz, 1H), 7.10 – 7.03 (m, 1H), 6.76 (d, J = 8.8 Hz, 2H), 3.79 (s, 3H).

(4-chlorophenyl)(2-(pyridin-2-yl)phenyl)methanone 3af.¹ Yield: 69% (40.5 mg). ¹H NMR (500 MHz, CDCl₃) δ 8.35 (d, J = 4.4 Hz, 1H), 7.78 (d, J = 7.7 Hz, 1H), 7.65 – 7.57 (m, 4H), 7.56 – 7.49 (m, 3H), 7.23 (d, J = 8.5 Hz, 2H), 7.09 – 7.02 (m, 1H).

(2-chlorophenyl)(2-(pyridin-2-yl) phenyl)methanone 3ag.² Yield: 57% (33.5 mg). ¹H NMR (500 MHz, CDCl₃) δ 8.51 (d, J = 2.6 Hz, 1H), 7.75 – 7.50 (m, 5H), 7.46 (d, J = 6.9 Hz, 1H), 7.35 – 7.27 (m, 1H), 7.25 – 7.20 (m, 1H), 7.18 (t, J = 7.0 Hz, 1H), 7.11 – 6.97 (m, 2H).

(3-chlorophenyl)(2-(pyridin-2-yl)phenyl)methanone 3ah.³ Yield: 65% (38.2 mg). ¹H NMR (500 MHz, CDCl₃) δ 8.37 (s, 1H), 7.79 (d, J = 7.6 Hz, 1H), 7.66 – 7.59 (m, 2H), 7.58 – 7.50 (m, 5H), 7.41 (d, J = 8.5 Hz, 2H), 7.11 – 7.03 (m, 1H).

(4-bromophenyl)(2-(pyridin-2-yl)phenyl)methanone 3ai.⁴ Yield: 63% (42.6 mg). ¹H NMR (500 MHz, CDCl₃) δ 8.37 (s, 1H), 7.78 (d, J = 7.6 Hz, 1H), 7.66 – 7.59 (m, 2H), 7.58 – 7.50 (m, 5H), 7.41 (d, J = 8.5 Hz, 2H), 7.11 – 7.05 (m, 1H).

(3-bromophenyl)(2-(pyridin-2-yl)phenyl)methanone 3aj.³ Yield: 68% (46.0 mg). ¹H NMR (500 MHz, CDCl₃) δ 8.34 (d, J = 4.1 Hz, 1H), 7.82 (s, 1H), 7.78 (d, J = 7.7 Hz, 1H), 7.62 (t, J = 6.8 Hz, 2H), 7.59 – 7.51 (m, 5H), 7.49 (d, J = 7.9 Hz, 1H), 7.13 (t, J = 7.8 Hz, 1H), 7.06 – 7.00 (m, 1H).

benzo[h]quinolin-10-yl(phenyl)methanone 3ba.¹ Yield: 84% (47.6 mg). ¹H NMR (500 MHz, CDCl₃) δ 8.51 (dd, J = 4.4, 1.7 Hz, 1H), 8.11 (dd, J = 8.0, 1.7 Hz, 1H), 8.06 (dd, J = 8.0, 0.9 Hz, 1H), 7.91 (d, J = 8.8 Hz, 1H), 7.83 – 7.73 (m, 4H), 7.63 (dd, J = 7.2, 1.1 Hz, 1H), 7.45 – 7.39 (m, 1H), 7.34 (dd, J = 8.0, 4.4 Hz, 1H), 7.30 (t, J = 7.7 Hz, 2H).

(2-(1H-pyrazol-1-yl)phenyl)(phenyl)methanone 3ca.⁵ Yield: 70% (34.7 mg). ¹H NMR (500 MHz, CDCl₃) δ 7.69 – 7.60 (m, 5H), 7.60 – 7.56 (m, 1H), 7.51 – 7.47 (m, 1H), 7.45 – 7.41 (m, 1H), 7.40 (d, J = 1.6 Hz, 1H), 7.32 – 7.27 (m, 2H), 6.21 – 6.14 (m, 1H).

(5-methyl-2-(pyridin-2-yl)phenyl)(phenyl)methanone 3da.¹ Yield: 81% (44.3 mg). ¹H NMR (500 MHz, CDCl₃) δ 8.36 (d, J = 4.8 Hz, 1H), 7.73 – 7.67 (m, 3H), 7.58 – 7.53 (m, 1H), 7.49 (d, J = 7.9 Hz, 1H), 7.45 – 7.36 (m, 3H), 7.29 – 7.25 (m, 2H), 7.00 (dd, J = 6.9, 5.4 Hz, 1H), 2.47 (s, 3H).
References
4. $^1$H NMR and $^{13}$C NMR Spectra of the Products

$^1$H NMR of phenyl(2-(pyridin-2-yl)phenyl)methanone 3aa

$^1$H NMR of (2-(pyridin-2-yl)phenyl)(p-tolyl)methanone 3ab
$^1$H NMR of (2-(pyridin-2-yl)phenyl)(o-tolyl)methanone 3ac

$^1$H NMR of (2-(pyridin-2-yl)phenyl)(m-tolyl)methanone 3ad
$^1$H NMR of (4-methoxyphenyl)(2-(pyridin-2-yl)phenyl)methanone 3ae

$^1$H NMR of (4-chlorophenyl)(2-(pyridin-2-yl)phenyl)methanone 3af
$^1$H NMR of (2-chlorophenyl)(2-(pyridin-2-yl)phenyl)methanone 3ag

$^1$H NMR of (3-chlorophenyl)(2-(pyridin-2-yl)phenyl)methanone 3ah
$^1$H NMR of (4-bromophenyl)(2-(pyridin-2-yl)phenyl)methanone 3ai

$^1$H NMR of (3-bromophenyl)(2-(pyridin-2-yl)phenyl)methanone 3aj
$^1$H NMR of (4-iodophenyl)(2-(pyridin-2-yl)phenyl)methanone 3ak

$^1$H NMR of benzo[h]quinolin-10-yl(phenyl)methanone 3ba
$^1$H NMR of (2-(1H-pyrazol-1-yl)phenyl)(phenyl)methanone 3ca

$^1$H NMR of (5-methyl-2-(pyridin-2-yl)phenyl)(phenyl)methanone 3da