

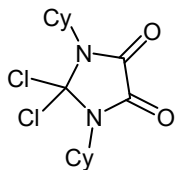
Supporting Information

DCID-Mediated Heck Cross-Coupling of Phenols *via* C-O Bond activation

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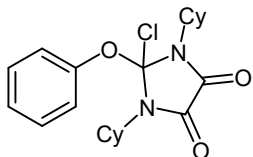
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Dichloroimidazolidinedione (DCID) 2:



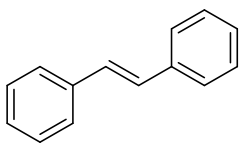
Yield 97%, White solid, m.p =174 -176 °C (lit. [1] mp: 174-176 °C); ¹HNMR (500 MHz, CDCl₃): δ (ppm) 1.17-1.36 (m, 6H), 1.66- 1.69 (m, 2H), 1.71-1.75 (m, 4H), 1.73-1.87 (m, 4H), 2.02- 2.10 (m, 4H), 3.97- 4.0 (m, 2H).

2-chloro-1,3-dicyclohexyl-2-phenoxyimidazolidine-4,5-dione (Ph-OMCID) (3a):



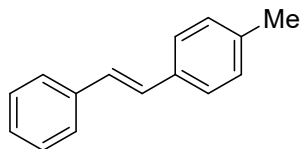
¹HNMR (500 MHz, CDCl₃): δ (ppm) 1.15 (m, 4H), 1.18(m, 4H), 1.65 (m, 2H), 1.71 (m, 4H), 1.79 ppm (m, 6H), 3.95 (m, 1H), 6.76 (d, ³J=7.59, 2H), 6.82 (t, ³J= 8.14, 2H), 7.16 (t, 3J =7.44, 1H). ¹³C-NMR: (125.66 MHz, CDCl₃) δ 24.41, 28.73, 28.94, 31.87, 114.74, 116.35, 121.22, 128.93, 156.27, 156.79. EI-MS m/z: 393 [M+2]. (lit. [1])

(E)-Stilbene (5a):



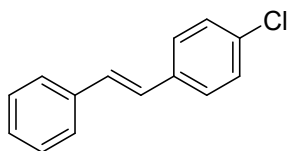
Yield 52 %, white solid, mp 122-124 °C (lit. [2] mp:124-126 °C); ¹H NMR (500 MHz, CDCl₃): δ (ppm) 7.17 (s, 2H), 7.32 (d, J = 7.4 Hz, 2H), 7.41 (t, J = 7.5 Hz, 4H), 7.57 (d, J = 7.5 Hz, 4H).

(E)-4-Methylstilbene (5b):



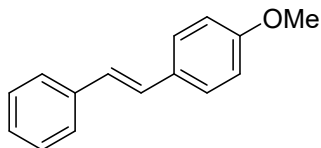
Yield 51 %, white solid, mp 116-118 °C (lit. [2] mp: 120-121 °C); ¹H NMR (500 MHz, CDCl₃): δ (ppm): 2.40 (s, 3H), 7.08-7.16 (m, 2H), 7.21 (d, J = 7.9 Hz, 2H), 7.29 (t, J = 7.2 Hz 1H), 7.40 (t, J = 7.7 Hz, 2H), 7.46 (d, J = 8.3 Hz, 2H), 7.55 (d, J = 8.3 Hz, 2H).

(E)-4-Chlorostilbene (5c):



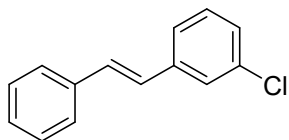
Yield 56%, white solid, mp 127-129 °C (lit. [3] mp: 126-128 °C); ¹H NMR (500 MHz, CDCl₃): δ (ppm) 7.04-7.14 (m, 2H), 7.28-7.32 (m, 1H), 7.32-7.36 (m, 2H), 7.39 (t, J = 7.7 Hz, 2H), 7.43-7.49 (m, 2H), 7.50-7.56 (m, 2H).

(E)-4-Methoxostilbene (5d):



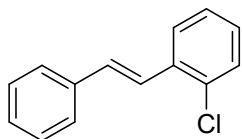
Yield 50%, white solid, mp 130-132 °C (lit. [2] mp: 135-136 °C); ¹H NMR (500 MHz, CDCl₃): δ (ppm) 3.85 (s, 3H), 6.88-6.94 (m, 2H), 7.00 (d, J = 16.4 Hz, 1H), 7.09 (d, J = 16.4 Hz, 1H), 7.25 (t, J = 7.4 Hz, 1H), 7.37 (t, J = 7.7 Hz, 2H), 7.52-7.46 (m, 4H).

(E)-3-Chlorostilbene (5e):



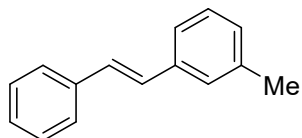
Yield: 52%; white solid; mp: 72-74 °C (lit. [4] mp: 74-76 °C); ¹H NMR (500 MHz, CDCl₃): δ (ppm) 7.07 (q, J = 16.2 Hz, 2H); 7.26 (t, J = 7.4 Hz, 3H), 7.34-7.40 (m, 3H), 7.51 (d, J = 7.2 Hz, 3H).

(E)-2-Chlorostilbene (5f):



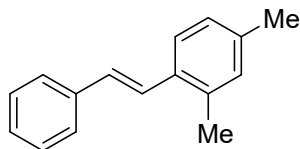
Yield: 51 %; white solid; mp: 60-62 °C (lit. [4] mp: 64-66 °C); ¹H NMR (500 MHz, CDCl₃): δ (ppm) 7.07 (d, J = 16.0 Hz, 1H), 7.18 (t, J = 7.6 Hz, 1H), 7.31-7.25 (m, 2H), 7.37 (t, J = 7.6 Hz, 3H), 7.53 (m, 3H), 7.68 (d, J = 7.8 Hz, 1H).

(E)-3-Methylstilbene (5g):



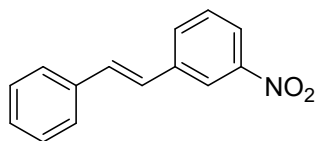
Yield 55 %, white solid, mp 45-47 °C (lit. [4] mp: 48-49 °C); ¹H NMR (500 MHz, CDCl₃): δ (ppm) 2.41 (s, 3H), 7.09-7.13 (m, 3H), 7.27-7.31 (m, 2H), 7.35-7.40 (m, 4H), 7.56-7.54 (m, 2H).

(E)-2,4-Dimethylstilbene (5h):



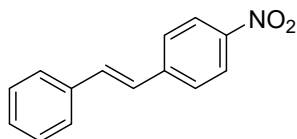
Yield 26 %, white solid, mp 121-124 °C; ¹H NMR (500 MHz, CDCl₃): δ (ppm) 2.30 (s, 3H), 2.40 (s, 3H), 7.08-7.16 (m, 2H), 7.21 (d, J = 7.9 Hz, 2H), 7.29 (t, J = 7.2 Hz 1H), 7.40 (t, J = 7.7 Hz, 2H), 7.46 (d, J = 8.3 Hz, 1H), 7.55 (d, J = 8.3 Hz, 2H).

(E)-3-Nitrostilbene (5i):



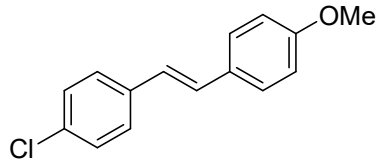
Yield 10 %, off-white solid, mp 102-104 °C; ¹H NMR (500 MHz, CDCl₃): δ (ppm) 7.16 (d, J = 16.4 Hz, 1H), 7.22 (d, J = 16.4 Hz, 1H), 7.28 (t, J = 7.4 Hz, 1H), 7.40 (t, J = 7.6 Hz, 2H), 7.48 (t, J = 7.7 Hz, 1H), 7.55 (d, J = 7.5 Hz, 2H), 7.73 (d, J = 7.7 Hz, 1H), 7.86 (d, J = 7.7 Hz, 1H), 8.12 (s, 1H).

(E)-4-Nitrostilbene (5j):



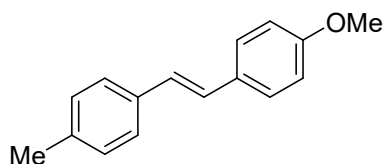
Pale yellow solid, mp 154-156 °C (lit. [5] mp: 157 °C); ¹H NMR (500 MHz, CDCl₃): δ (ppm) 7.05 (d, J = 16.2 Hz, 1H), 7.20 (d, J = 16.2 Hz, 1H), 7.24 (t, J = 7.2 Hz, 1H), 7.31 (t, J = 7.4 Hz, 2H), 7.46 (d, J = 7.4 Hz, 2H), 7.54 (d, J = 8.6 Hz, 2H), 8.13 (d, J = 8.6 Hz, 2H).

(E)-4-Chloro-4'-methoxystilbene (5k):



White solid, mp 182-184°C (lit. [6] mp: 181-184°C); ¹H NMR (500 MHz, CDCl₃): δ (ppm) 2.62 (s, 3H), 7.10 (d, J = 16.4 Hz, 1H), 7.18 (d, J = 16.4 Hz, 1H), 7.36 (d, J = 8.5 Hz, 2H), 7.47 (d, J = 8.5 Hz, 2H), 7.58 (d, J = 8.4 Hz, 2H), 7.97 (d, J = 8.4 Hz, 2H).

(E)-4'-Methoxy-4-methylstilbene (5l):



Off white solid, mp 164-166 °C (lit. [7] mp: 166-167 °C); ¹H NMR (500 MHz, CDCl₃) δ (ppm) 2.62 (s, 3H), 3.86 (s, 3H), 6.93 (d, J = 8.7 Hz, 2H), 7.01 (d, J = 16.3 Hz, 1H), 7.20 (d, J = 16.3 Hz, 1H), 7.50 (d, J = 8.7 Hz, 2H), 7.57 (d, J = 8.3 Hz, 2H), 7.87 (d, J = 8.3 Hz, 2H).

References

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