Supporting Information

for

Direct arylation catalysis with chloro[8-

(dimesitylboryl)quinoline-κN]copper(l)

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NMR spectra and GC–MS data of the products

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Experimental

General Conditions

Compound 1 and Chloro[8-(dimesitylboryl)quinoline- κ N]copper(I) was prepared according to the literature [1]. All organic reagents and solvents were obtained from commercial sources and used without further purification. A GCMS-QP2010SE gas chromatograph-mass spectrometer (Shimadzu Corp., Kyoto, Japan) was used for GCMS analyses. NMR spectra were recorded on an Avance 400 MHz spectrometer (Bruker, Billerica, MA, USA).

Experimental Conditions

A 50 mL roundbottom flask was charged with 0.5 mmol of aryl halide, benzene (4mL) and 1.5 mmol of KOtBu. The flask was fitted with a reflux condenser left open to air. Then, a solution of catalyst dissolved in 420 μ L DMF was added to the reaction. The reaction was then stirred and refluxed for 40 hrs. The reaction was worked up by extraction with ether and washing with DI H₂O. The organic phase was collected and dried over anhydrous sodium sulfate. The residue was purified by flash column chromatography. NMR spectra of isolated products matched well with the literature.

[1] Son, J.H.; Pudenz, M.A.; Hoefelmeyer, J.D. Dalton Trans. 2010, 39, 11081-11090.

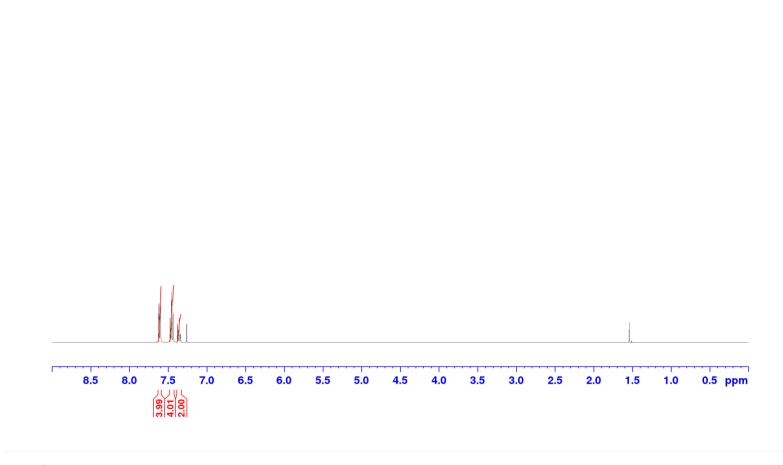


Figure S1: ¹H NMR of biphenyl in CDCl₃.

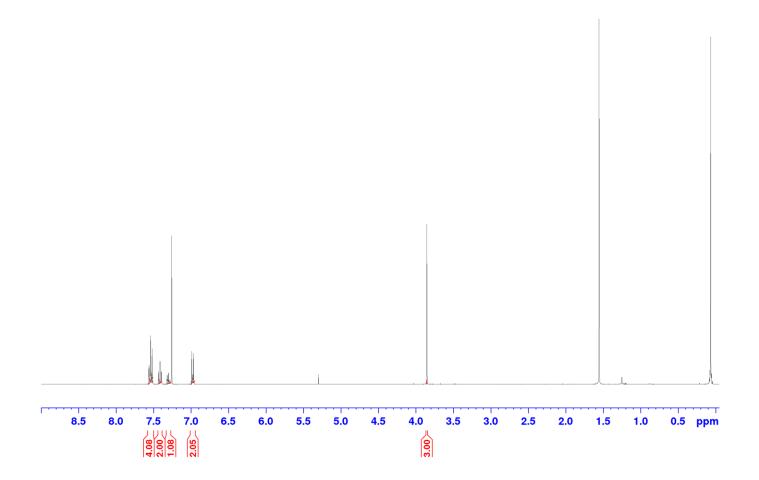


Figure S2: ¹H NMR of 4-methoxybiphenyl in CDCl₃.

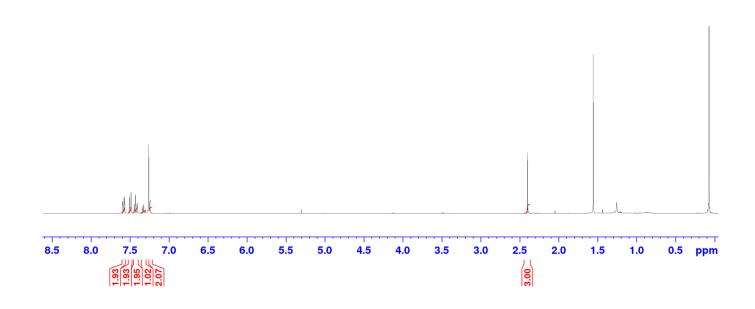


Figure S3: ¹H NMR of 4-methylbiphenyl in CDCl₃.

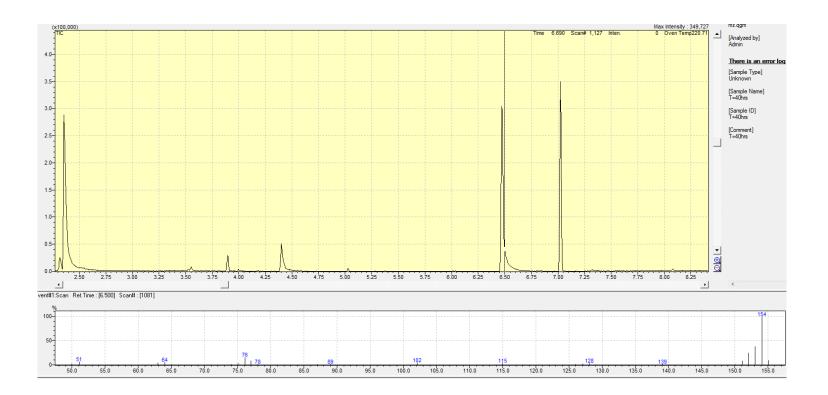


Figure S4: GC–MS data of biphenyl. m/z = 154.

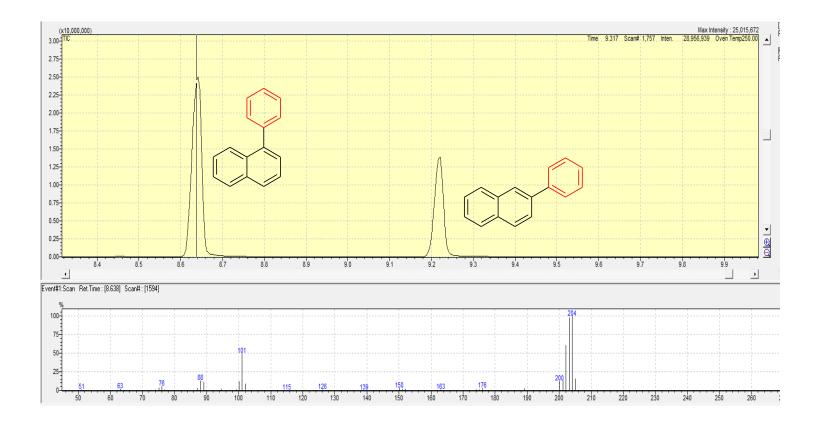


Figure S5: GC–MS data of direct arylation at 1 and 2 position of naphthalene. m/z = 204.

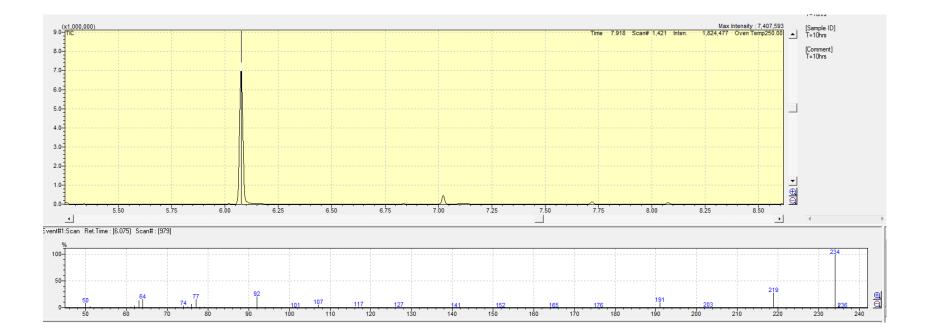


Figure S6: GC–MS data for *p*-methoxybiphenyl. m/z = 234.

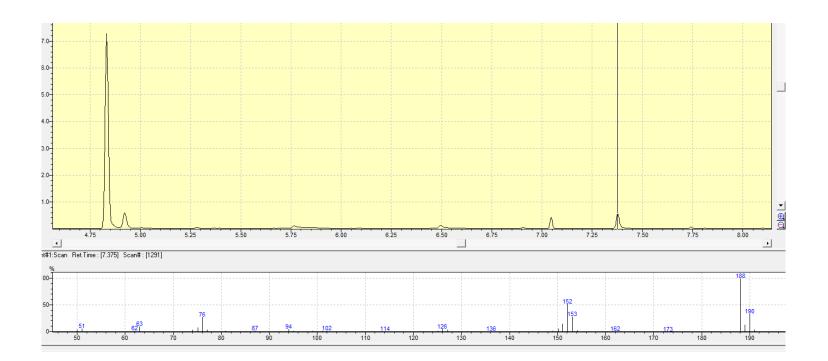


Figure S7: GC–MS data for *m*-chlorobiphenyl. m/z = 188.

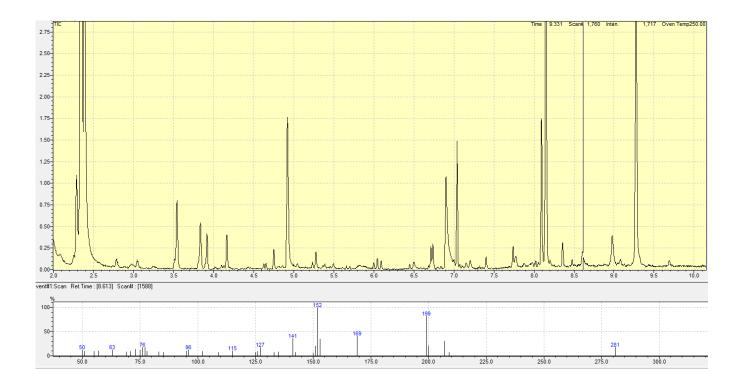


Figure S8: GC–MS data for *p*-nitrobiphenyl. m/z = 199.

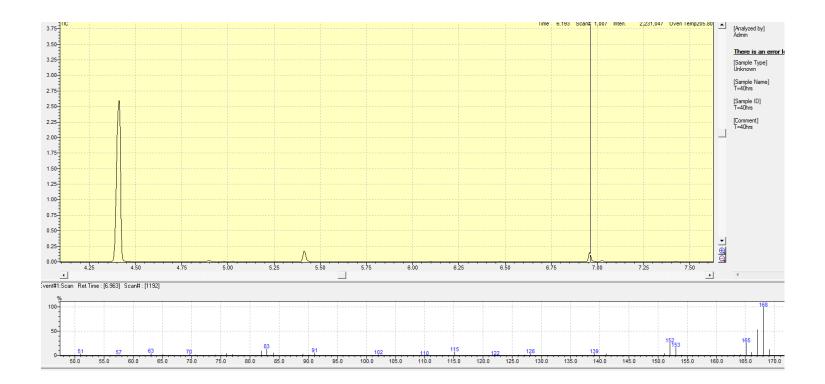


Figure S9: GC–MS data for *m*-methylbiphenyl. m/z = 168.