Compound Information

Name:
- 4-Chloro-3-methoxy-biphenyl
- 3-Methoxy-4-chloro-biphenyl

Chemical formula: $C_{13}H_{11}ClO$

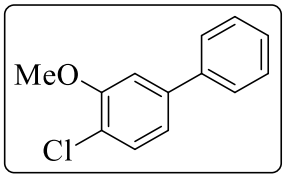
Molecular weight: 218.6800

PubChem CID: 46314681 (https://pubchem.ncbi.nlm.nih.gov/compound/46314681)

InChl Key: GZNUGXLDNUTRHC-UHFFFAOYSA-N

CAS number: 74447-81-7

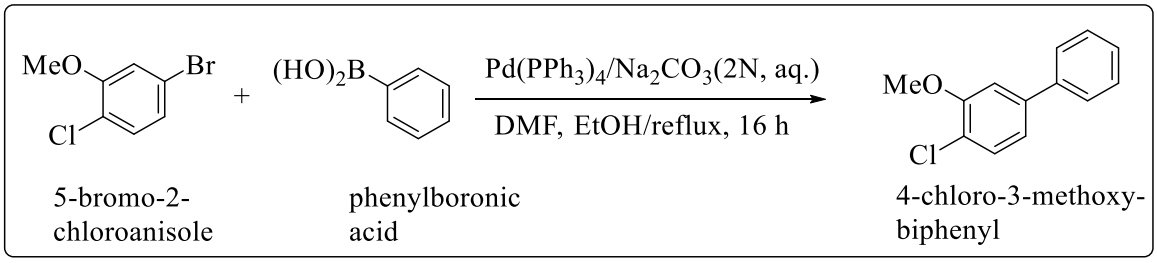
Structure:



Synthetic route: Suzuki cross coupling

Synthesis: 5-Bromo-2-chloroanisole reacted with phenyl boronic acid in the presence of $Pd(PPh_4)_2$ and aqueous solution of sodium carbonate (2N) to provide 4-chloro-3-methoxy-biphenyl

Reaction:



^{1}H NMR: 500 MHz, $CDCl_3$, δ = 7.60 – 7.54 (m, 2H), 7.49 – 7.34 (m, 4H), 7.16 – 7.09 (m, 2H), 3.97 (s, 3H) ppm (1)

^{13}C NMR: 126 MHz, $CDCl_3$, δ = 155.3, 141.5, 140.7, 130.5, 129.0, 127.9, 127.3, 121.8, 120.2, 111.2, 56.3 ppm (1)

GC-MS:	*m/z* (relative abundance %): 218.1 (M^{+}, 100), 175.0 (59), 152.1 (15), 139.1 (39) (1)
Purification:	Flash column chromatography (silica gel and hexane) and recrystallization (1:7; chloroform/hexane)
Purity:	>99% (determined based on relative peak area by GC-MS)
State:	Colorless oil
R_f:	0.63 (3:1; hexane/ethyl acetate, silica-gel TLC glass plate)

Reference:

1. Zhai, G.; Lehmler, H.-J.; Schnoor, J. L. (2011) New hydroxylated metabolites of 4-monochlorobiphenyl in whole poplar plants. *Chem Cent J* **5:**87

*Instruments and software used to record and process raw data for **4-chloro-3-methoxy-biphenyl***

Files	Instruments for raw data	Software to process raw data
^{1}HNMR raw.rar	Bruker AV500 spectrometer in the University of Iowa Central NMR Research Facility (Iowa City, IA, USA)	Spectrometer software: Vnmr Varian, Vnmr J Varian, TopSpin Bruker Other software: Mnova, NMRPipe, ACD, SpinWorks, matNMR
^{13}CNMR raw.rar	Bruker AV500 spectrometer in the University of Iowa Central NMR Research Facility (Iowa City, IA, USA)	Spectrometer software: Vnmr Varian, Vnmr J Varian, TopSpin Bruker Other software: Mnova, NMRPipe, ACD, SpinWorks, matNMR
GC-MS raw.D.rar	Mass spectra of all compounds were recorded on an Agilent 7890A gas chromatograph equipped with an Agilent 5975C Inert Mass Selective Detector (Agilent Technologies, CA, USA)	Agilent ChemStation is commonly used to process the raw data in .d format. Raw data can be converted into the desired format using ProteoWizard software.