Compound Information

Name:
- 4-Chloro-2-methoxy-biphenyl
- 2-Methoxy-4-chloro-biphenyl
- 4-Chloro-2-methoxy-1-phenylbenzene

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

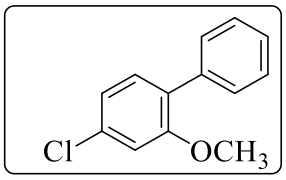
Molecular weight: 218.0498

PubChem CID: 46314680 (https://pubchem.ncbi.nlm.nih.gov/compound/46314680)

InChl Key: FLJUCQWJTRGSLN-UHFFFAOYSA-N

CAS number: 1214380-13-8

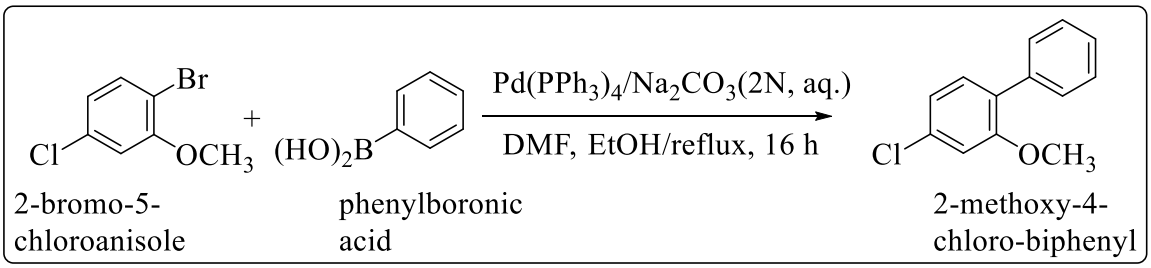
Structure:



Synthetic route: Suzuki cross coupling

Synthesis: 2-Bromo-5-chloroanisole undergoes Suzuki cross-coupling with phenylboronic acid to give 2-methoxy-4-chloro-biphenyl

Reaction:



^{1}H NMR: 500 MHz, $CDCl_3$ δ = 7.54 – 7.49 (dm, 2H), 7.44 (pseudo t, *J* = 7.6 Hz, 2H), 7.37 (pseudo t, *J* = 7.3 Hz, 1H), 7.28 (d, *J* = 2.8 Hz, 1H), 7.05 (dd, *J* = 8.1, 2.0 Hz, 1H), 7.00 (d, *J* = 1.8 Hz, 1H), 3.84 (s, 3H) ppm

^{13}C NMR: 126 MHz, $CDCl_3$ δ = 157.1, 137.6, 134.1, 131.7, 129.6, 129.4, 128.2, 127.4, 121.0, 112.0, 55.9 ppm

GC-MS:	*m/z* (relative abundance %): 218.1 (90), 203.0 (15), 168.1 ($M^{\cdot+}$ - CH_3Cl, 100), 152.1 (15), 139.1 (54)
Purification:	Flash column chromatography (silica-gel and hexane)
R_f:	0.375 (9:1; hexane/ethyl acetate, silica-gel TLC glass plate)
Purity:	>99% (determined based on relative peak area by GC-MS)
State:	White solid
Melting point:	37-38 °C (literature m.p. 37-42 °C)

References:

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

2. Quibell, J. M.; Duan, G.; Perry, G. J. P.; Larrosa, I. (2019) Decarboxylative Suzuki–Miyaura coupling of (hetero)aromatic carboxylic acids using iodine as the terminal oxidant. *Chem Commun* **55**, 6445-6448

Instruments and software used to record and process raw data for ***4-chloro-2-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.