Supporting Information

[Pd(Phbz)(X)(PPh_3)] palladacycles promote the base-free homocoupling of arylboronic acids in air at room temperature.

Anant R. Kapdi,*[a] Gopal Dhangar,[a] Jose Luis Serrano,[b] Jose A. De Haro,[c] Pedro Lozano,[d] Ian J. S. Fairlamb[e]

[a] Department of Chemistry, Institutite of Chemical Technology
Nathalal Parekh road, Matunga, Mumbai-400019, India
E-mail: ar.kapdi@ictmumbai.edu.in

[b] Departamento de Ingeniería Minera, Geológica y Cartográfica.
Universidad Politécnica de Cartagena. Área de Química Inorgánica, Regional Campus of International Excellence "Campus Mare Nostrum"30203 Cartagena, Spain.

[c] Villapharma Research, Parque Tecnológico de Fuente Álamo, 30320, Murcia, Spain.

[d] Departamento de BioQuímica Biologia Molecular, Universidad de Murcia, 30071 Murcia, Spain.

[e] Department of Chemistry, University of York, Heslington. York-YO105DD, United Kingdom

Table of Contents

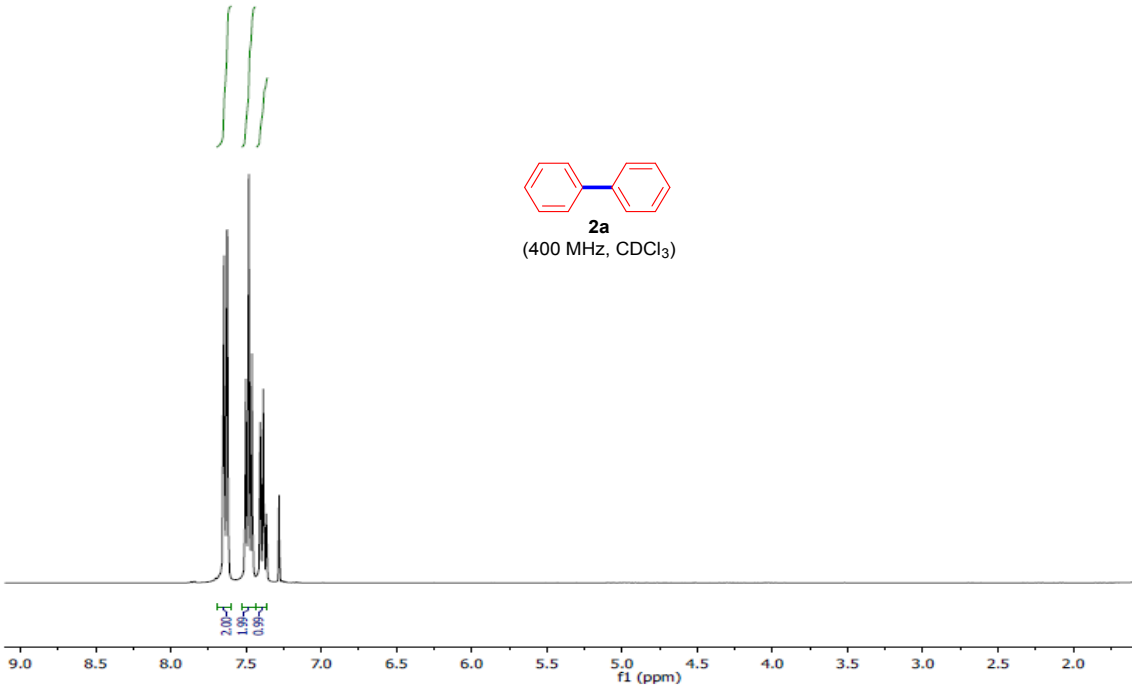
General Remarks:

Aryl boronic acids and other chemicals were obtained from commercial sources, and were used without further purification. Yields refer to isolated compounds, estimated to be >95 % pure as determined by ^{1}H-NMR. Flash chromatography: silica gel 60 (70-230 mesh). NMR data (^{1}H, ^{13}C) were recorded on Bruker 400 spectrometers. LC-MS analyses were performed on an Agilent VL mass-spectrometer. GC-MS used for analysis was Shimadzu QP-2010. Water content of THF solvents was estimated by using Metrohm Volumetric Karl Fischer titrator. All the palladacyclic complexes employed in the study were synthesised according to literature procedures.[18,23]

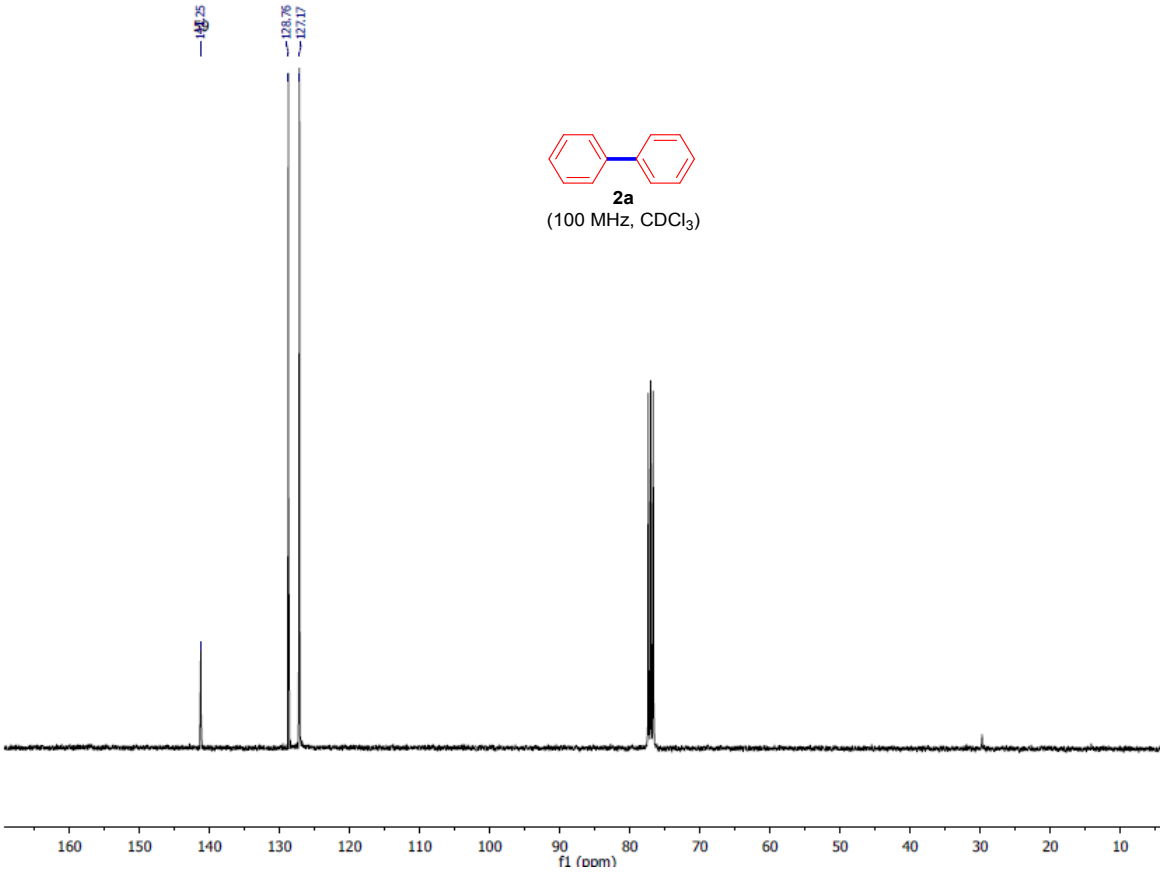
GC parameters: Analysis was performed using a Varian CP-3800 GC equipped with an Autosampler. A DB-1 column (30m x 0.32mm, 0.25 μm film thickness) with carrier gas N_2 flow rate of 5 ml min^{-1} and a temperature ramp from 50 ºC to 250 ºC at 15 ºC min^{-1}. The injection volume was 1 μL.

^{1}H and ^{13}C NMR for all the homocoupled products 2a-2w

Biphenyl (2a)

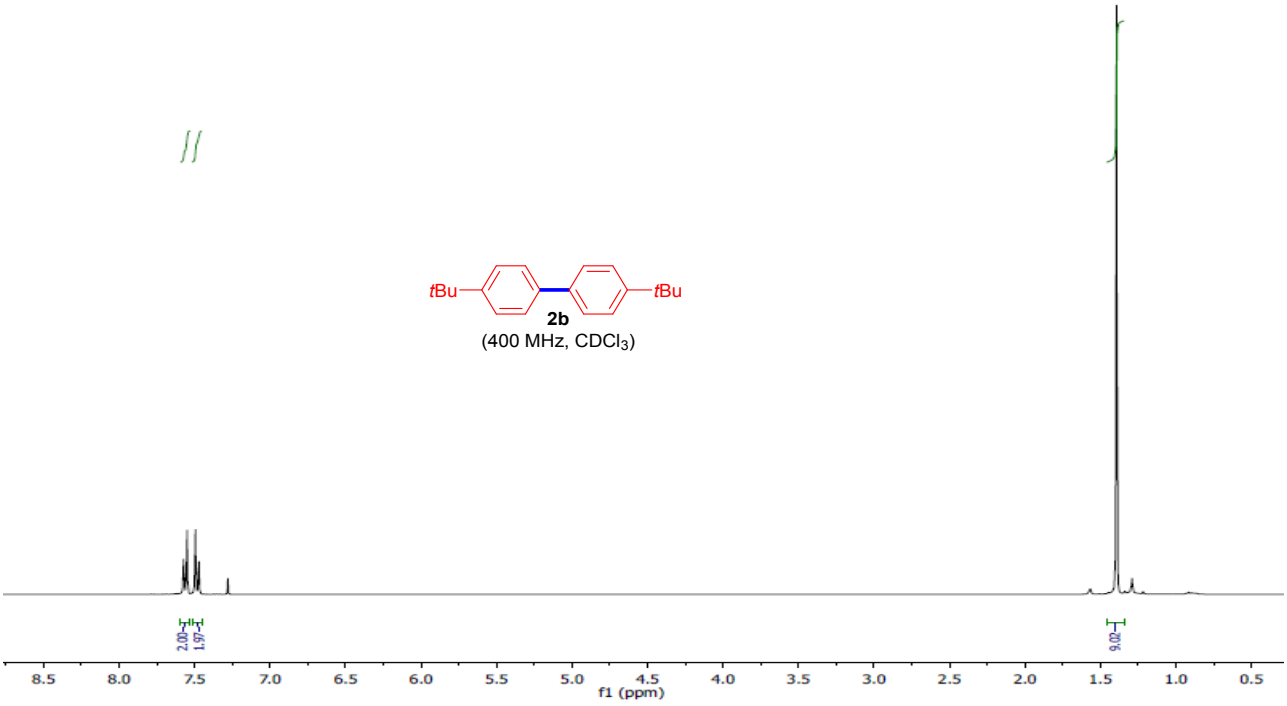


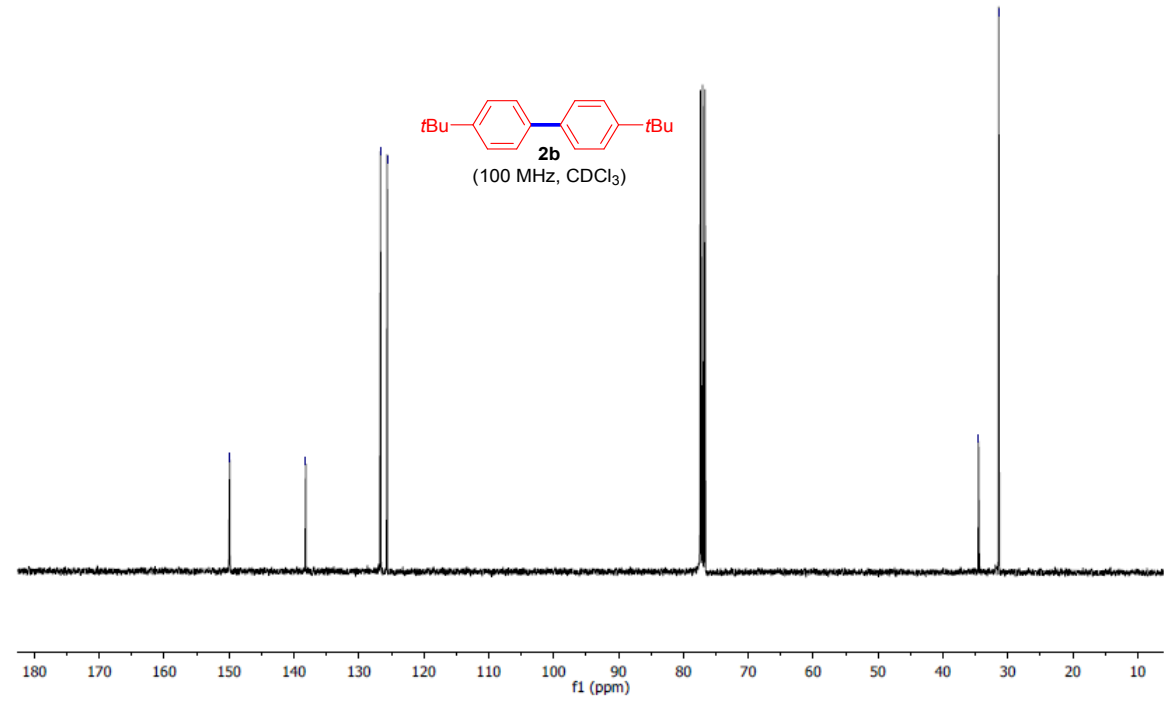
2a
(400 MHz, $CDCl_3$)



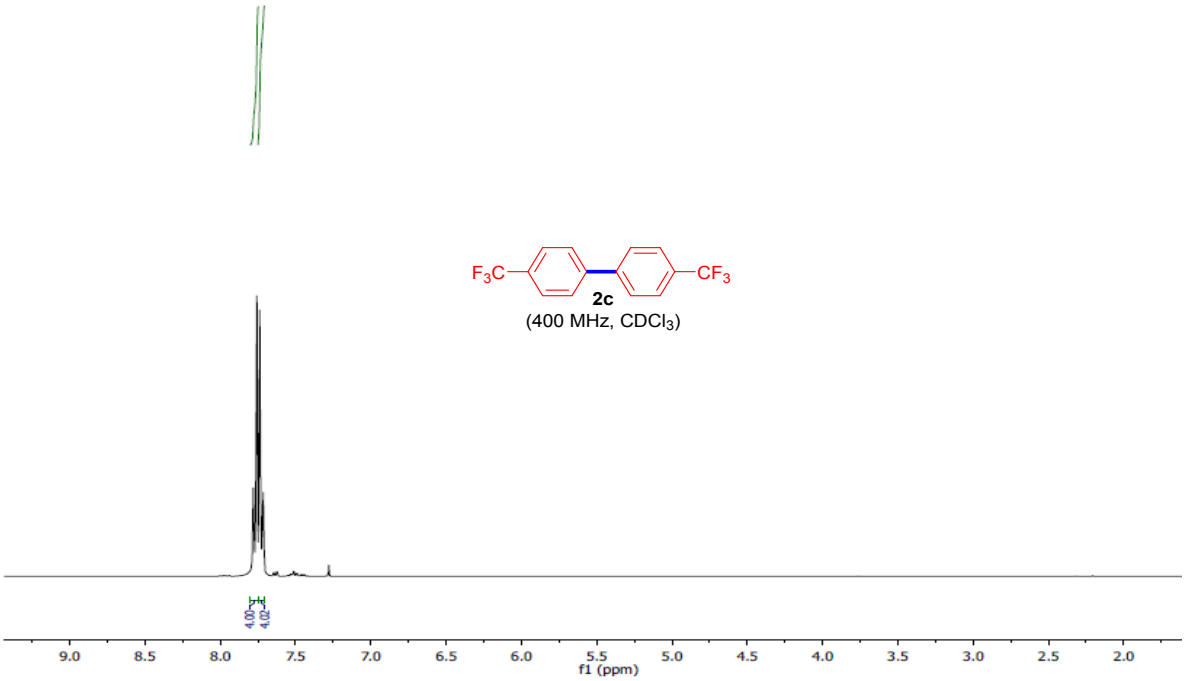
2a
(100 MHz, $CDCl_3$)

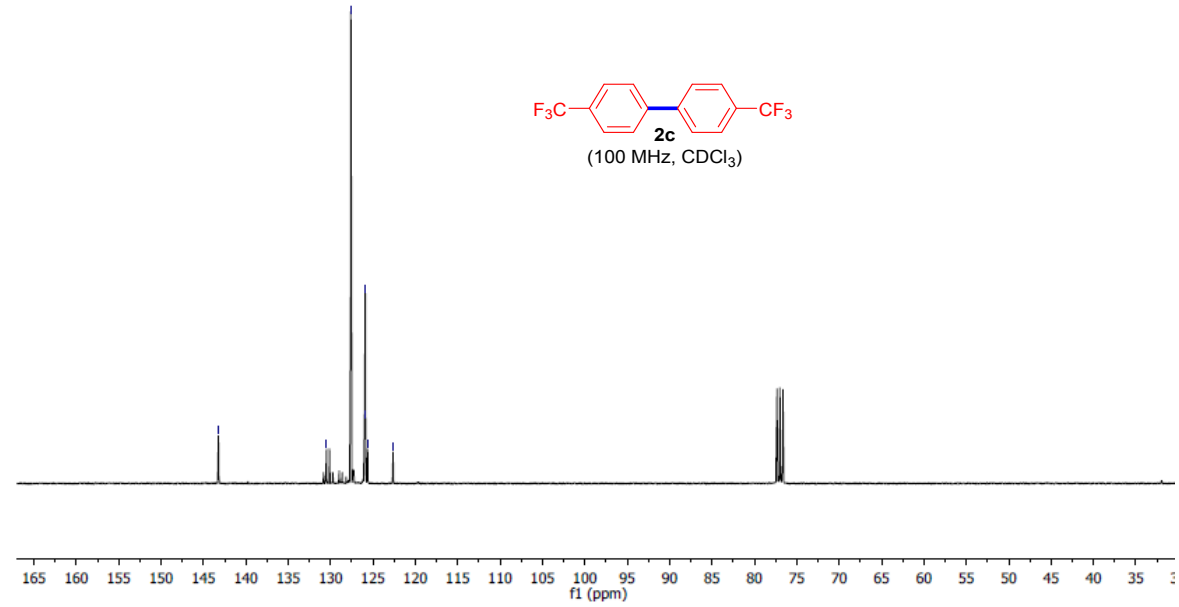
4,4'-Bis*tert*butyl biphenyl (2b)

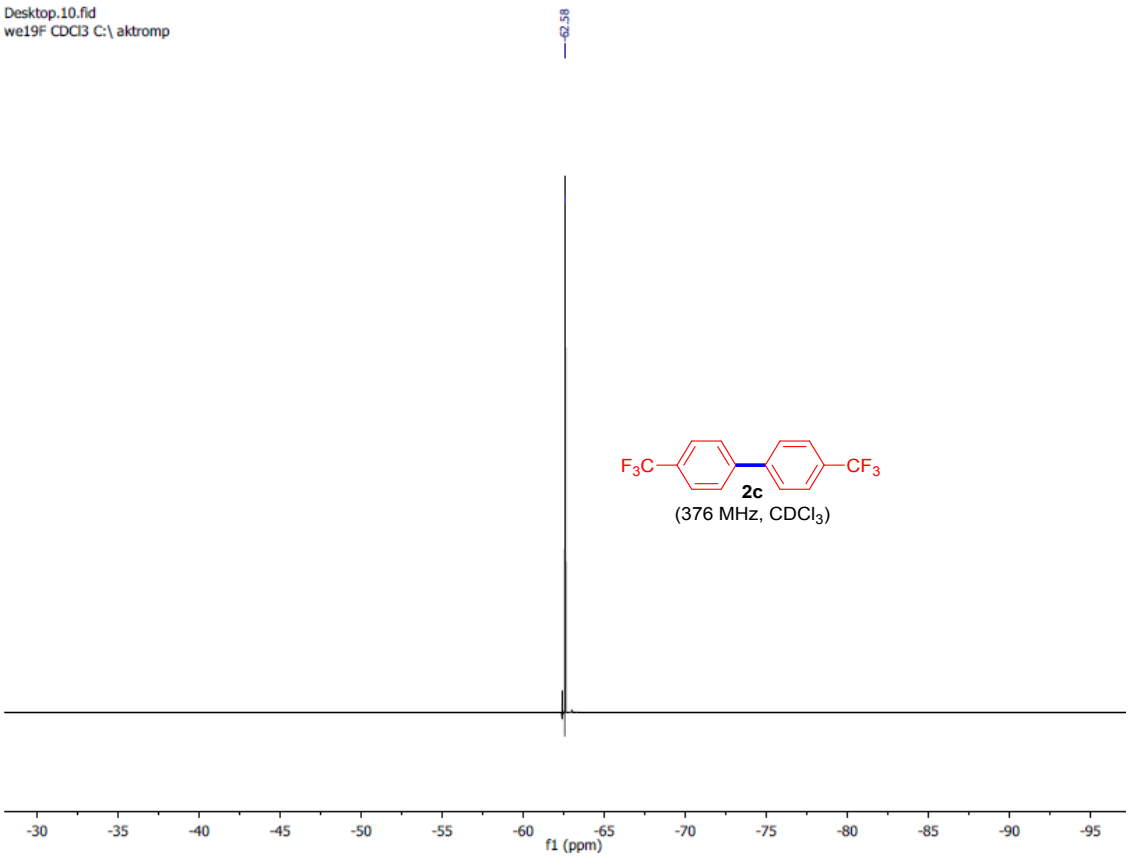




4,4'-Bistrifluoromethylbiphenyl (2c)



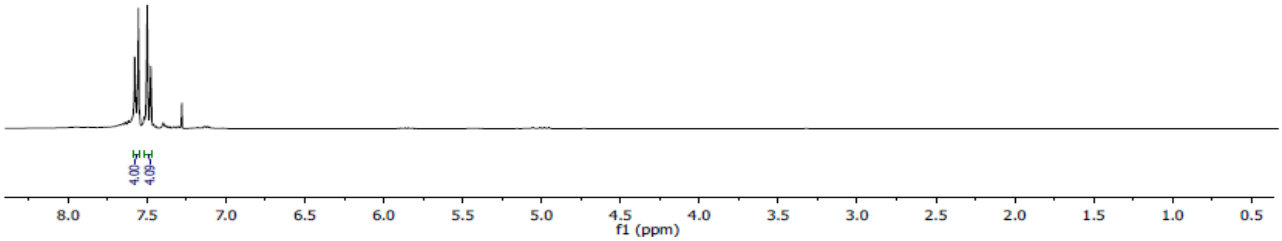


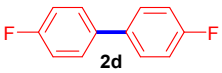

Desktop.10.fid
we19F CDCl3 C:\ aktromp
-62.58
F3C
CF3
2c
(376 MHz, CDCl3)
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
f1 (ppm)

4,4’-Difluorobiphenyl (2d)

2d

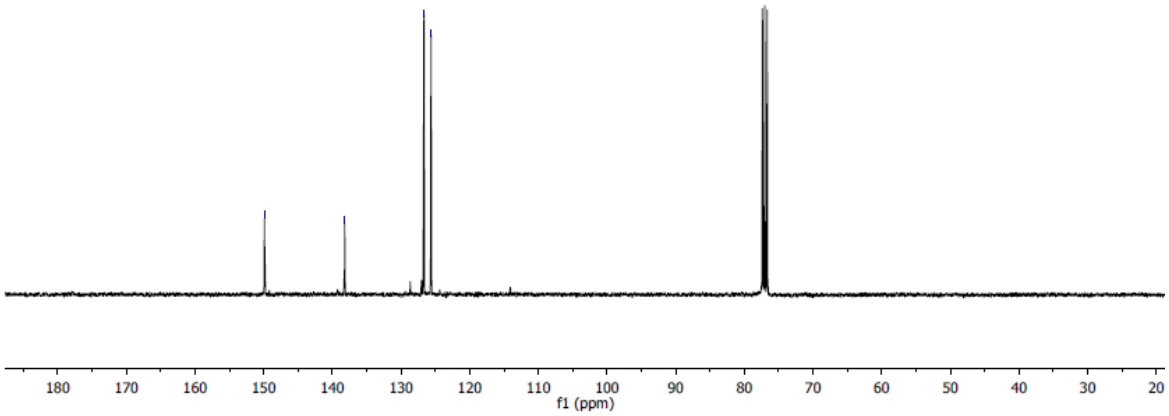
(400 MHz, $CDCl_3$)





2d

(100 MHz, $CDCl_3$)

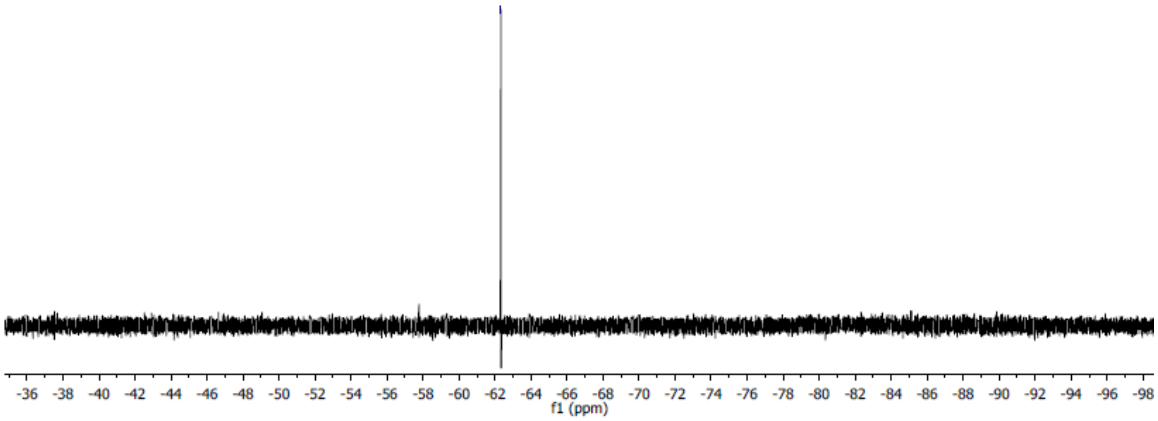


GDA-8.10.fid
we19F CDCl3 C:\ aktromp

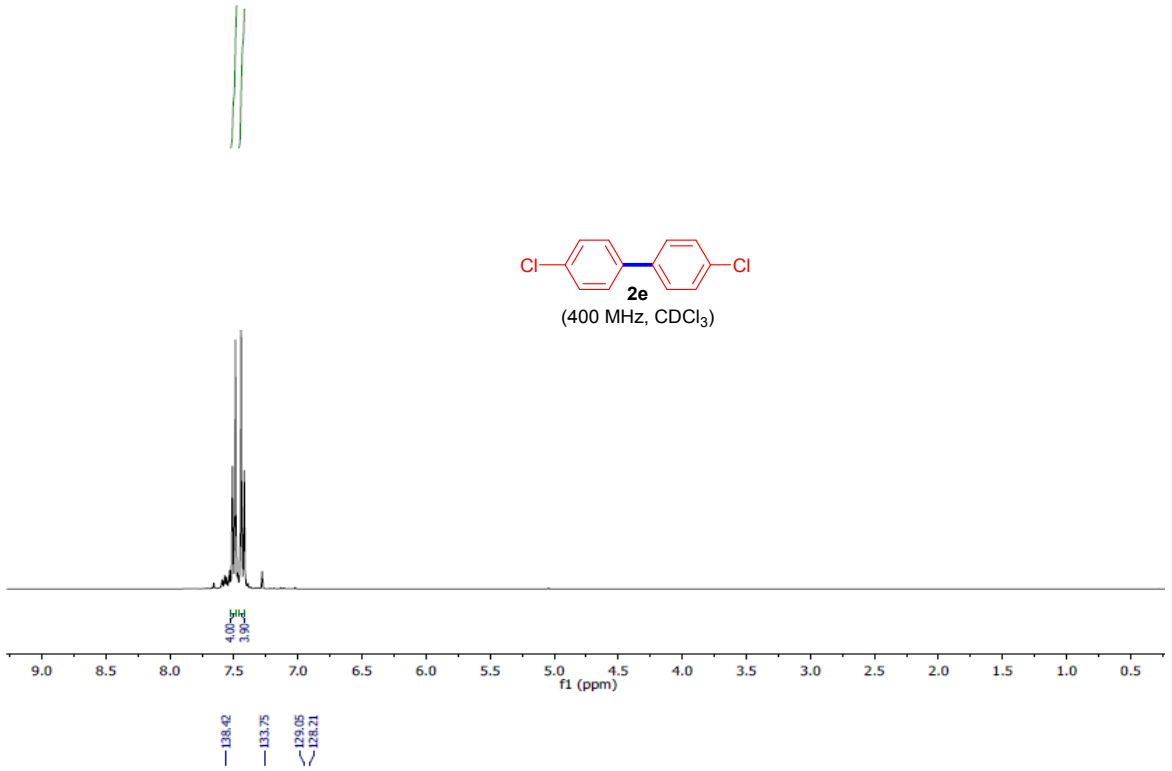
-62.33

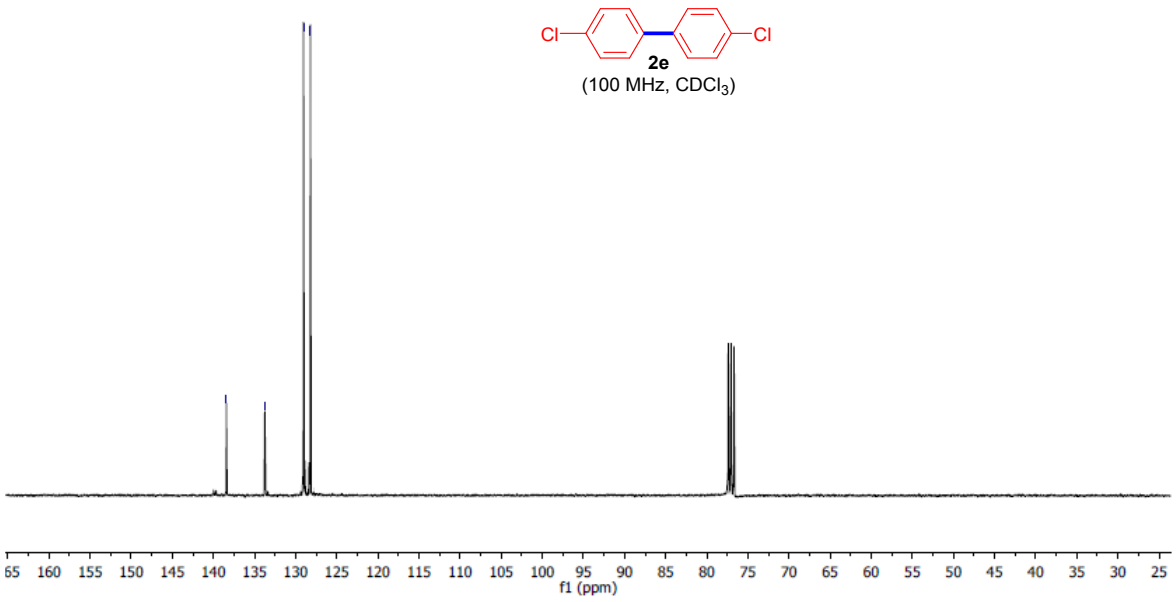
2d

(376 MHz, $CDCl_3$)

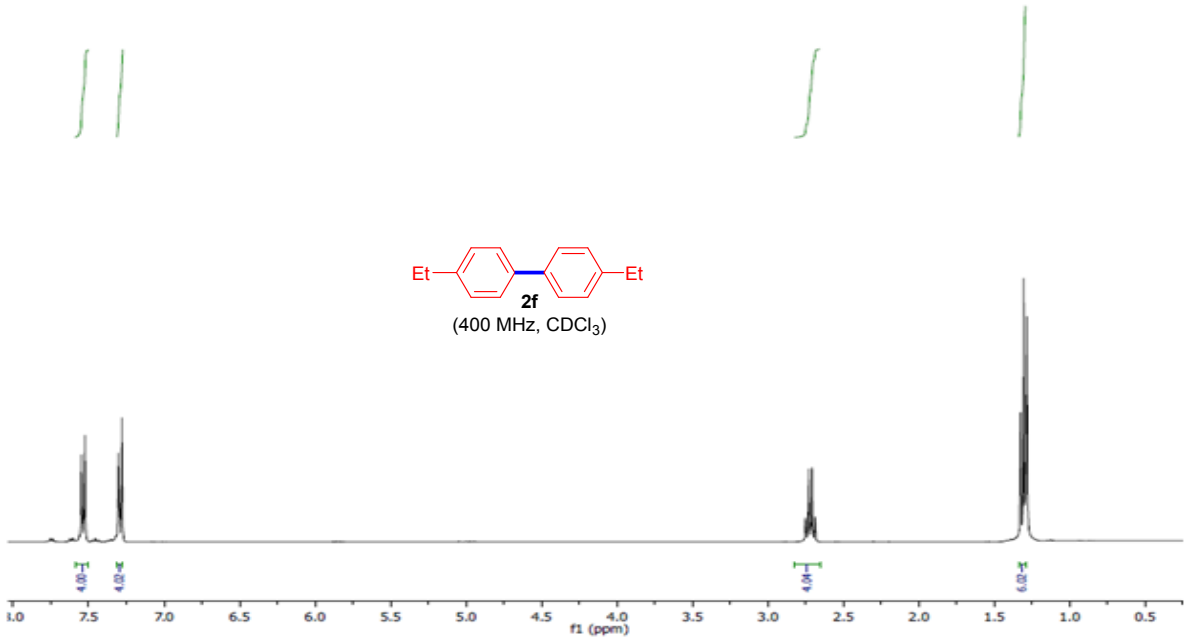


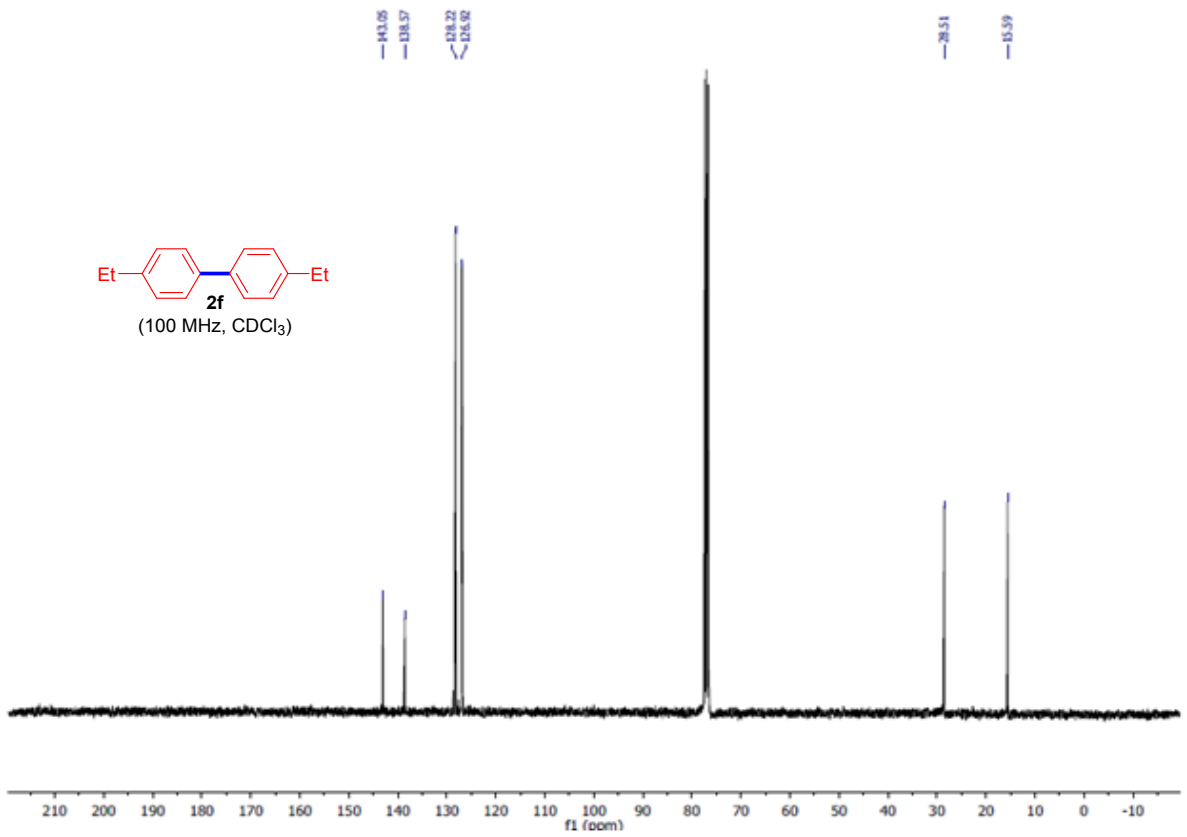
4,4'-Dichlorobiphenyl (2e)



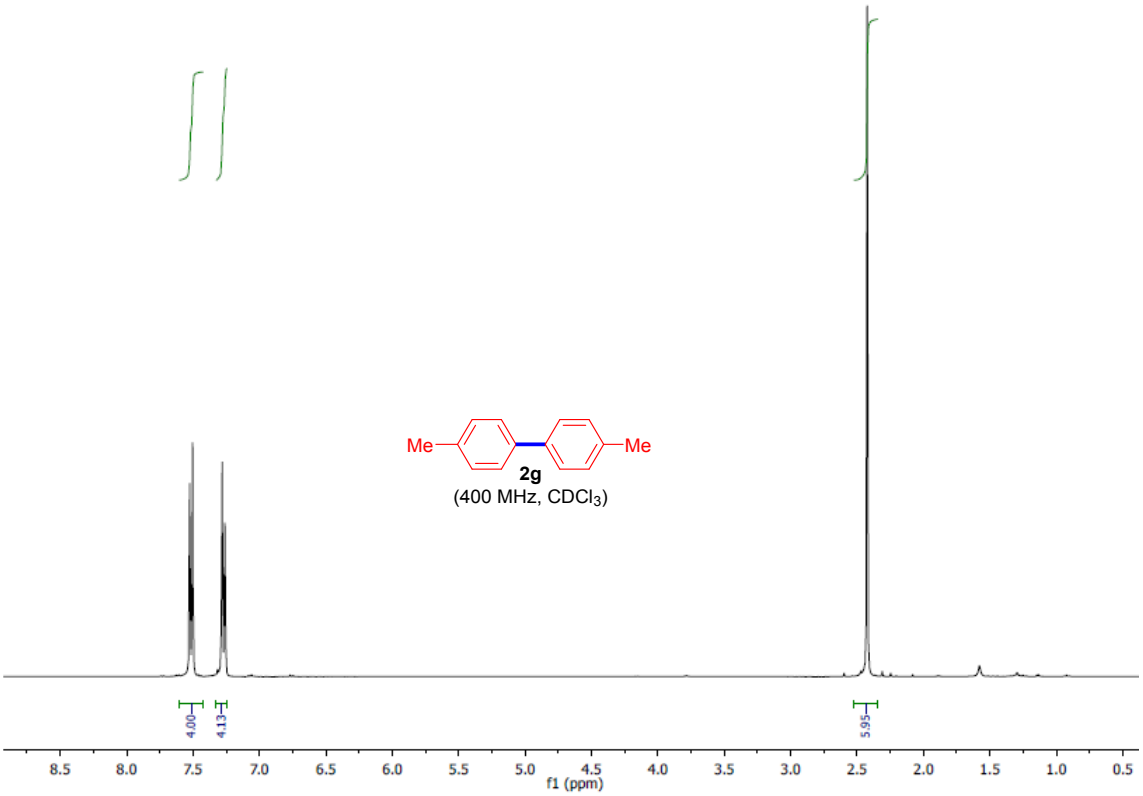


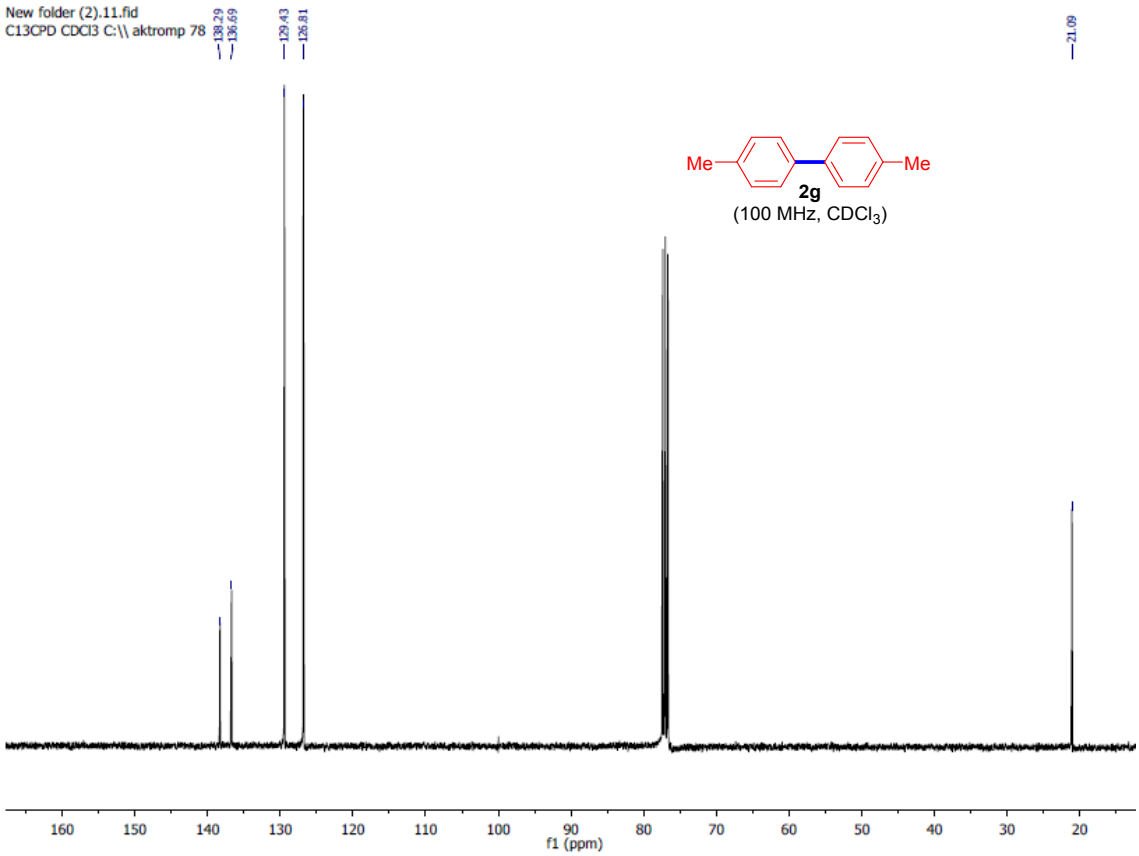
4,4'-Diethylbiphenyl (2f)



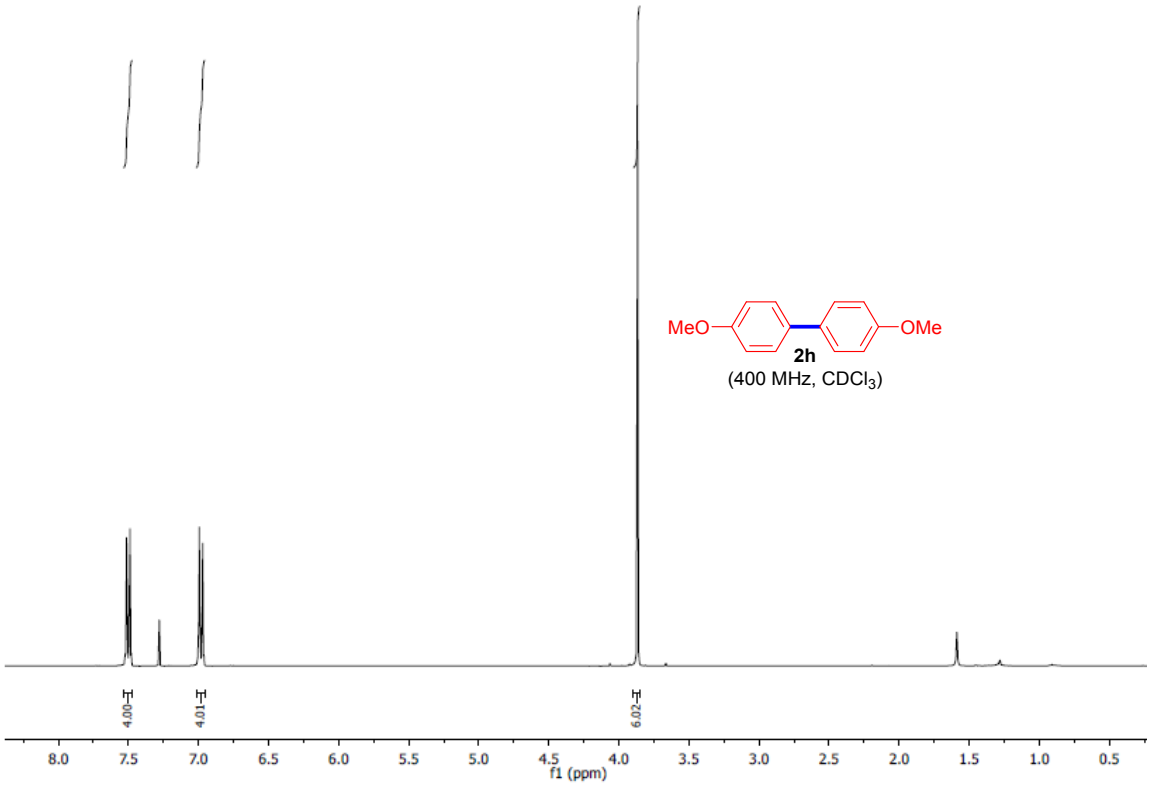


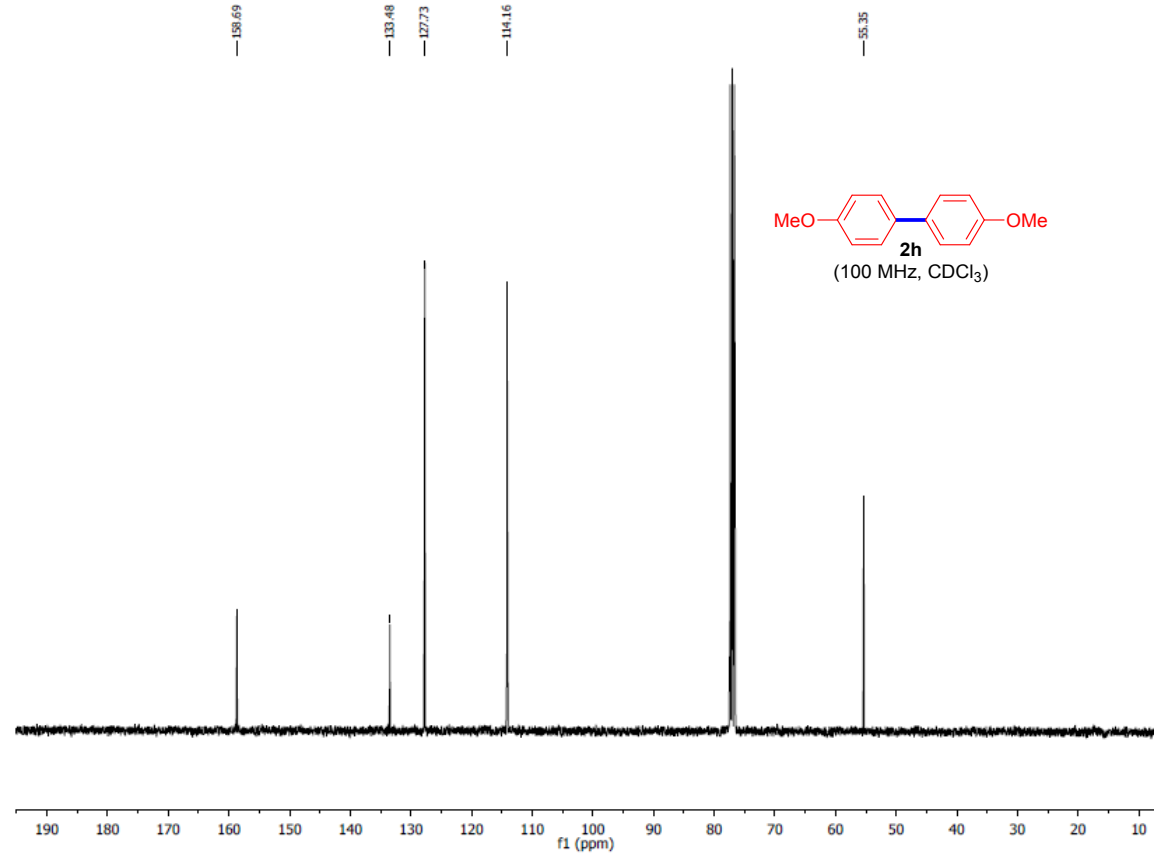
4,4'-Dimethylbiphenyl (2g)



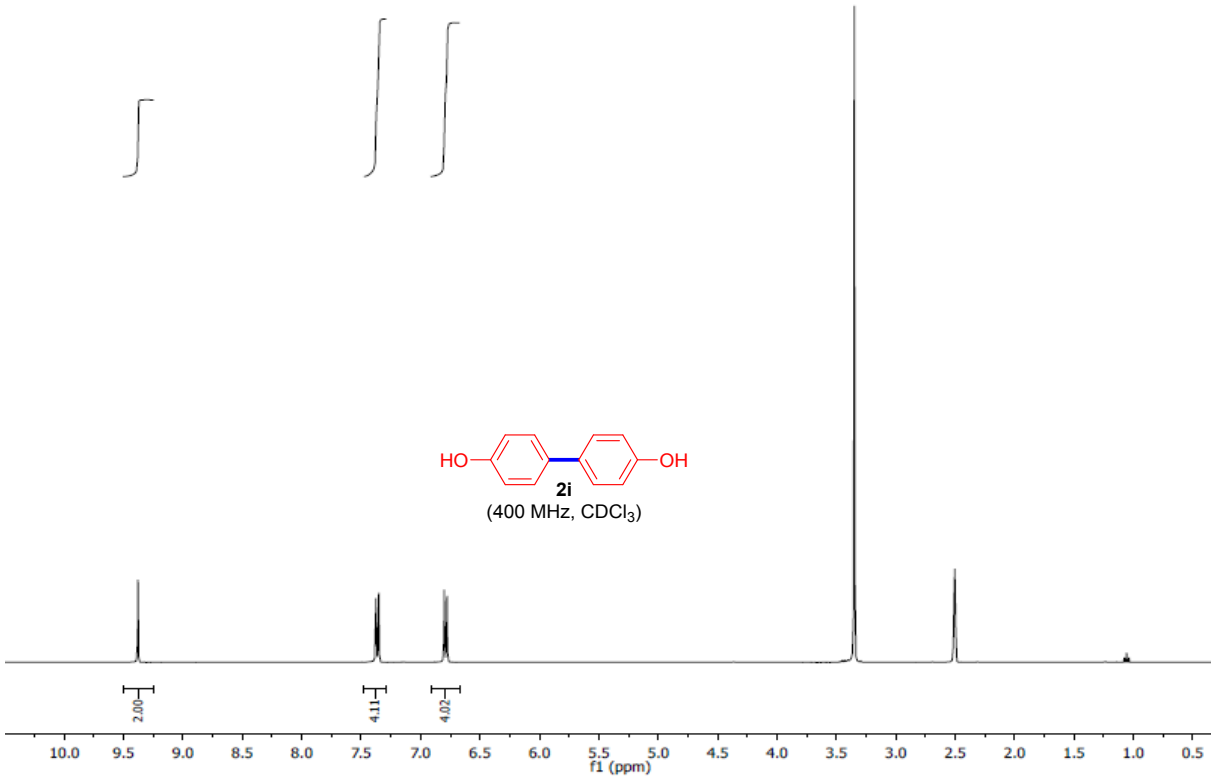


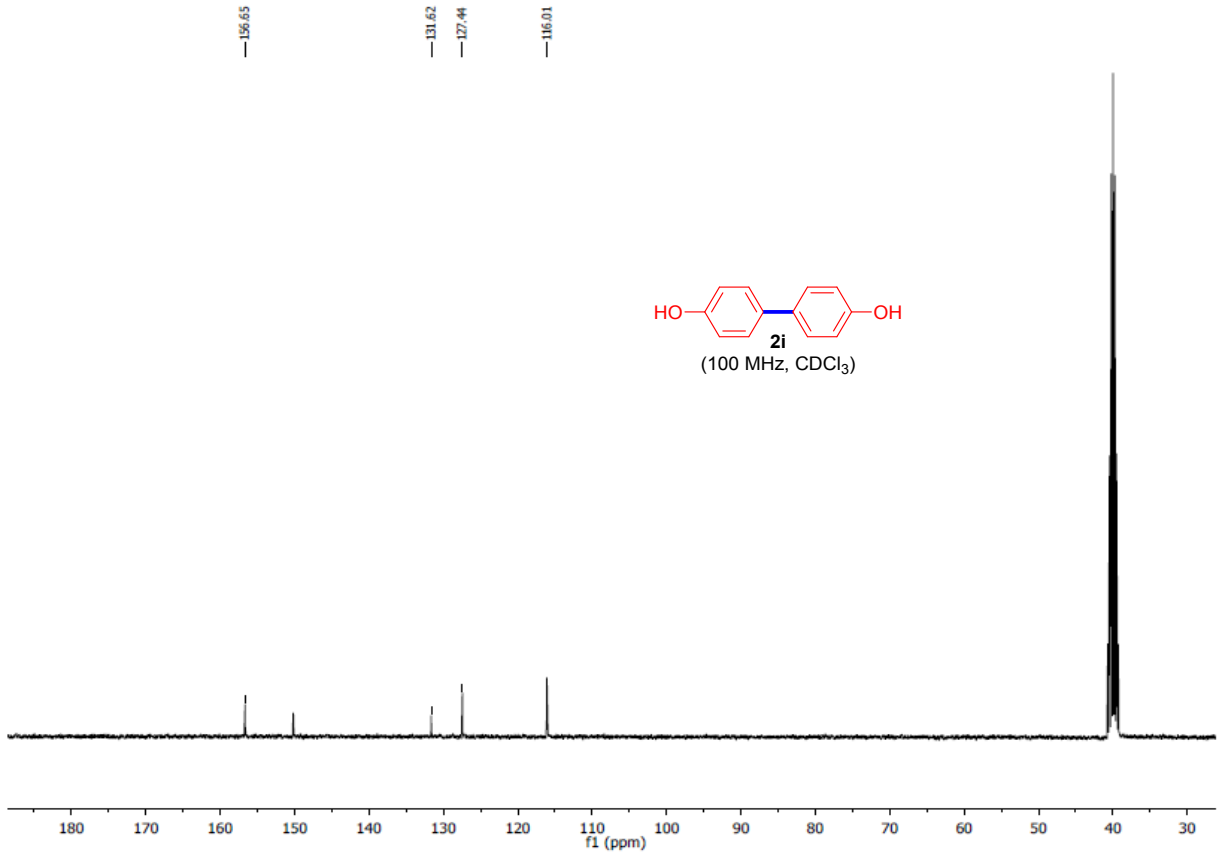
4,4’-Dimethoxybiphenyl (2h)



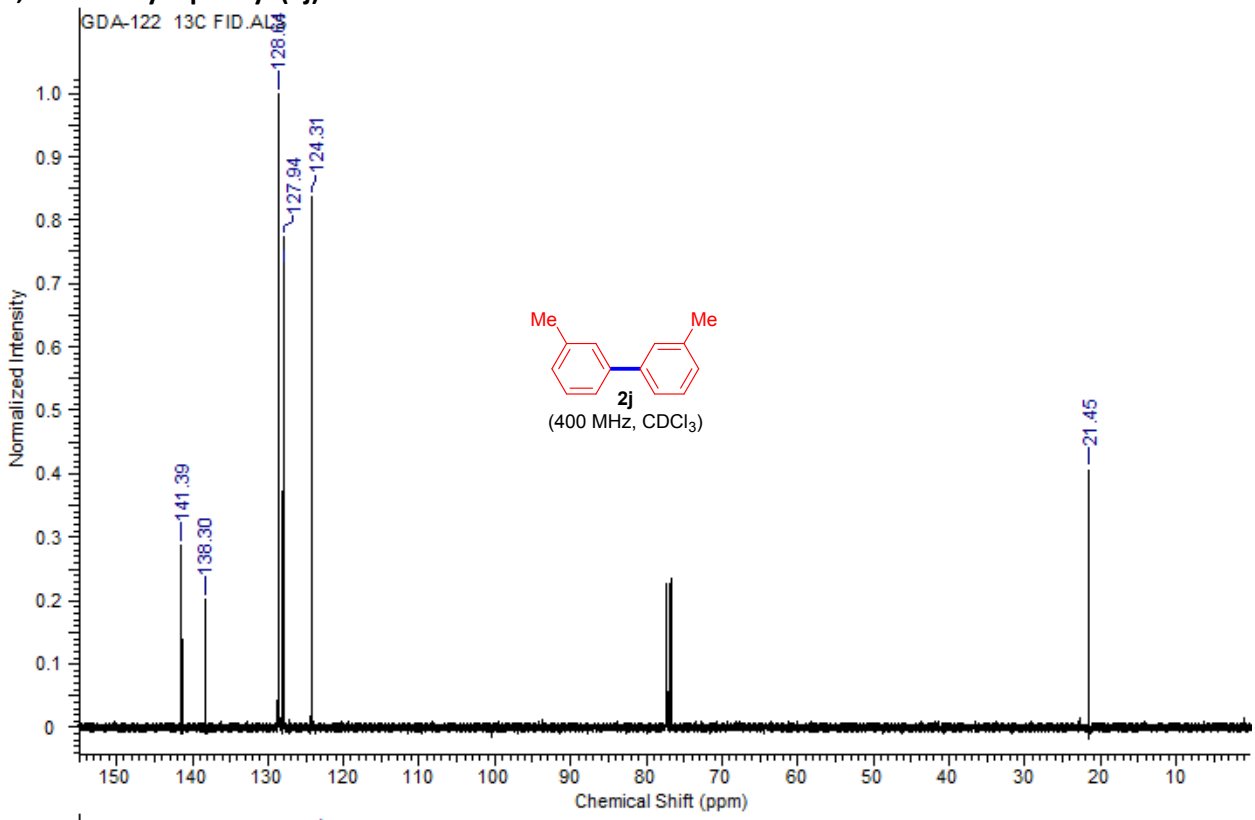


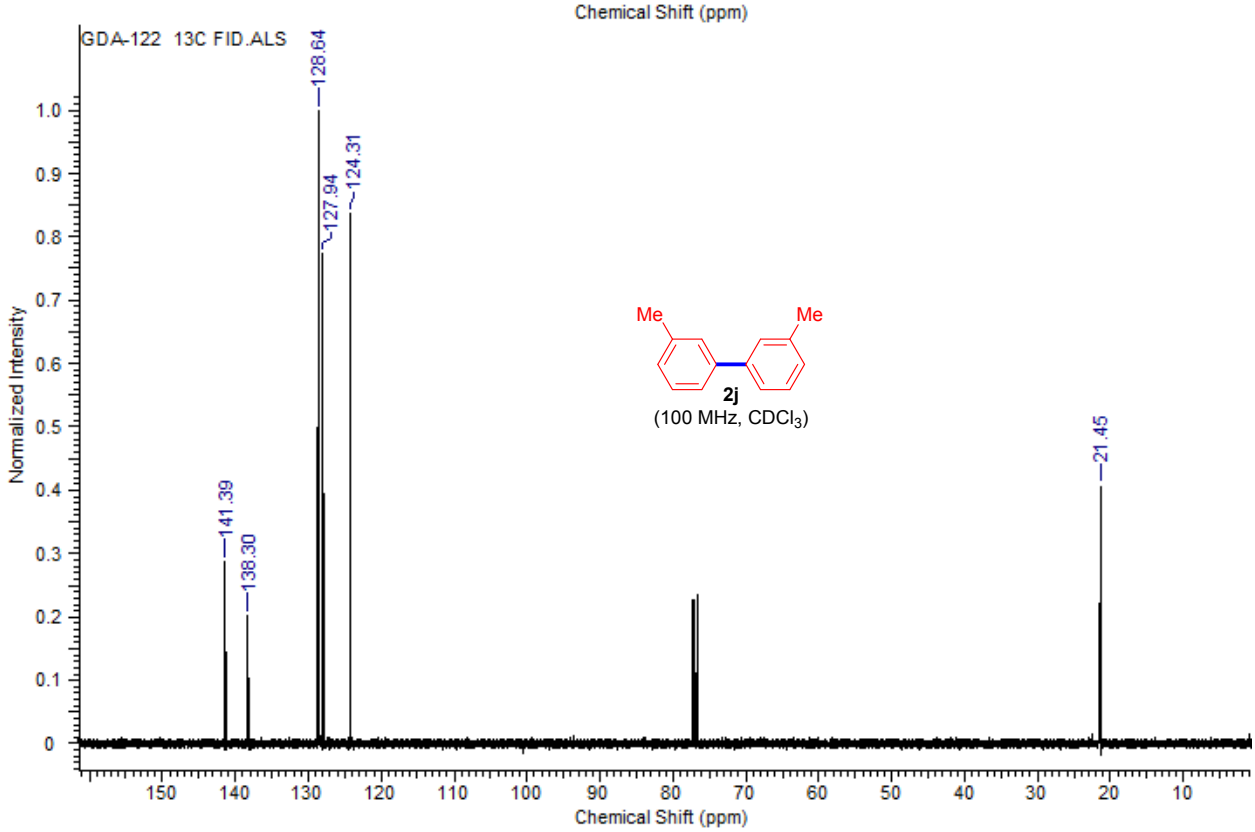
4,4'-Dihydroxybiphenyl (2i)



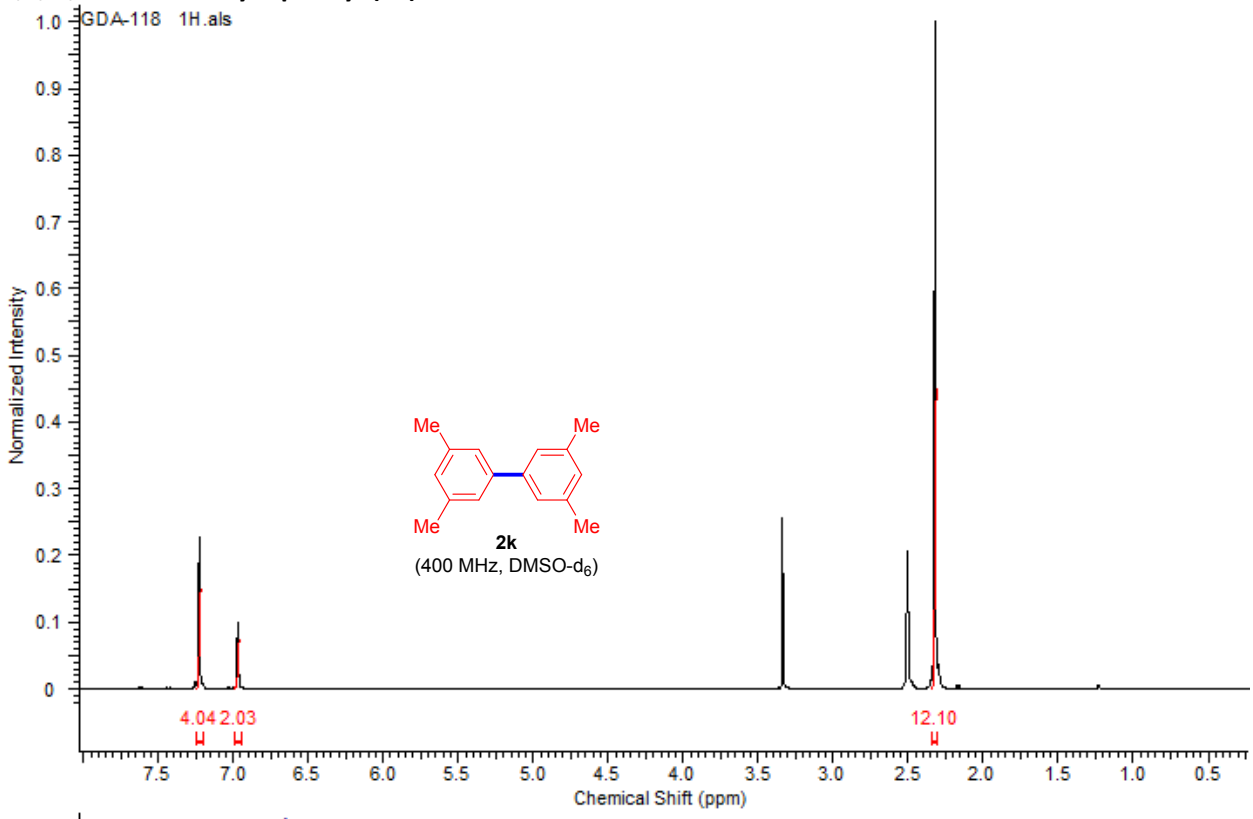


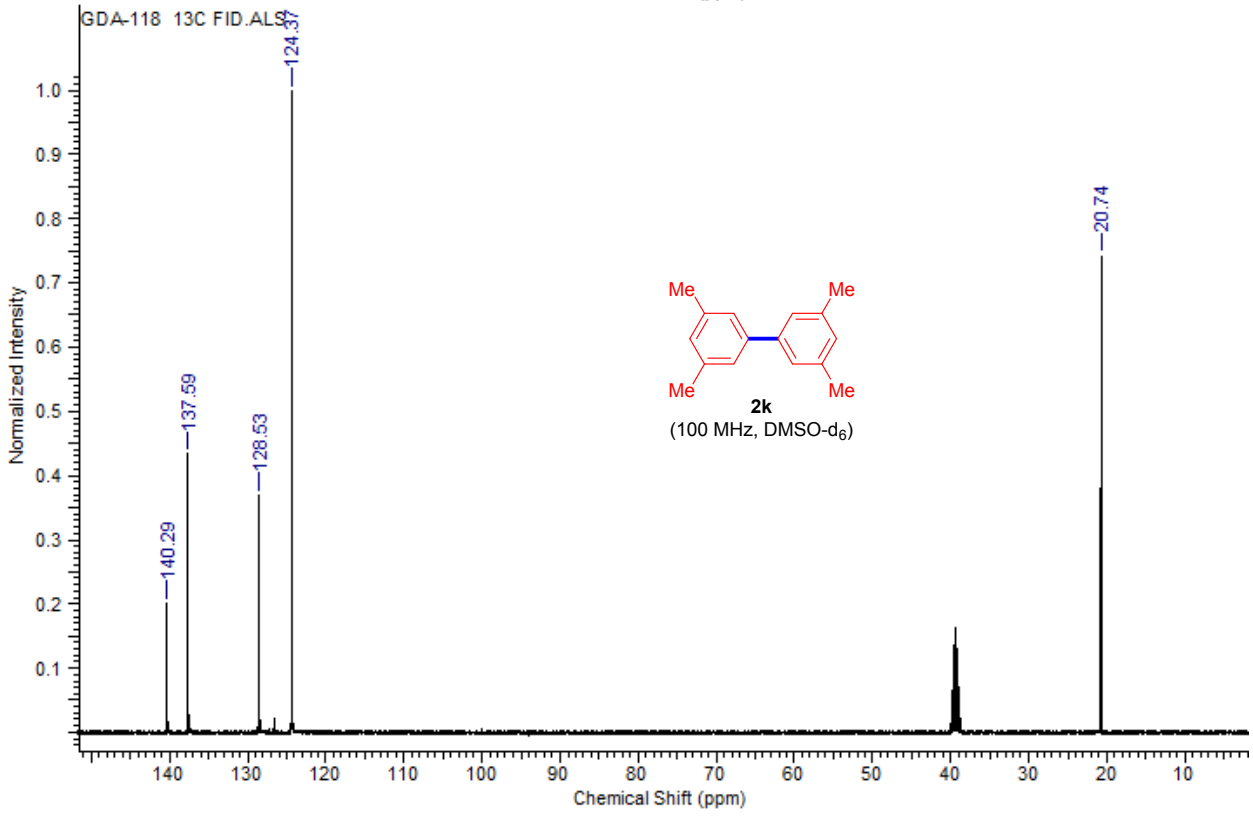
3,3'-Dimethylbiphenyl (2j)



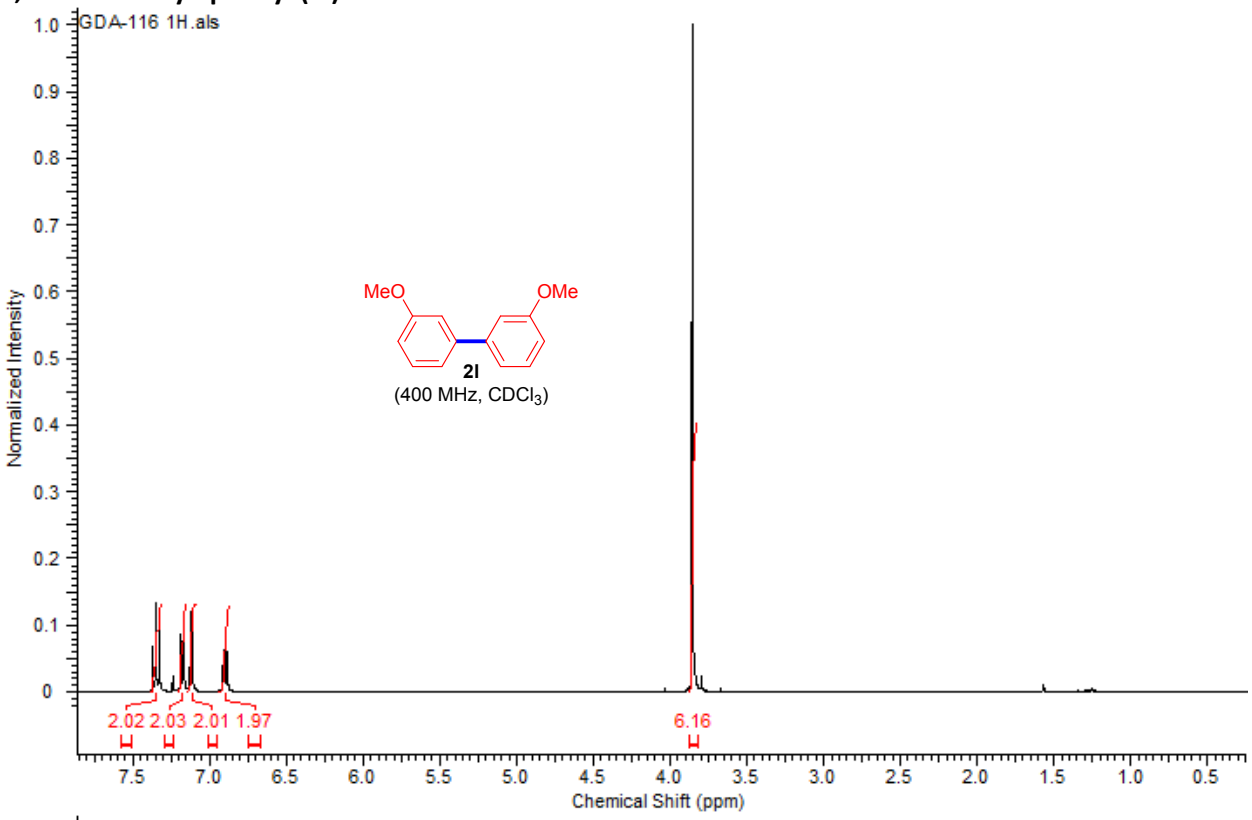


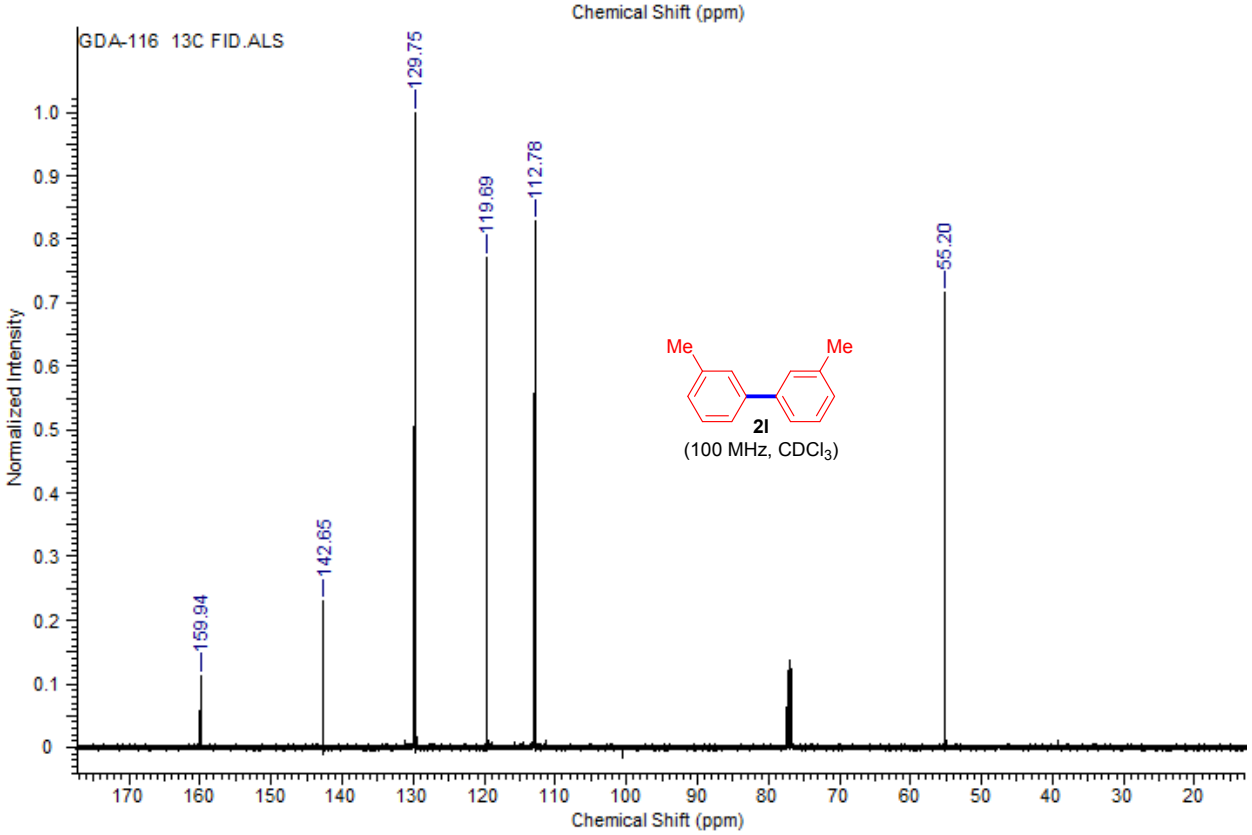
3,5,3’,5’-Tetramethylbiphenyl (2k)



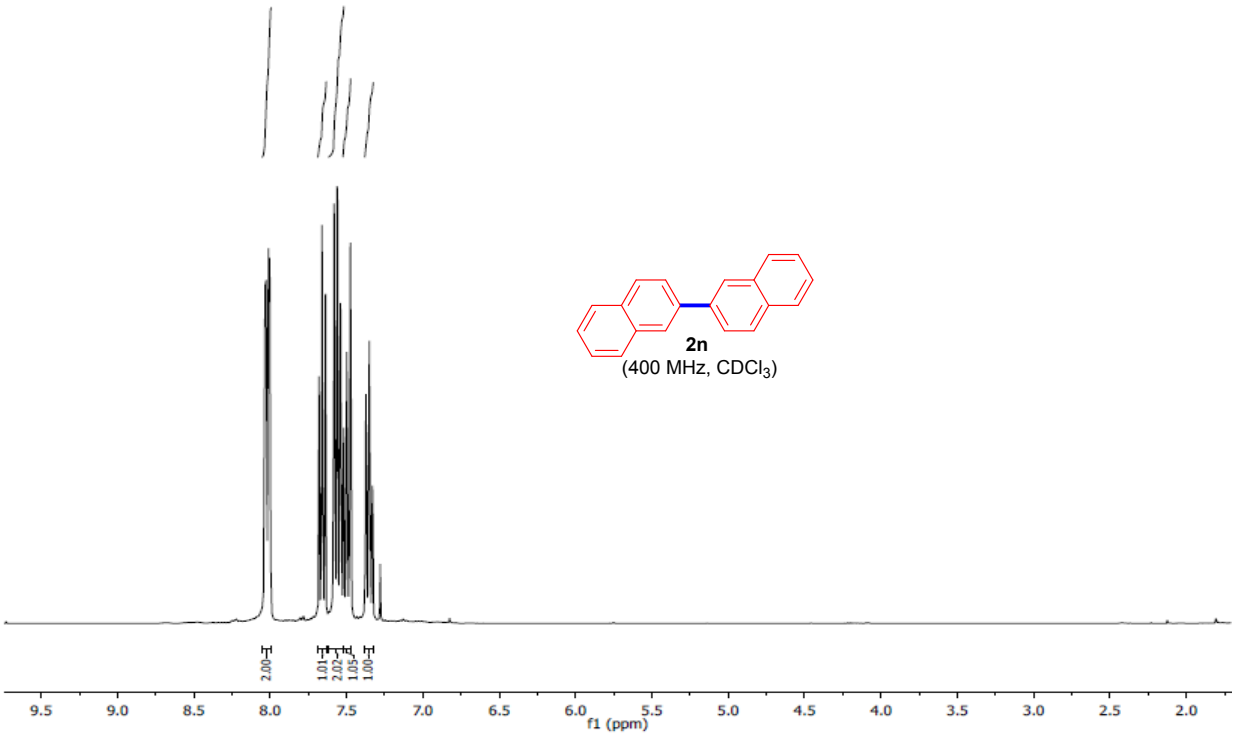


3,3'-Dimethoxybiphenyl (2l)

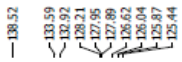


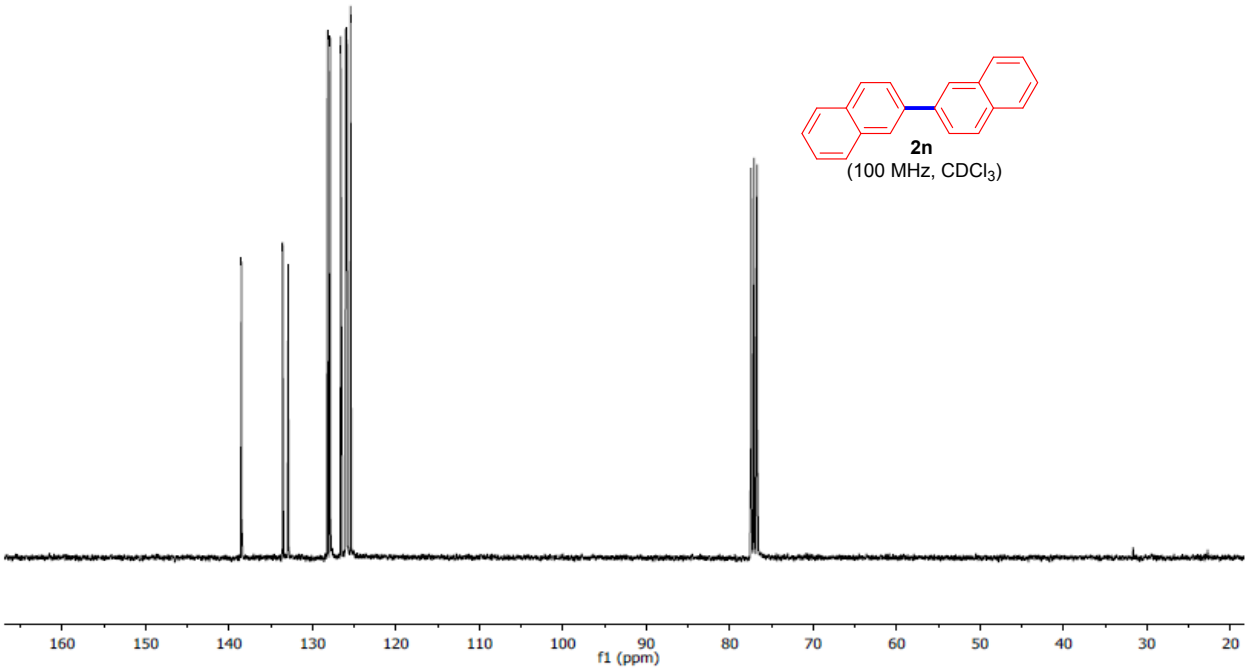


2,2’-Binaphthyl (2n)



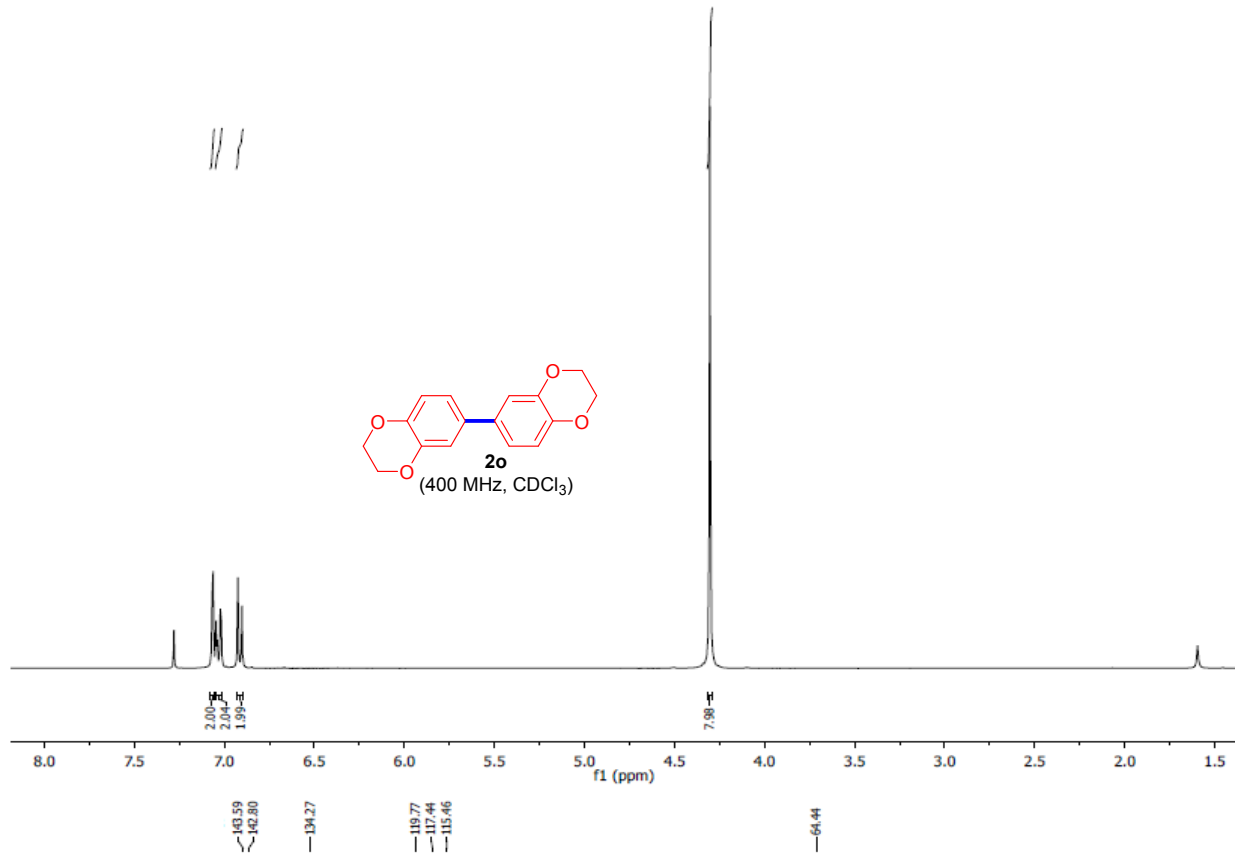
2n
(400 MHz, $CDCl_3$)

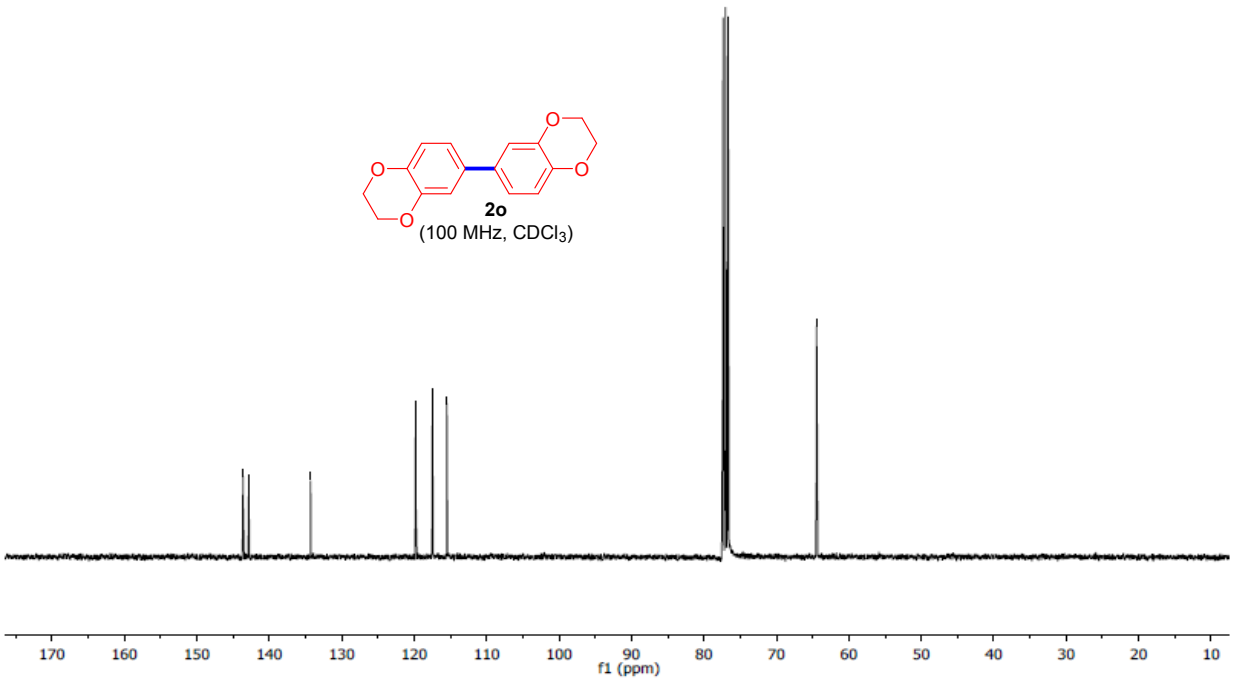




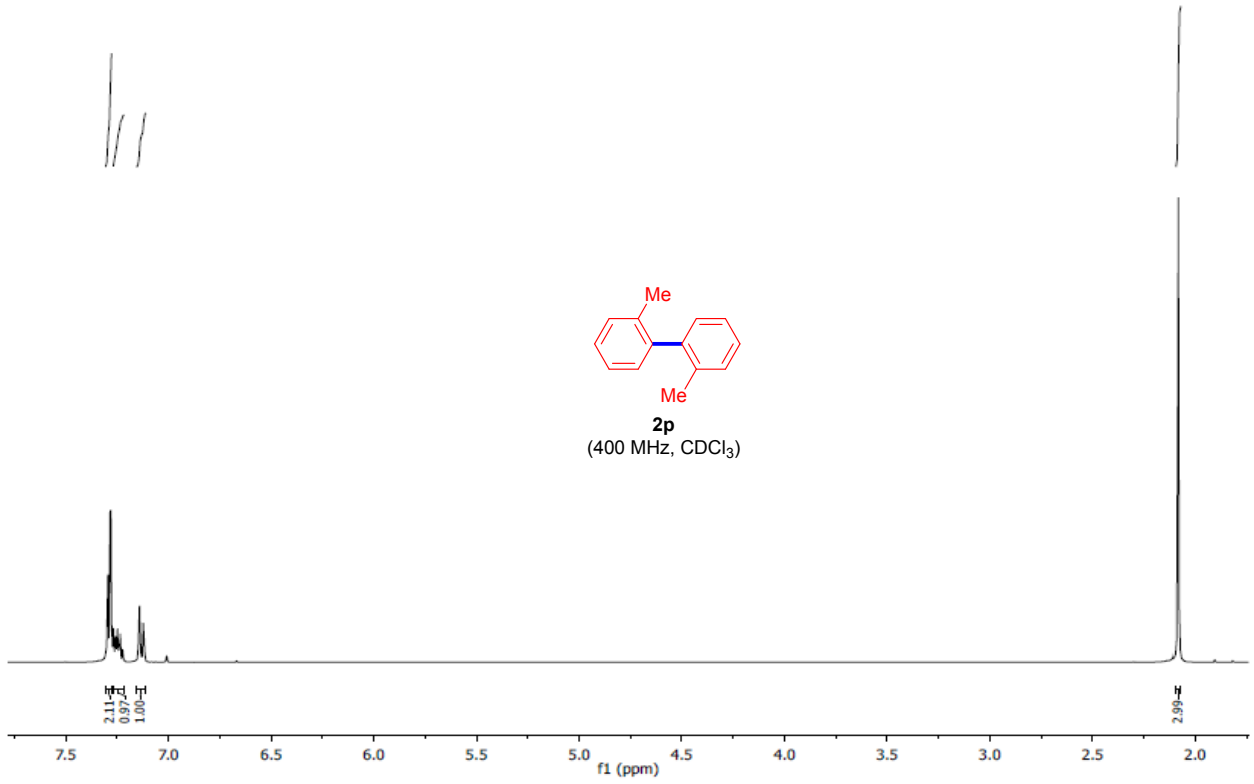
2n
(100 MHz, $CDCl_3$)

4,4'-Di-1,4-dioxolanebiphenyl (2o)

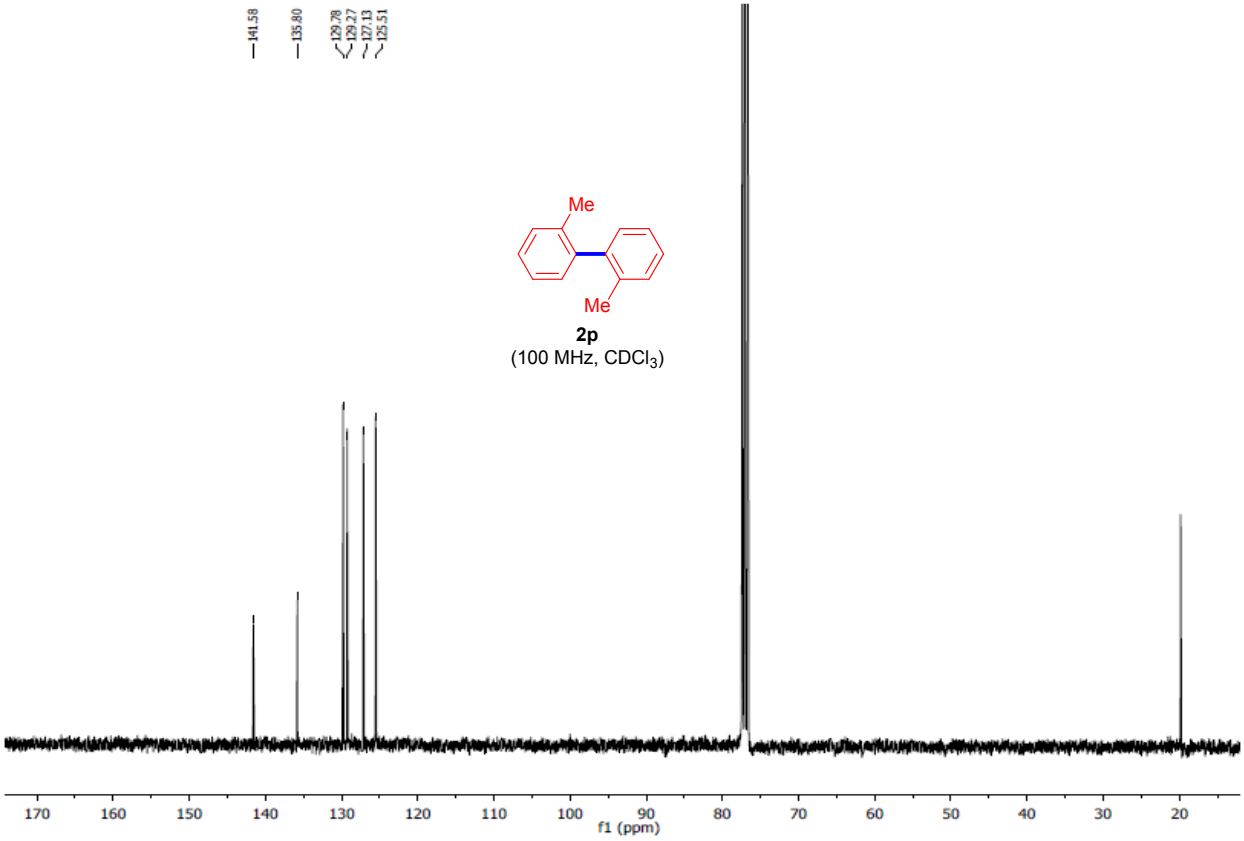




2,2'-Dimethylbiphenyl (2p)

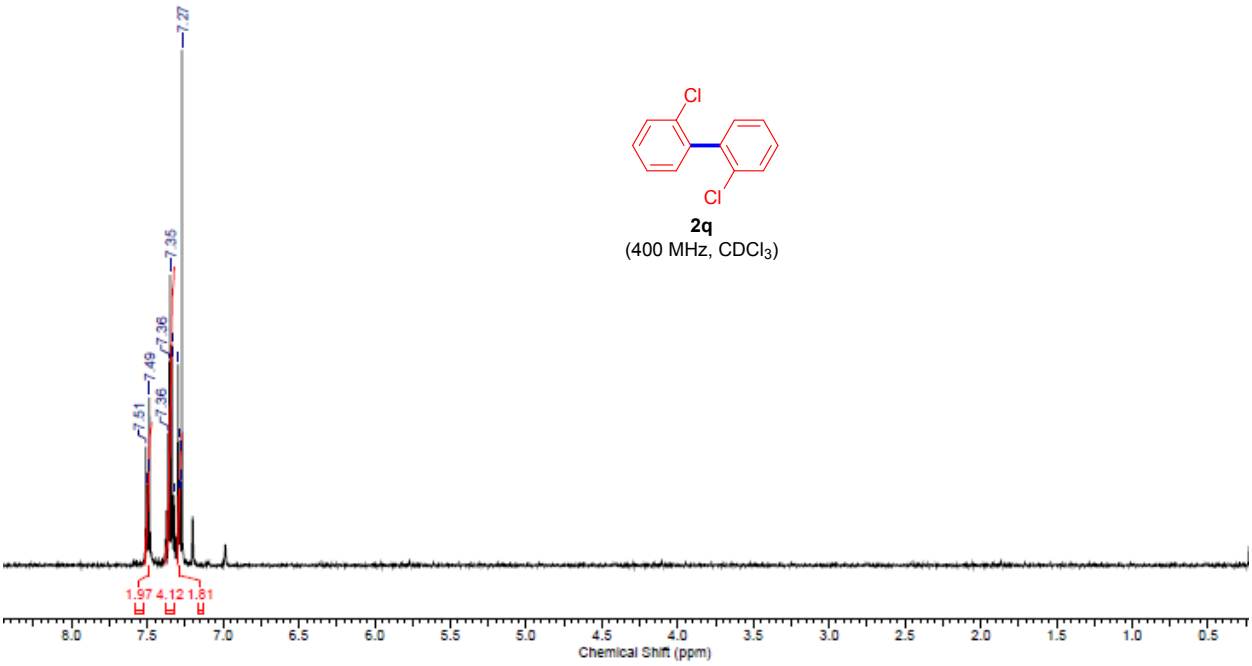


2p
(400 MHz, $CDCl_3$)



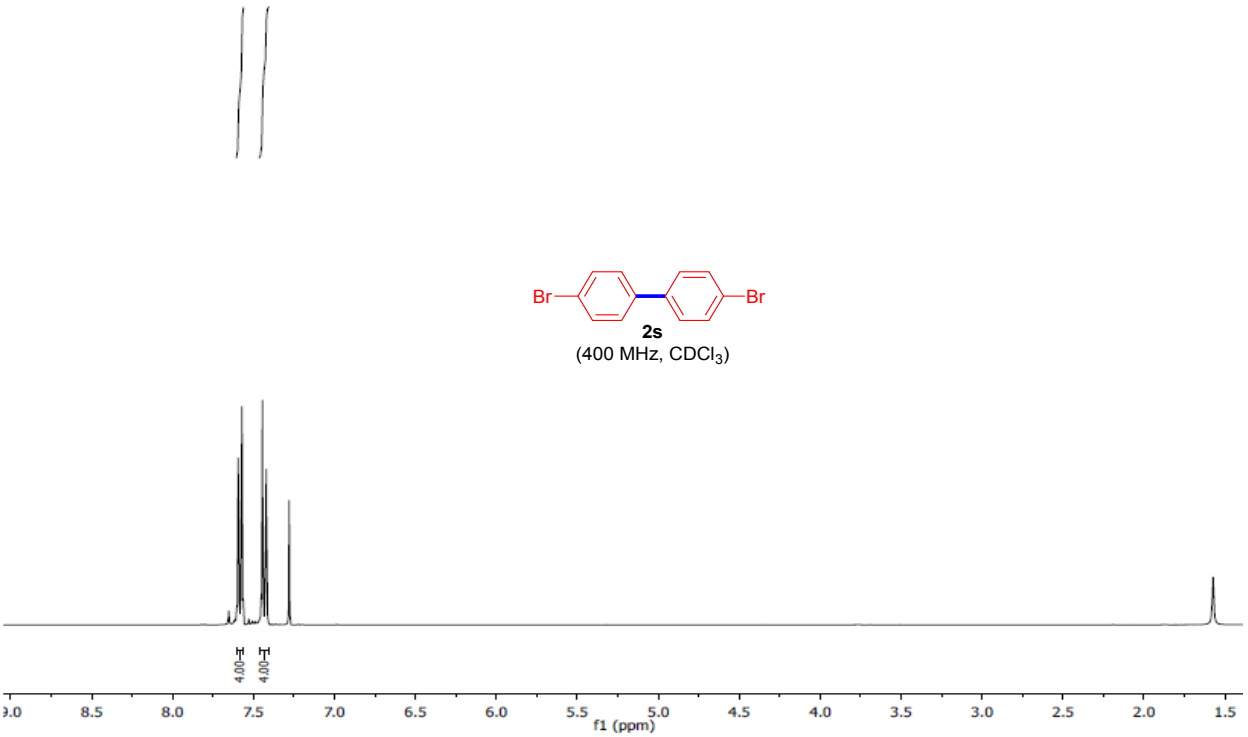
2p
(100 MHz, $CDCl_3$)

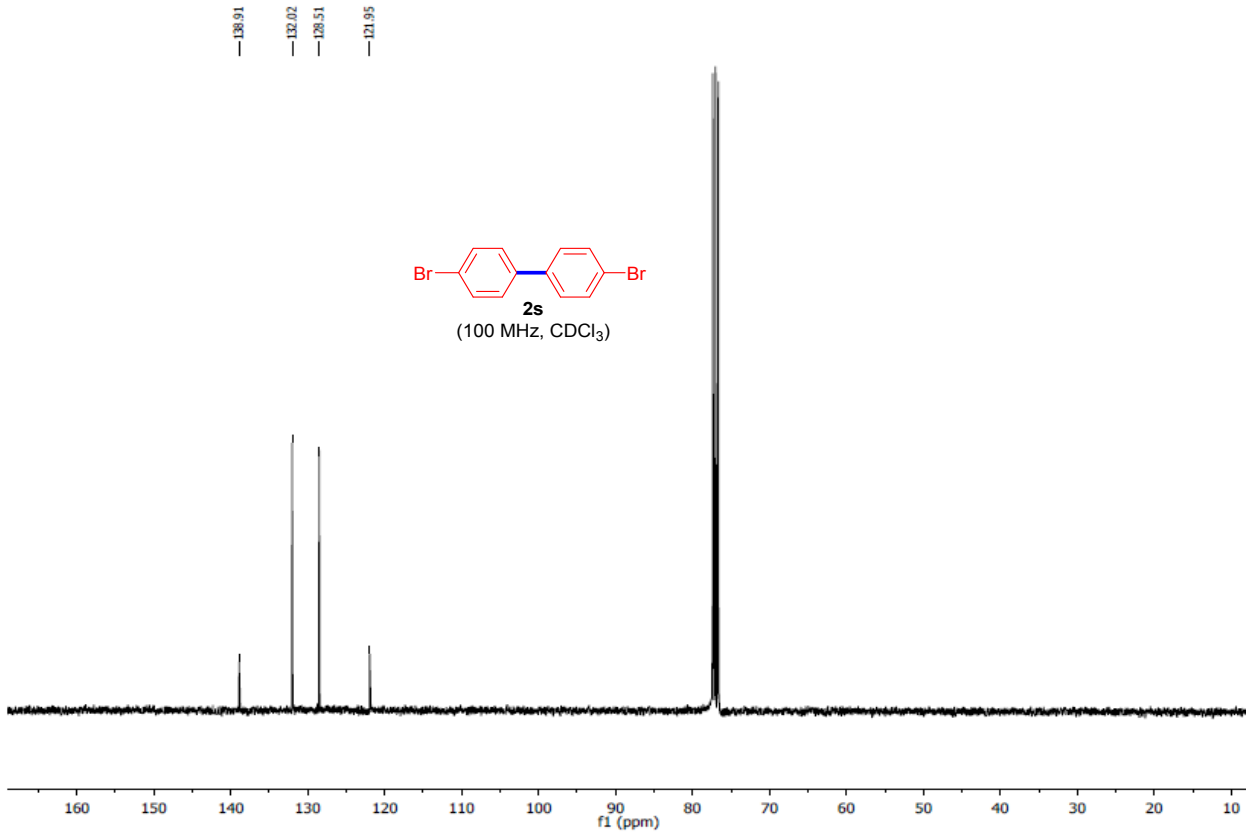
2,2'-Dichlorbiphenyl (2q)



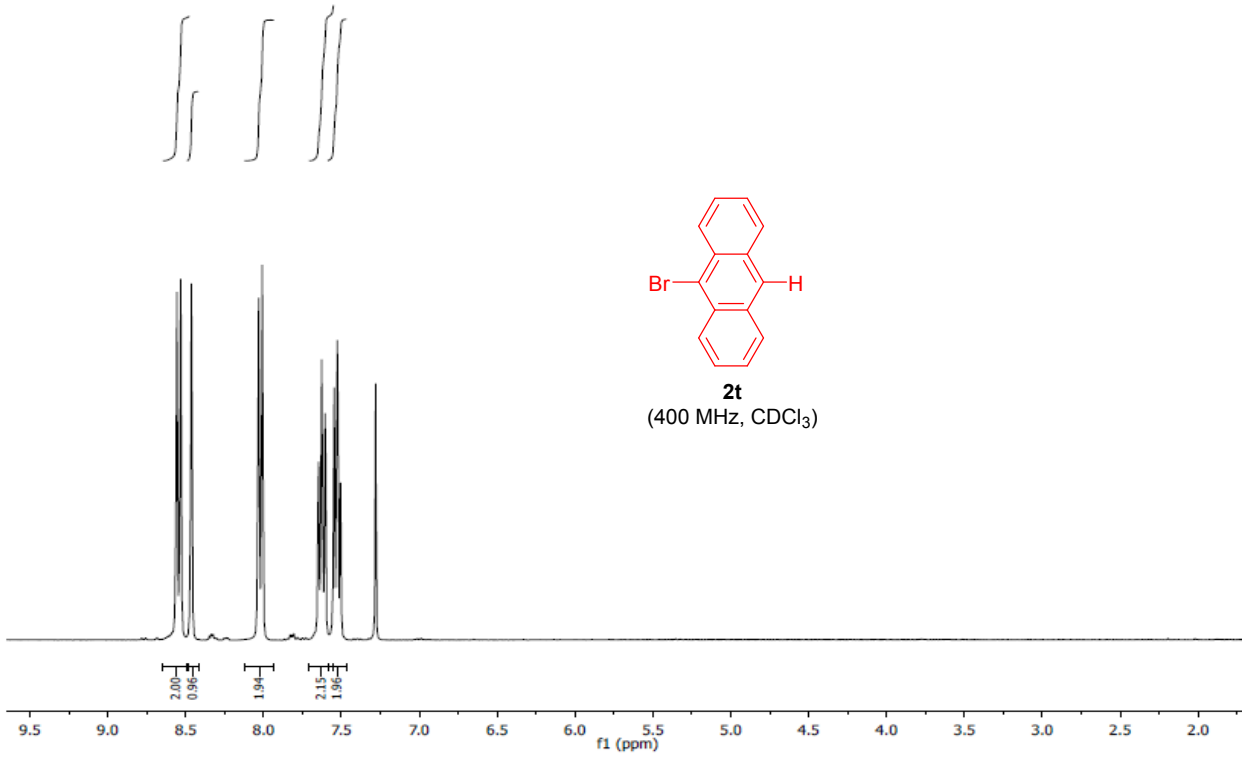
2q
(400 MHz, $CDCl_3$)

4,4'-Dibromobiphenyl (2s)

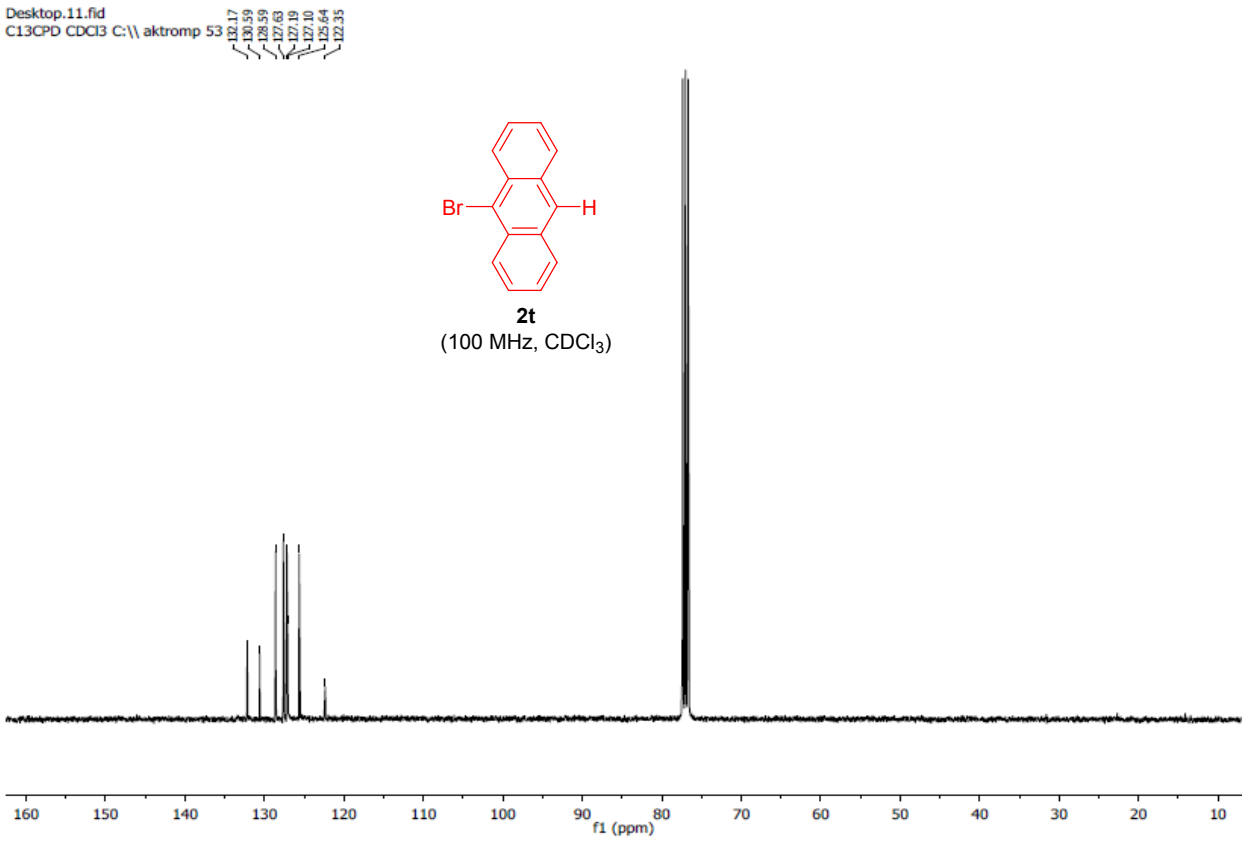




9-Bromoanthracene (2t)

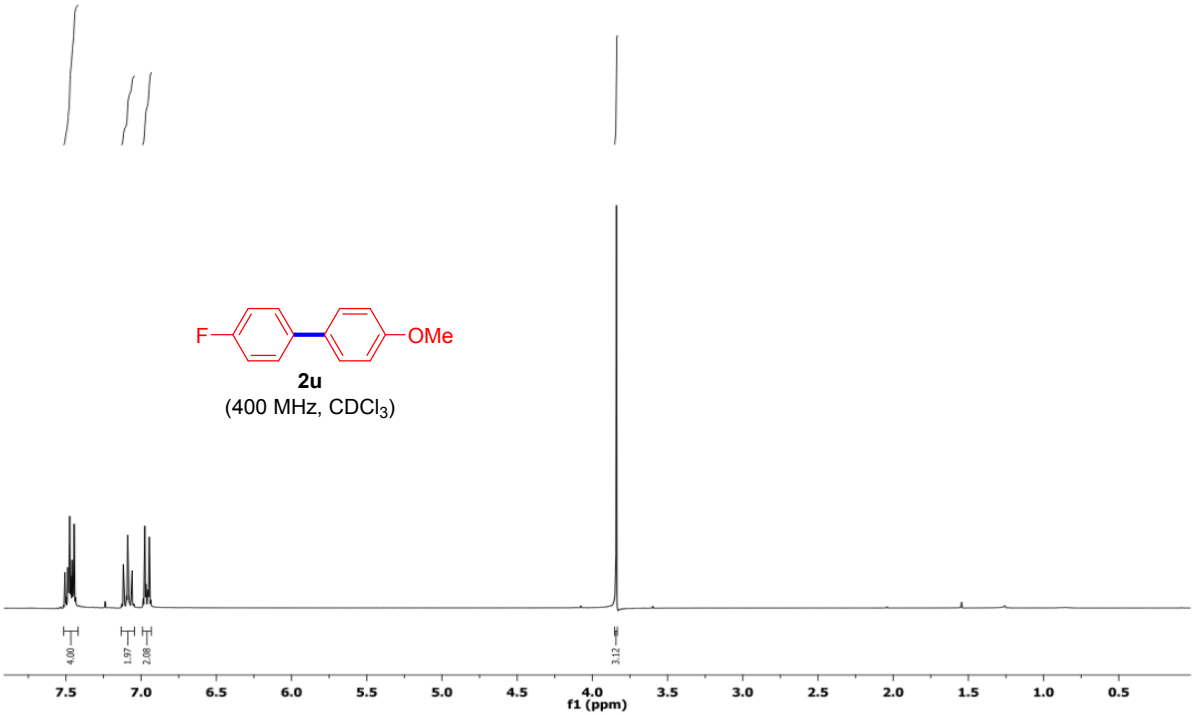


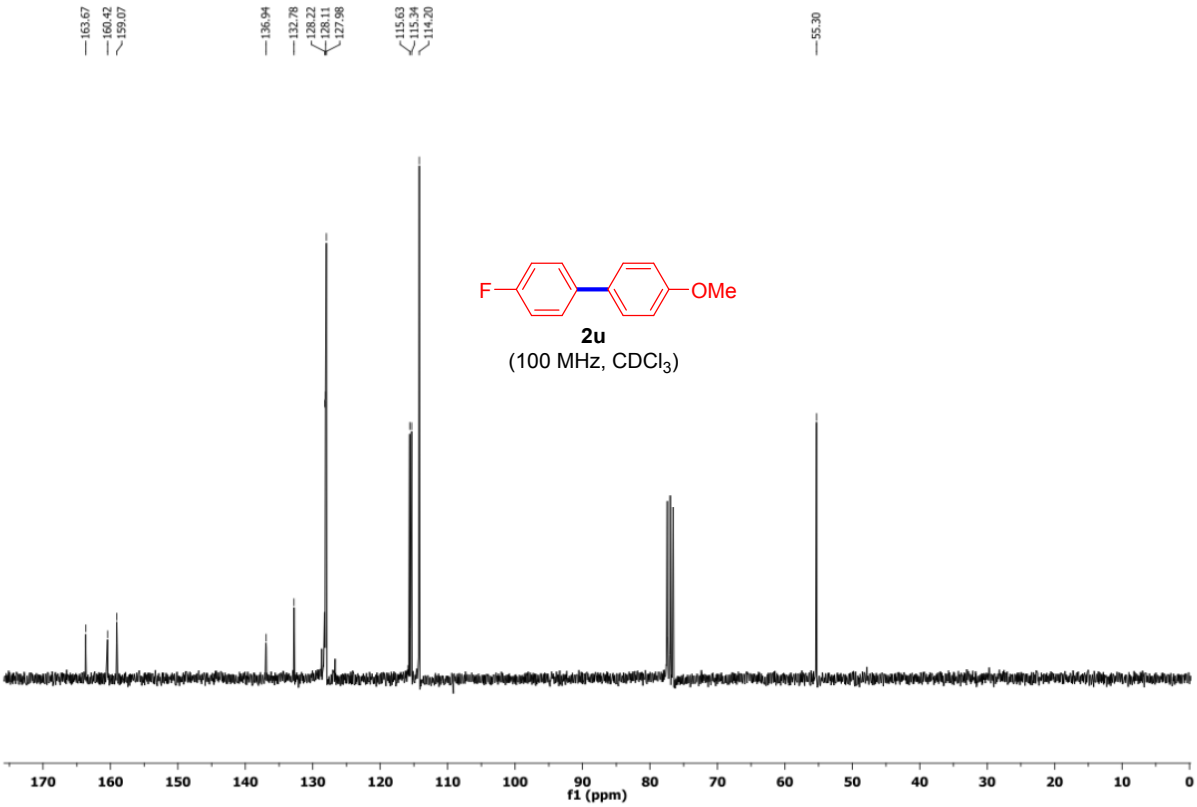
2t
(400 MHz, $CDCl_3$)

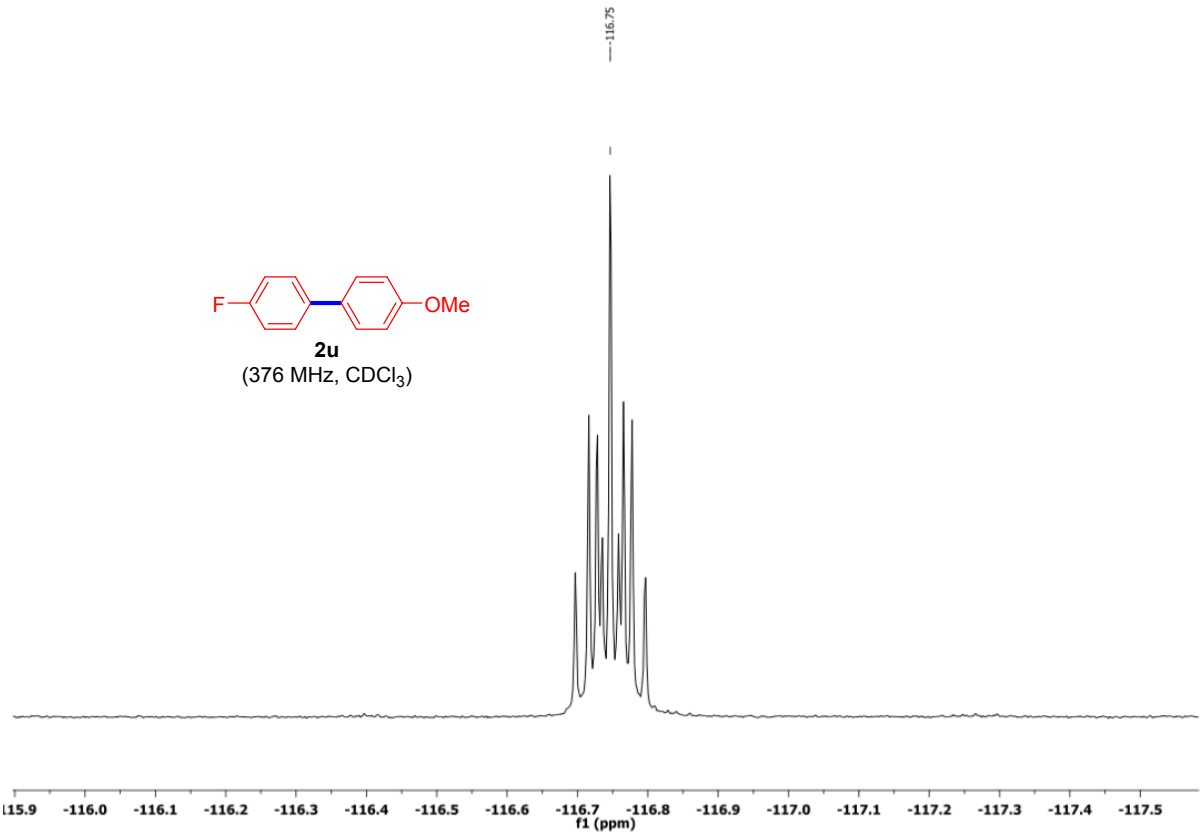


2t
(100 MHz, $CDCl_3$)

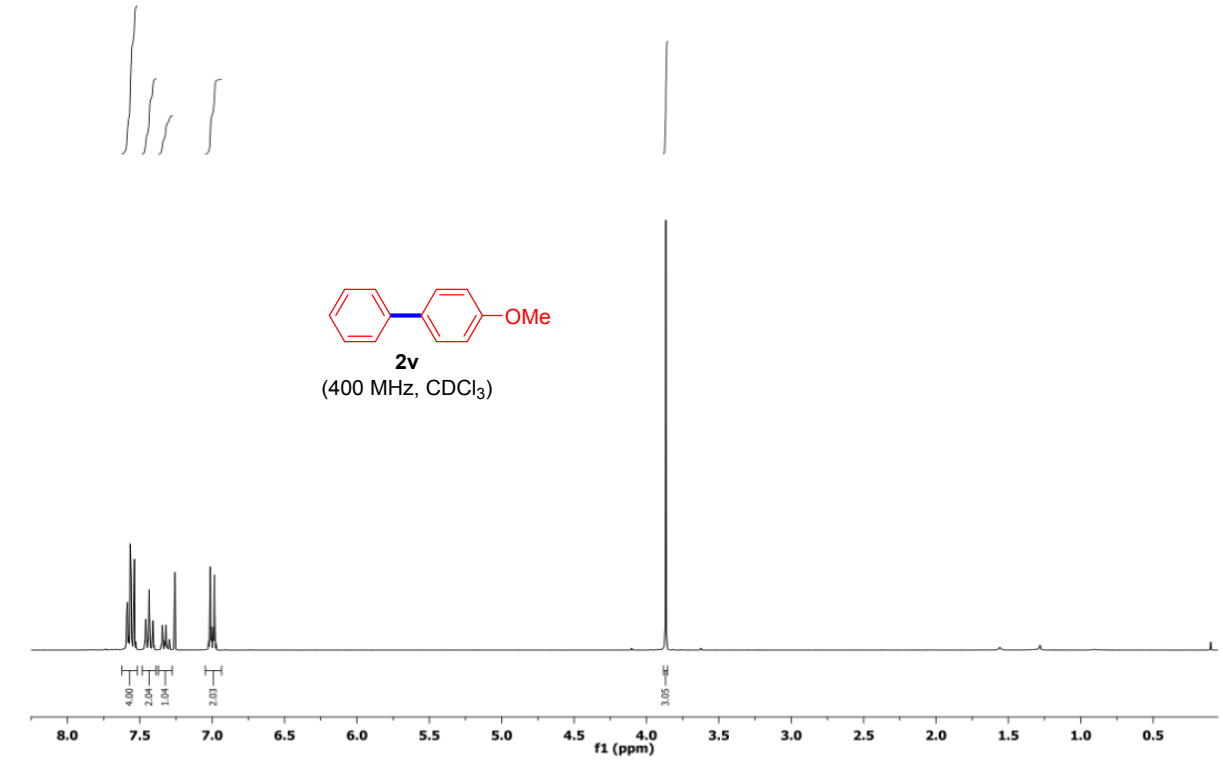
4-Fluoro-4'-methoxybiphenyl (2u)

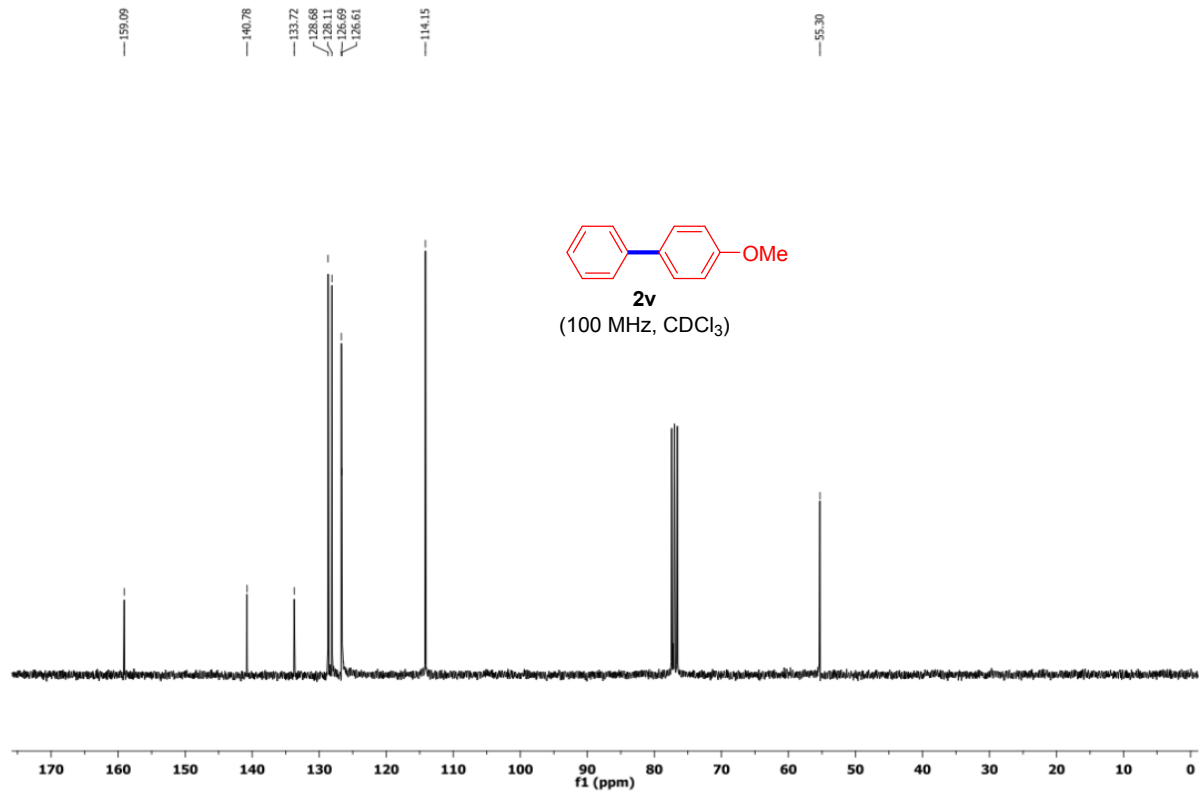




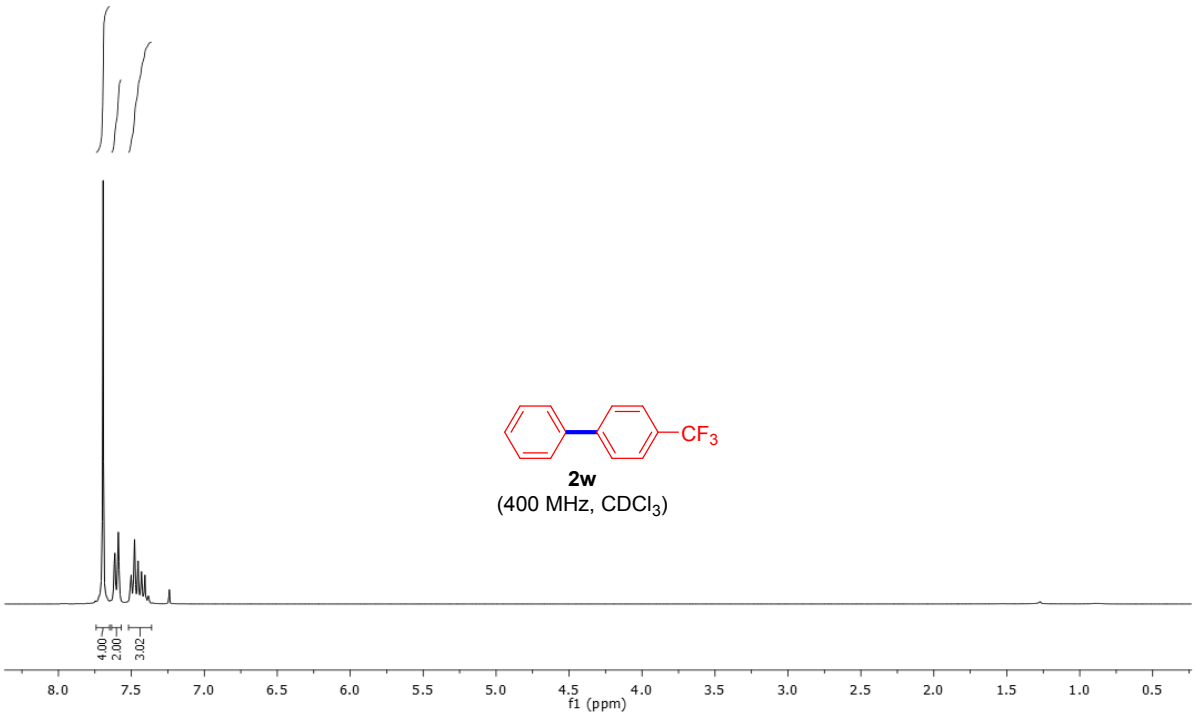

F
OMe
2u
(376 MHz, CDCl3)
-116.75
-115.9
-116.0
-116.1
-116.2
-116.3
-116.4
-116.5
-116.6
-116.7
-116.8
-116.9
-117.0
-117.1
-117.2
-117.3
-117.4
-117.5
f1 (ppm)

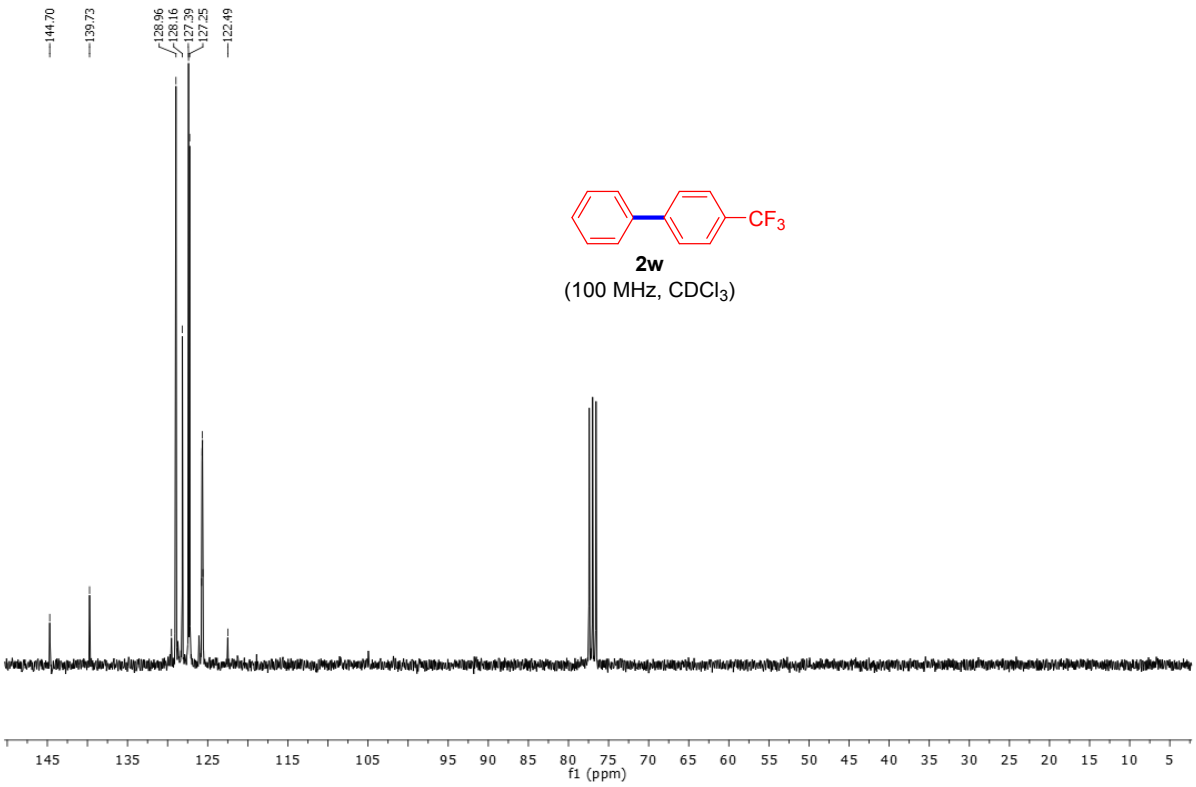
4-Methoxybiphenyl (2v)

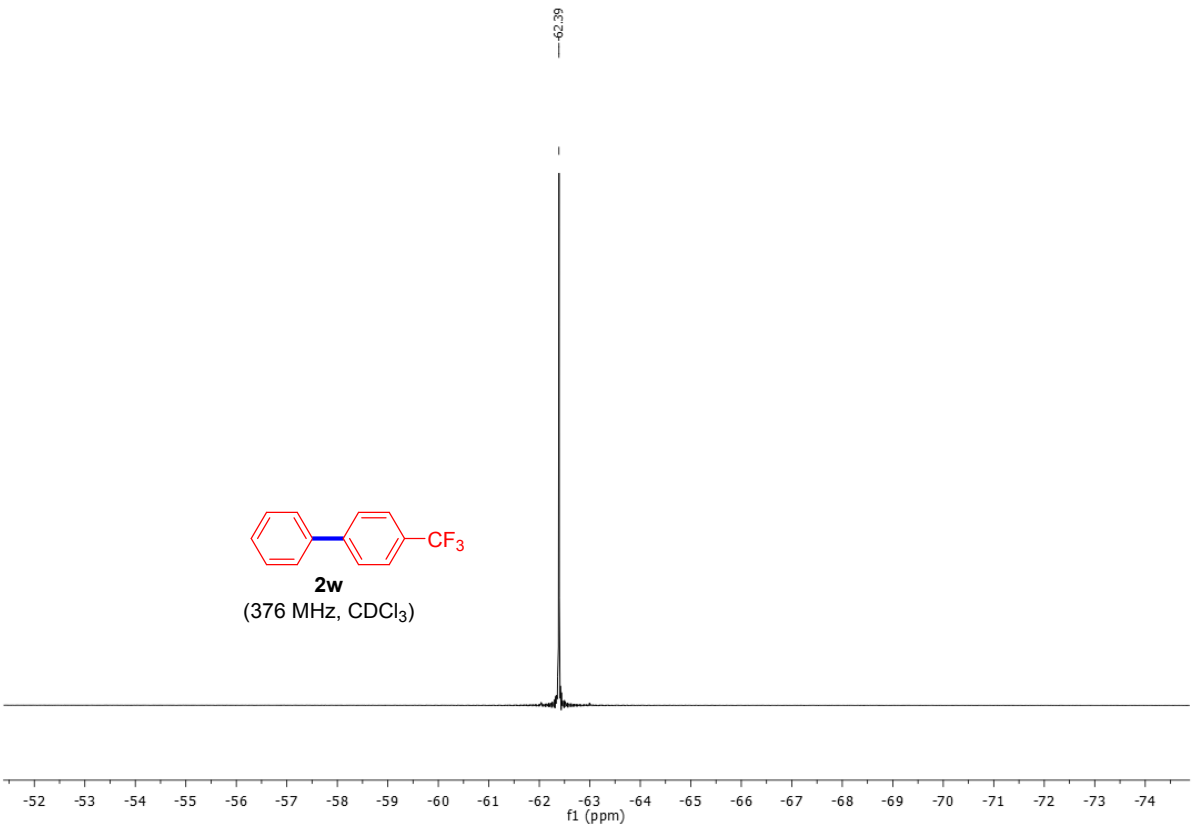




4-Trifluoromethylbiphenyl (2w)






-62.39
CF3
2w
(376 MHz, CDCl3)
-52 -53 -54 -55 -56 -57 -58 -59 -60 -61 -62 -63 -64 -65 -66 -67 -68 -69 -70 -71 -72 -73 -74
f1 (ppm)