

Supplementary Material

Synthesis of novel pyridine and pyrimidine derivatives as potential inhibitors of HIV-1 reverse transcriptase using palladium-catalysed C-N cross-coupling and nucleophilic aromatic substitution reactions

Charles R. K. Changunda,^a Amanda L. Rousseau,^a Adriaan E. Basson,^b and Moira L. Bode^{a*}

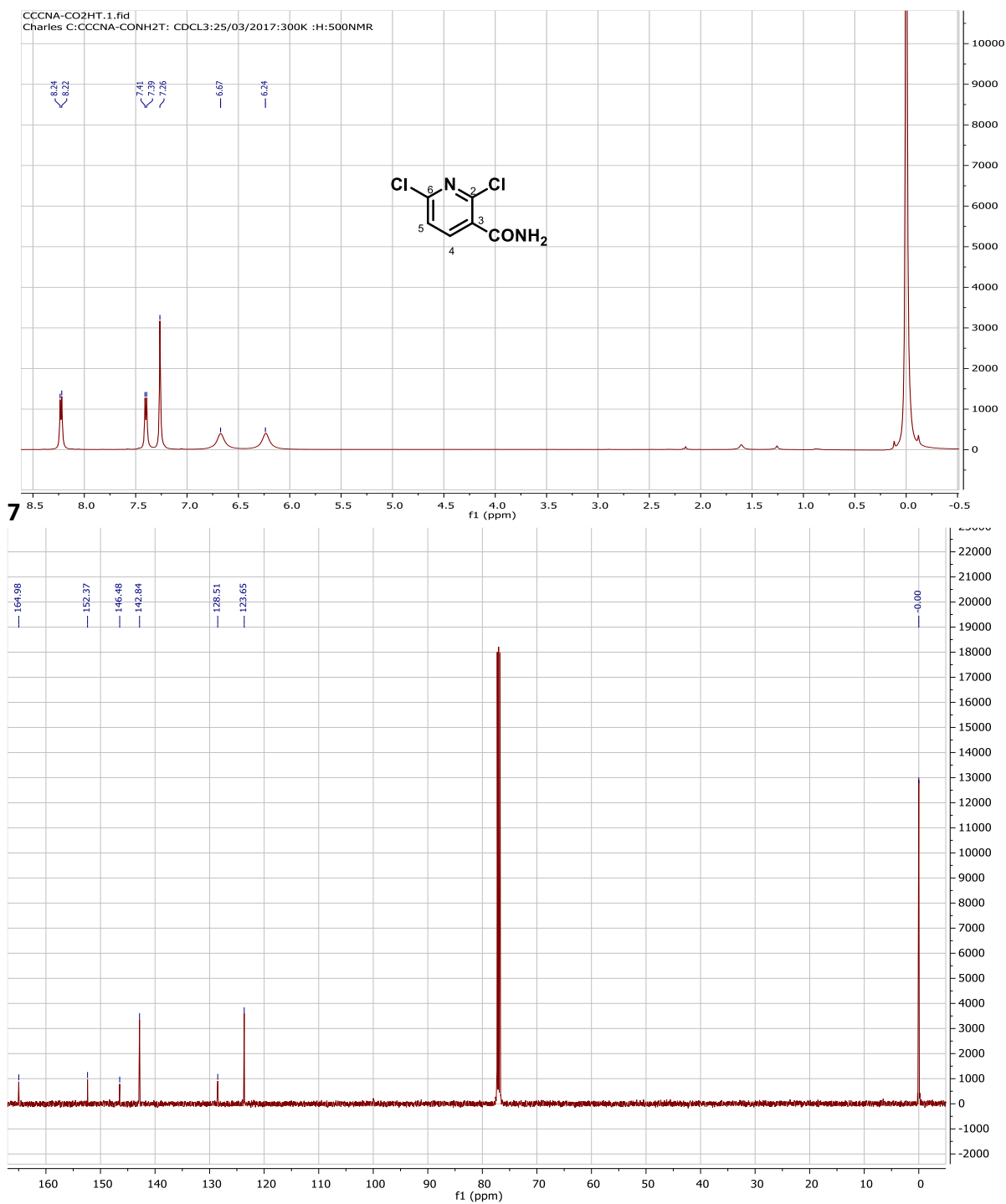
^a *Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Private Bag 3, PO WITS, 2050, South Africa*

^b *School of Pathology, Department of Molecular Medicine and Haematology, Faculty of Health Sciences, University of the Witwatersrand, Medical School, Parktown, JHB, Private Bag 3, WITS 2050, South Africa*

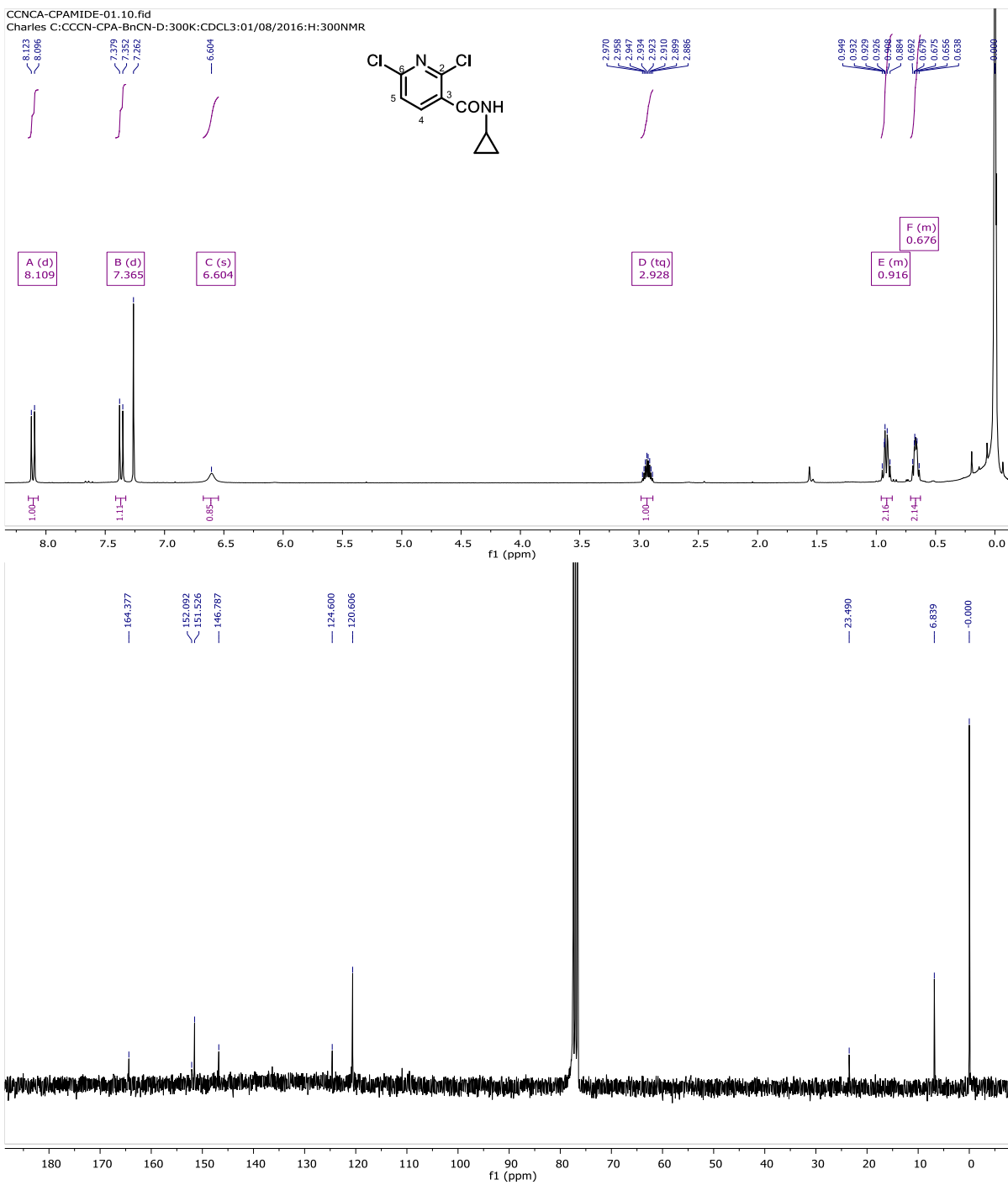
Email: moira.bode@wits.ac.za

Table of Contents

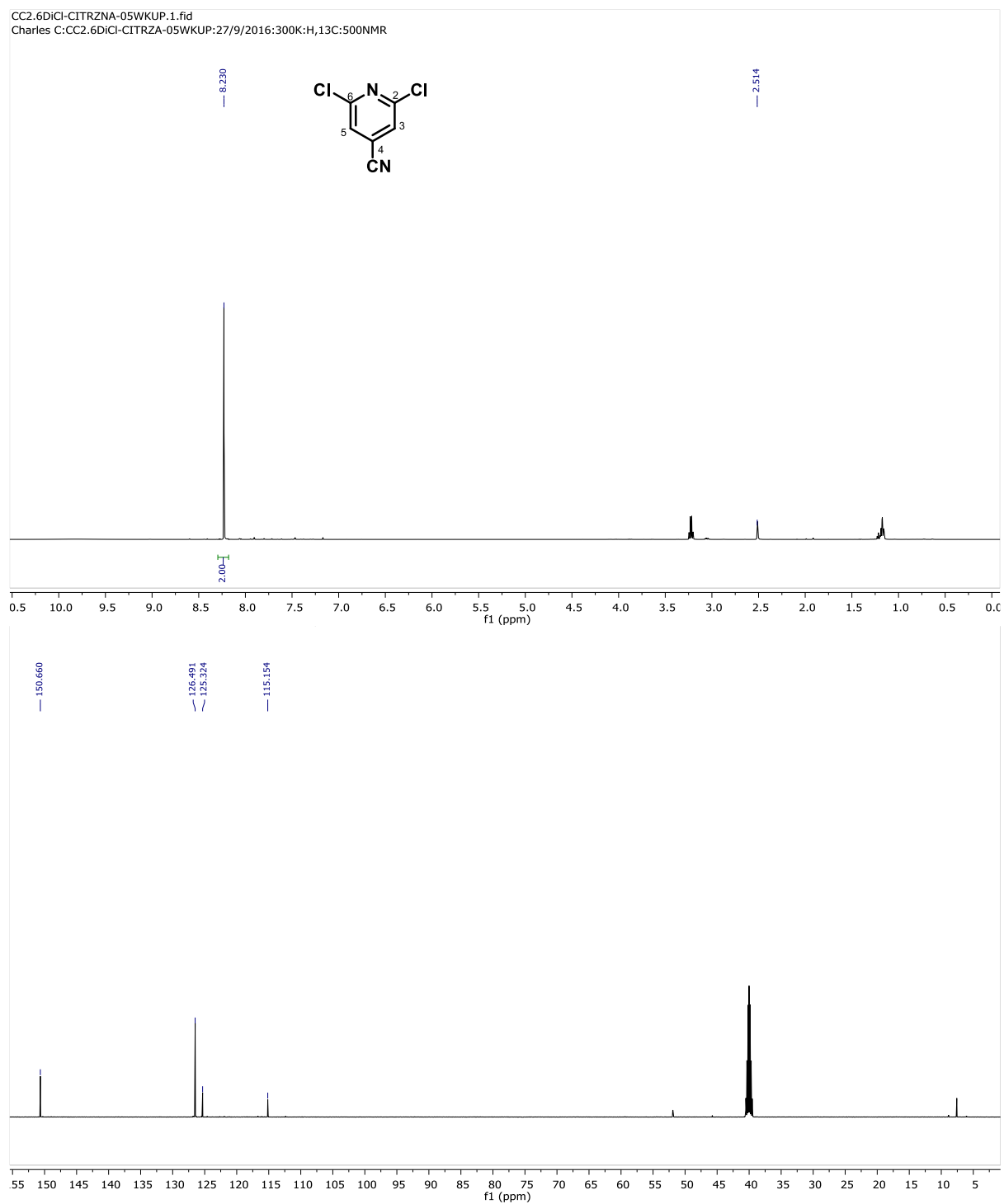
1. NMR spectra of compounds 7 , 10 , 14 , 16 and 19	S2
2. NMR spectra of compounds 3a , 3c , 3d and 3e	S7
3. NMR spectra of compounds 4a , 4c and 4d	S11
4. NMR spectra of compounds 5a-5k	S14

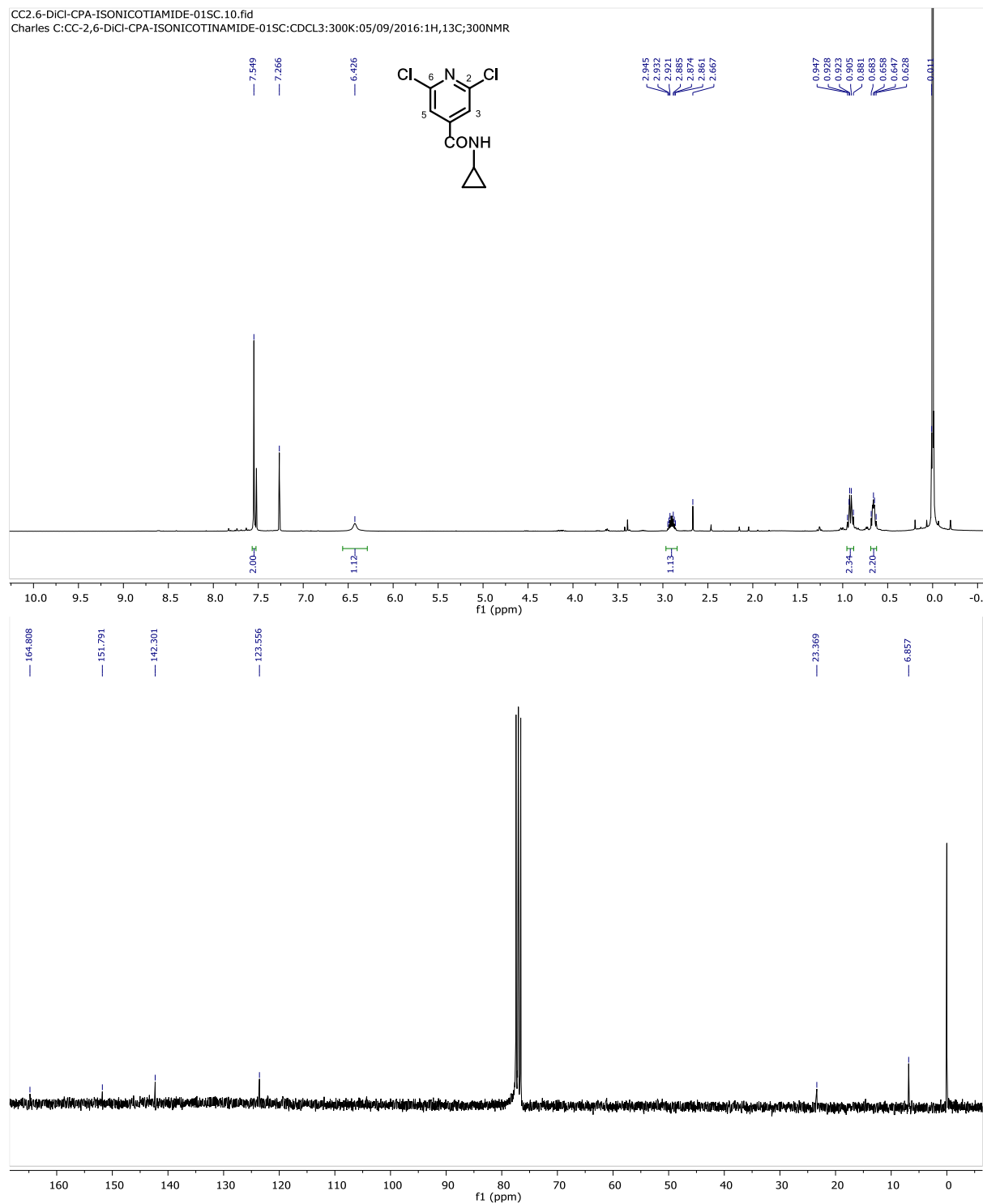


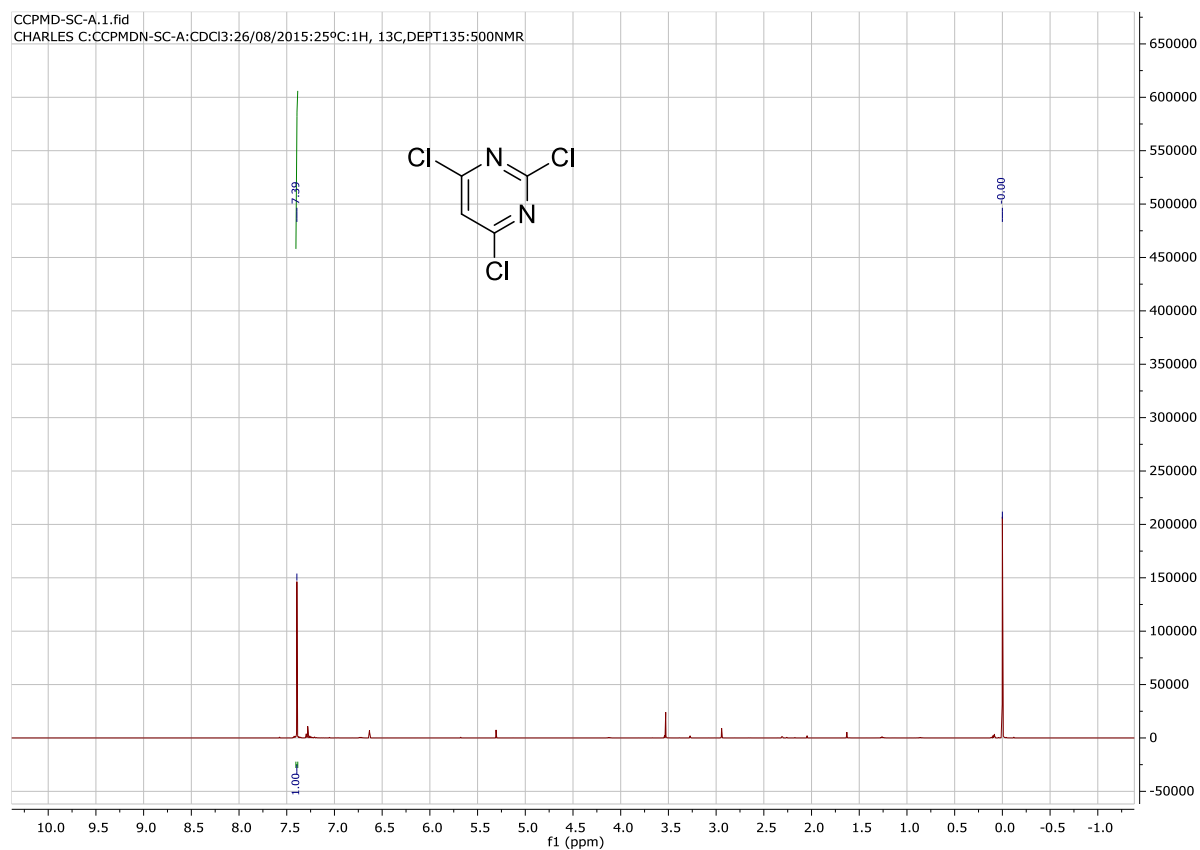
10



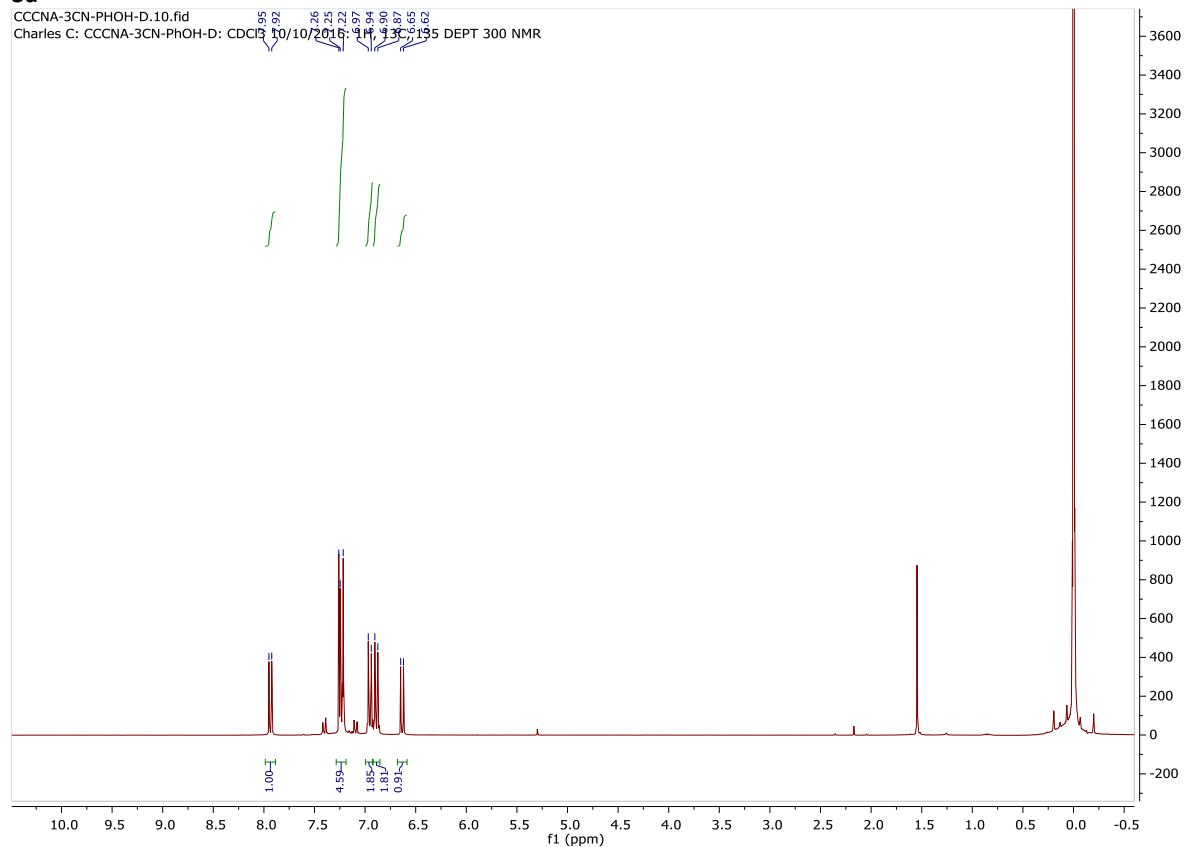
14



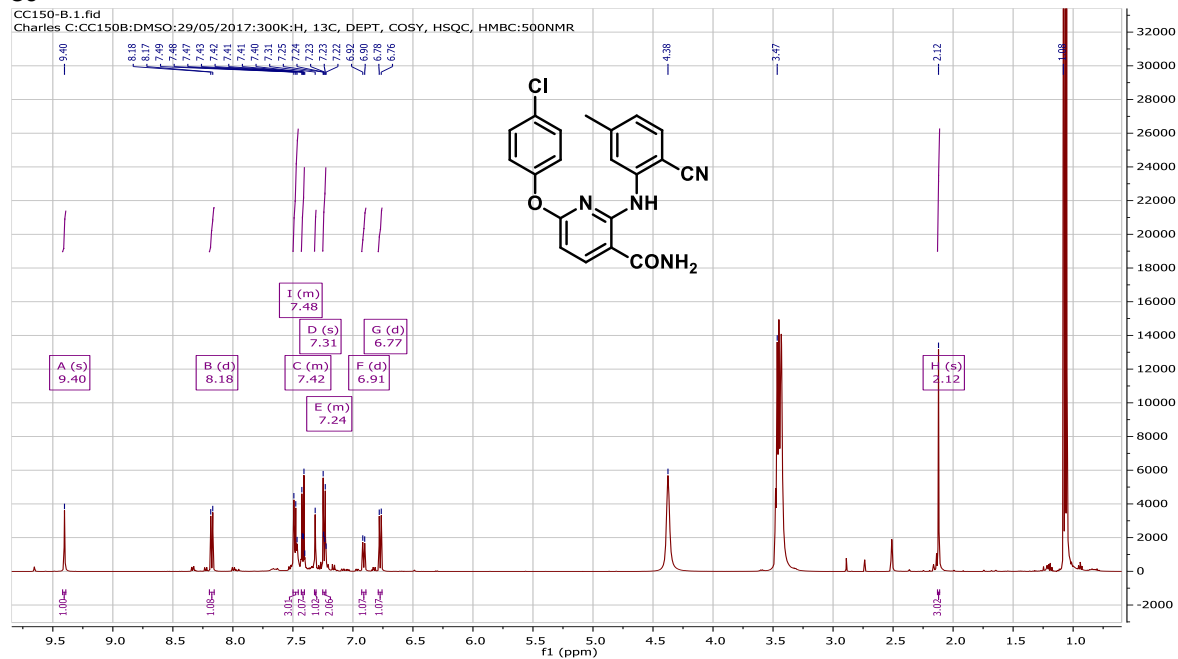


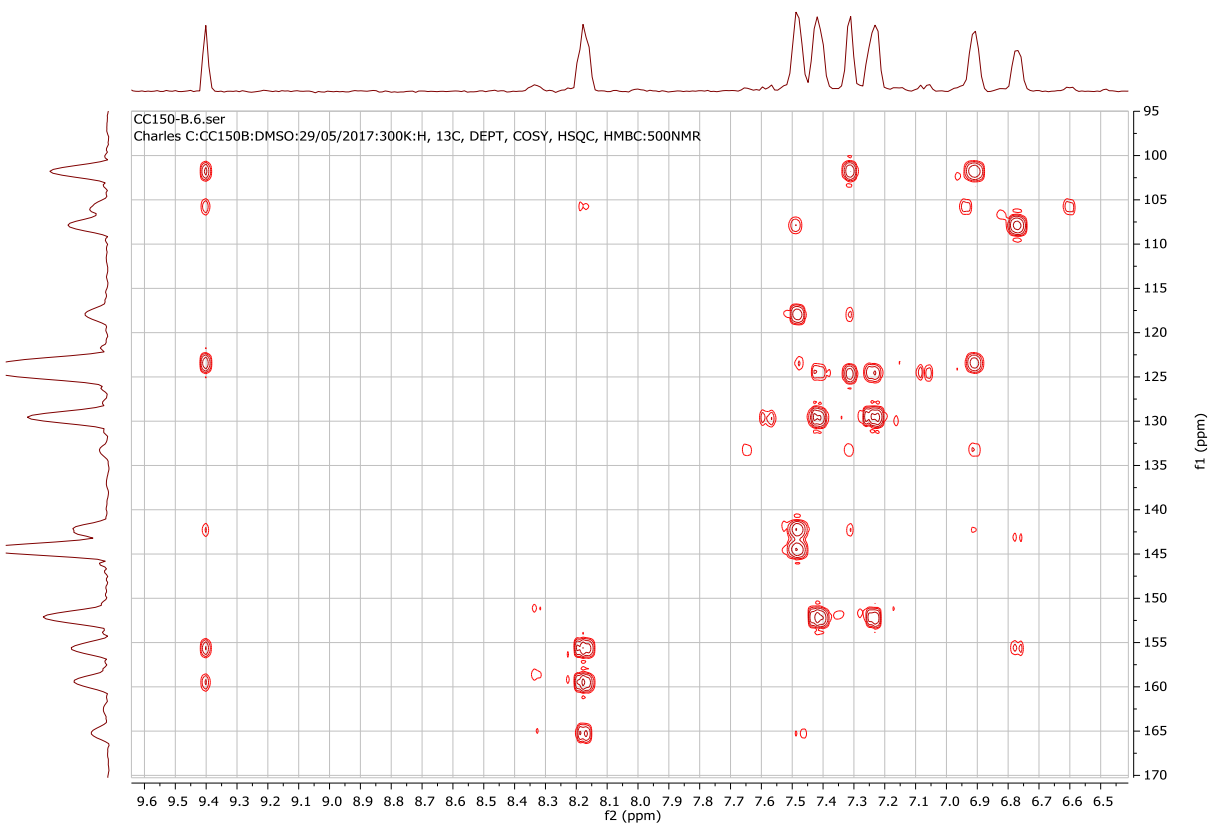
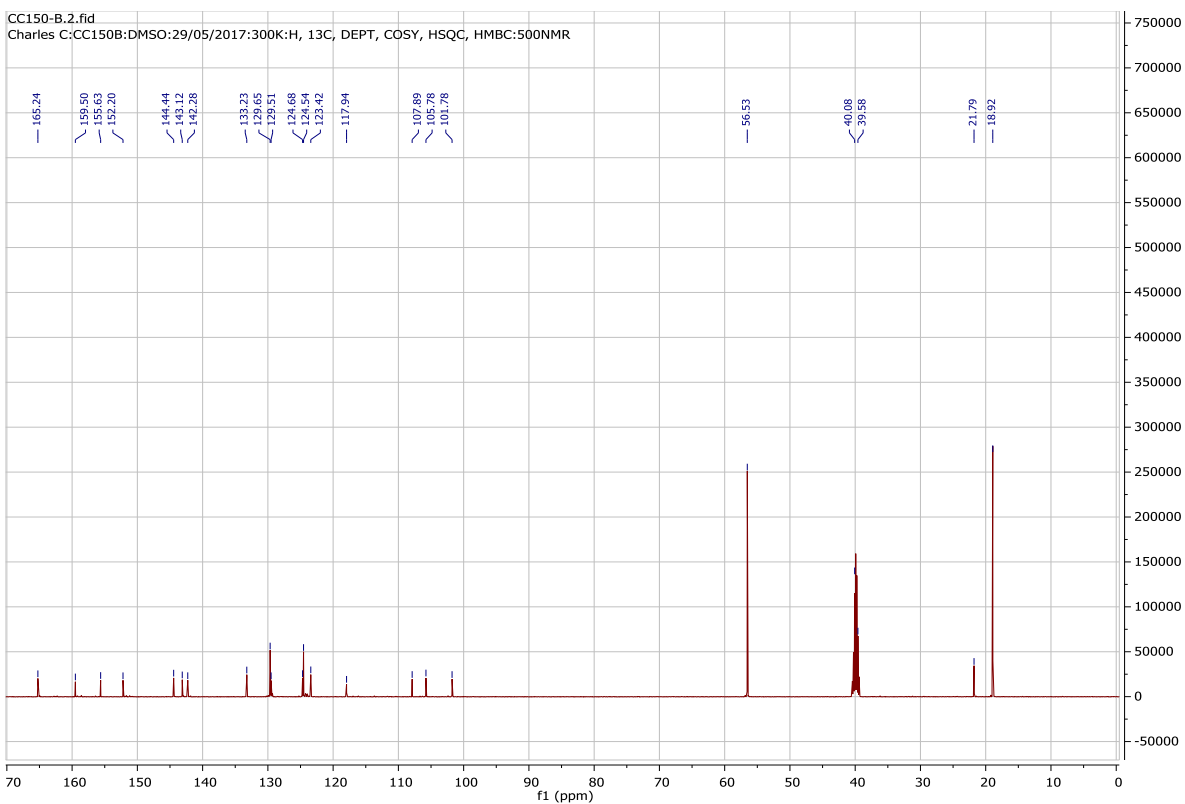


3a



3c



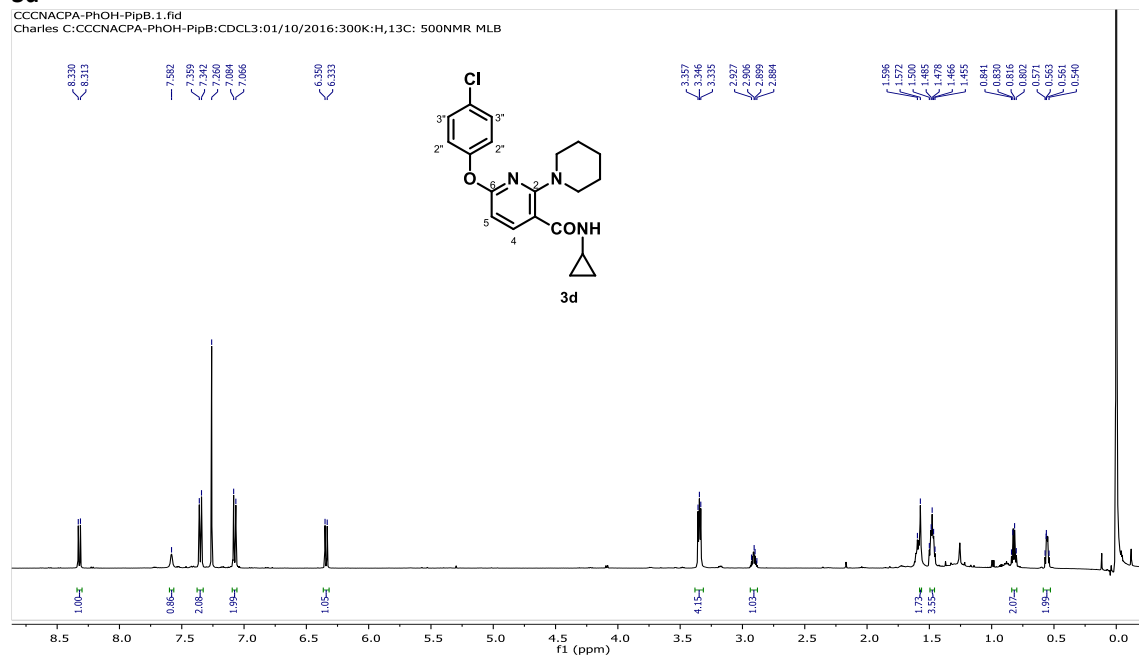


HMBC spectrum of 3c

3d

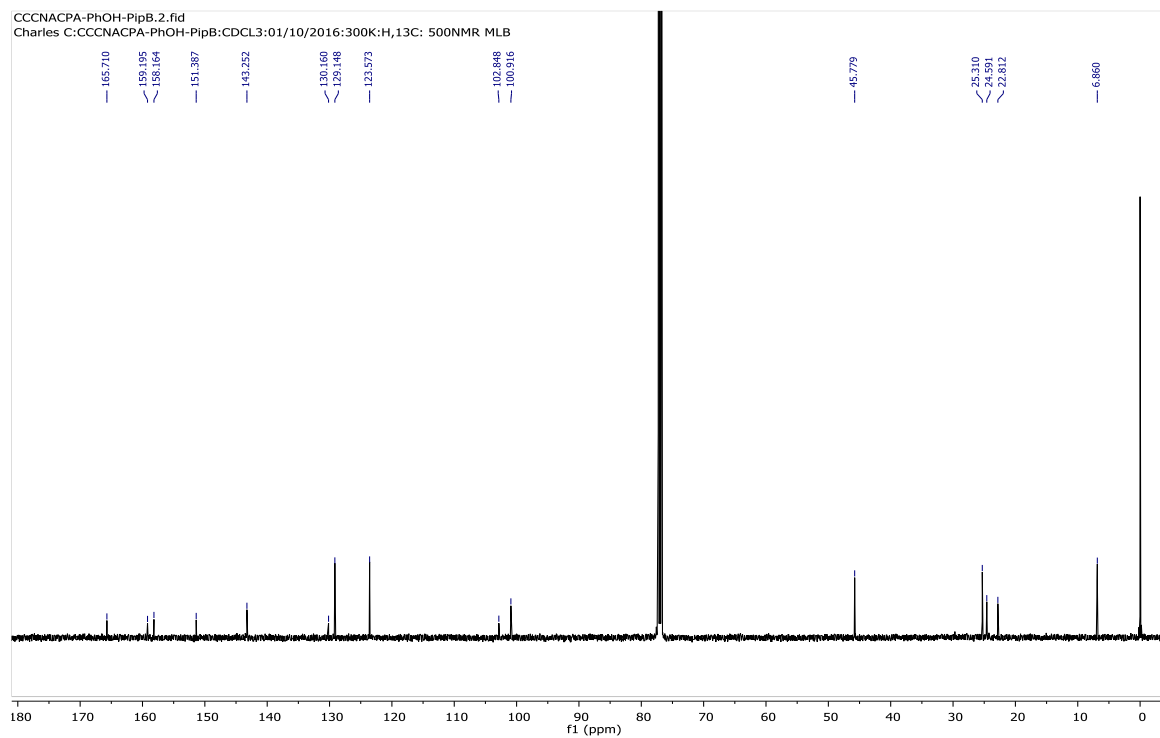
CCCNACPA-PhOH-PipB.1.fid

Charles C:CCCNACPA-PhOH-PipB:CDCL3:01/10/2016:300K:H,13C: 500NMR MLB



CCCNACPA-PhOH-PipB.2.fid

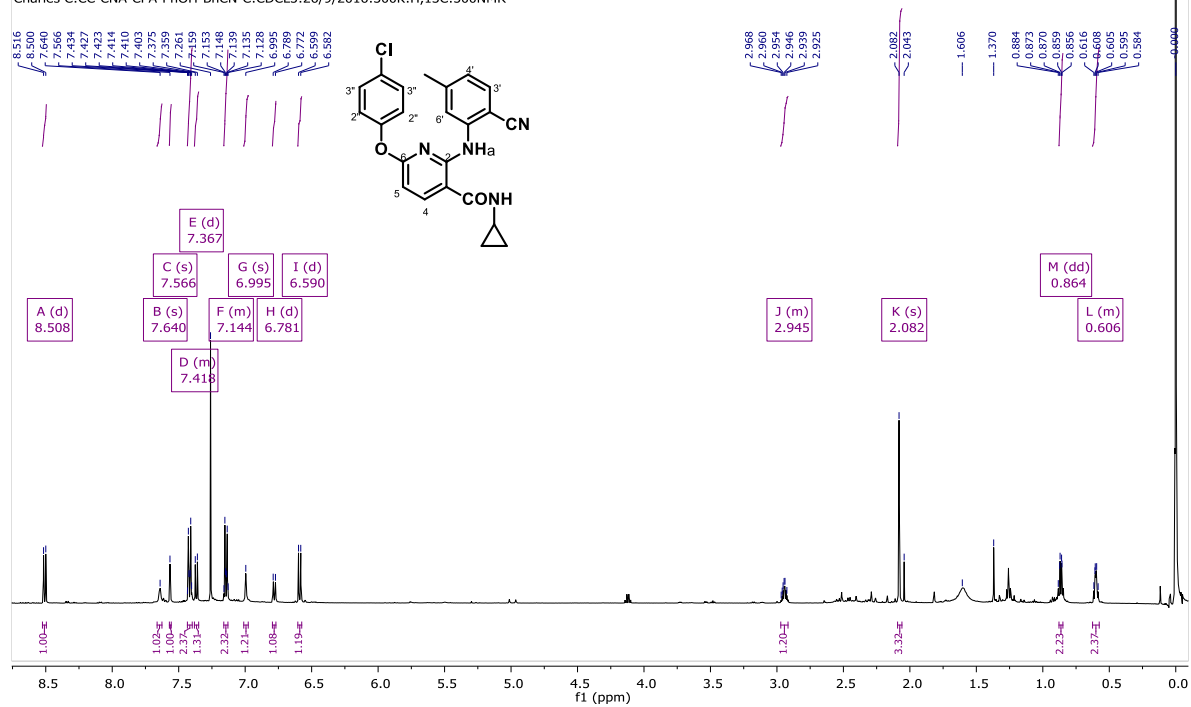
Charles C:CCCNACPA-PhOH-PipB:CDCL3:01/10/2016:300K:H,13C: 500NMR MLB



3e

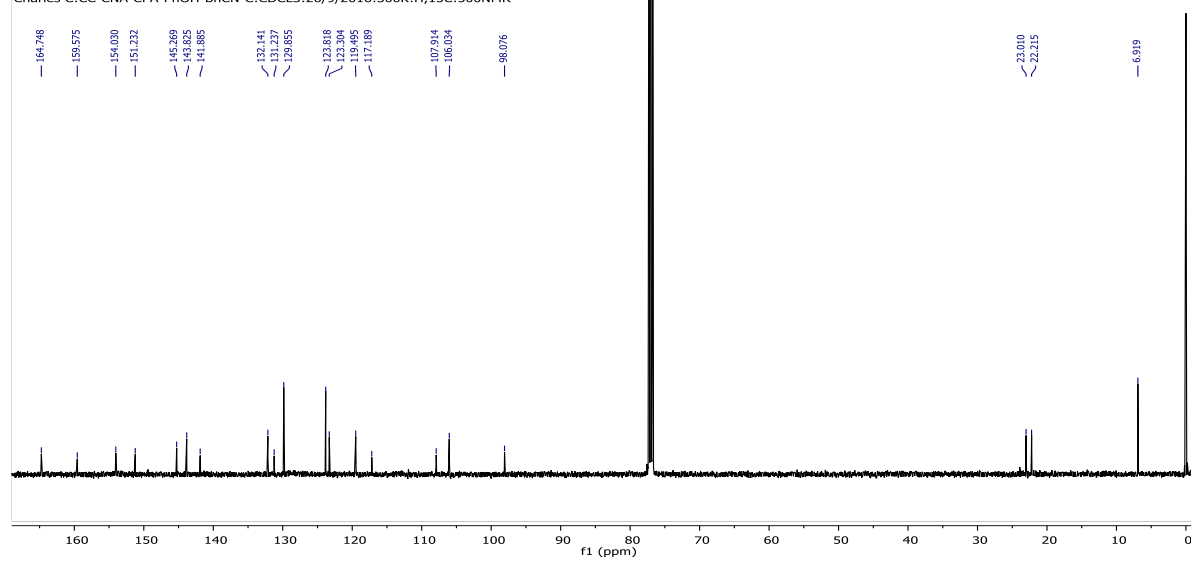
CC-CNA-CPA-PhOH-BnCN-C.1.fid

Charles C:CC-CNA-CPA-PhOH-BnCN-C:CDCL3:26/9/2016:300K:H,13C:500NMR

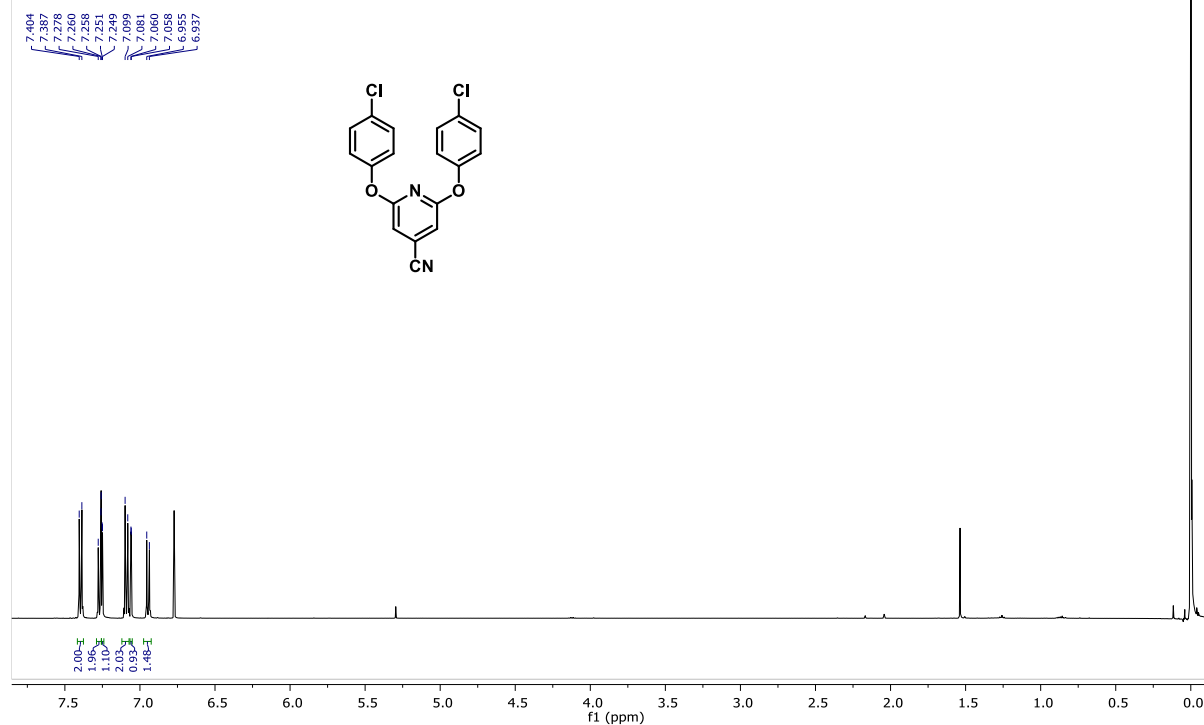


CC-CNA-CPA-PhOH-BnCN-C.2.fid

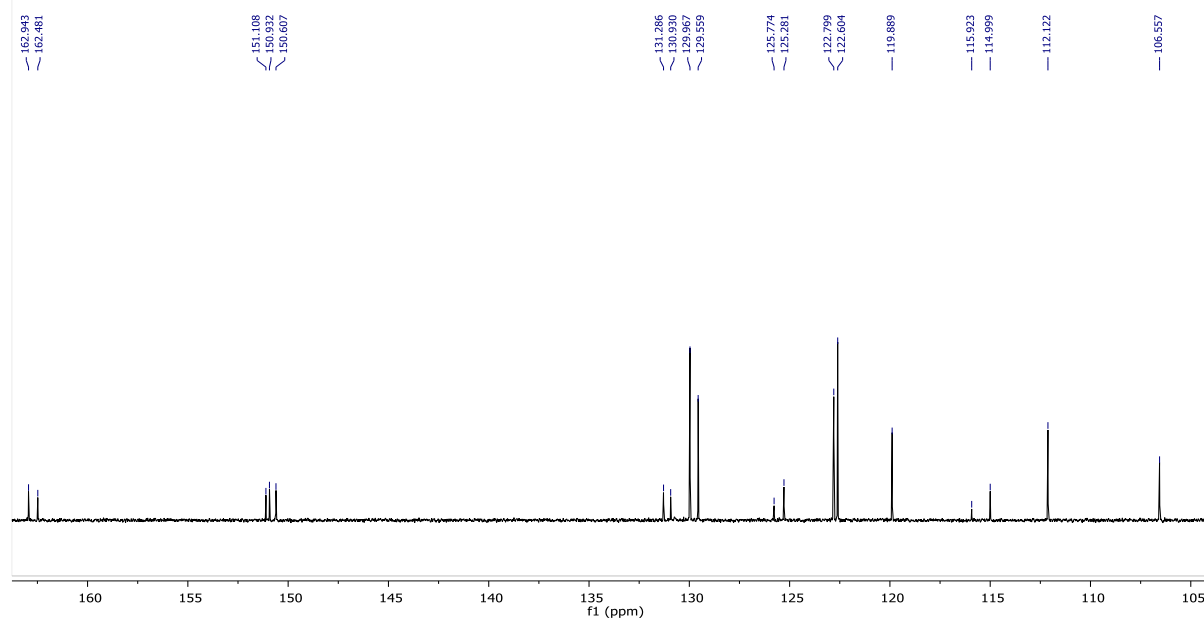
Charles C:CC-CNA-CPA-PhOH-BnCN-C:CDCL3:26/9/2016:300K:H,13C:500NMR



Charles C:CC2.6DiClPyD-4-CN-PhOH-A:CDCL3:29/9/2016:300K:H,13C:500NMR



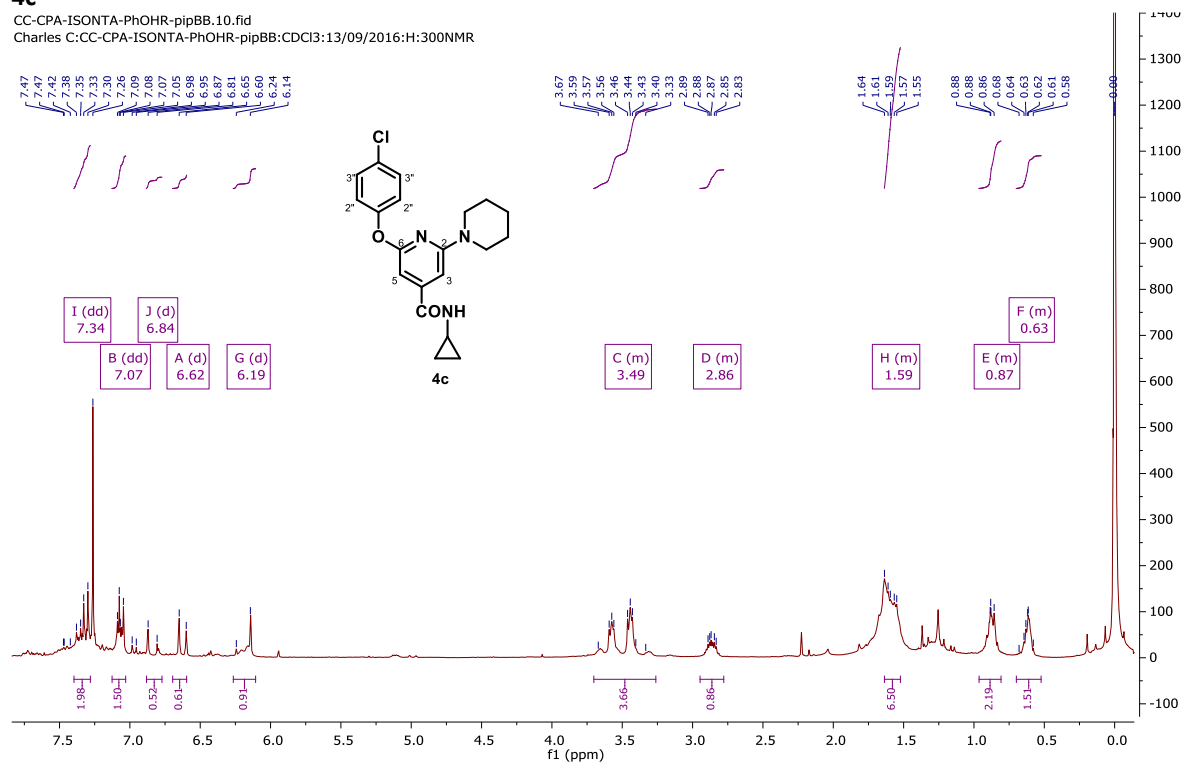
Charles C:CC2.6DiClPyD-4-CN-PhOH-A:CDCL3:29/9/2016:300K:H,13C:500NMR



4c

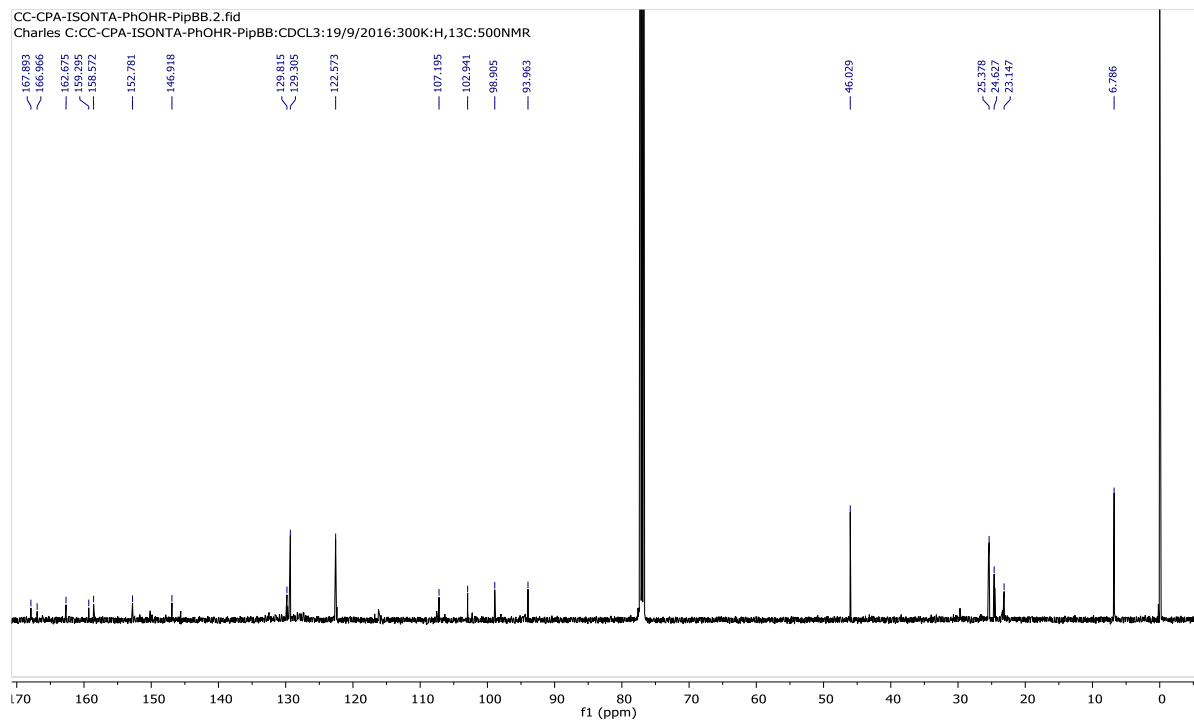
CC-CPA-ISONTA-PhOHR-pipBB.10.fid

Charles C:CC-CPA-ISONTA-PhOHR-pipBB:CDCl3:13/09/2016:H:300NMR

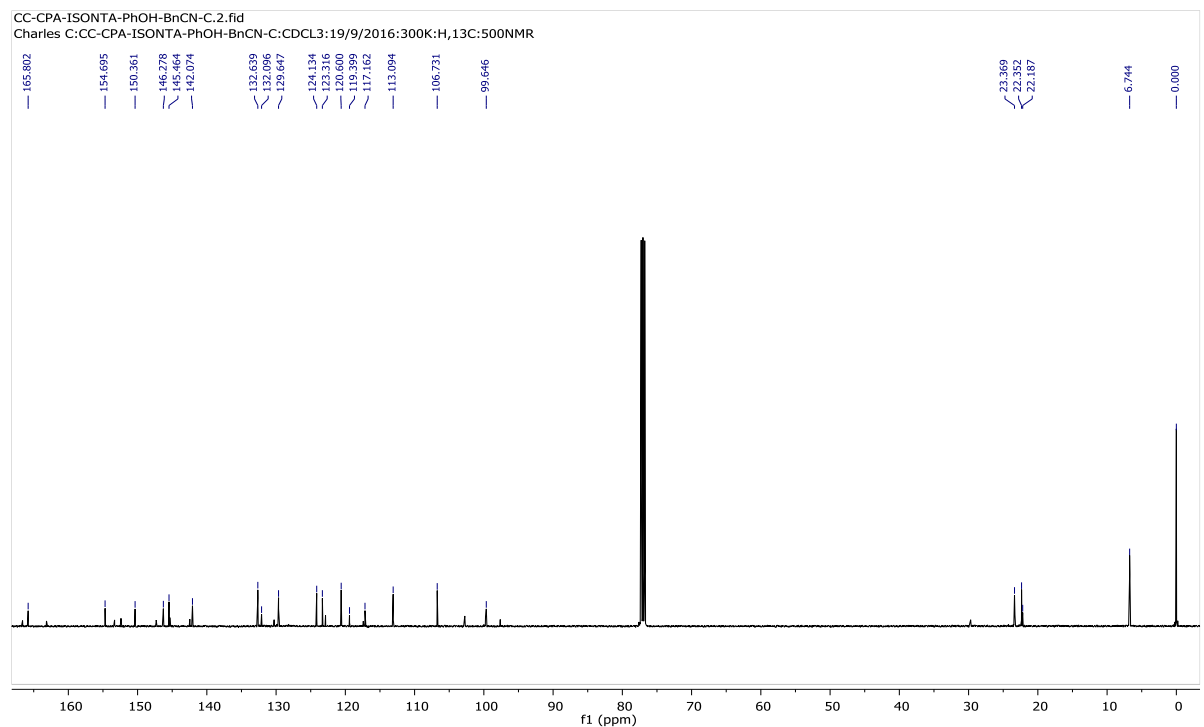
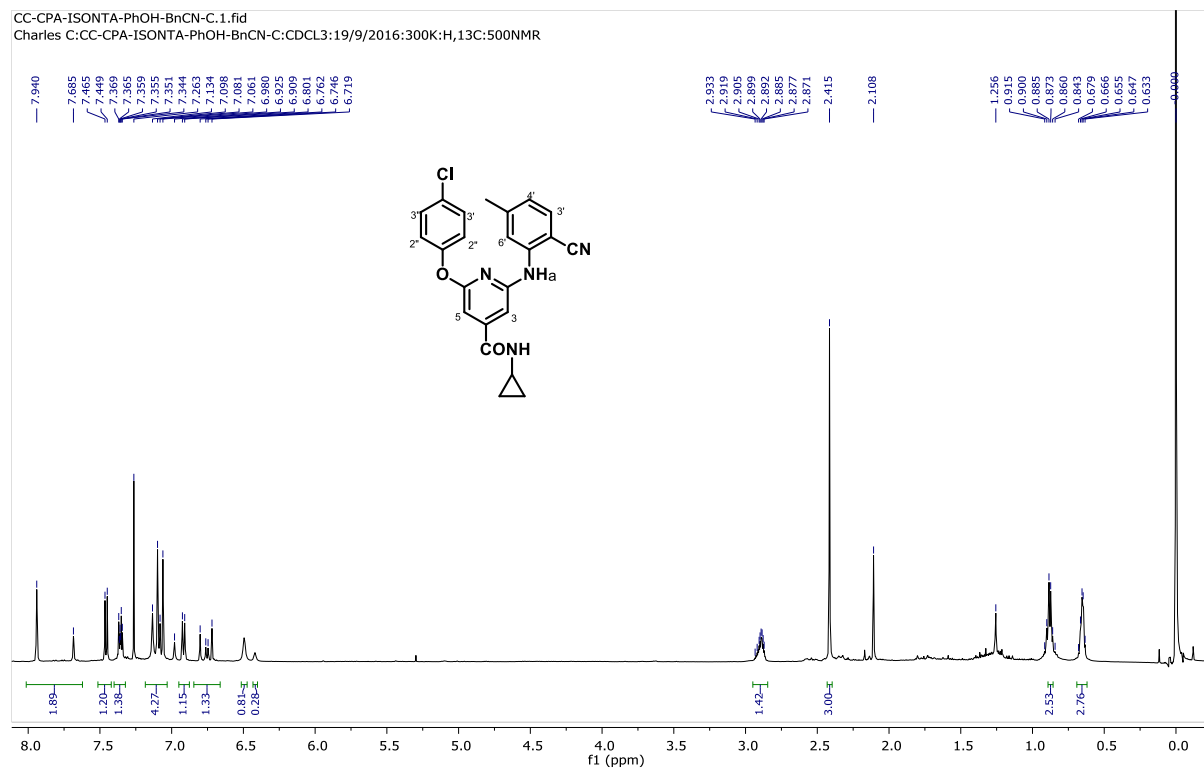


CC-CPA-ISONTA-PhOHR-PipBB.2.fid

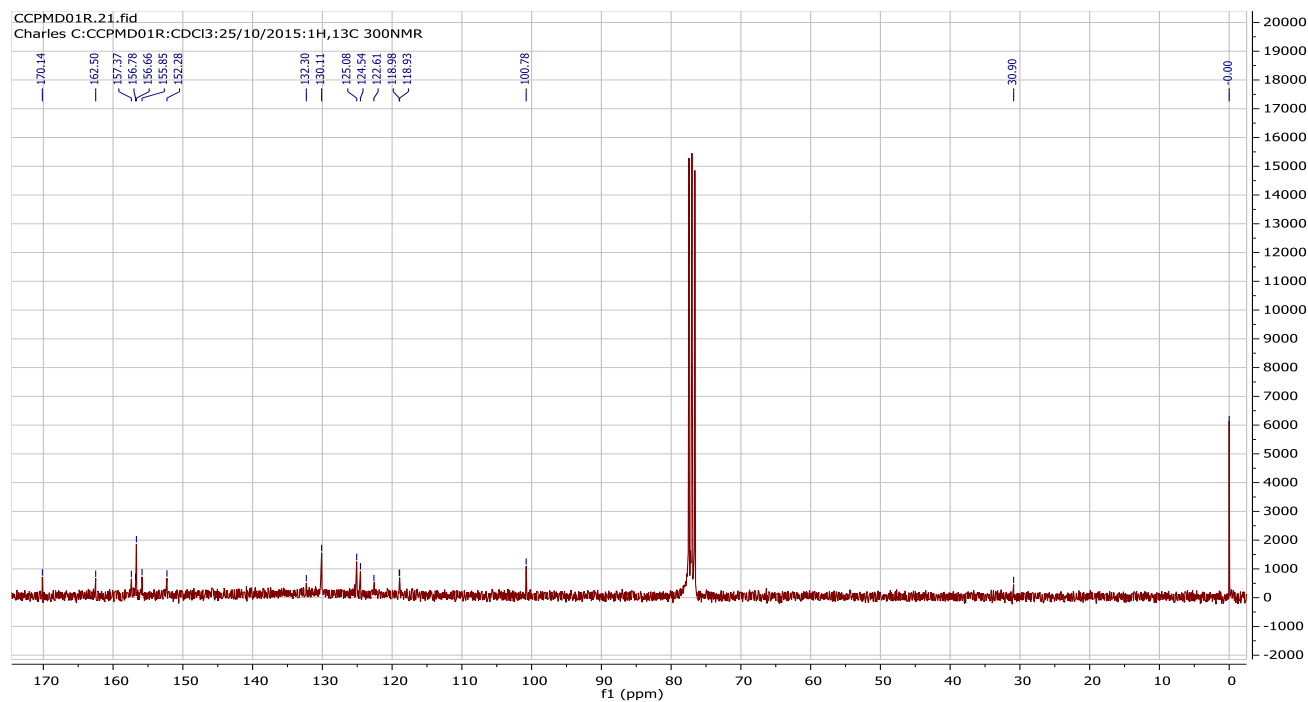
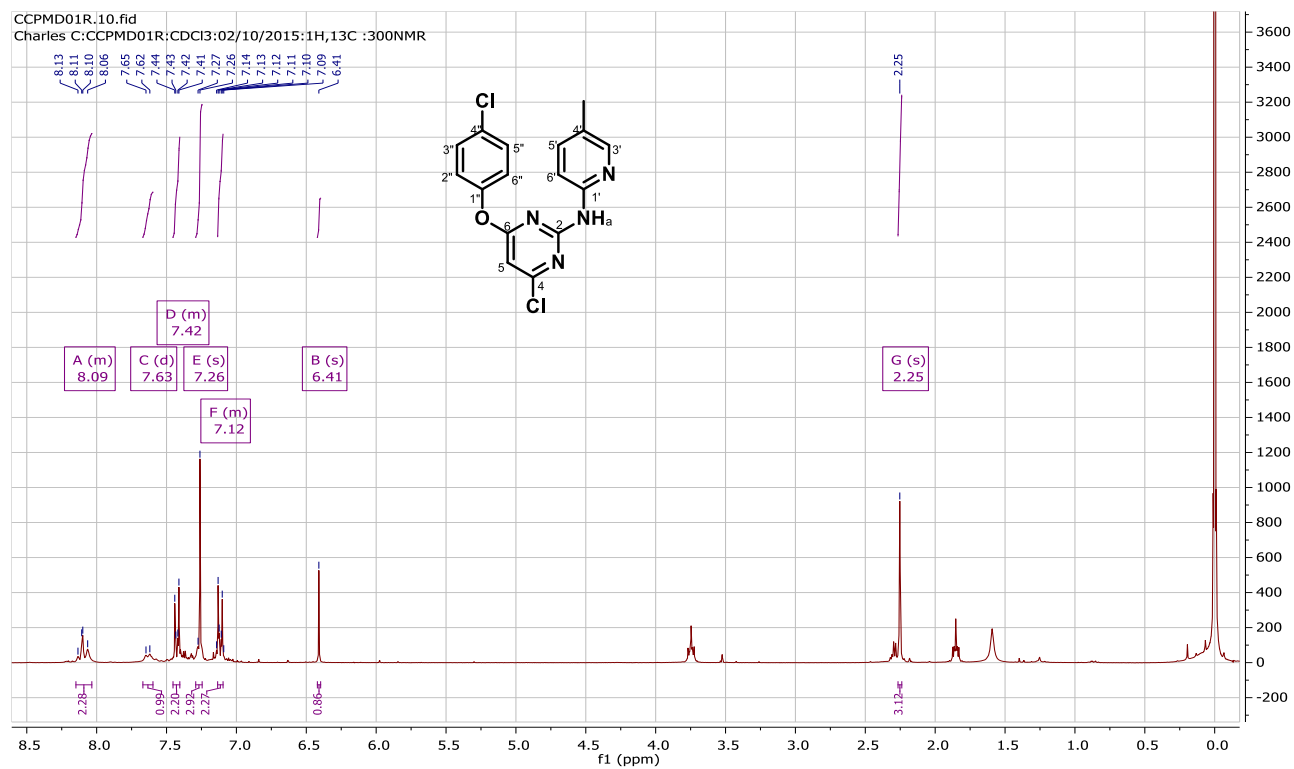
Charles C:CC-CPA-ISONTA-PhOHR-PipBB:CDCl3:19/9/2016:300K:H,13C:500NMR



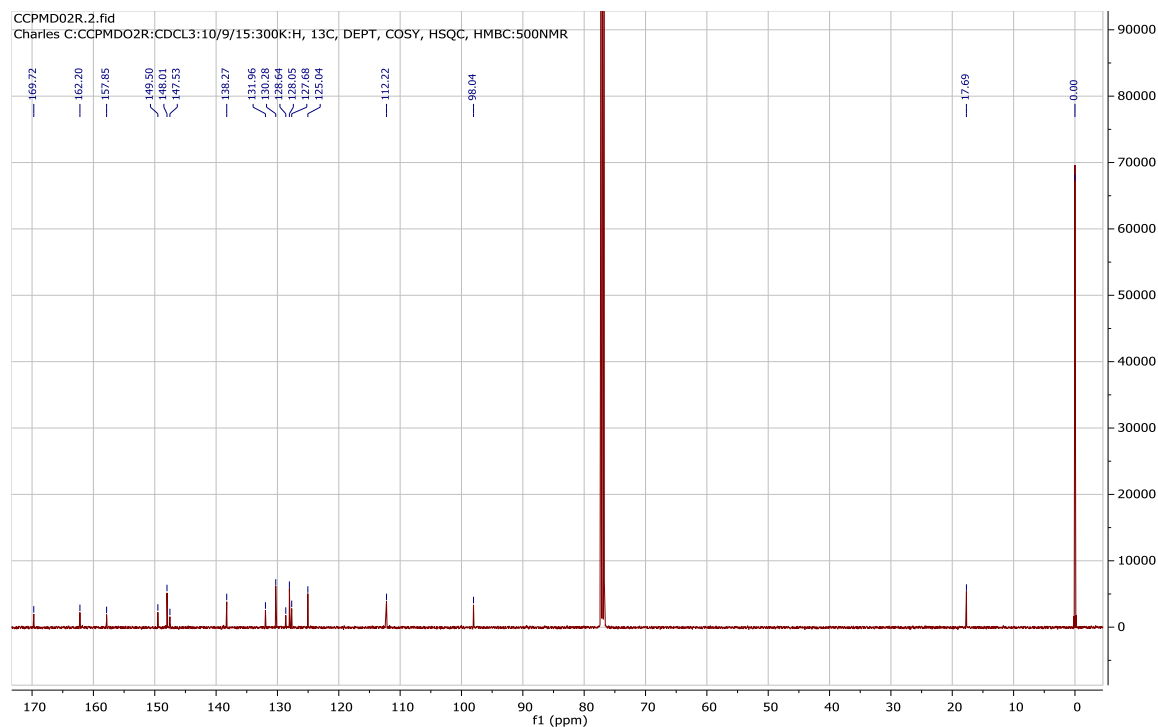
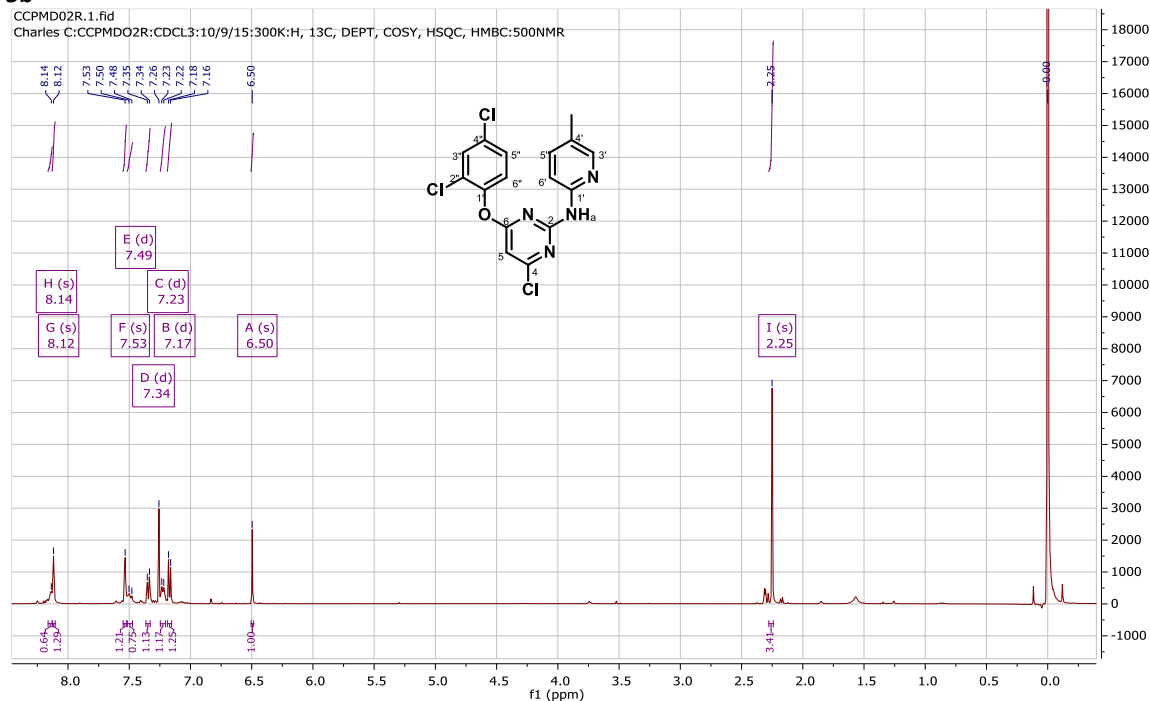
4d



5a

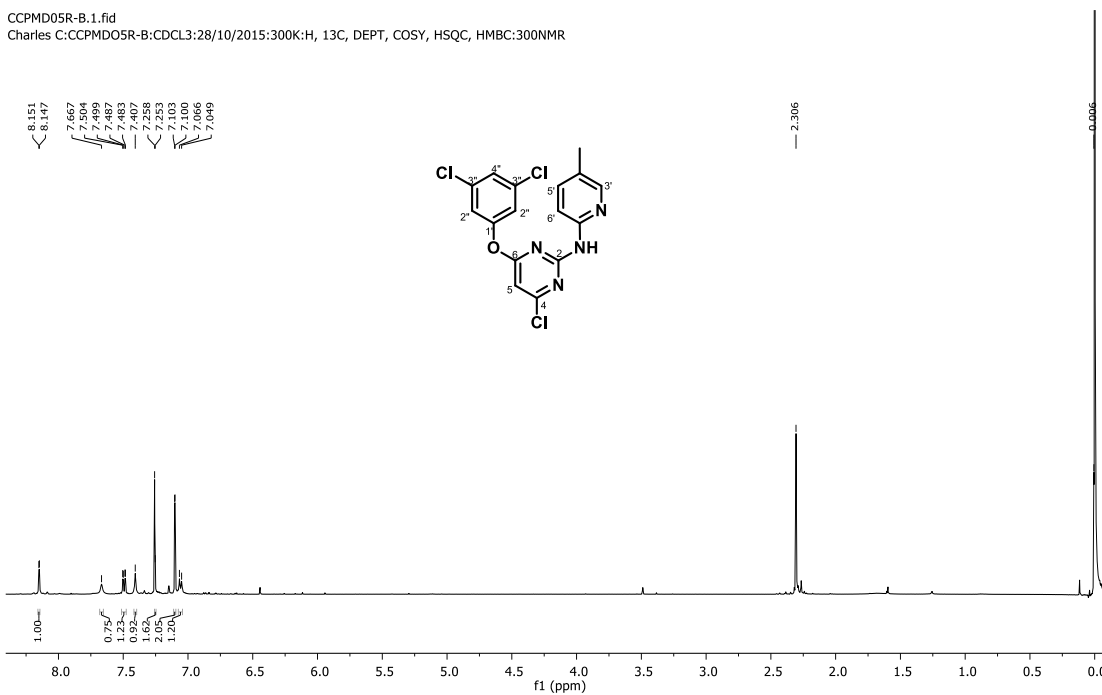


5b

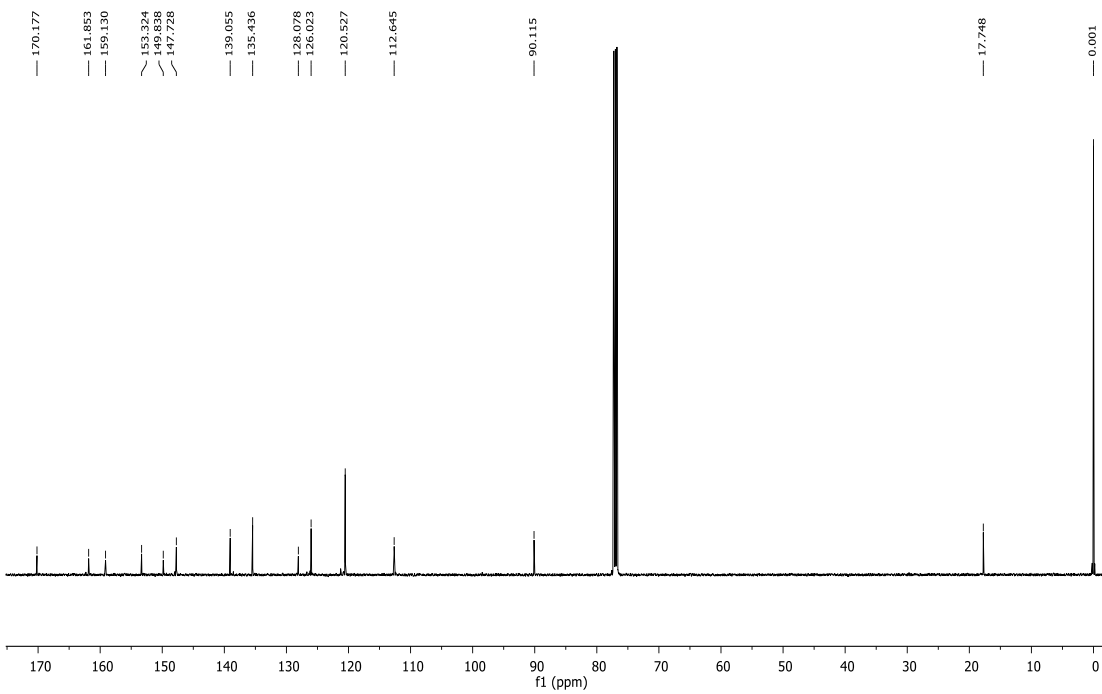


5c

CCPMD05R-B.1.fid
Charles C:CCPMD05R-B:CDCL3:28/10/2015:300K:H, ¹³C, DEPT, COSY, HSQC, HMBC:300NMR

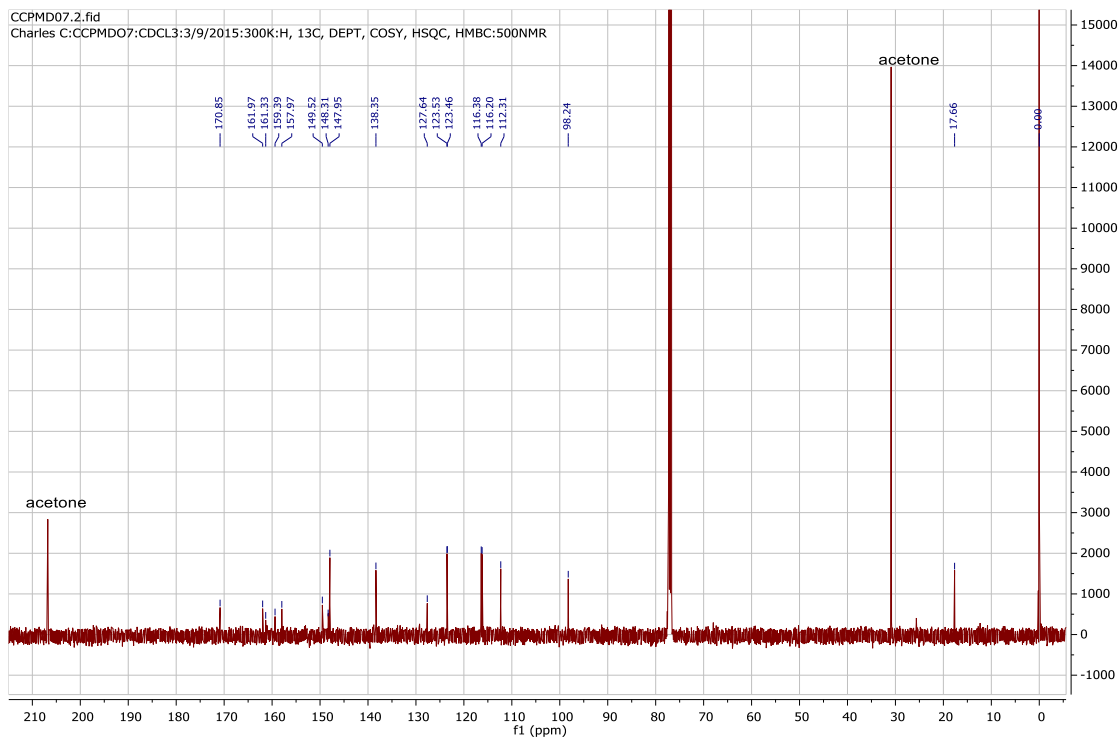
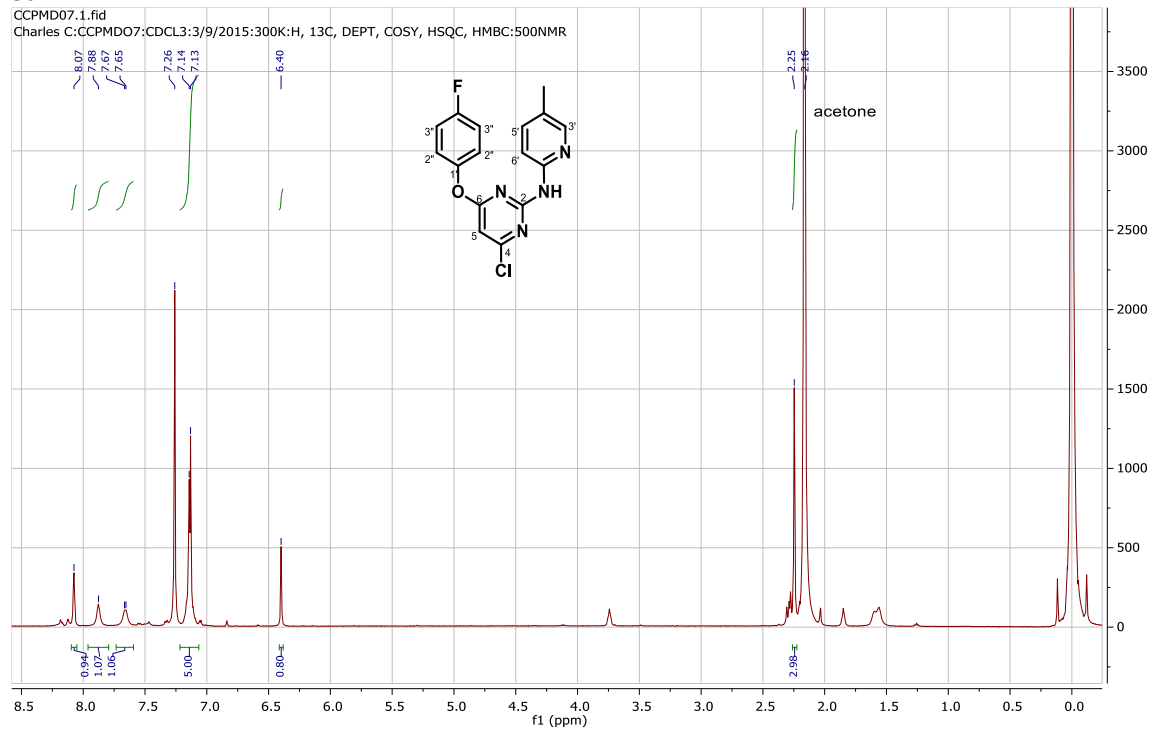


CCPMD05R-B.2.fid
Charles C:CCPMD05R-B:CDCL3:28/10/2015:300K:H, ¹³C, DEPT, COSY, HSQC, HMBC:300NMR



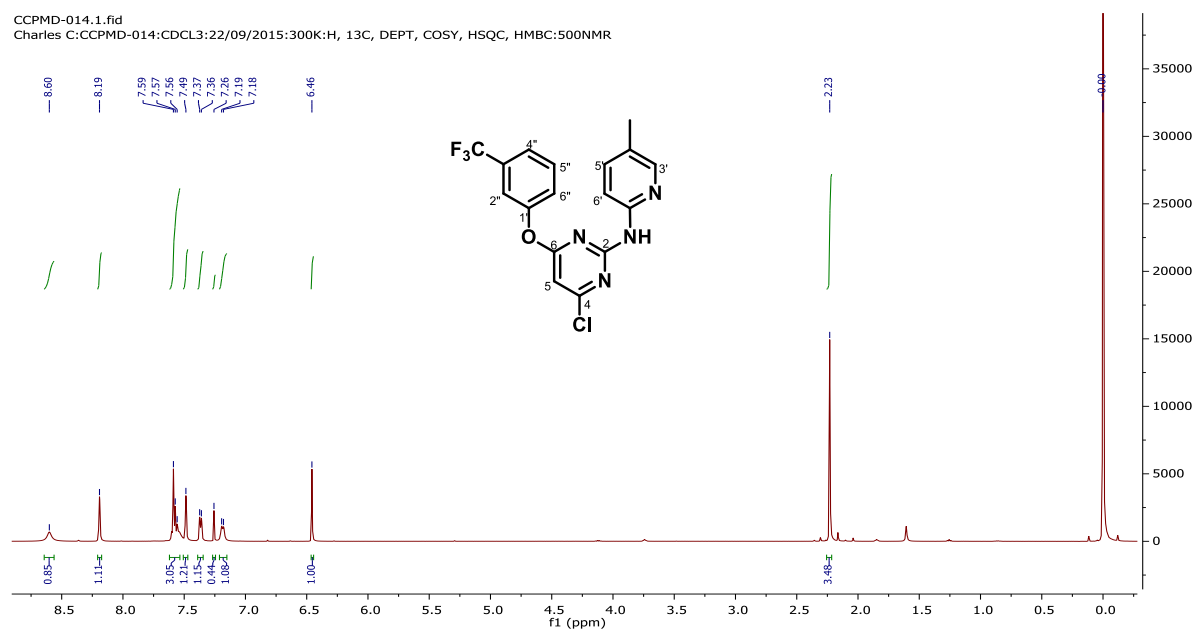
5d

CCPMD07.1.fid
Charles C:CCPMD07:CDCL3:3/9/2015:300K:H, 13C, DEPT, COSY, HSQC, HMBC:500NMR

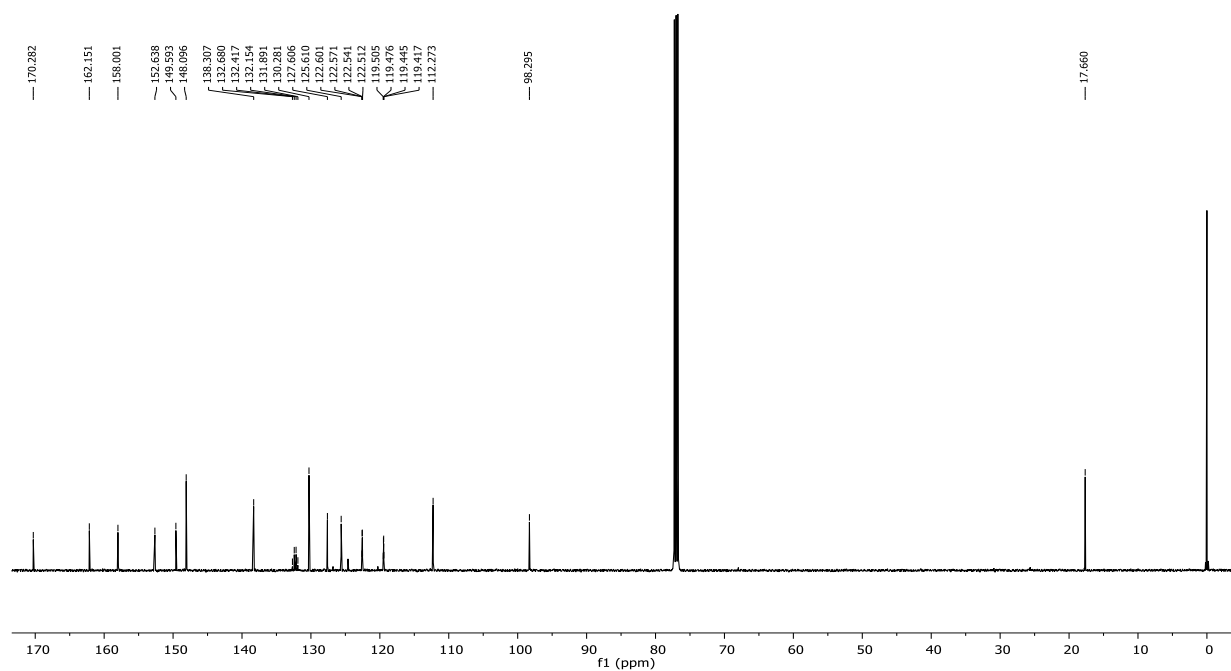


5e

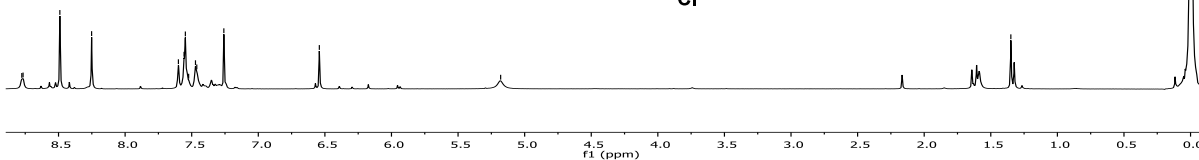
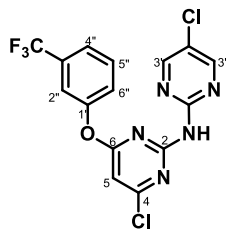
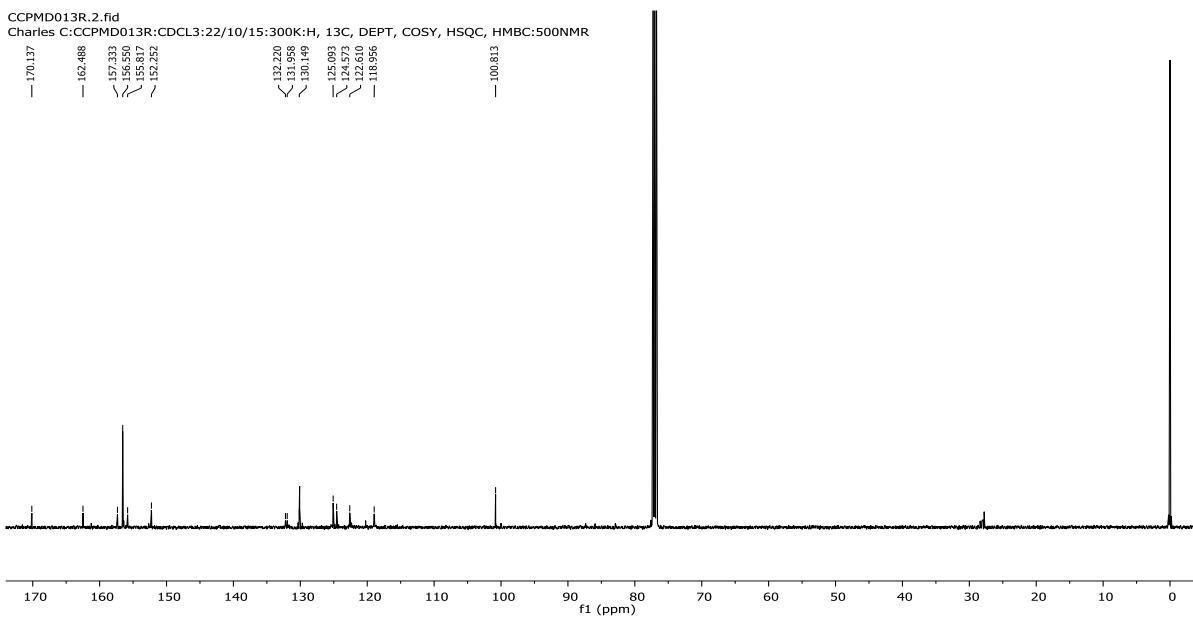
CCPMD-014.1.fid
Charles C:CCPMD-014:CDCL3:22/09/2015:300K:H, 13C, DEPT, COSY, HSQC, HMBC:500NMR



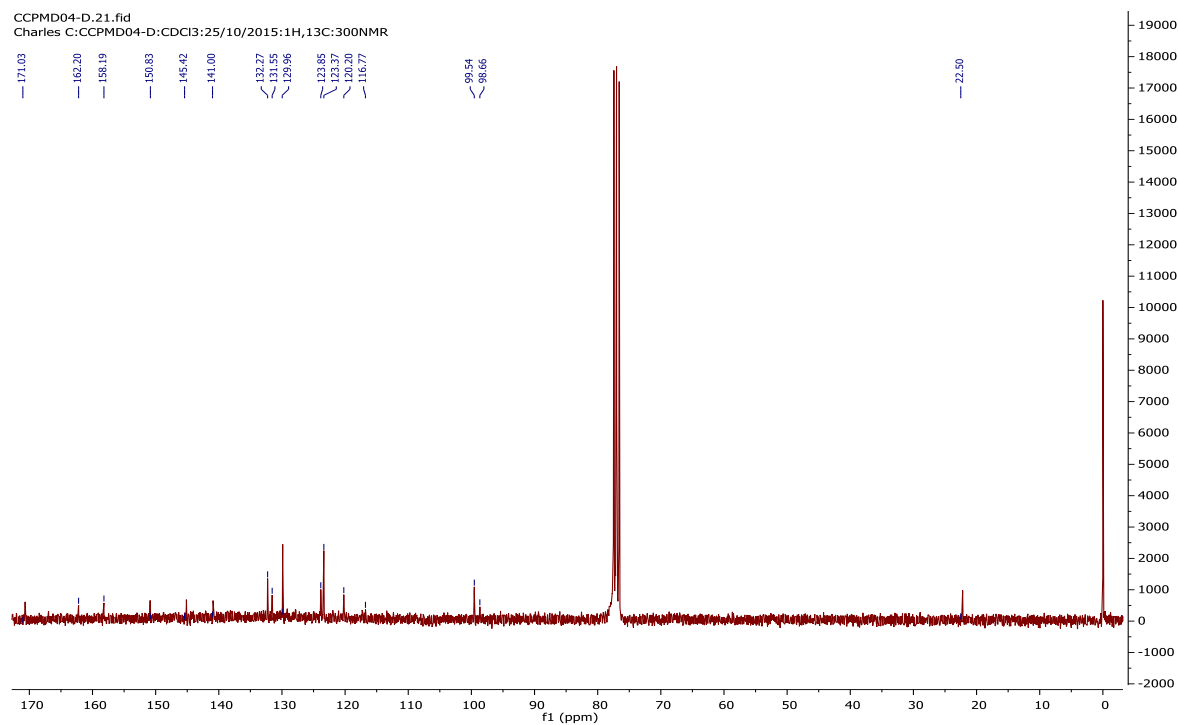
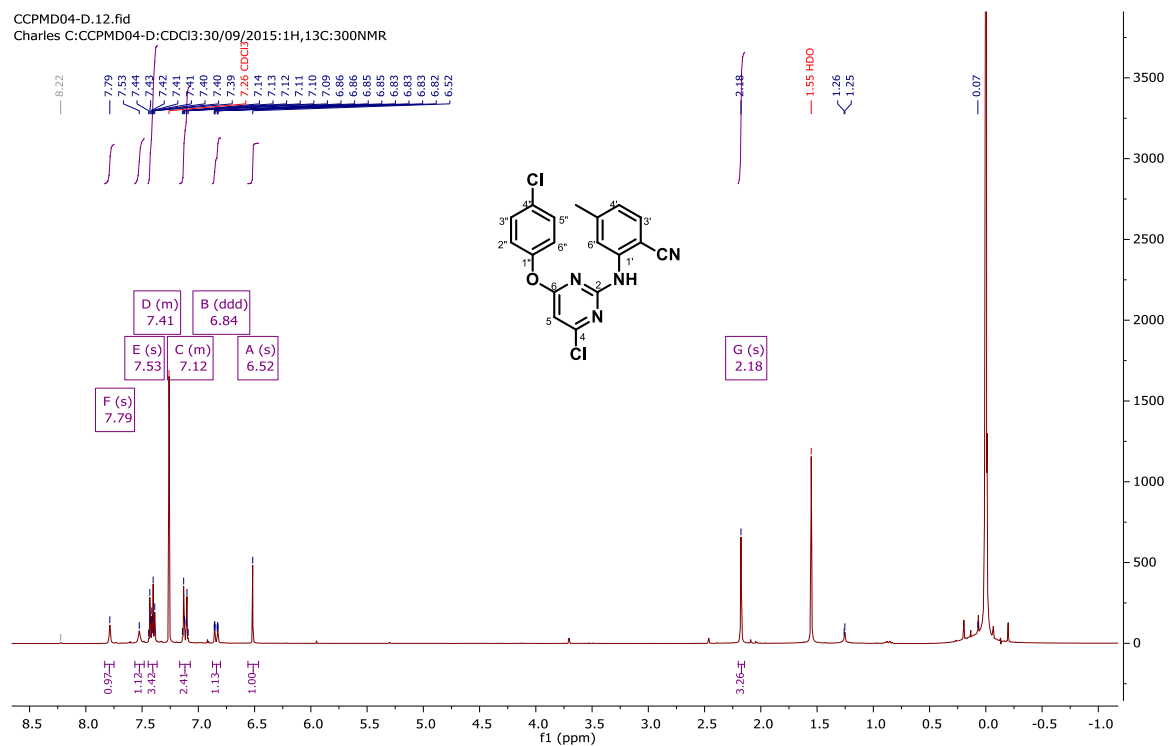
CCPMD-014.2.fid
Charles C:CCPMD-014:CDCL3:22/09/2015:300K:H, 13C, DEPT, COSY, HSQC, HMBC:500NMR



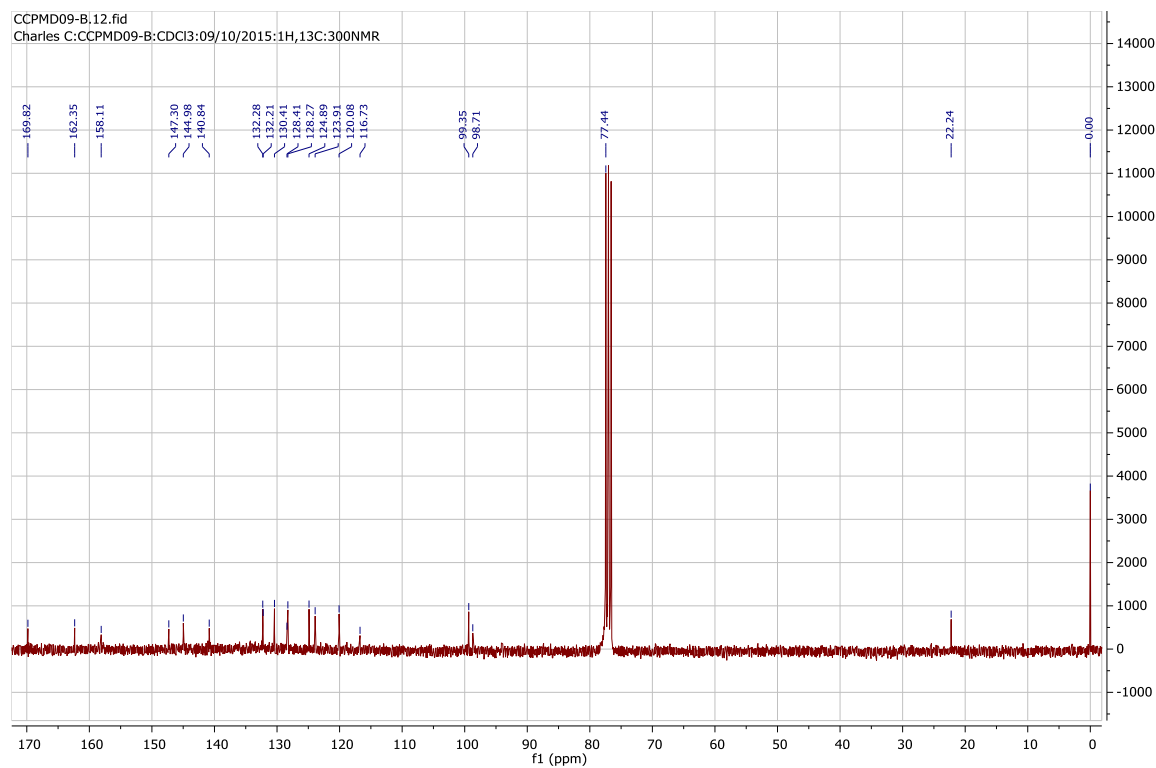
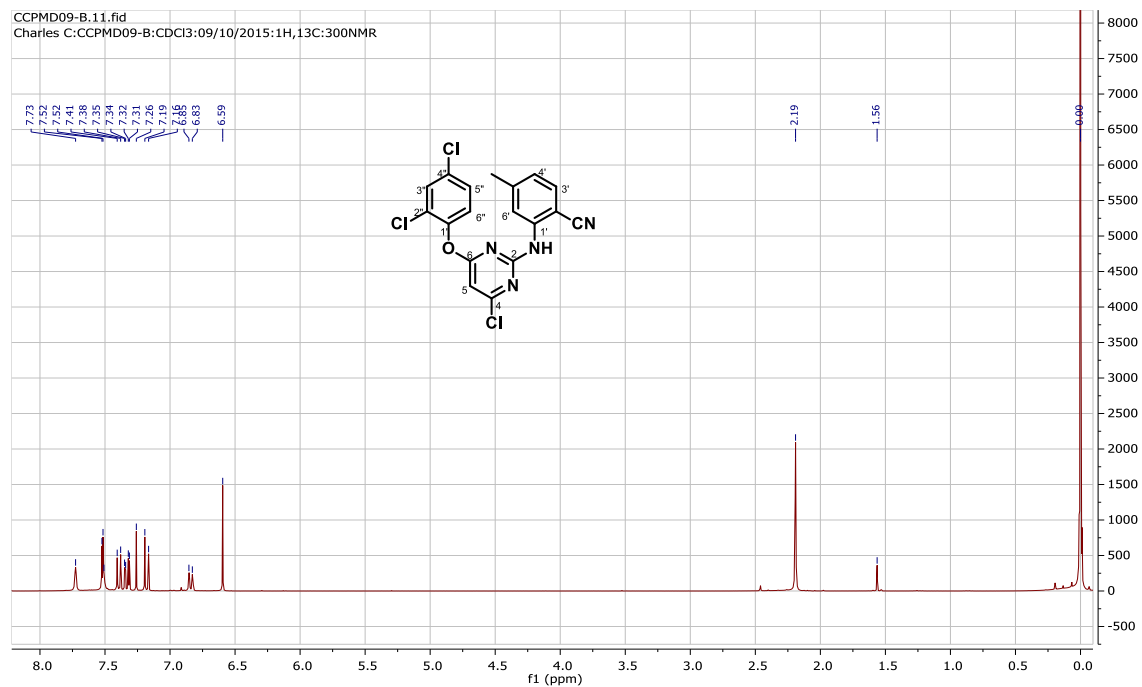
5f

CCPMD013R.1.fid
Charles C:CCPMD013R:CDCL3:22/10/15:300K:H, 13C, DEPT, COSY, HSQC, HMBC:500NMR8.776
8.766
8.490
8.352
7.600
7.557
7.548
7.523
7.472
7.462
7.259
6.542
5.180
1.389CCPMD013R.2.fid
Charles C:CCPMD013R:CDCL3:22/10/15:300K:H, 13C, DEPT, COSY, HSQC, HMBC:500NMR170.137
162.488
157.333
156.550
155.817
152.252
132.220
131.986
130.149
125.093
124.573
122.610
116.996
100.813

5g

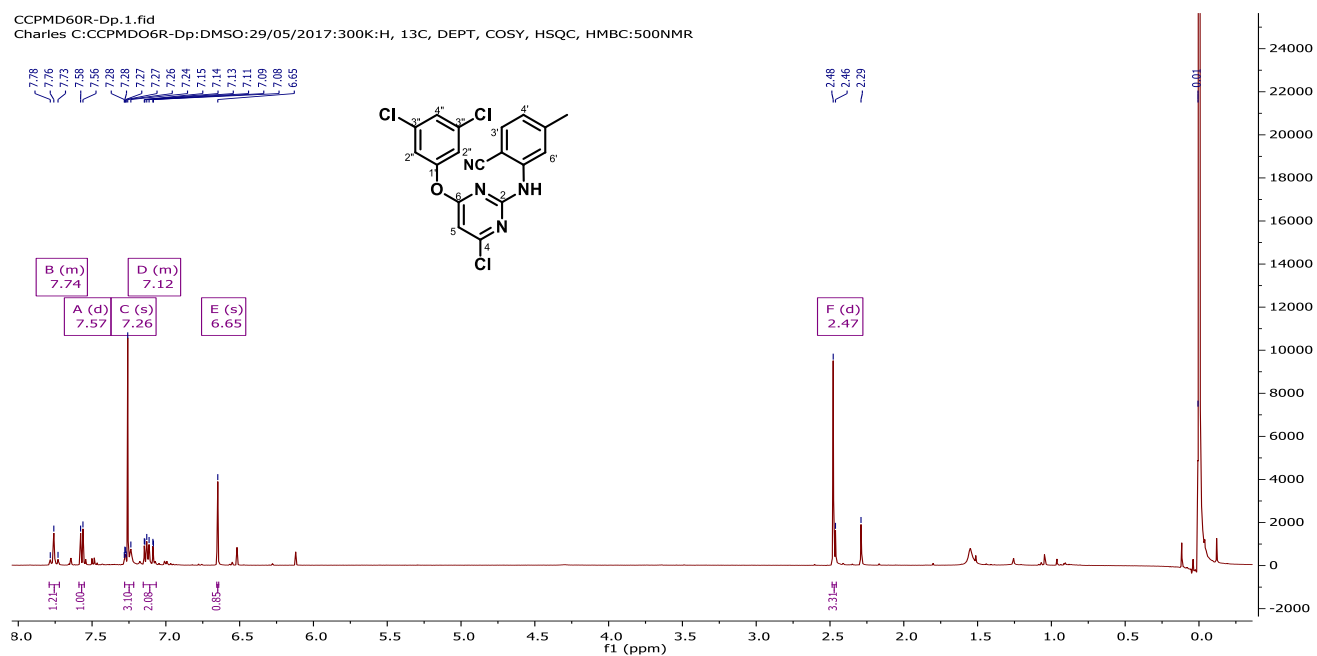


5h

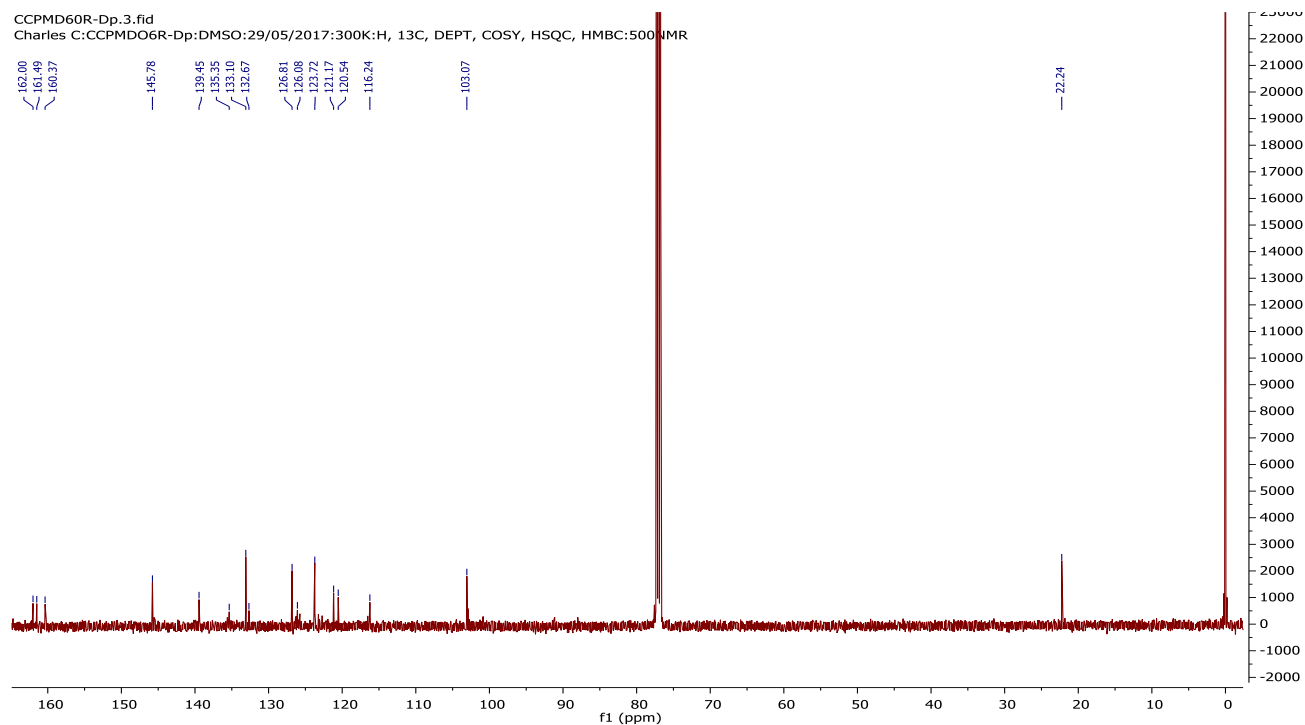


5i

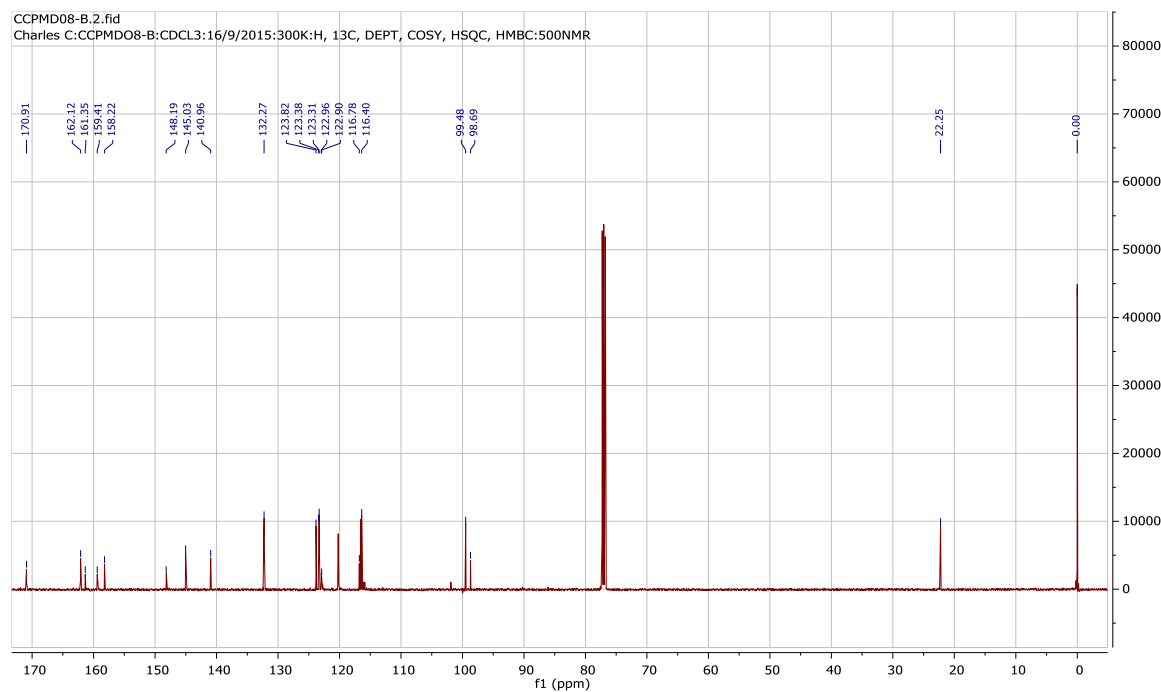
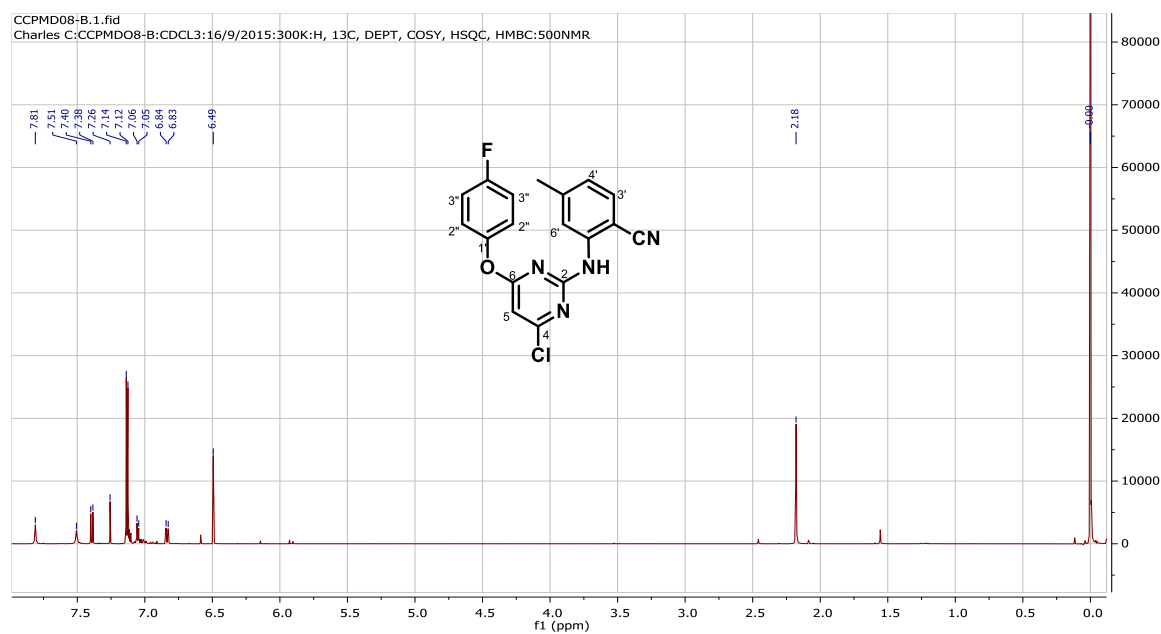
CCPMD60R-Dp.1.fid
Charles C:CCPMD06R-Dp:DMSO:29/05/2017:300K:H, 13C, DEPT, COSY, HSQC, HMBC:500NMR



CCPMD60R-Dp.3.fid
Charles C:CCPMD06R-Dp:DMSO:29/05/2017:300K:H, 13C, DEPT, COSY, HSQC, HMBC:500NMR



5j



5k

