

Palladium-Catalyzed Hydroxylation of Aryl and Heteroaryl Halides Enabled by the Use of a Palladacycle Precatalyst

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Supporting Information

Content	Page no.
General Information	S2
List of Spectra of Compounds (¹ H and ¹³ C NMR): Phenols and Hydroxylated Heteroaryl Compounds Synthesized from the Cross-Coupling of KOH (3a-n) Phenols Synthesized from the Cross-Coupling of CsOH at Room Temperature (5a-f)	S3

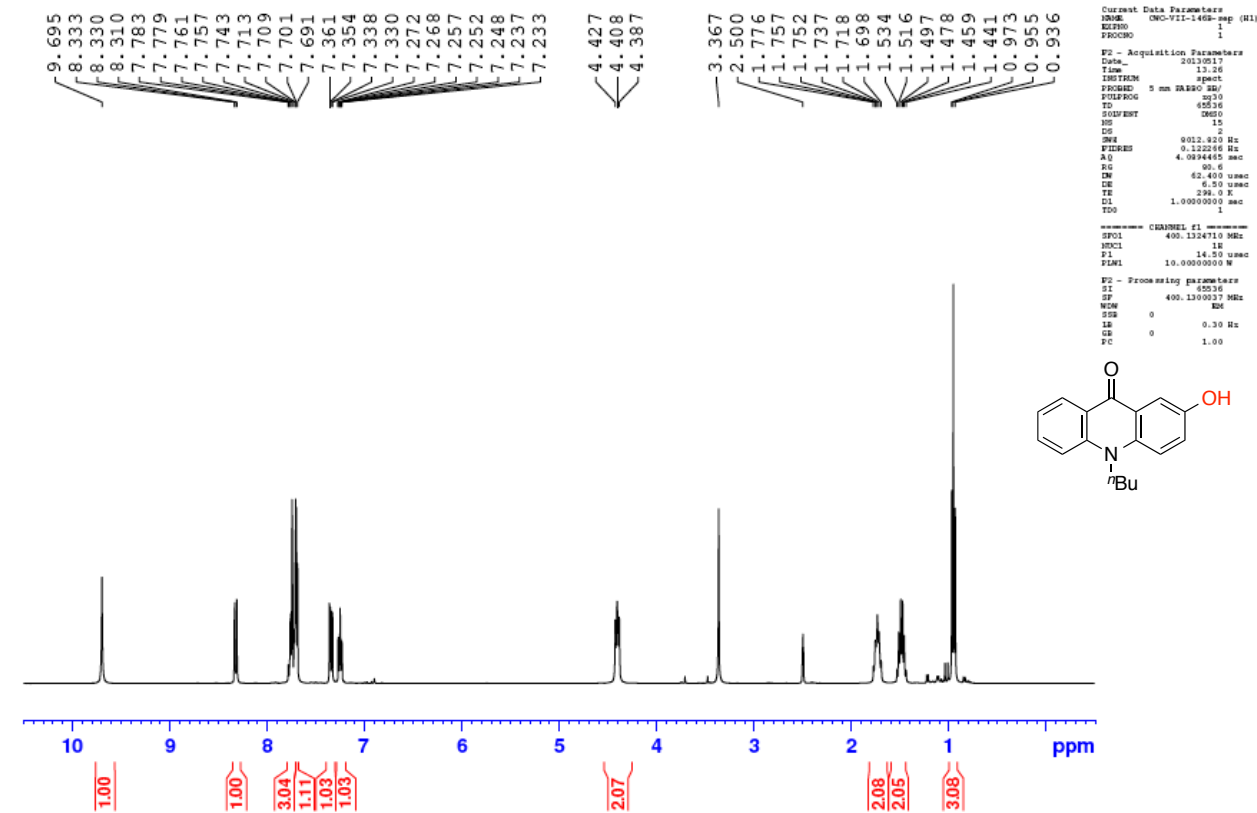
General Information

General Analytical Information. Nuclear magnetic resonance spectra were recorded on a 400 MHz NMR instrument at ambient temperature. All ^1H NMR spectra were measured in parts per million (ppm) relative to the signals for residual DMSO in DMSO- d_6 (2.50 ppm) unless otherwise stated. Data for ^1H NMR were reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, qu = quintet, sex = sextet, m = multiplet, ovrlp = overlap, br = broad), coupling constants, and integration. All ^{13}C NMR spectra were reported in ppm relative to DMSO- d_6 (39.52 ppm) unless otherwise stated, and were obtained with complete ^1H decoupling.

General Reagent Information. Unless otherwise noted, all chemicals used in the preparations of (hetero)aryl halides, and all the (hetero)aryl halides used in the coupling reactions with alkali metal hydroxides, were commercially available and were used as received without further purification. THF was purchased from J.T. Baker in CYCLE-TAINER® solvent-delivery kegs and vigorously purged with argon for 1 h, followed by further purification by passing it under argon pressure through two packed columns of neutral alumina. Anhydrous 1,4-dioxane (99.8%) was purchased from Aldrich Chemical Co. in a Seal-Seal® bottle and stored under argon. Potassium hydroxide (KOH) pellets were crushed into smaller granules before use. Cesium hydroxide monohydrate ($\text{CsOH}\cdot\text{H}_2\text{O}$) was stored in a nitrogen-filled glove-box. Compounds were purified by flash chromatography using Silicycle SiliaFlash® F60 (230-400 mesh) silica gel.

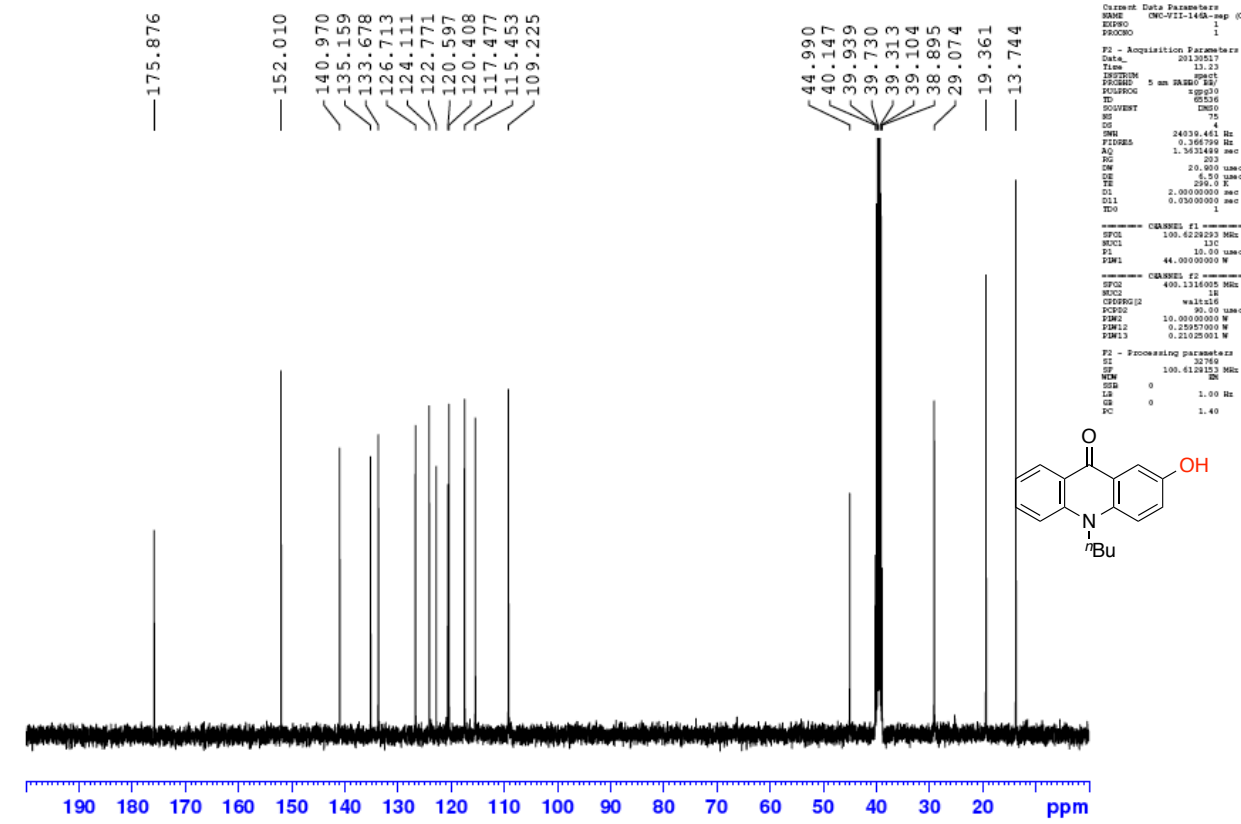
General Consideration. The solvent system as an eluent for column chromatography is presented as a ratio of solvent volumes. Yields reported in the publication are of isolated materials. The isolated yields of the products represent averages of two independent runs unless otherwise noted. All products were characterized by ^1H NMR and ^{13}C NMR spectroscopies, elemental analyses / high-resolution mass spectrometry, and IR spectroscopy. All solid products were further characterized by melting point determination.

¹H and ¹³C NMR spectra of 10-*n*-butyl-2-hydroxyacridin-9(10*H*)-one (3a)



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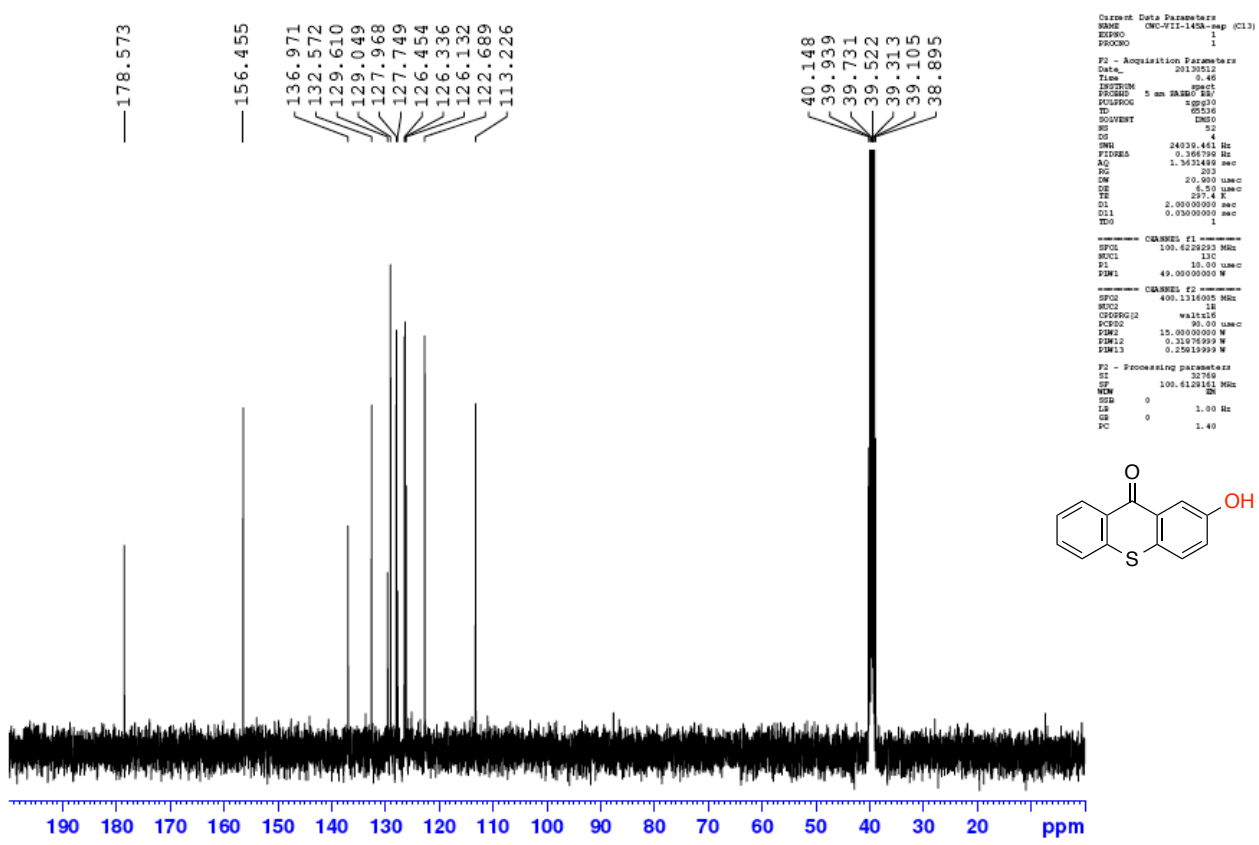
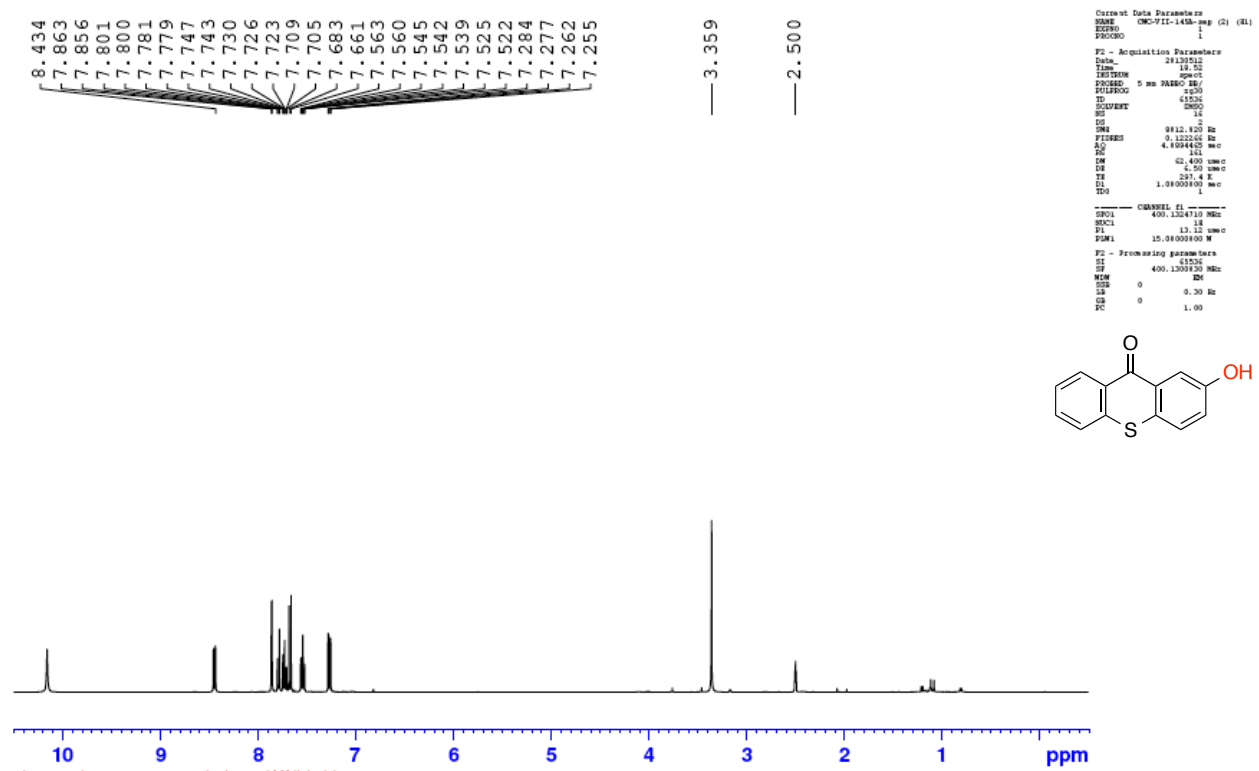
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SOLVENT  DMSO
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AQ        0.122316 Hz
RG        4.0994445 sec
RG        90.6
DE        62.400 umsec
TE        294.0 K
CL        1.0000000 sec
TD0       1
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NUC1      1H
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PDM1     10.0000000 M
----- Processing parameters
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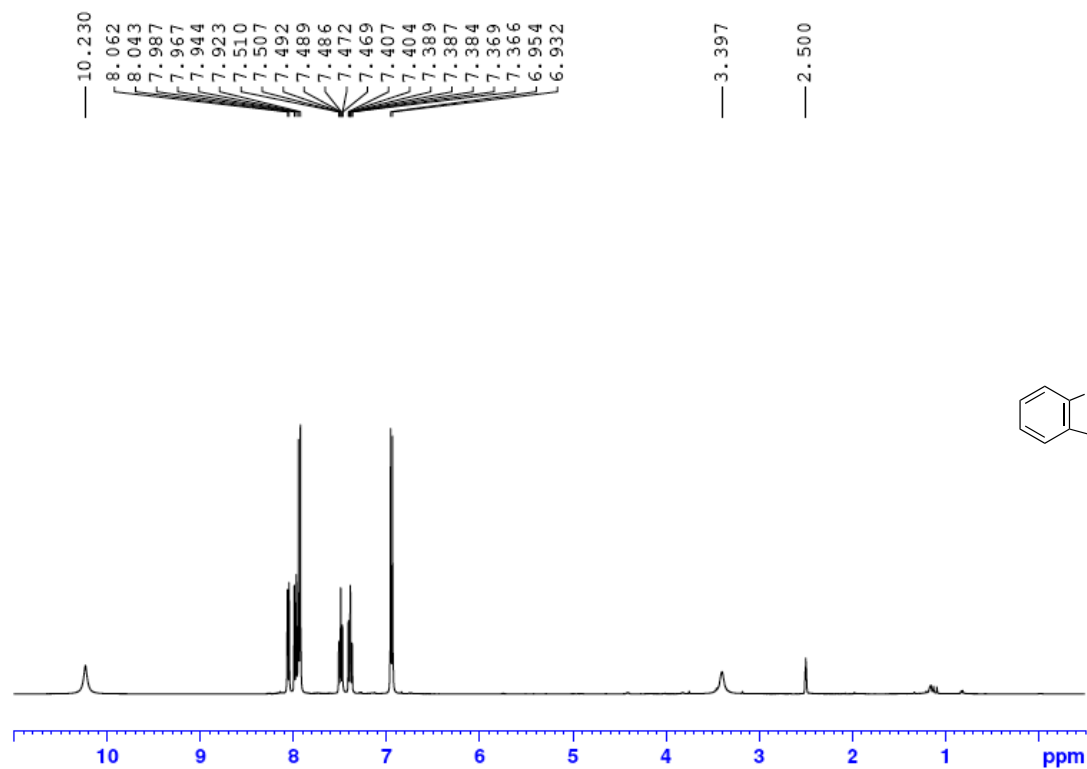
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TE        294.0 K
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TD0       1
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NUC2      1H
P2        14.50 umsec
PDM2     10.0000000 M
SFO3     0.250270000 MHz
P3        0.21025001 M
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SSB       0
LB        0.30 Hz
GB        0
PC        1.40
    
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¹H and ¹³C NMR spectra of 2-hydroxy-9H-thioxanthen-9-one (3b)



¹H and ¹³C NMR spectra of 4-(benzothiazol-2-yl)phenol (3c)



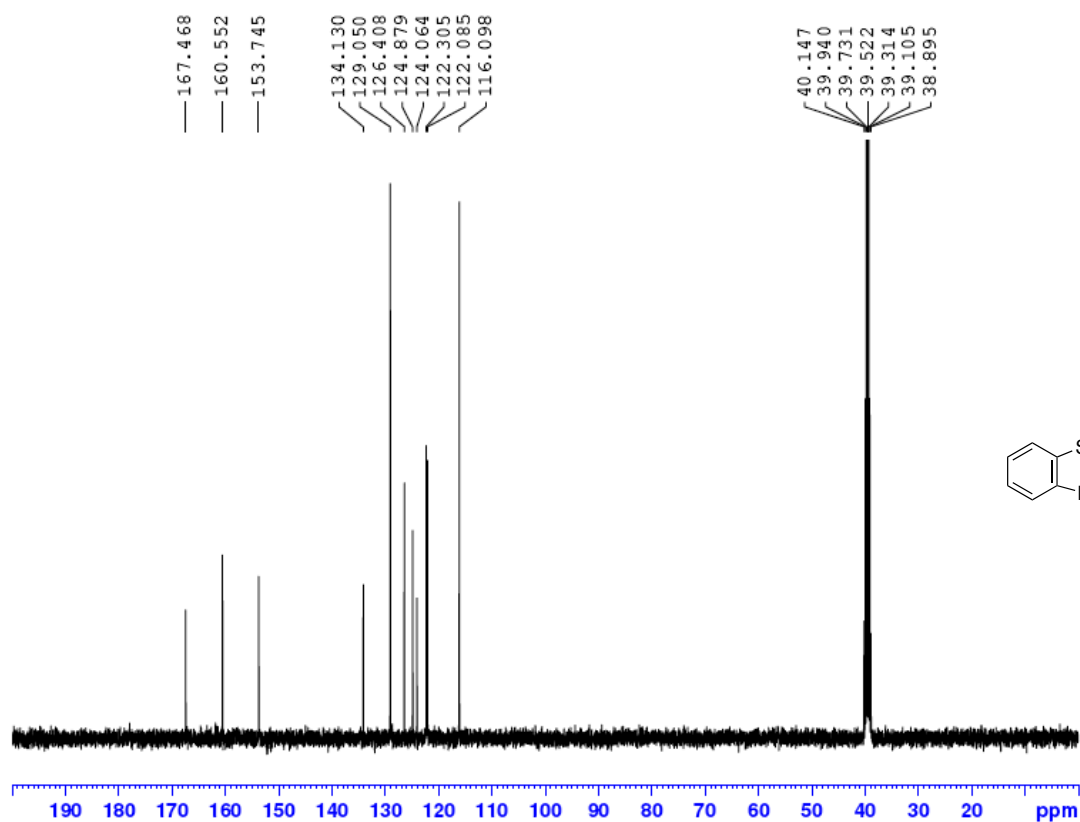
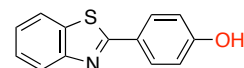
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PULPROG zg30
TC       303.2
SOLVENT DMSO
NS       12
DS       2
SFO      400.1324710 Hz
FIDRES   0.122266 Hz
AQ       4.0284405 sec
RG       39.5
DM       62.400 umsec
DE       6.50 umsec
TE       300.2 K
D1       1.00000000 sec
TD0      1

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NUC1     13C
P1       14.50 umsec
PL1      10.00000000 W

F2 - Processing parameters
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SSB      0
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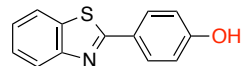
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PULPROG zgpg30
TC       303.2
SOLVENT DMSO
NS       34
DS       4
SFO      24020.461 Hz
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AQ       1.3531489 sec
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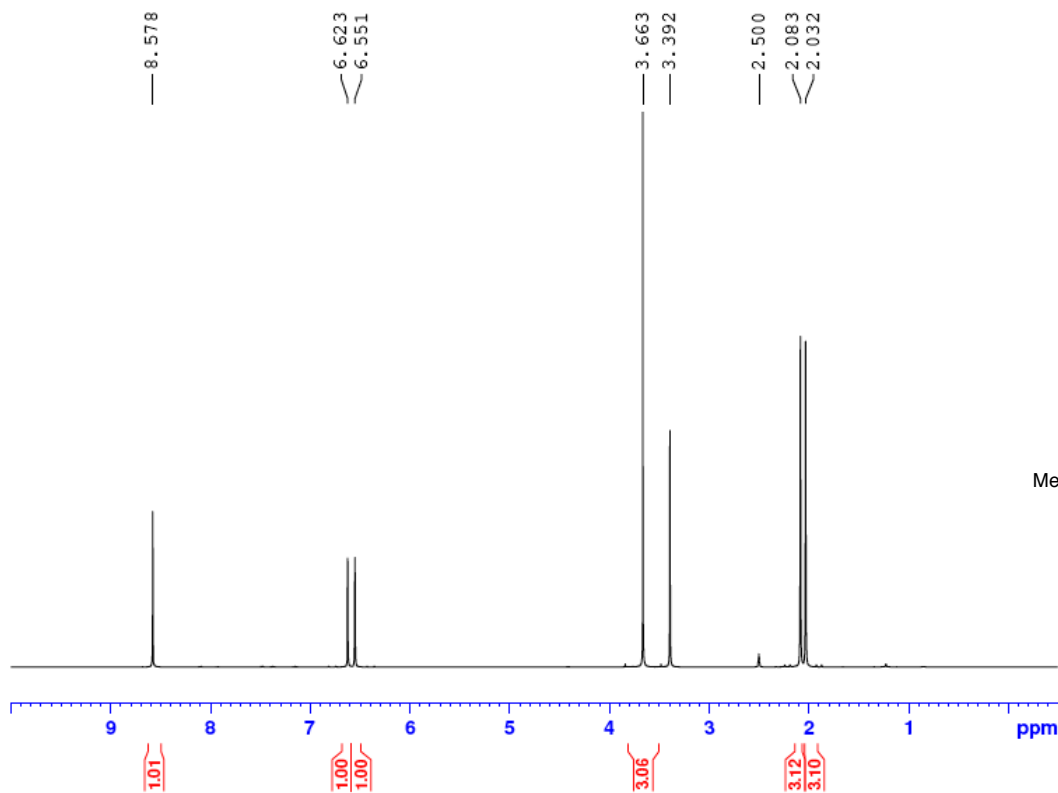
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CHRGNG[2] wait16
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PMD12   0.20070000 W
PMD13   0.21025001 W

F2 - Processing parameters
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¹H and ¹³C NMR spectra of 4-methoxy-2,5-dimethylphenol (3d)



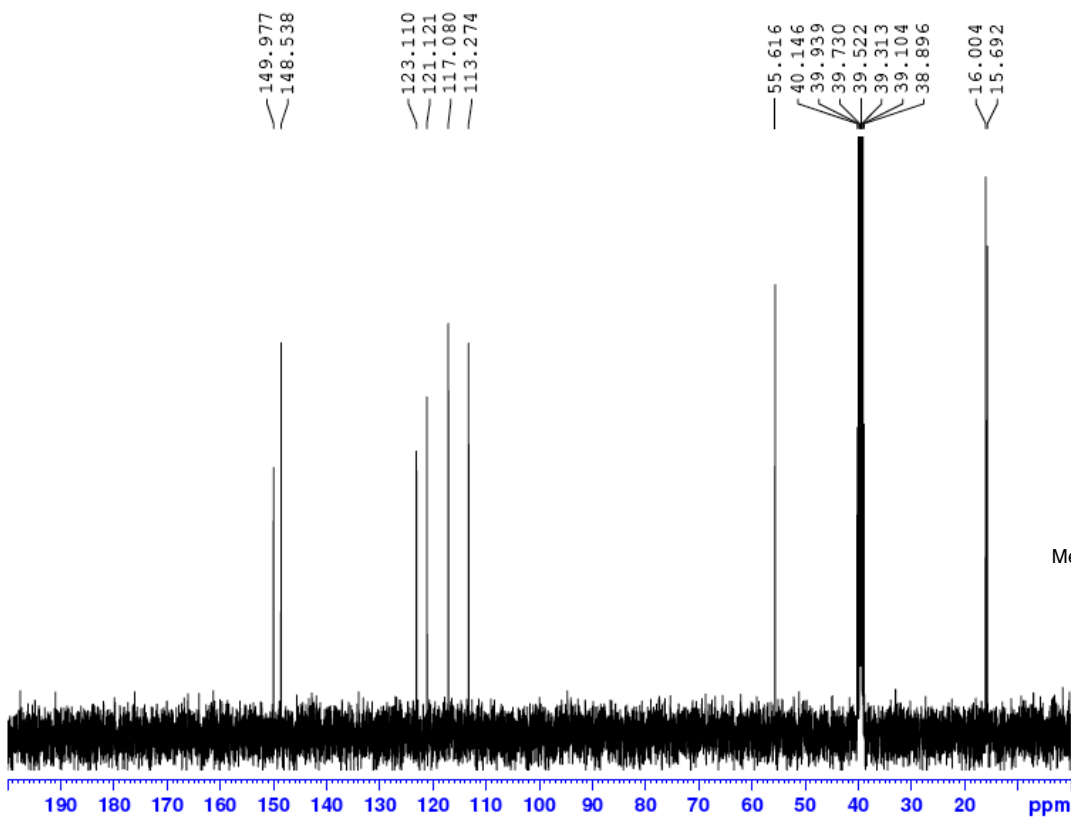
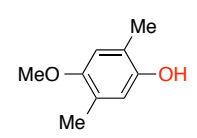
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EXPNO    1
PROCNO   1

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PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       10
DS       2
SWH      9012.810 Hz
FIDRES   0.122246 Hz
AQ       4.934445 sec
RG       57
CM       62.400 usec
DE       6.50 usec
TE       296.0 K
DQ       1.0000000 sec
TDO      1

===== CHANNEL f1 =====
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NUC1     1H
P1       14.50 usec
PLM1     10.0000000 W

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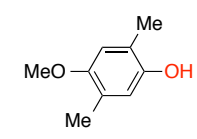
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TD       65536
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DS       4
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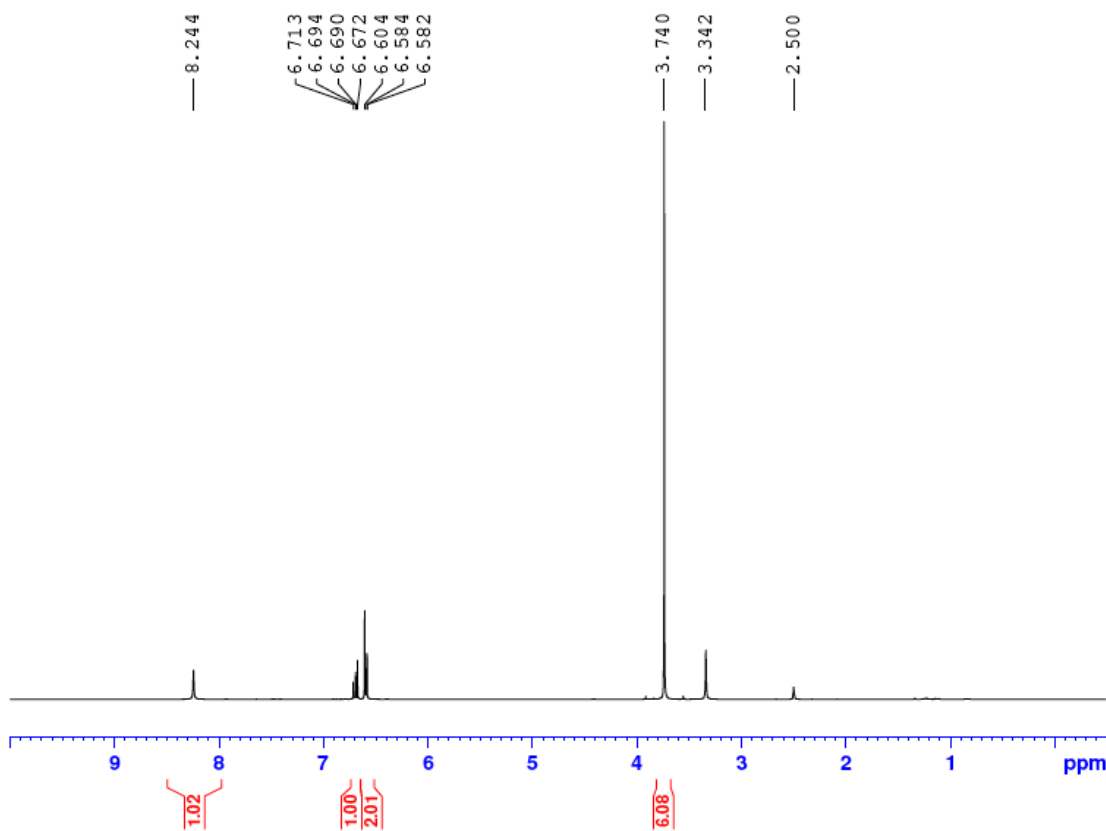
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===== CHANNEL f3 =====
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NUC3     13C
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SFO4     100.6126112 MHz
NUC4     13C

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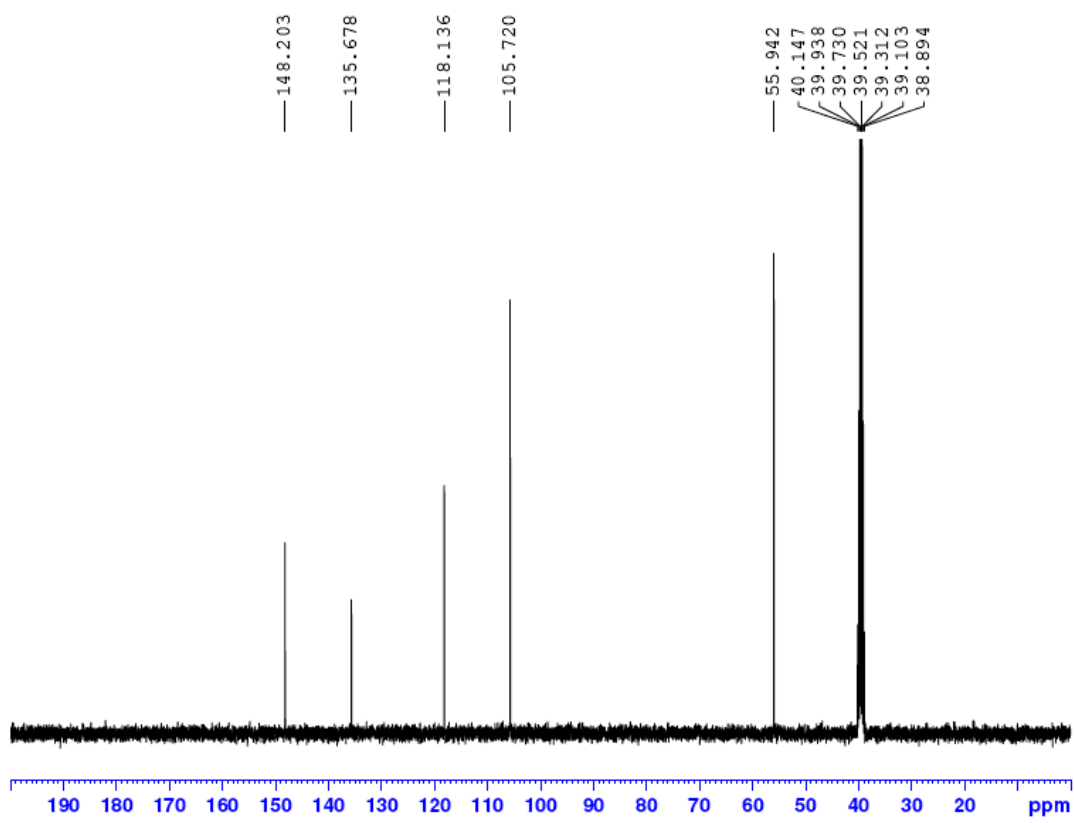
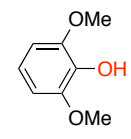


¹H and ¹³C NMR spectra of 2,6-dimethoxyphenol (3e)



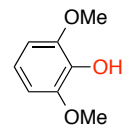
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EXPNO 1
PROCNO 1
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Time 20.24
INSTRUM spect
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 14
DS 2
SWH 9012.820 Hz
FIDRES 0.122286 Hz
AQ 4.081445 sec
RG 101
DM 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
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NUC1 1H
P1 14.50 usec
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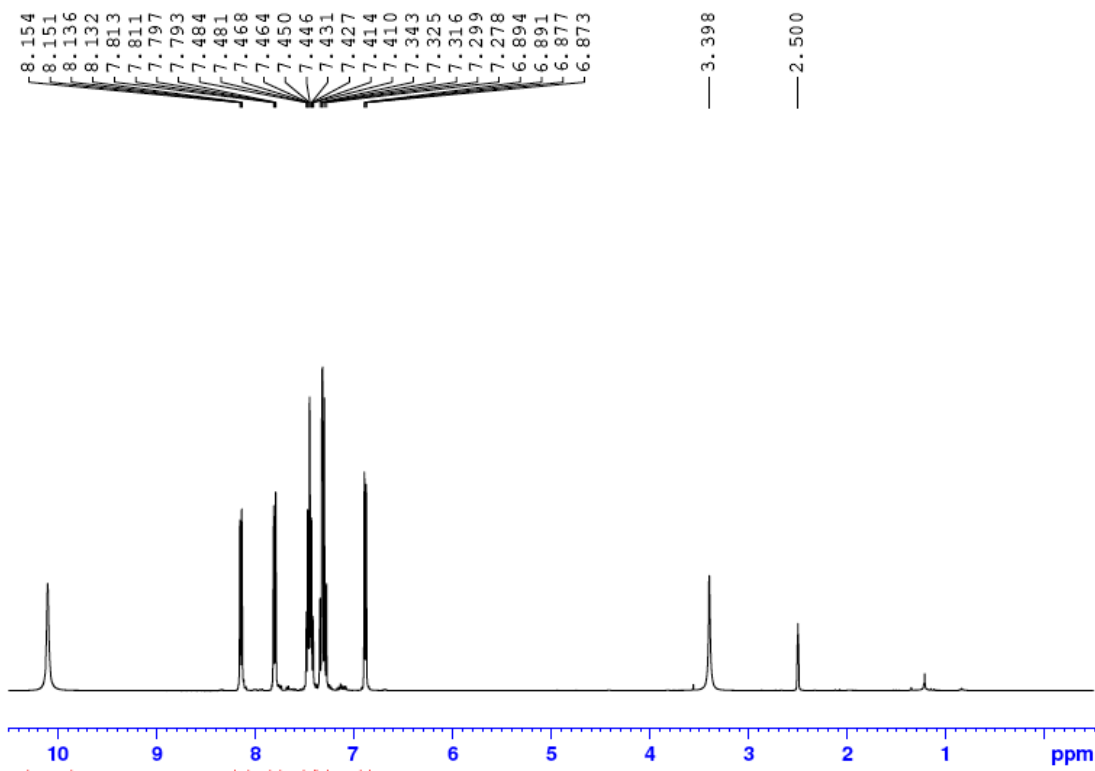


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Current Data Parameters
NAME 06C-VII-1458-np (c13)
EXPNO 1
PROCNO 1
----- Acquisition Parameters
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Time 20.27
INSTRUM spect
PROBHD 5 mm HASTE BBI/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 37
DS 4
SWH 24830.461 Hz
FIDRES 0.368700 Hz
AQ 1.3621480 sec
RG 101
DM 20.000 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
----- CHANNEL f1 -----
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NUC1 13C
P1 15.00 usec
P1M1 44.00000000 W
----- CHANNEL f2 -----
SFO2 400.1314005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
P1M2 10.00000000 W
P1M12 0.23957000 W
P1M13 0.21020001 W
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GB 0
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¹H and ¹³C NMR spectra of naphthalen-1-ol (3f)



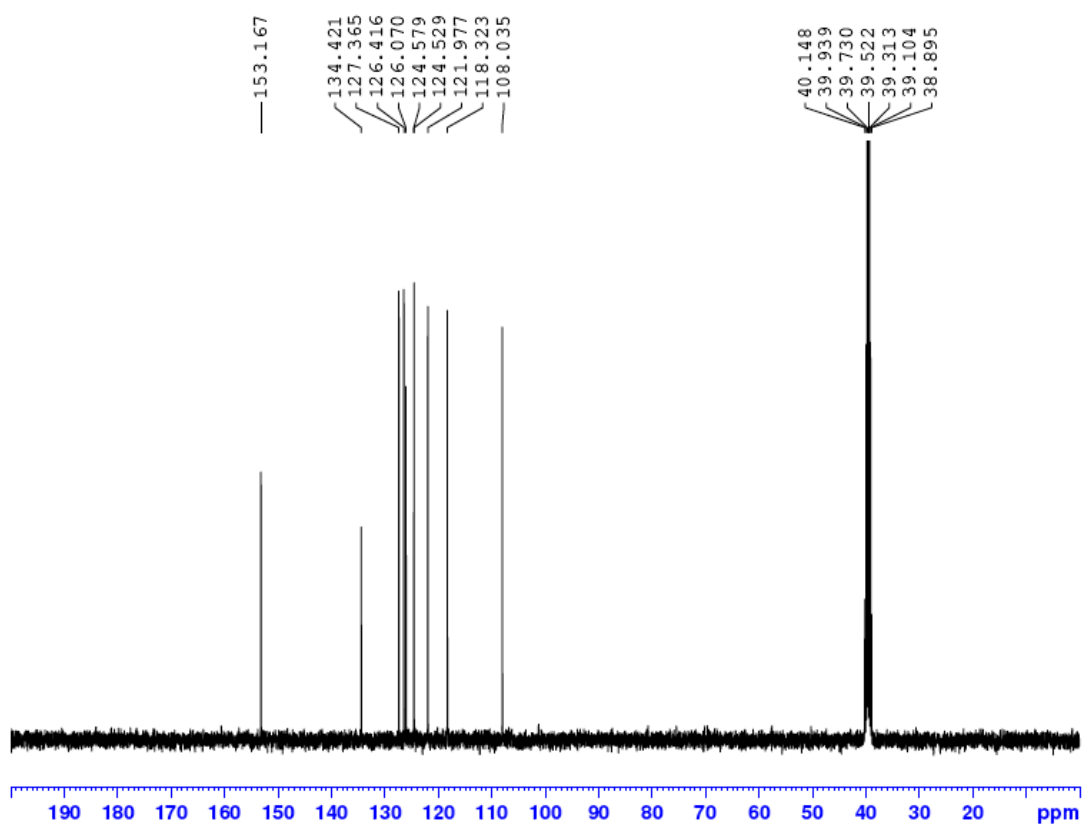
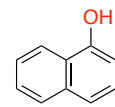
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PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
NS        2
DS        2
SWH       8012.820 Hz
FIDRES    0.122266 Hz
AQ        4.9894465 sec
RG        50.5
DM        62.400 usec
DE        6.50 usec
TE        296.0 K
D1        1.0000000 sec
TD0

===== CHANNEL f1 =====
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NUC1      1H
P1        14.50 usec
PLM1     10.0000000 W

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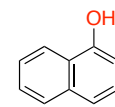
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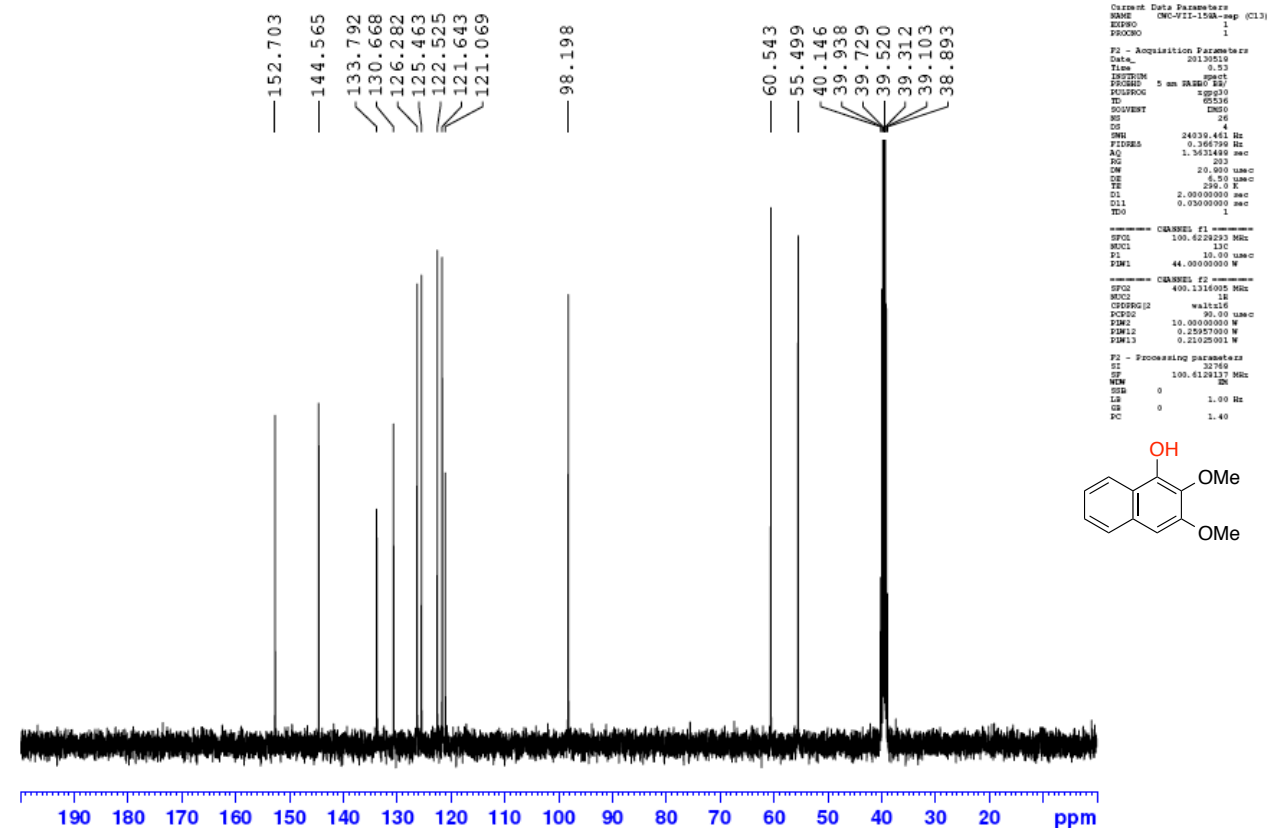
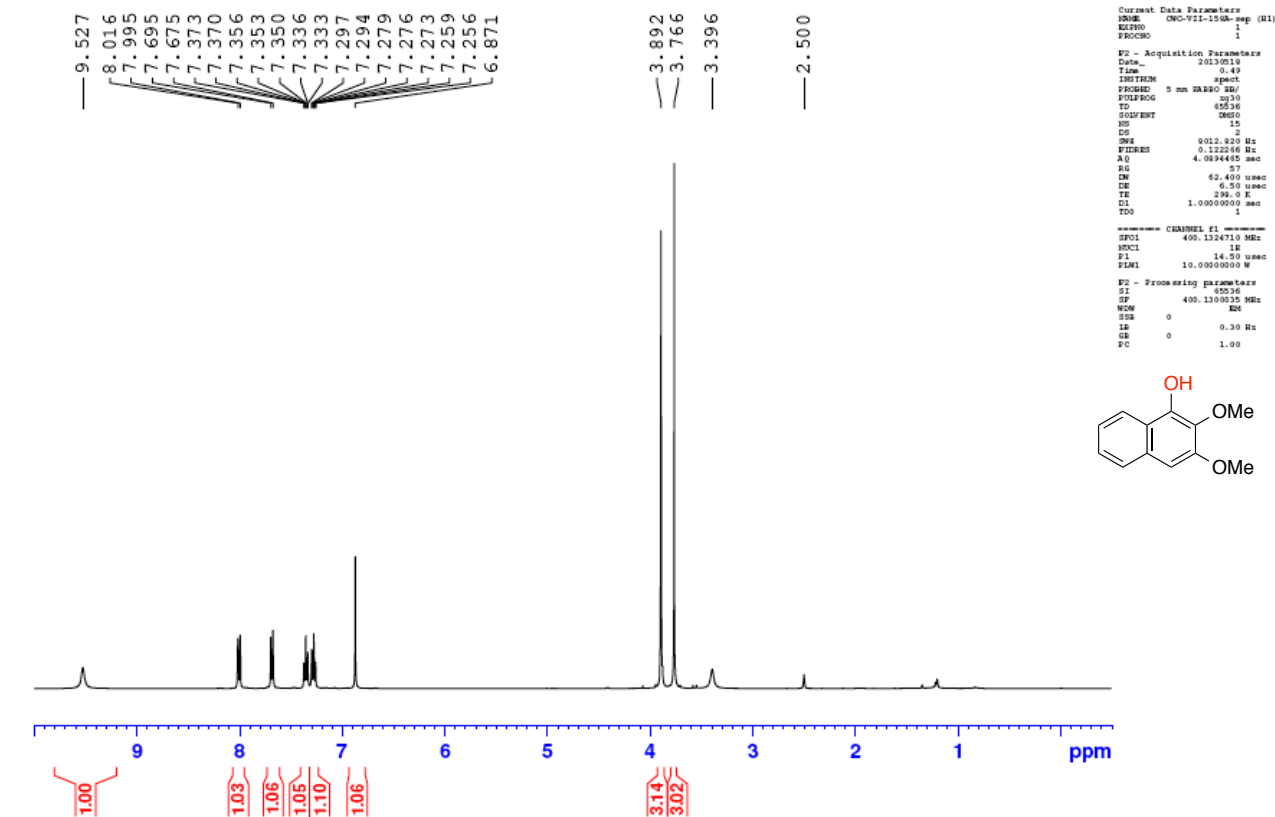
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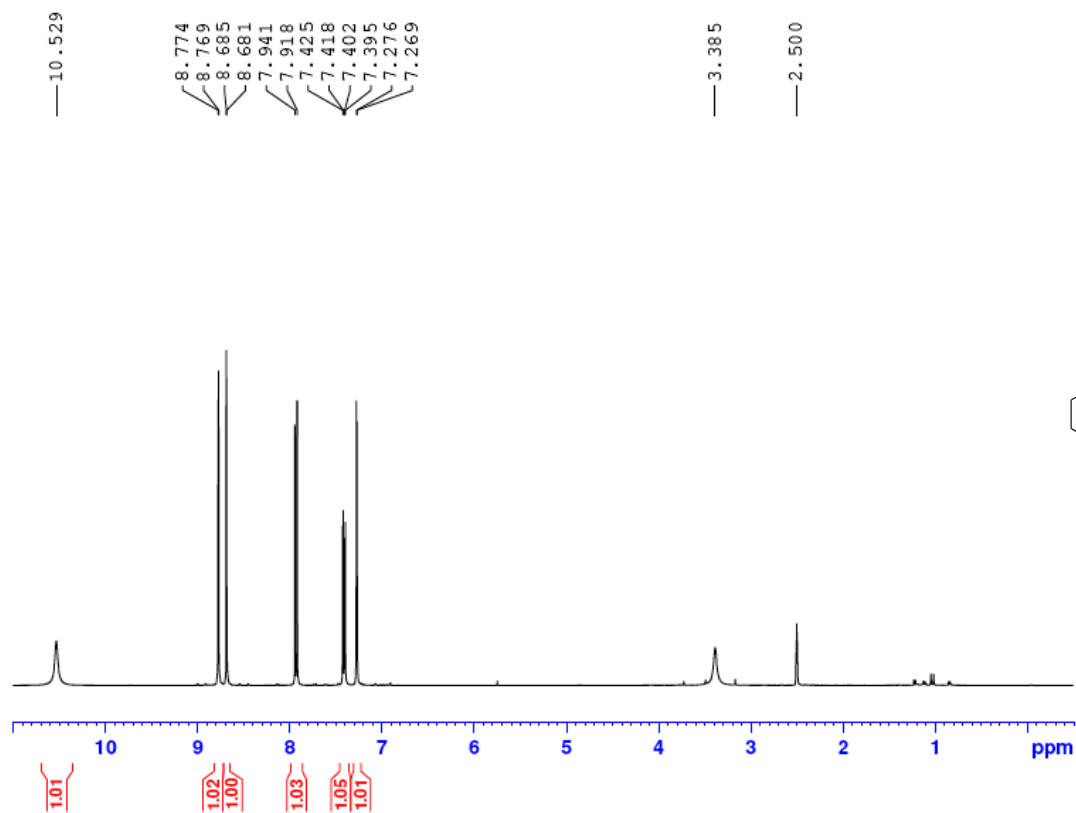
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^1H and ^{13}C NMR spectra of 2,3-dimethoxynaphthalen-1-ol (3g)



^1H and ^{13}C NMR spectra of quinoxalin-6-ol (3h)



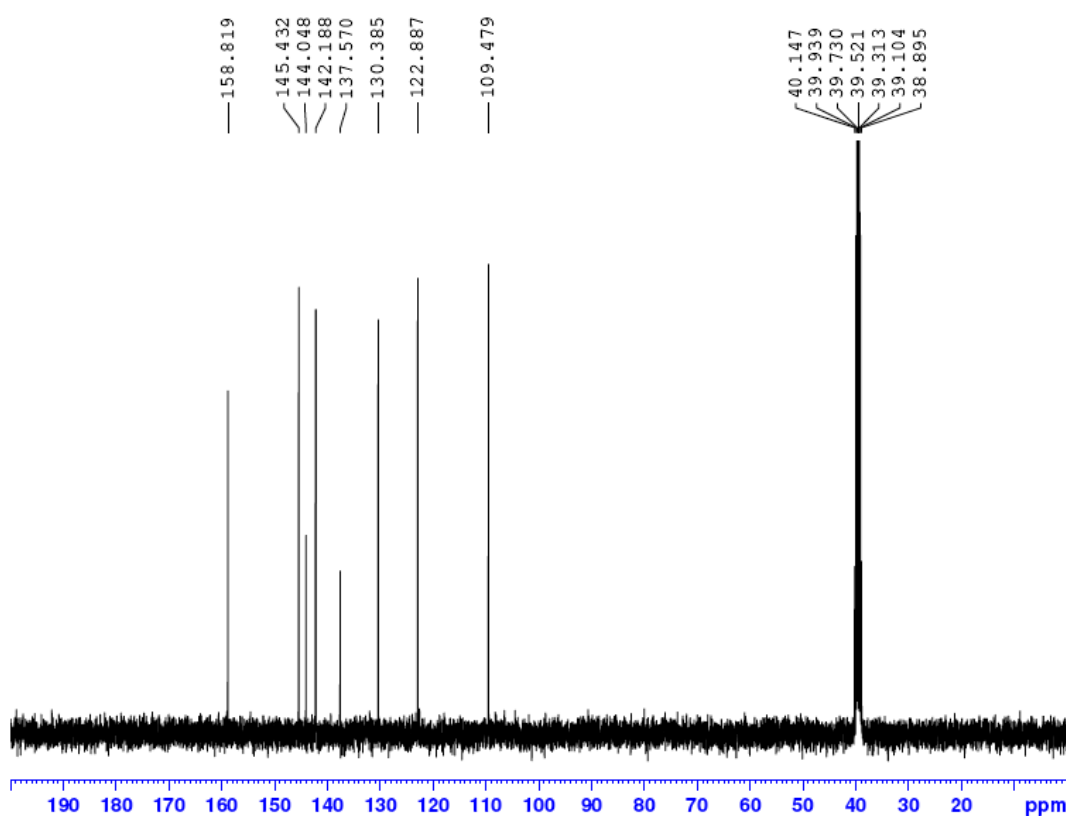
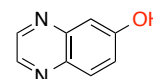
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PROCNO   1

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PULPROG  zg30
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DS        2
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FIDRES   0.122266 Hz
AQ        4.0924465 sec
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TE        298.0 K
DQ        1.00000000 sec
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NUC1     1H
P1        14.50 umsec
PL1      10.00000000 W

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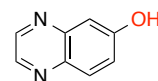
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RG        203
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DE        6.00 umsec
TE        298.0 K
DQ        2.00000000 sec
TD0       1

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NUC1     13C
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SFO2     400.1314005 MHz
NUC2     1H
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SFO3     100.6129140 MHz
NUC3     13C
===== CHANNEL f4 =====
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NUC4     13C

F2 - Processing parameters
SI        65536
SF        100.6129140 MHz
WDW       EM
SS        0
LB        1.00 Hz
GB        0
PC        1.40
    
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¹H and ¹³C NMR spectra of 1-benzyl-1H-indol-6-ol (3i)

8.993
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7.325
7.322
7.318
7.304
7.301
7.285
7.267
7.259
7.254
7.251
7.242
7.236
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7.214
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7.161
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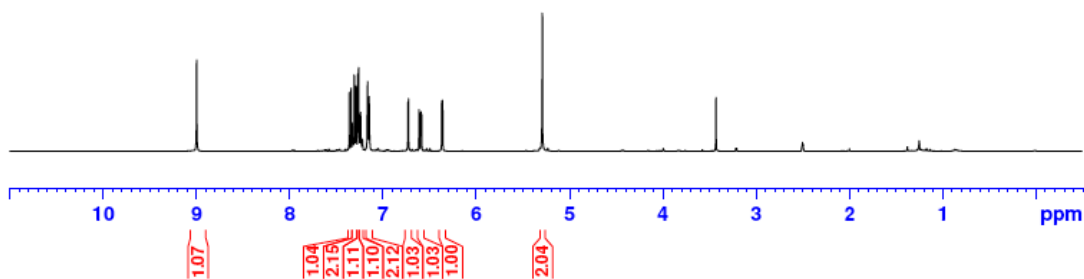
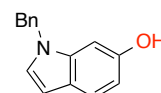
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PROCNO  1

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DE  2
SWH  9012.820 Hz
FIDRES  0.122246 Hz
AQ  4.094445 sec
RG  32
IN  62.400 usec
DE  6.50 usec
TE  298.0 K
D1  1.00000000 sec
TD0  1

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NUC1  1H
P1  14.50 usec
PL1  10.00000000 W

F2 - Processing parameters
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WDW  EM
SSB  0
LB  0.30 Hz
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PC  1.00
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136.891
128.508
127.348
127.218
126.830
121.642
120.884
109.742
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40.147
39.939
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39.522
39.313
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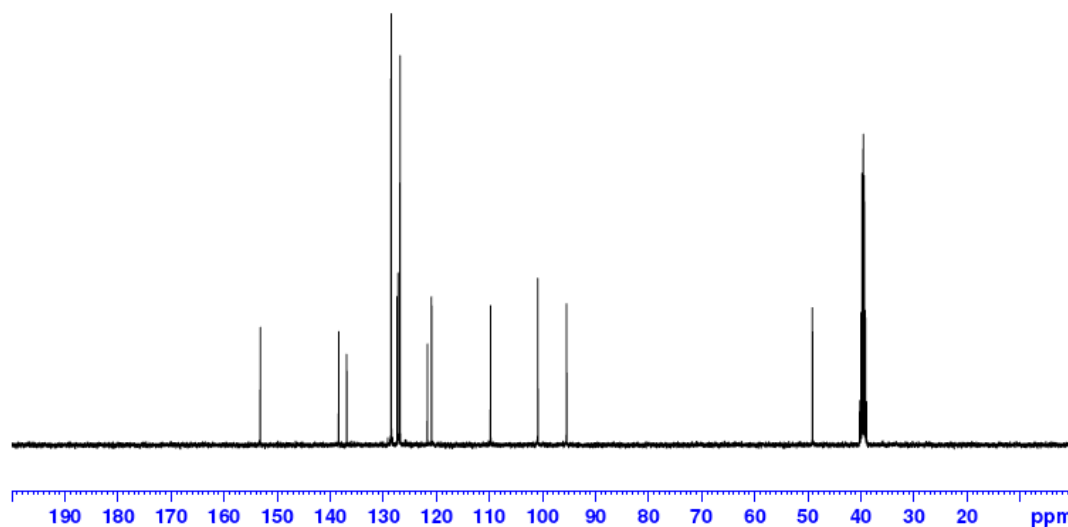
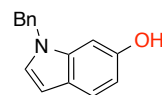
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EXPNO  1
PROCNO  1

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PULPROG  zgpg30
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DE  24038.444 Hz
FIDRES  0.366790 Hz
AQ  1.3621460 sec
RG  203
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DE  6.50 usec
TE  298.0 K
D1  2.00000000 sec
D11  0.03000000 sec
TD0  1

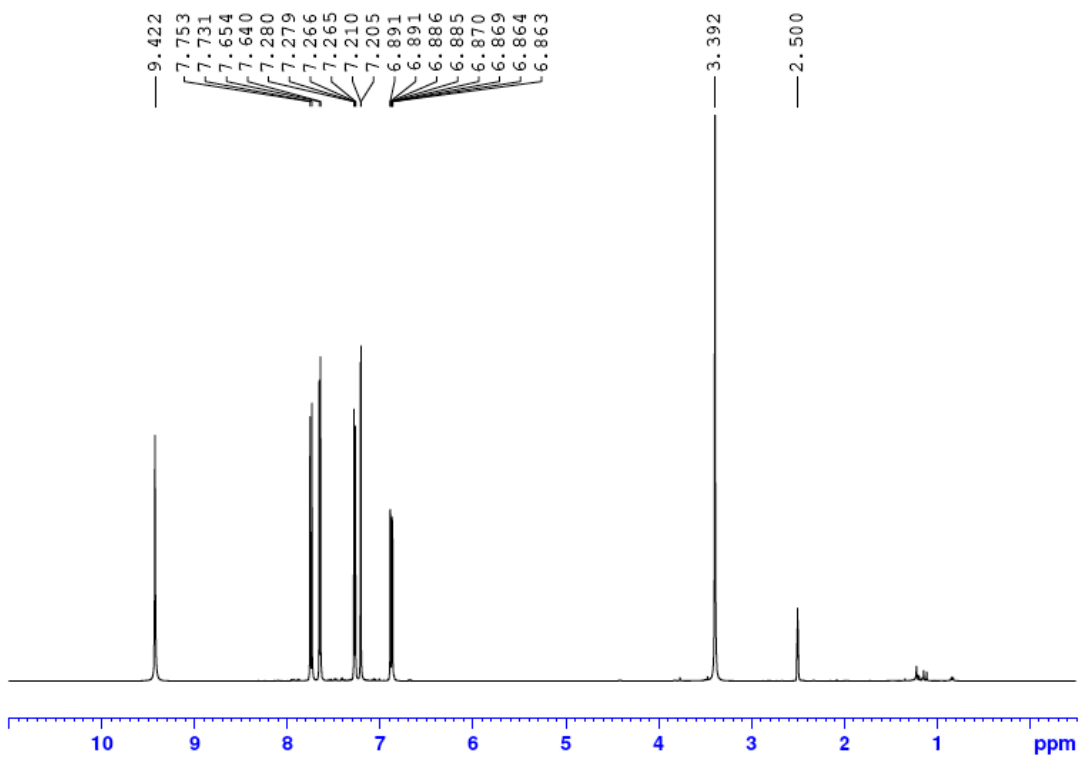
===== CHANNELS f1 =====
SFO1  100.6228293 MHz
NUC1  13C
P1  10.50 usec
PL1  44.00000000 W

===== CHANNELS f2 =====
SFO2  400.1316095 MHz
NUC2  1H
===== CHANNELS f3 =====
SFO3  90.480 usec
===== CHANNELS f4 =====
SFO4  0.25957000 W
===== CHANNELS f5 =====
SFO5  0.21029011 W

F2 - Processing parameters
SI  32768
SF  100.6181264 MHz
WDW  EM
SSB  0
LB  1.00 Hz
GB  0
PC  1.40
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¹H and ¹³C NMR spectra of benzothiophen-5-ol (3j)



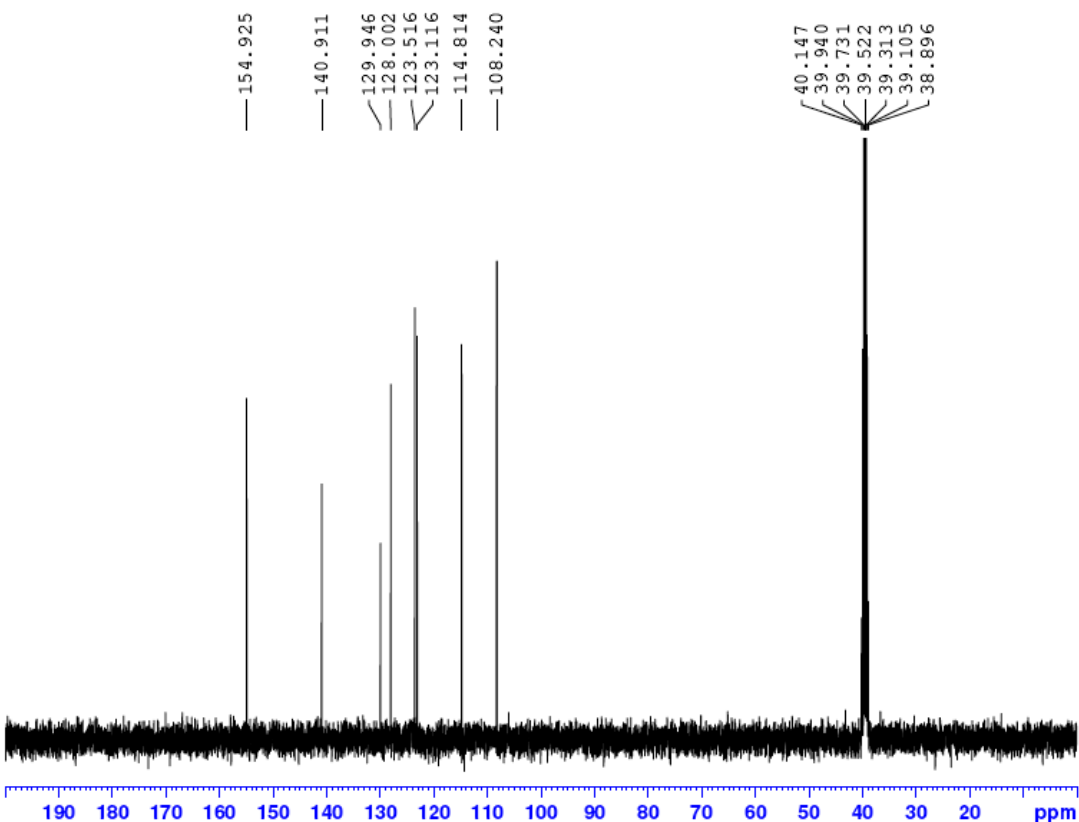
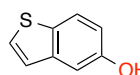
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Current Data Parameters
NAME      CMC-VII-118a-np (H1)
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20130524
Time     0.39
INSTRUM  spect
PROBHD   5 mm HASTE 5H/
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
DS        4
DE        2
OH1      9012.820 Hz
FIDRES   0.122266 Hz
AQ       4.0294415 sec
RG        114
IN       62.400 usec
DE       6.50 usec
TE       298.0 K
D1       1.00000000 sec
TD0      1

===== CHANNEL f1 =====
SFO1     400.1324710 MHz
NUC1     1H
P1       14.50 usec
P1M1     10.00000000 W

F2 - Processing parameters
SI       32768
SF       400.1300030 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
    
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```

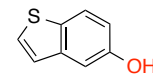
Current Data Parameters
NAME      CMC-VII-118a-np (C13)
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20130523
Time     1.06
INSTRUM  spect
PROBHD   5 mm HASTE 5H/
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
DS        4
DE        2
OH1      24039.461 Hz
FIDRES   0.366790 Hz
AQ       1.3021490 sec
RG        233
IN       20.000 usec
DE       6.50 usec
TE       298.1 K
D1       2.00000000 sec
D11      0.03000000 sec
TD0      1

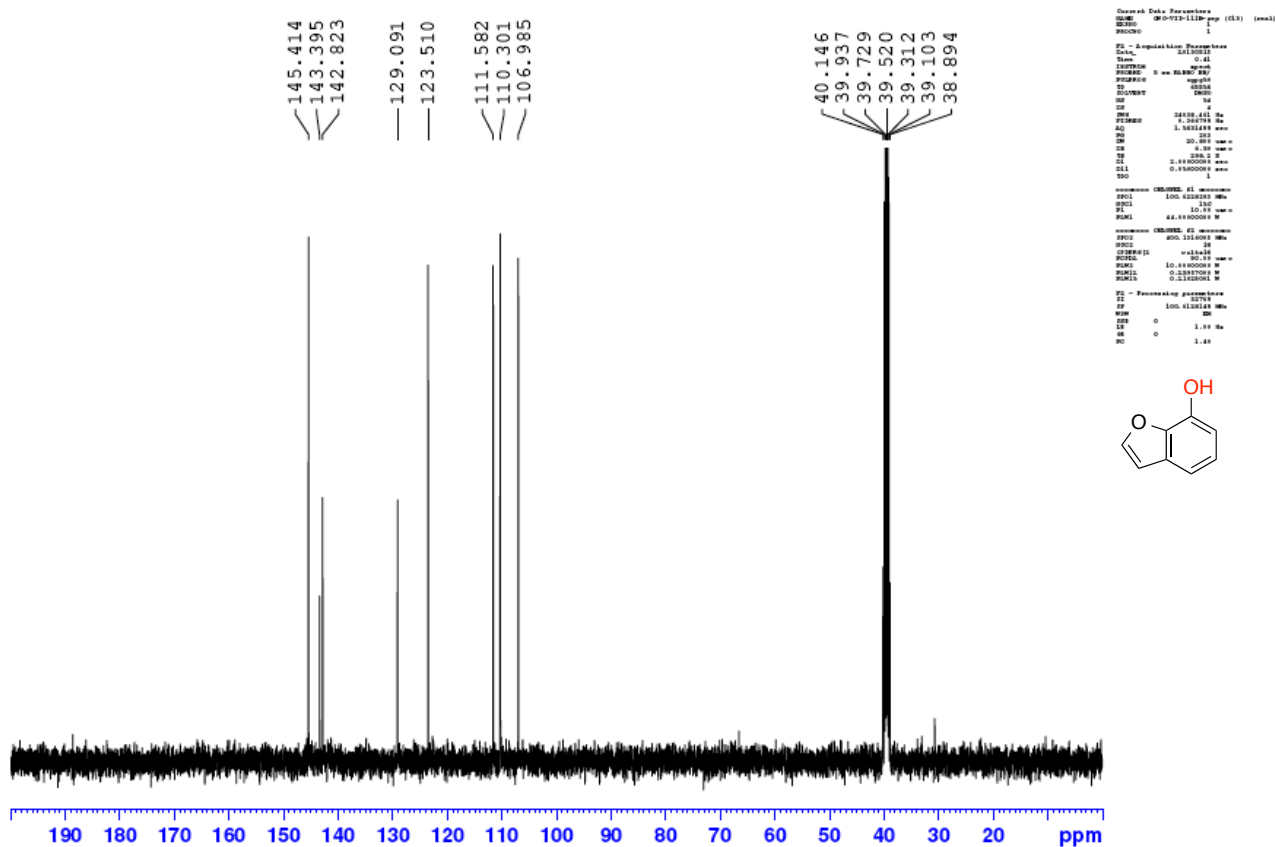
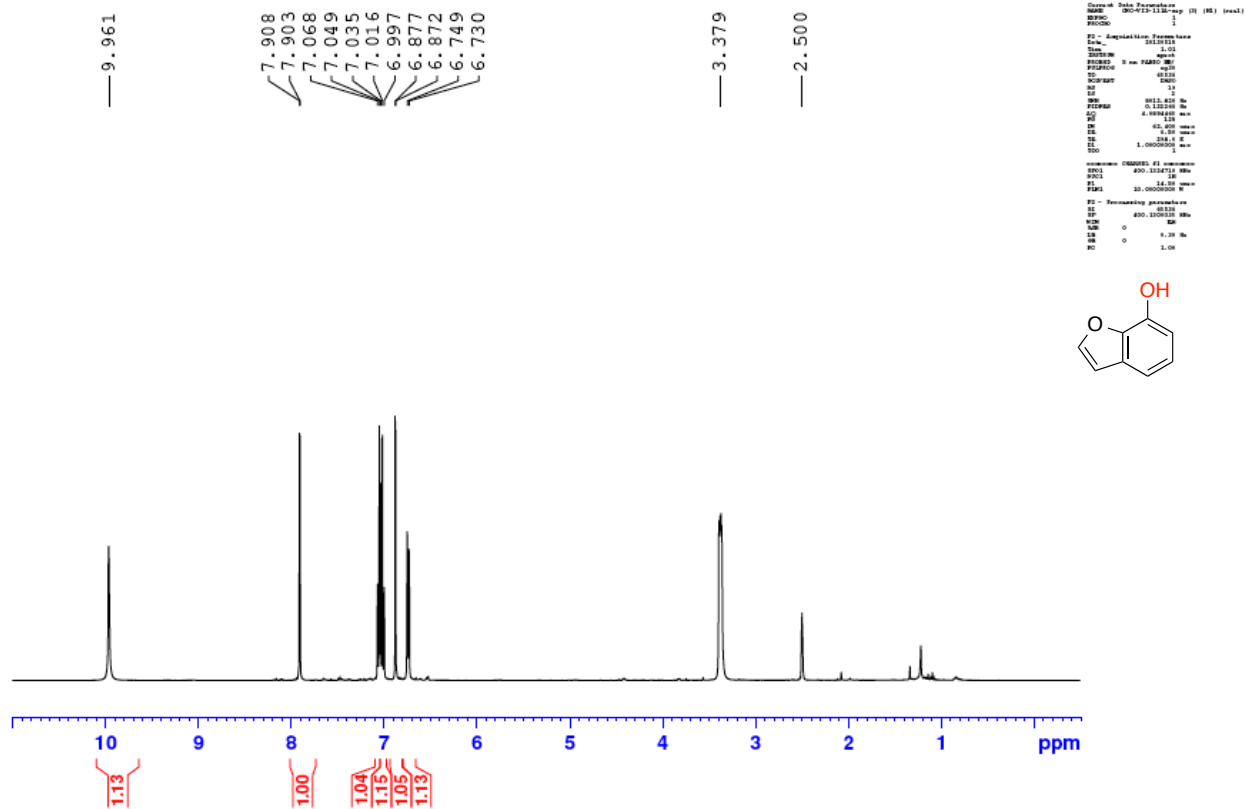
===== CHANNEL f1 =====
SFO1     100.6229250 MHz
NUC1     13C
P1       10.00 usec
P1M1     44.00000000 W

===== CHANNEL f2 =====
SFO2     400.1316005 MHz
NUC2     1H
CPDPRG2  waltz16
P2       90.00 usec
P2M2     10.00000000 W
P2M12    0.25957000 W
P2M13    0.21025001 W

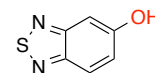
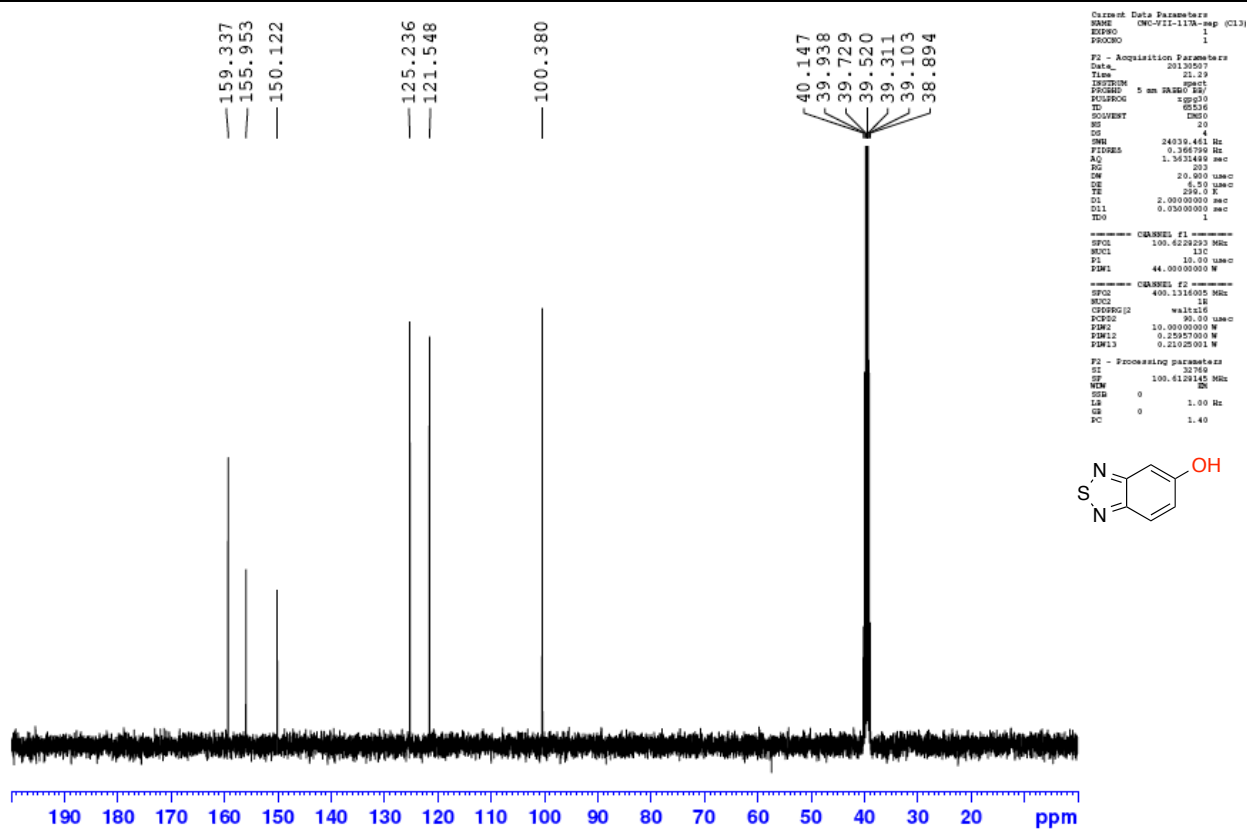
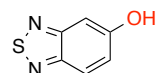
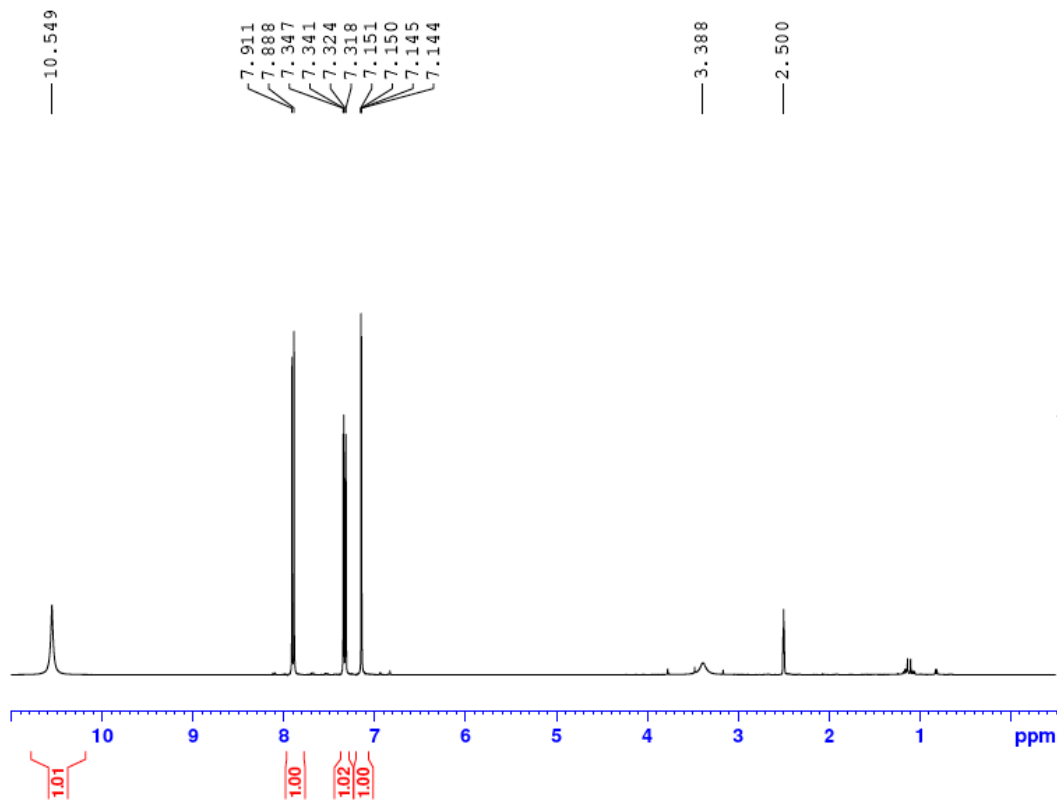
F2 - Processing parameters
SI       32768
SF       100.6128092 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
    
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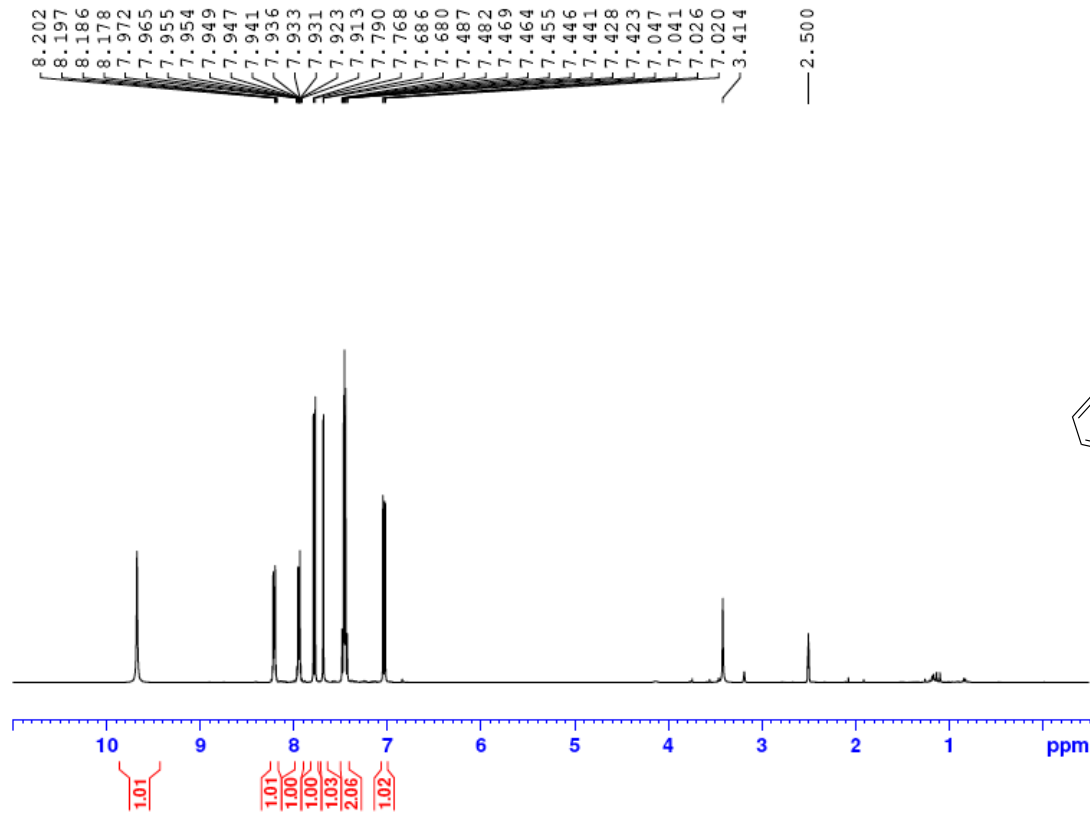
¹H and ¹³C NMR spectra of benzofuran-7-ol (3k)



¹H and ¹³C NMR spectra of benzo-2,1,3-thiadiazol-5-ol (3l)

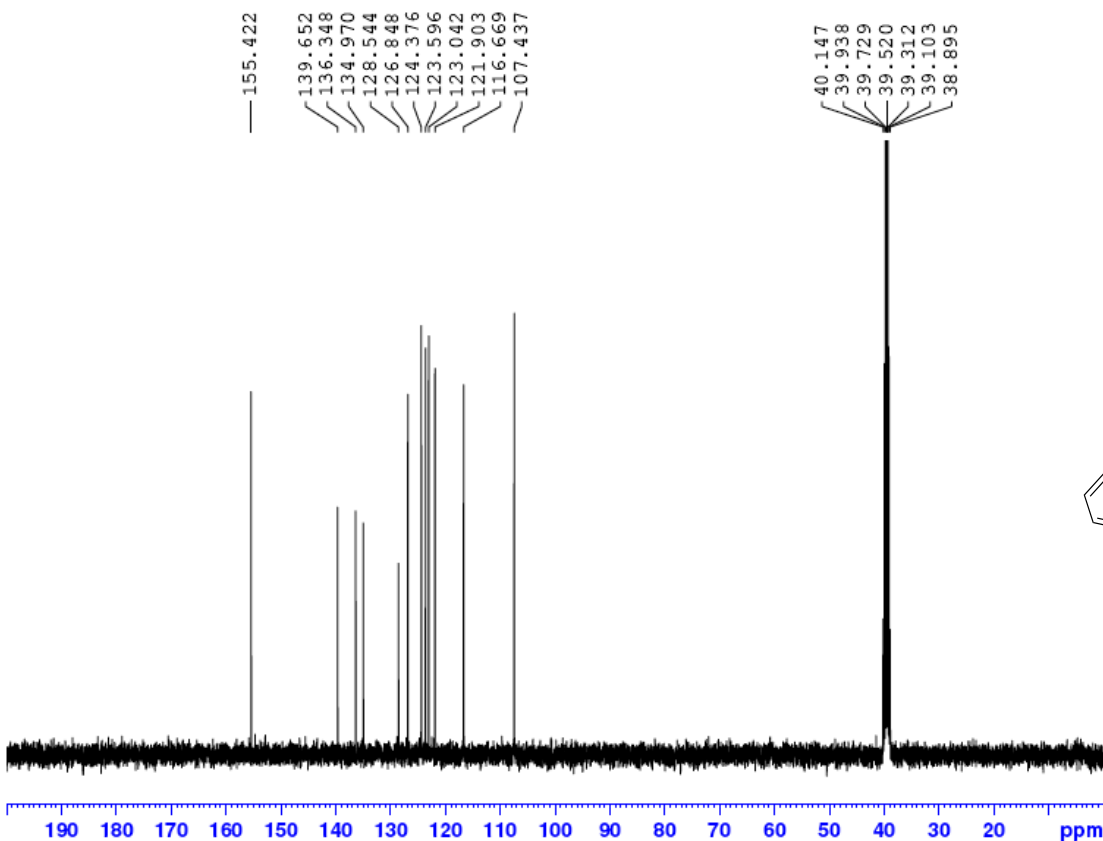
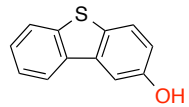


¹H and ¹³C NMR spectra of dibenzothiophen-2-ol (3m)



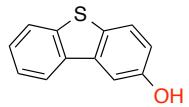
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Current Data Parameters
NAME      OMC-VII-112A-exp (H1)
EXPNO    1
PROCNO   1
F2 - Acquisition Parameters
Date_    20130112
Time     0.30
INSTRUM  spect
PROBHD   5 mm BBO-500
PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       19
DS       4
SWH      8011.875 Hz
FIDRES   0.122266 Hz
AQ       4.094445 sec
RG       101
DM       62.400 usec
DE       6.50 usec
TE       298.2 K
DQ       1.0000000 sec
TD0      1
===== CHANNEL f1 =====
SFO1     400.132410 MHz
NUC1     1H
P1       13.12 usec
PL1      15.0000000 W
F2 - Processing parameters
SI       65536
SF       400.130030 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
  
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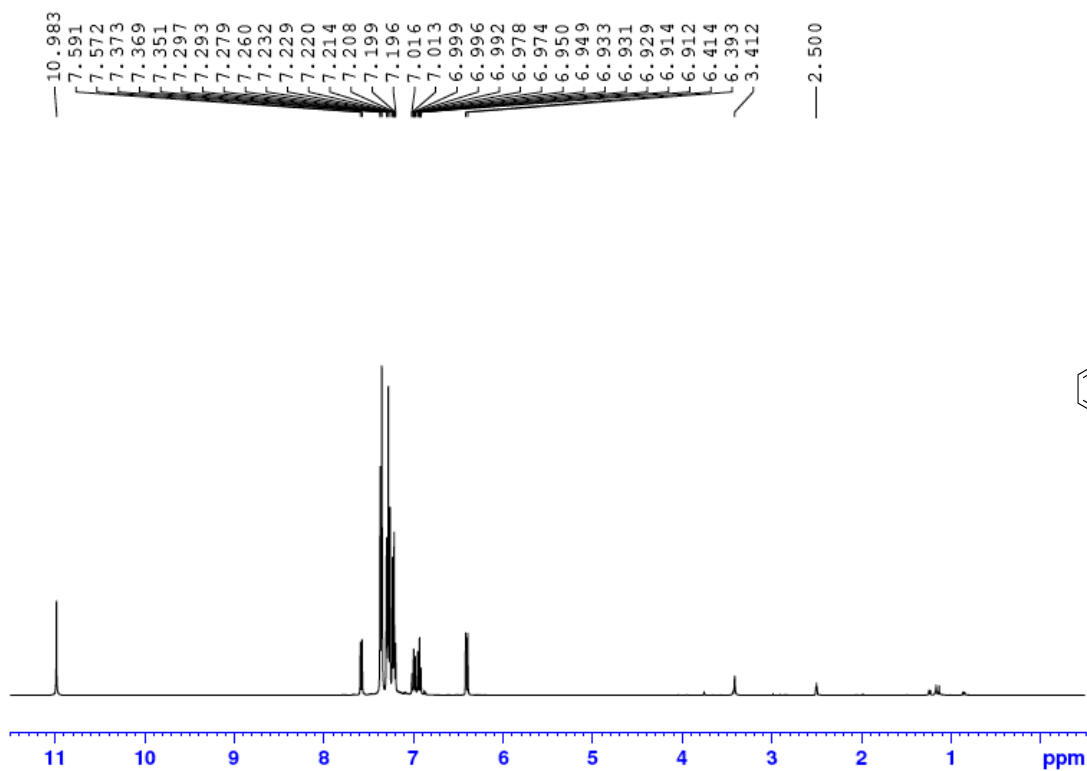


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Current Data Parameters
NAME      OMC-VII-112A-exp (C13)
EXPNO    1
PROCNO   1
F2 - Acquisition Parameters
Date_    20130512
Time     0.34
INSTRUM  spect
PROBHD   5 mm BBO-500
PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       19
DS       4
SWH      24030.461 Hz
FIDRES   0.366790 Hz
AQ       1.563160 sec
RG       203
DM       20.900 usec
DE       6.50 usec
TE       297.3 K
DQ       2.0000000 sec
D11      0.0300000 sec
TD0      1
===== CHANNEL f1 =====
SFO1     100.6228293 MHz
NUC1     13C
P1       10.00 usec
PL1      49.0000000 W
F2 - Processing parameters
SI       65536
SF       100.6128145 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
  
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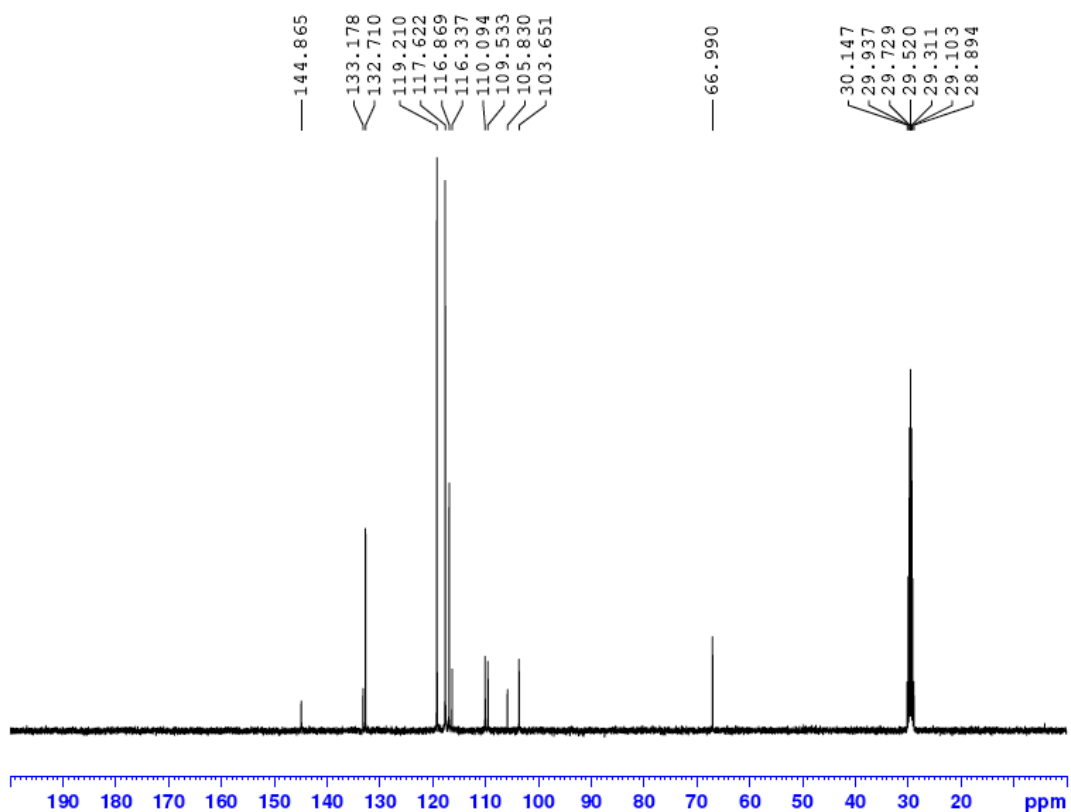
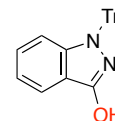


¹H and ¹³C NMR spectra of 1-trityl-1H-indazol-3-ol (3n)



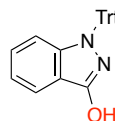
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Current Data Parameters
NAME  CMC-111-1418-imp (3) (1)
EXPNO  1
PROCNO  1
F2 - Acquisition Parameters
Date_  20130514
Time  17:03:47
INSTRUM  spect
PROBHD  5 mm BBO-1H/
PULPROG  zgpg30
TD  65536
SOLVENT  DMSO
DS  11
SFO  400.142000 MHz
FIDRES  0.122245 Hz
AQ  1.180148 sec
RG  327
SF  400.142000 MHz
AQ  1.180148 sec
DE  4.50 umec
TE  298.0 K
DQ  1.99000000 sec
SFO  400.142000 MHz
===== CHANNEL f1 =====
NUC1  13C
P1  12.00 umec
SFO1  101.625300 MHz
===== CHANNEL f2 =====
NUC2  1H
P2  4.00 umec
SFO2  400.142000 MHz
===== CHANNEL f3 =====
NUC3  1H
P3  0.30 sec
SFO3  0.000000 MHz
===== CHANNEL f4 =====
NUC4  13C
P4  0.30 sec
SFO4  0.000000 MHz
  
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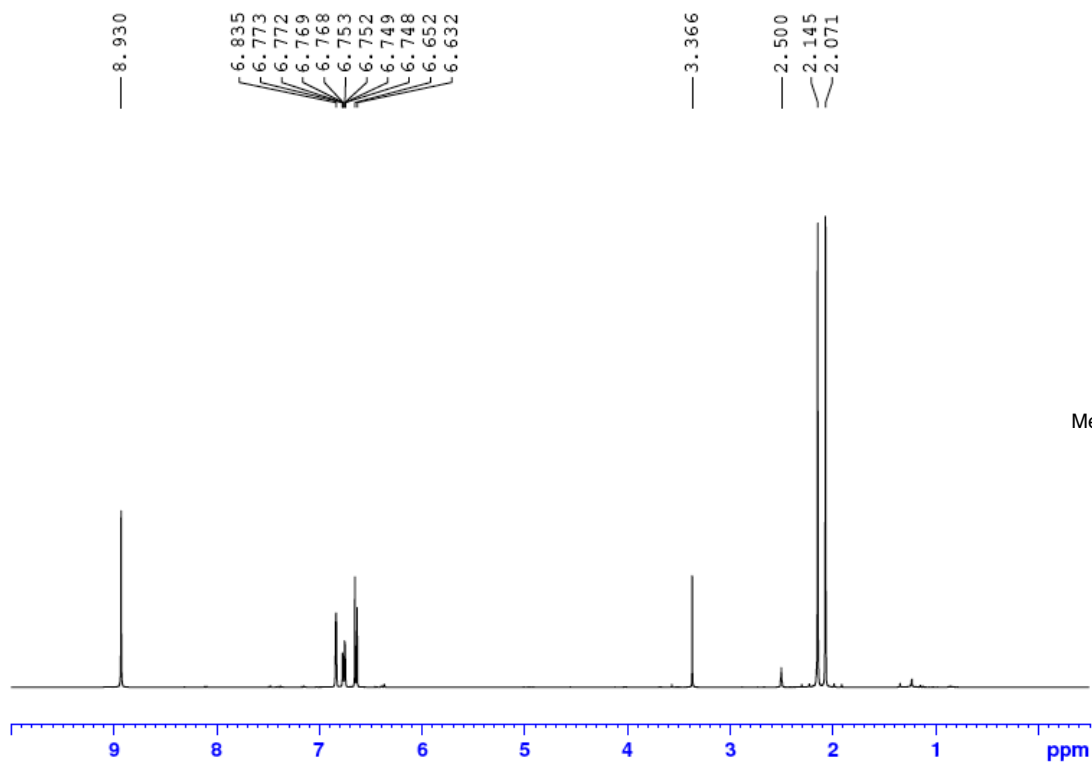


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Current Data Parameters
NAME  CMC-111-1418-imp (3) (1)
EXPNO  1
PROCNO  1
F2 - Acquisition Parameters
Date_  20130514
Time  17:03:47
INSTRUM  spect
PROBHD  5 mm BBO-1H/
PULPROG  zgpg30
TD  65536
SOLVENT  DMSO
DS  11
SFO  400.142000 MHz
FIDRES  0.122245 Hz
AQ  1.180148 sec
RG  327
SF  400.142000 MHz
AQ  1.180148 sec
DE  4.50 umec
TE  298.0 K
DQ  1.99000000 sec
SFO  400.142000 MHz
===== CHANNEL f1 =====
NUC1  13C
P1  12.00 umec
SFO1  101.625300 MHz
===== CHANNEL f2 =====
NUC2  1H
P2  4.00 umec
SFO2  400.142000 MHz
===== CHANNEL f3 =====
NUC3  1H
P3  0.30 sec
SFO3  0.000000 MHz
===== CHANNEL f4 =====
NUC4  13C
P4  0.30 sec
SFO4  0.000000 MHz
  
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¹H and ¹³C NMR spectra of 2,4-dimethylphenol (5a)



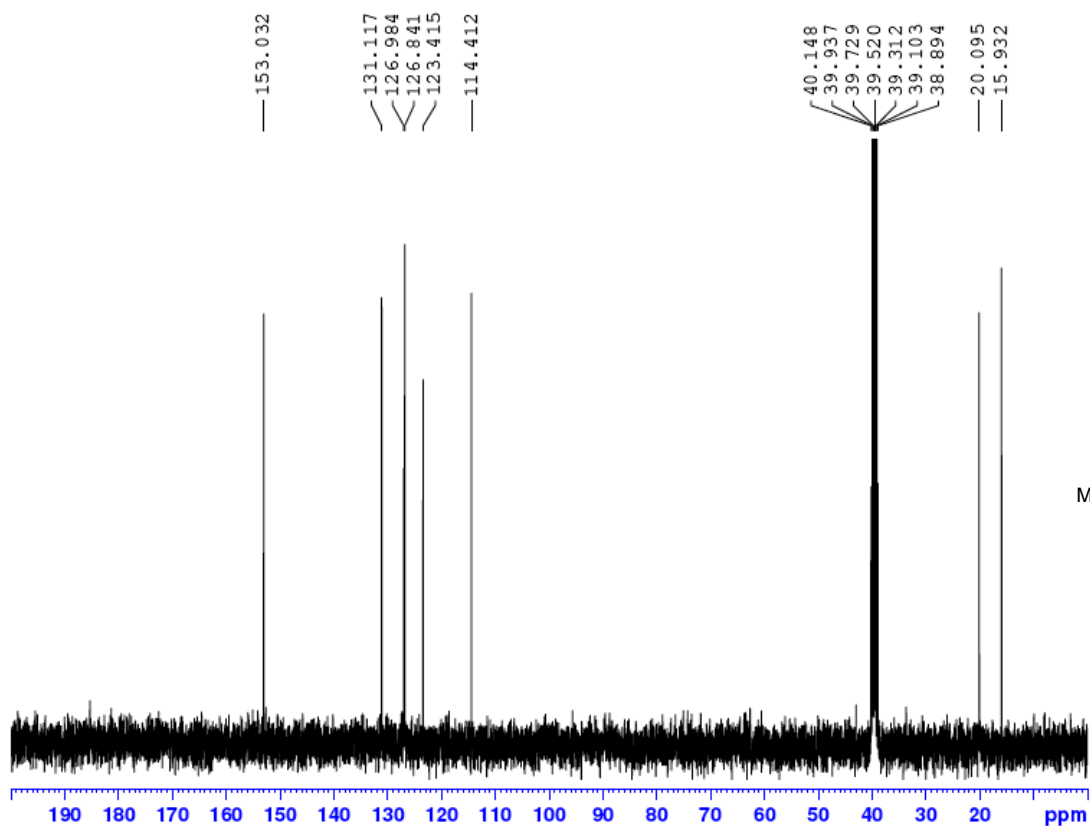
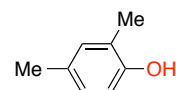
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Current Data Parameters
NAME  CMC-VII-167b-np (H1)
EXPNO  1
PROCNO  1

F2 - Acquisition Parameters
Date_  20130520
Time  14:30
INSTRUM  spect
PROBHD  5 mm BBOBO BBI/
PULPROG  zgpg30
TD  65536
SOLVENT  DMSO
NS  2
DS  2
SWH  9012.830 Hz
FIDRES  0.132266 Hz
AQ  4.0934485 sec
RG  30.5
IN  65.400 usec
DE  6.50 usec
TE  299.0 K
D1  1.0000000 sec
TD0  1

===== CHANNEL f1 =====
SFO1  400.132410 MHz
NUC1  1H
P1  13.12 usec
PLM1  15.0000000 W

F2 - Processing parameters
SI  400.130930 MHz
SF  400.130930 MHz
NOM  8M
SSB  0
LB  8M
GB  0
PC  1.00
    
```



```

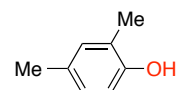
Current Data Parameters
NAME  CMC-VII-167b-np (C13)
EXPNO  1
PROCNO  1

F2 - Acquisition Parameters
Date_  20130520
Time  14:54
INSTRUM  spect
PROBHD  5 mm BBOBO BBI/
PULPROG  zgpg30
TD  65536
SOLVENT  DMSO
NS  2
DS  2
SWH  24039.461 Hz
FIDRES  0.366790 Hz
AQ  1.363488 sec
RG  20.0
IN  20.000 usec
DE  6.50 usec
TE  299.0 K
D1  2.0000000 sec
D11  0.0500000 sec
TD0  1

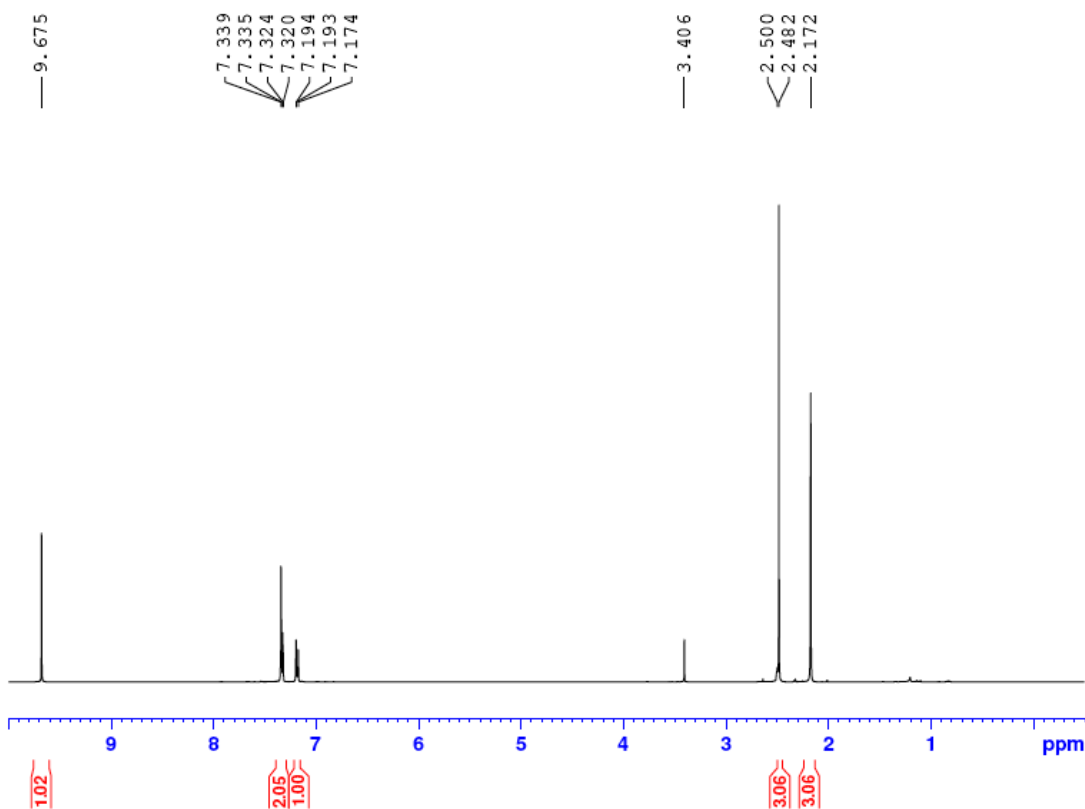
===== CHANNEL f1 =====
SFO1  100.622920 MHz
NUC1  13C
P1  15.00 usec
PLM1  49.0000000 W

===== CHANNEL f2 =====
SFO2  400.1316000 MHz
NUC2  1H
CPDPRG2  waltz16
PCPD2  90.00 usec
PDM2  15.0000000 W
PDM12  0.21019999 W
PDM13  0.25019999 W

F2 - Processing parameters
SI  100.6120144 MHz
SF  100.6120144 MHz
NOM  8M
SSB  0
LB  1.00 Hz
GB  0
PC  1.40
    
```

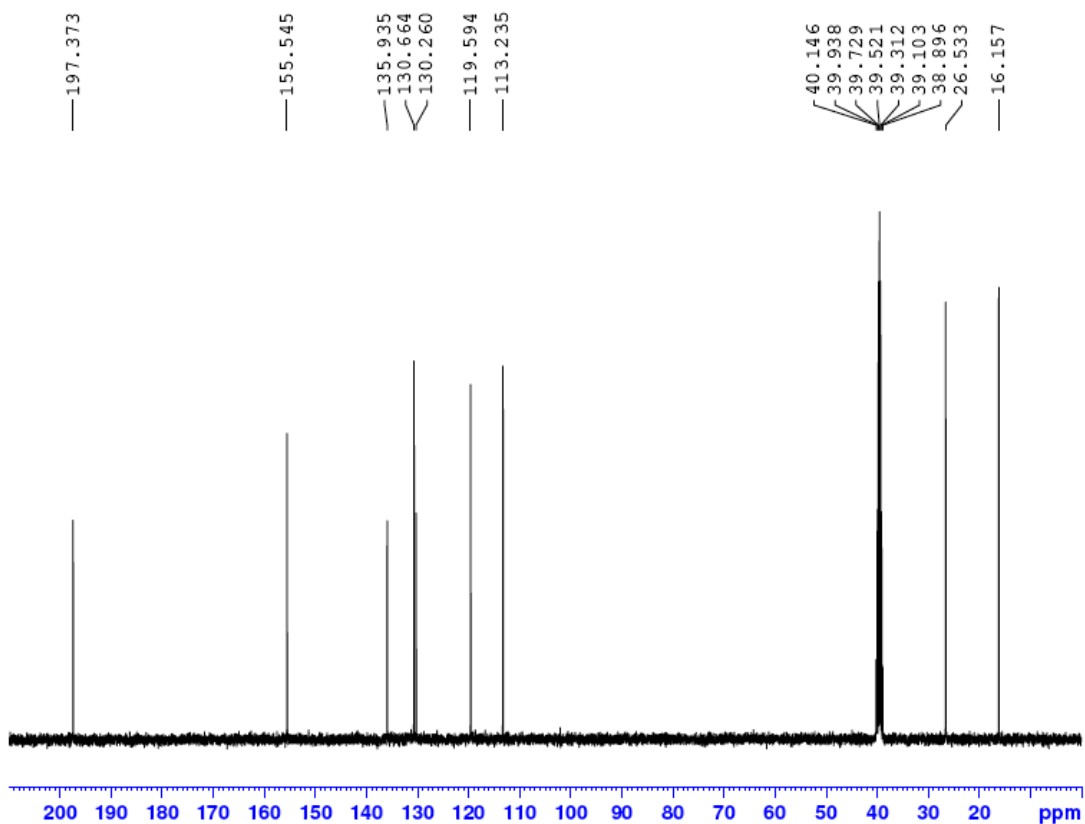
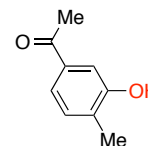


¹H and ¹³C NMR spectra of 3'-hydroxy-4'-methylacetophenone (5b)



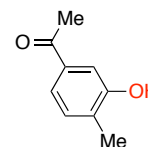
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Current Data Parameters
NAME 09C-VII-173A-exp (H1)
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130229
Time 16.00
INSTRUM spect
PROBHD 5 mm BBOBO 4B/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 23
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.094465 sec
RG 64
DM 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.0000000 sec
TD0 1
===== CHANNEL f1 =====
SFO1 400.124710 MHz
NUC1 1H
P1 13.12 usec
PLW1 15.0000000 W
F2 - Processing parameters
SI 65536
SF 400.130031 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
    
```

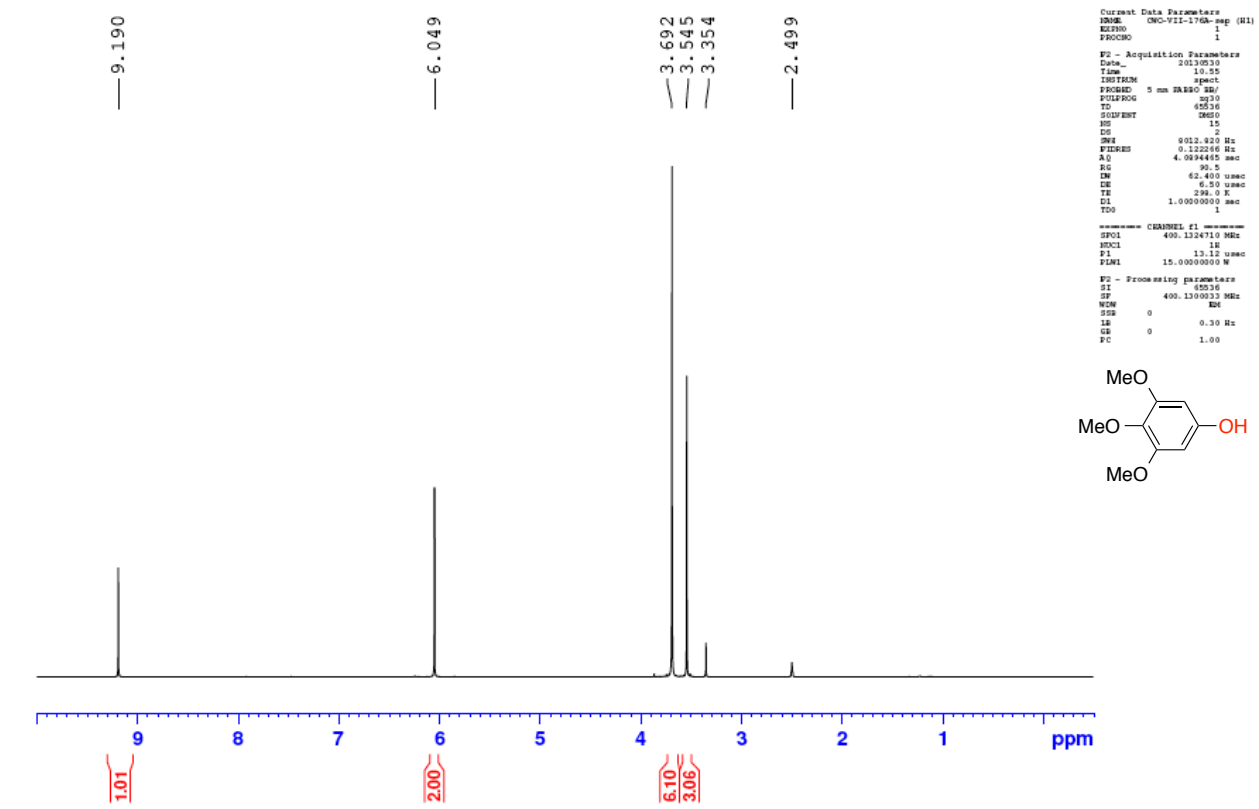


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Current Data Parameters
NAME 09C-VII-173A-exp (C13)
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130229
Time 16.00
INSTRUM spect
PROBHD 5 mm BBOBO 4B/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4
DS 4
SWH 24030.440 Hz
FIDRES 0.368798 Hz
AQ 1.5631480 sec
RG 203
DM 20.900 usec
DE 6.50 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 47.0000000 W
===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
PCPRG2 waltz16
PULPROG 15.0000000 W
PLW2 0.3187899 W
PLW3 0.2501399 W
F2 - Processing parameters
SI 32768
SF 100.6128110 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
    
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¹H and ¹³C NMR spectra of 3,4,5-trimethoxyphenol (5c)



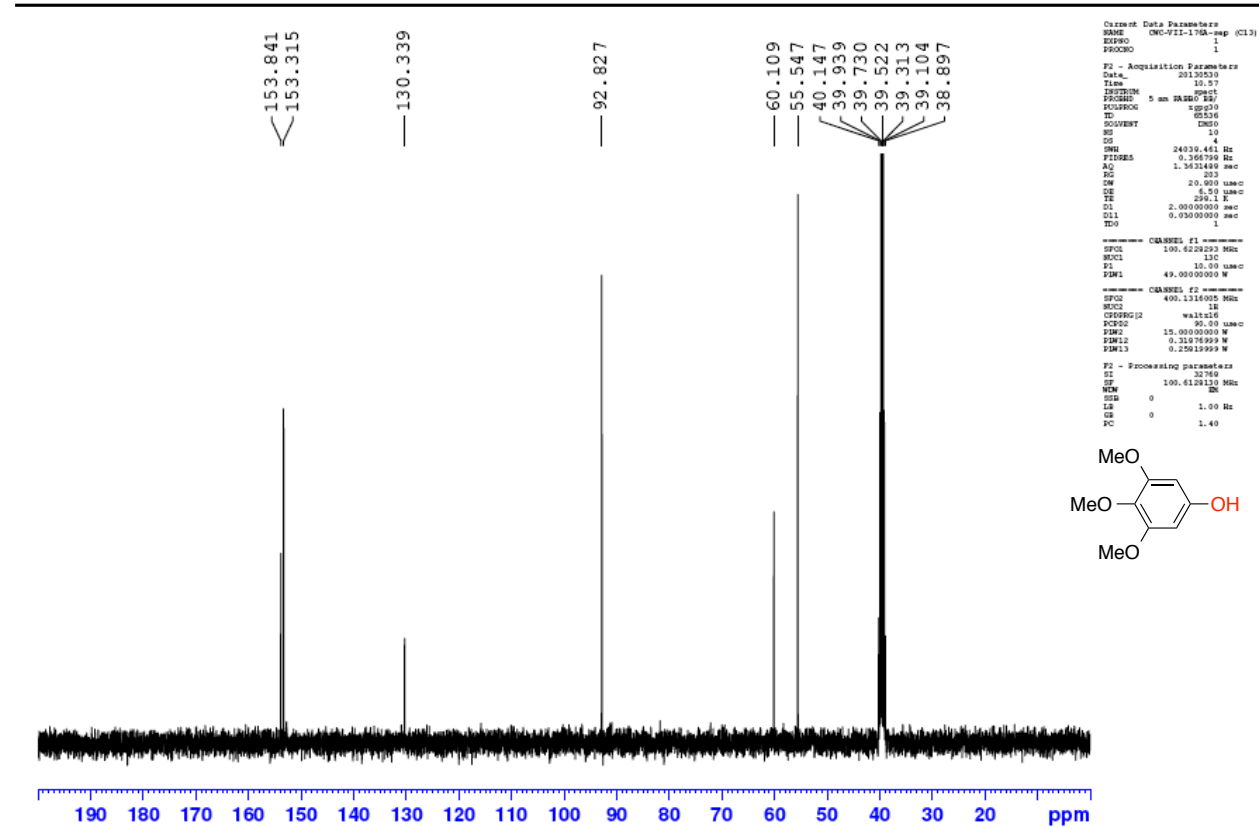
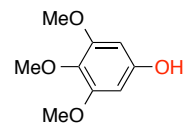
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Current Data Parameters
NAME  CMC-VII-176A-exp (H1)
EXPNO  1
PROCNO  1

F2 - Acquisition Parameters
Date_  20130310
Time  10.55
INSTRUM  spect
PROBHD  5 mm PABBO BBI
PULPROG  zgpg30
TD  65536
SOLVENT  DMSO
NS  15
DS  2
SWH  8012.810 Hz
FIDRES  0.132256 Hz
AQ  4.024445 sec
RG  39.5
DM  62.400 usec
DE  6.50 usec
TE  300.2 K
D1  1.0000000 sec
TD0  1

===== CHANNEL f1 =====
SFO1  400.126410 MHz
NUC1  1H
P1  13.12 usec
PLW1  15.0000000 W

F2 - Processing parameters
SI  32768
SF  400.1300013 MHz
WDW  EM
SSB  0
LB  0.30 Hz
GB  0
PC  1.00
    
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```

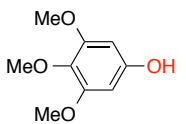
Current Data Parameters
NAME  CMC-VII-176A-exp (C13)
EXPNO  1
PROCNO  1

F2 - Acquisition Parameters
Date_  20130310
Time  10.57
INSTRUM  spect
PROBHD  5 mm PABBO BBI
PULPROG  zgpg30
TD  65536
SOLVENT  DMSO
NS  10
DS  4
SWH  24030.461 Hz
FIDRES  0.350796 Hz
AQ  1.3432489 sec
RG  203
DM  20.000 usec
DE  4.00 usec
TE  299.1 K
D1  2.0000000 sec
D11  0.0300000 sec
TD0  1

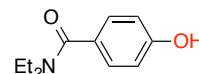
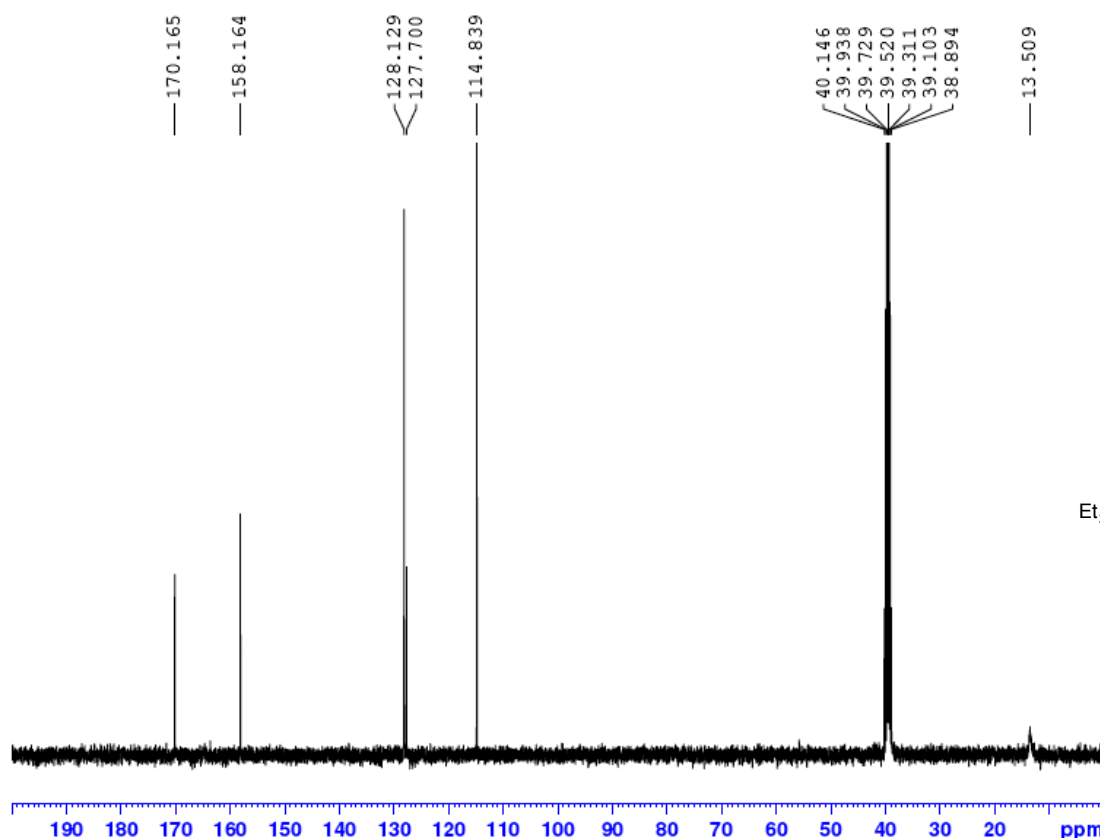
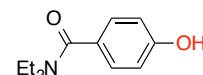
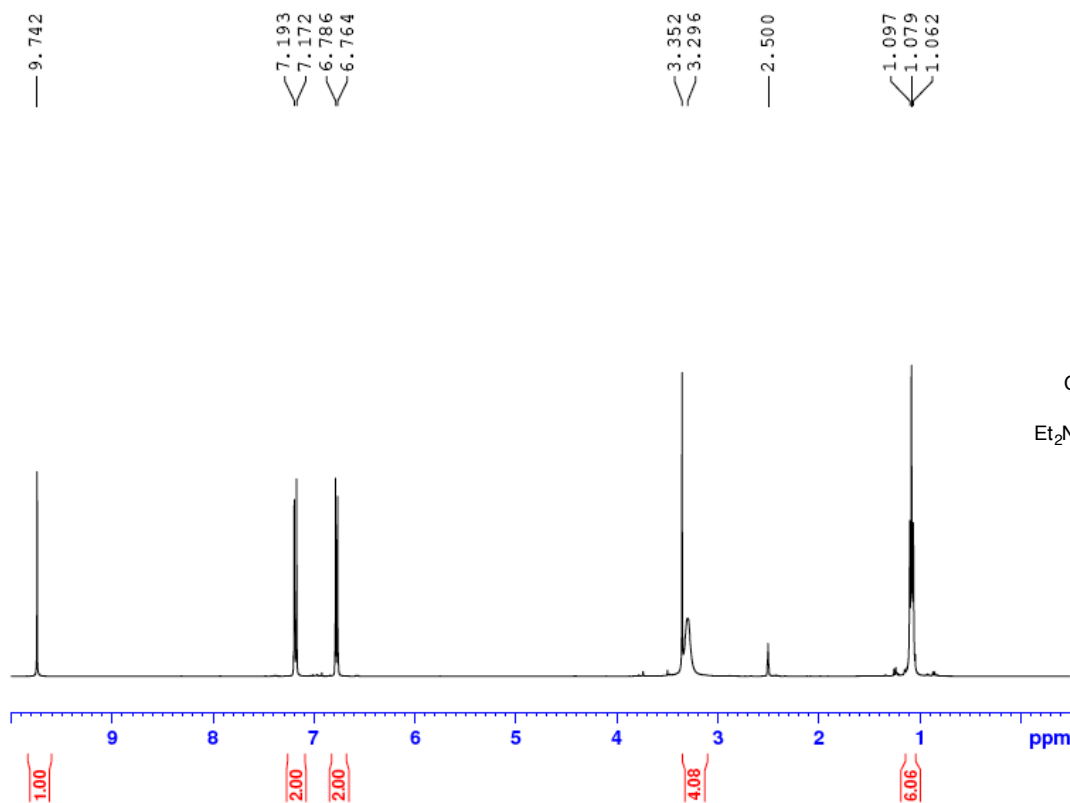
===== CHANNEL f1 =====
SFO1  100.6282823 MHz
NUC1  13C
P1  10.00 usec
PLW1  49.0000000 W

===== CHANNEL f2 =====
SFO2  400.1216000 MHz
NUC2  1H
CPDPRG2  waltz16
PCPD2  90.00 usec
PWR2  15.0000000 W
PWR12  0.31976999 W
PWR13  0.25019999 W

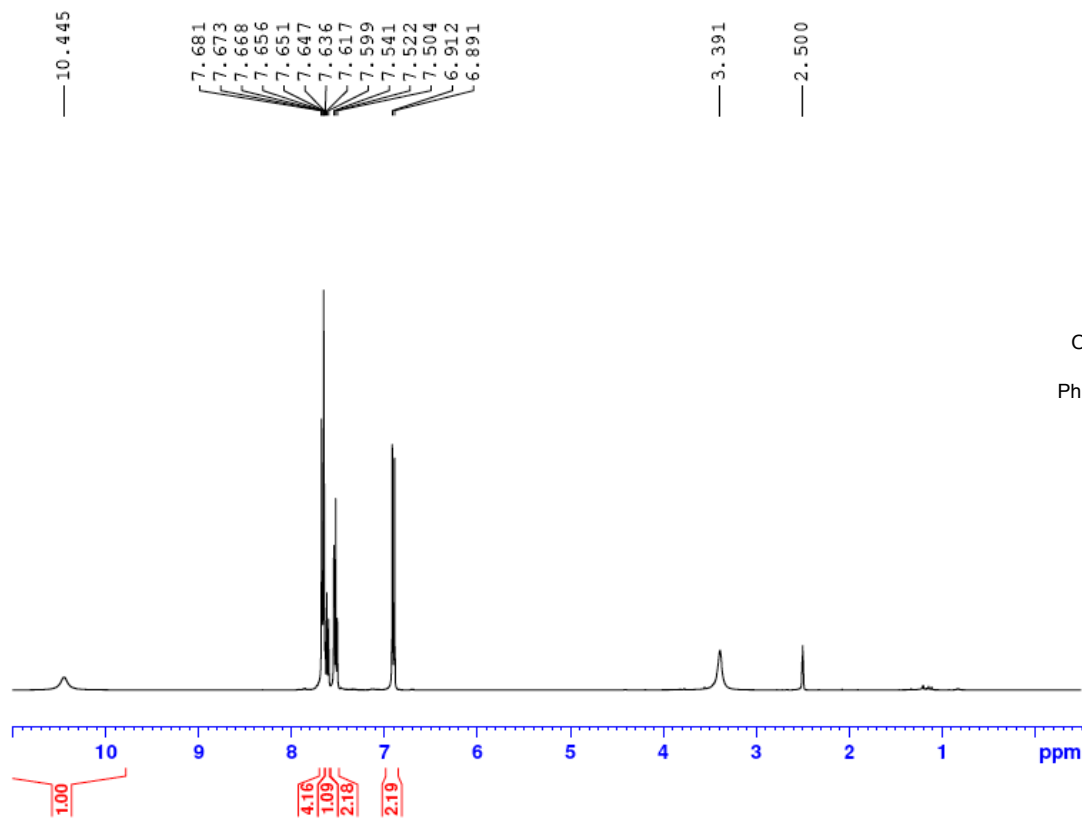
F2 - Processing parameters
SI  32768
SF  100.6126110 MHz
WDW  EM
SSB  0
LB  1.00 Hz
GB  0
PC  1.40
    
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¹H and ¹³C NMR spectra of *N,N*-diethyl-4-hydroxybenzamide (5d)

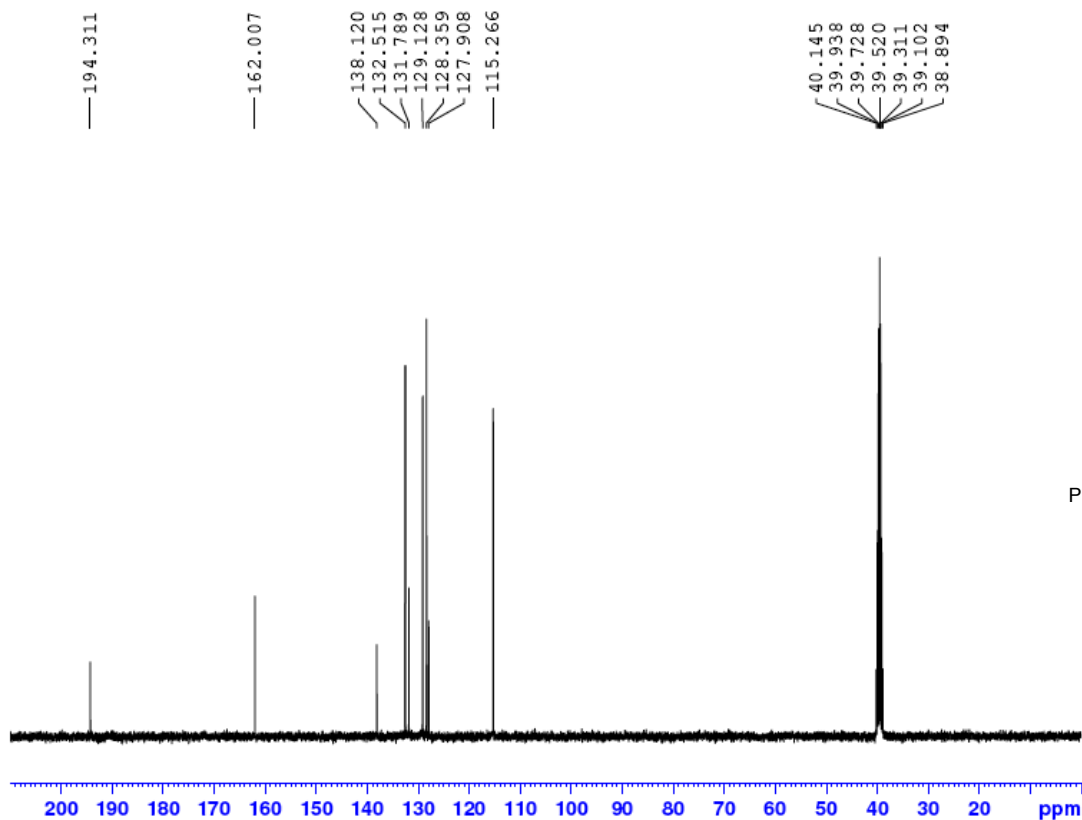
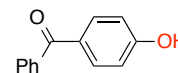


¹H and ¹³C NMR spectra of 4-hydroxybenzophenone (5e)



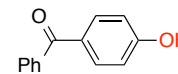
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Current Data Parameters
NAME      CMC-VII-17A-exp (s1) (f11)
EXPNO    1
PROCNO   1
F2 - Acquisition Parameters
Date_    20120523
Time     15:57
INSTRUM  spect
PROBHD   5 mm BBO
PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       40
DS       4
SWH      24019.461 Hz
FIDRES   0.366790 Hz
AQ       1.362480 sec
RG       303
SQ       20.900 usec
SE       6.50 usec
TE       300.2 K
D1       2.0000000 sec
d11      0.0300000 sec
D10      1
===== CHANNEL f1 =====
NUC1      13C
P1        10.00 usec
PL1       0.00 dB
SFO1      101.6253750 MHz
F2 - Processing parameters
SI        65536
SF        101.6253750 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
  
```

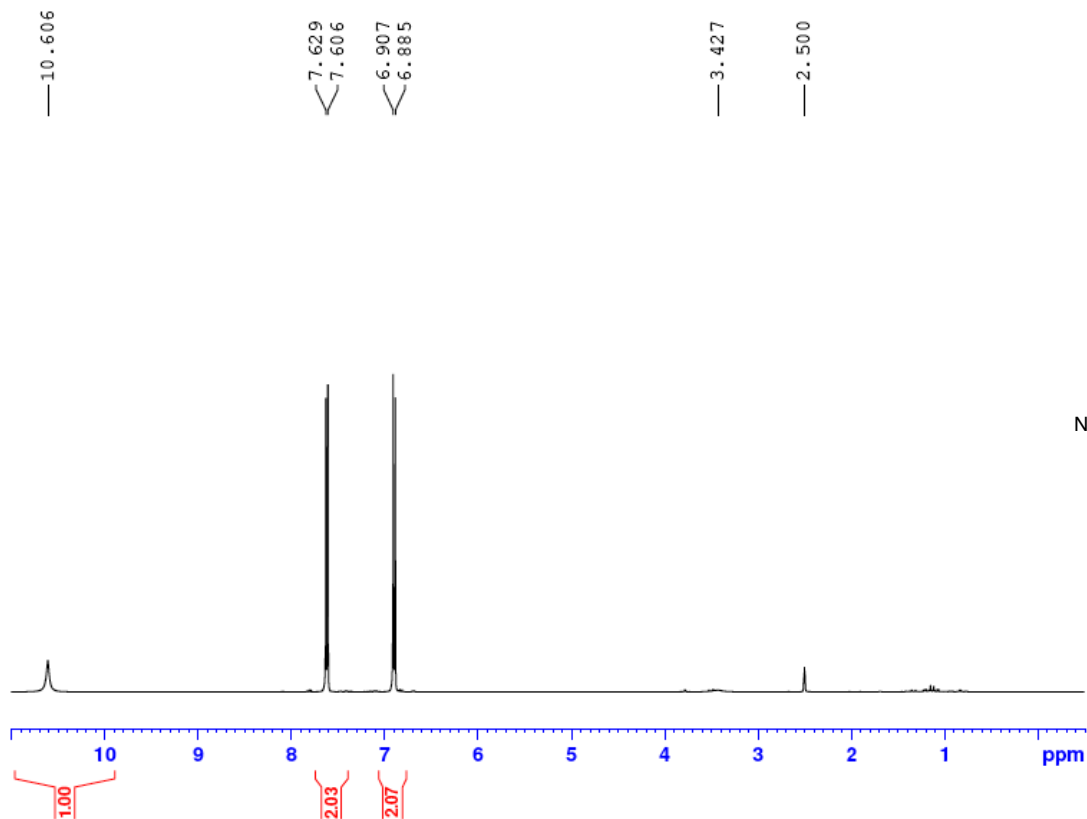


```

Current Data Parameters
NAME      CMC-VII-17A-exp (C13)
EXPNO    1
PROCNO   1
F2 - Acquisition Parameters
Date_    20120520
Time     15:55
INSTRUM  spect
PROBHD   5 mm BBO
PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       40
DS       4
SWH      24019.461 Hz
FIDRES   0.366790 Hz
AQ       1.362480 sec
RG       303
SQ       20.900 usec
SE       6.50 usec
TE       300.2 K
D1       2.0000000 sec
d11      0.0300000 sec
D10      1
===== CHANNEL f1 =====
SFO1      100.6229292 MHz
NUC1      13C
P1        10.00 usec
PL1       0.00 dB
SFO2      400.1314095 MHz
NUC2      13C
===== CHANNEL f2 =====
CPDPRG2  waltz16
PCPD2    90.00 usec
PDM2     10.0000000 W
PDM3     0.2297000 W
PDM13    0.2102001 W
F2 - Processing parameters
SI        65536
SF        100.6229292 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```



¹H and ¹³C NMR spectra of 4-hydroxybenzonitrile (5f)



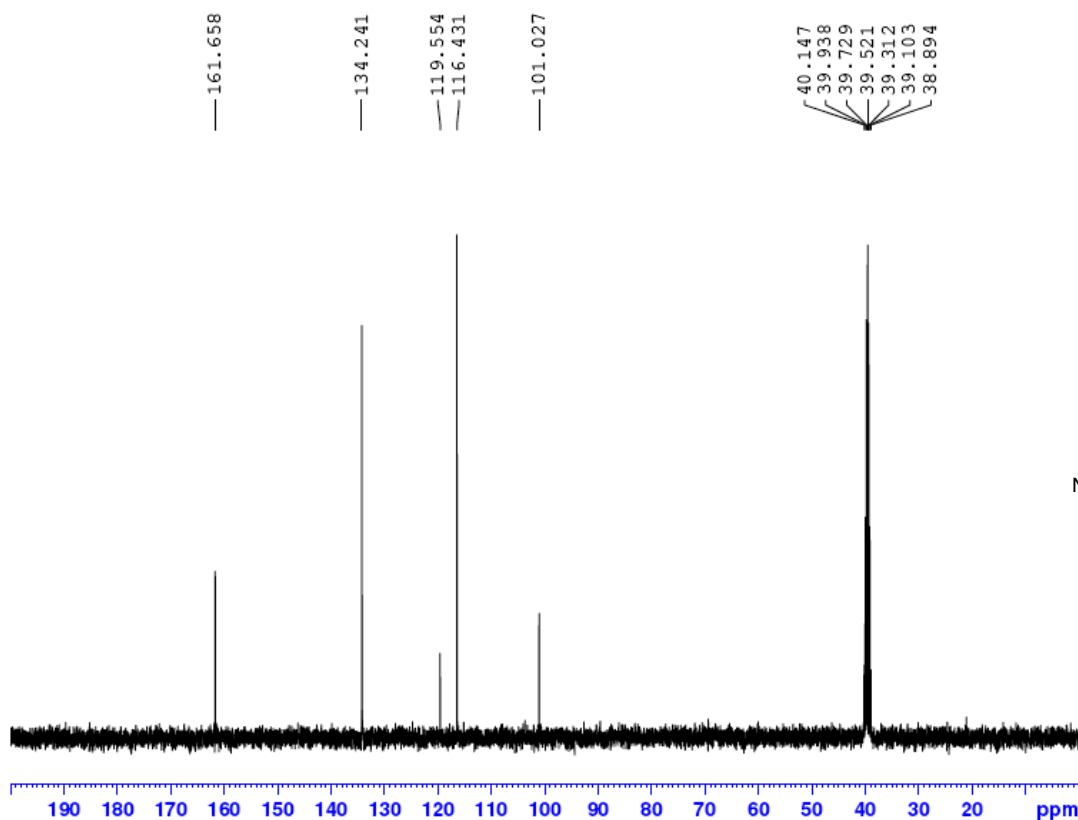
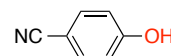
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Current Data Parameters
NAME  CNO-VII-175A-sep (H1)
EXPNO  1
PROCNO  1

F2 - Acquisition Parameters
Date_  20120310
Time  10.47
SYSTEM  spect
PROBHD  5 mm BBO BB/
PULPROG  zgpg30
TD  65536
SOLVENT  DMSO
NS  2
DS  13
SWH  9012.820 Hz
FIDRES  0.122266 Hz
AQ  4.0284465 sec
RG  90.5
DM  62.400 umax
DE  6.50 umax
TE  298.0 K
D1  1.0000000 sec
TD0  1

===== CHANNEL f1 =====
SFO1  400.134710 MHz
NUC1  1H
P1  13.12 umax
PL1  15.0000000 W

F2 - Processing parameters
SI  45536
SF  400.130027 MHz
WDW  EM
SSB  0
LB  0.30 Hz
GB  0
PC  1.00
    
```



```

Current Data Parameters
NAME  CNO-VII-175A-sep (C13)
EXPNO  1
PROCNO  1

F2 - Acquisition Parameters
Date_  20120310
Time  10.49
SYSTEM  spect
PROBHD  5 mm BBO BB/
PULPROG  zgpg30
TD  65536
SOLVENT  DMSO
NS  2
DS  13
SWH  24039.461 Hz
FIDRES  0.360790 Hz
AQ  1.3621480 sec
RG  203
DM  20.900 umax
DE  6.50 umax
TE  298.1 K
D1  2.0000000 sec
D11  0.0300000 sec
TD0  1

===== CHANNEL f1 =====
SFO1  100.628293 MHz
NUC1  13C
P1  10.00 umax
PL1  49.0000000 W

===== CHANNEL f2 =====
SFO2  400.134000 MHz
NUC2  1H
CPCPRG2  waltz16
PCPD2  90.00 umax
PMD2  15.0000000 W
PMD12  0.31976999 W
PMD13  0.25019999 W

F2 - Processing parameters
SI  32768
SF  100.612113 MHz
WDW  EM
SSB  0
LB  1.00 Hz
GB  0
PC  1.40
    
```

