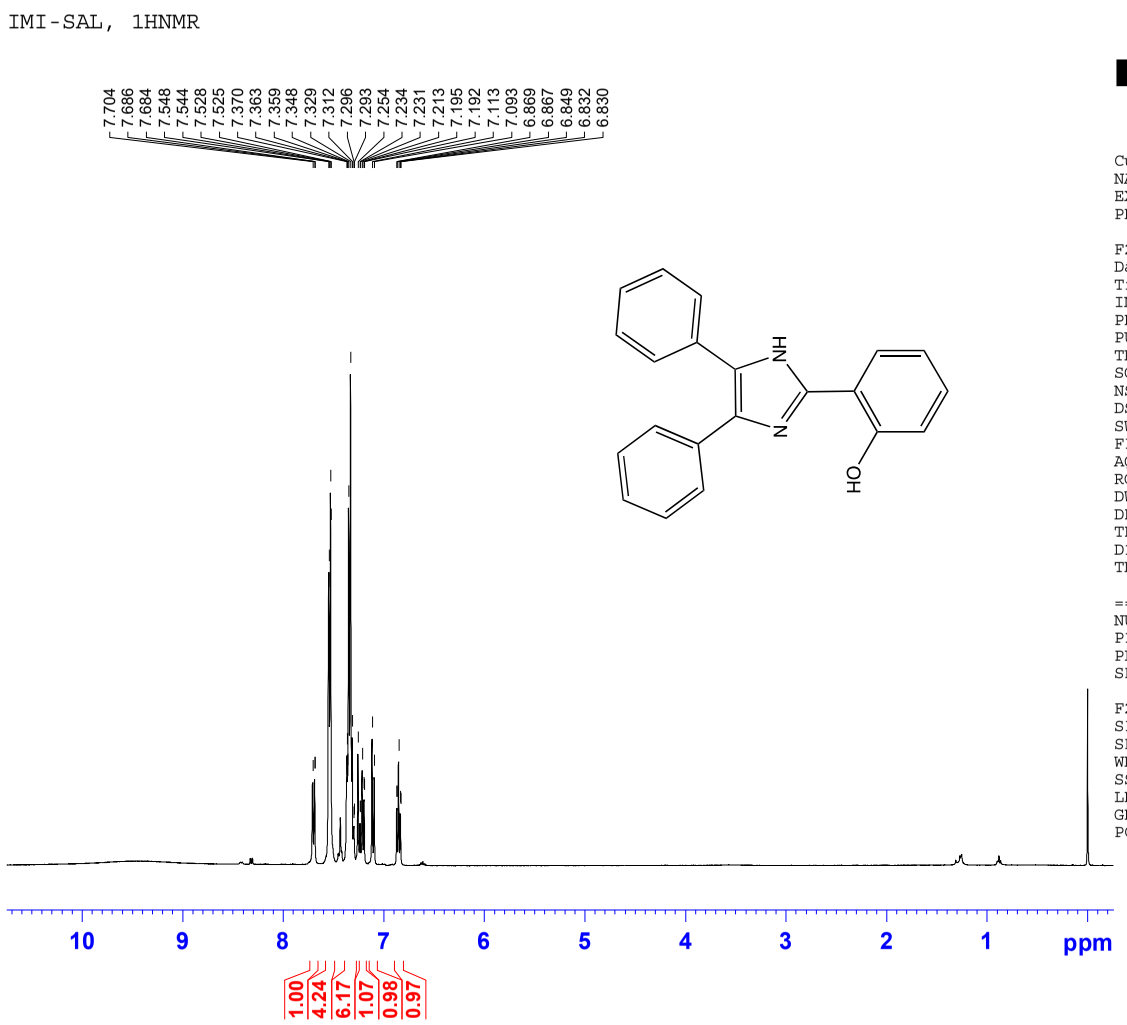
SUPPLEMENTARY INFORMATION

"*In vitro* and *in silico* screening of 2,4,5-trisubstituted imidazole derivatives as potential xanthine and cholinesterase inhibitors, antioxidant, and cytotoxic agents"

Representative Nuclear Magnetic Resonance Spectra

IMI-SAL, 1HNMR



Current Data Parameters

NAME	IMI-SAL
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20111110
Time	17.27
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8250.825 Hz
FIDRES	0.125898 Hz
AQ	3.9715316 sec
RG	362
DW	60.600 usec
DE	6.00 usec
TE	683.2 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	1H
P1	12.50 usec
PL1	-4.20 dB
SFO1	400.1324710 MHz

F2 - Processing parameters

SI	32768
SF	400.1300119 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

Figure S1. ^{1}H-NMR Compound 2.

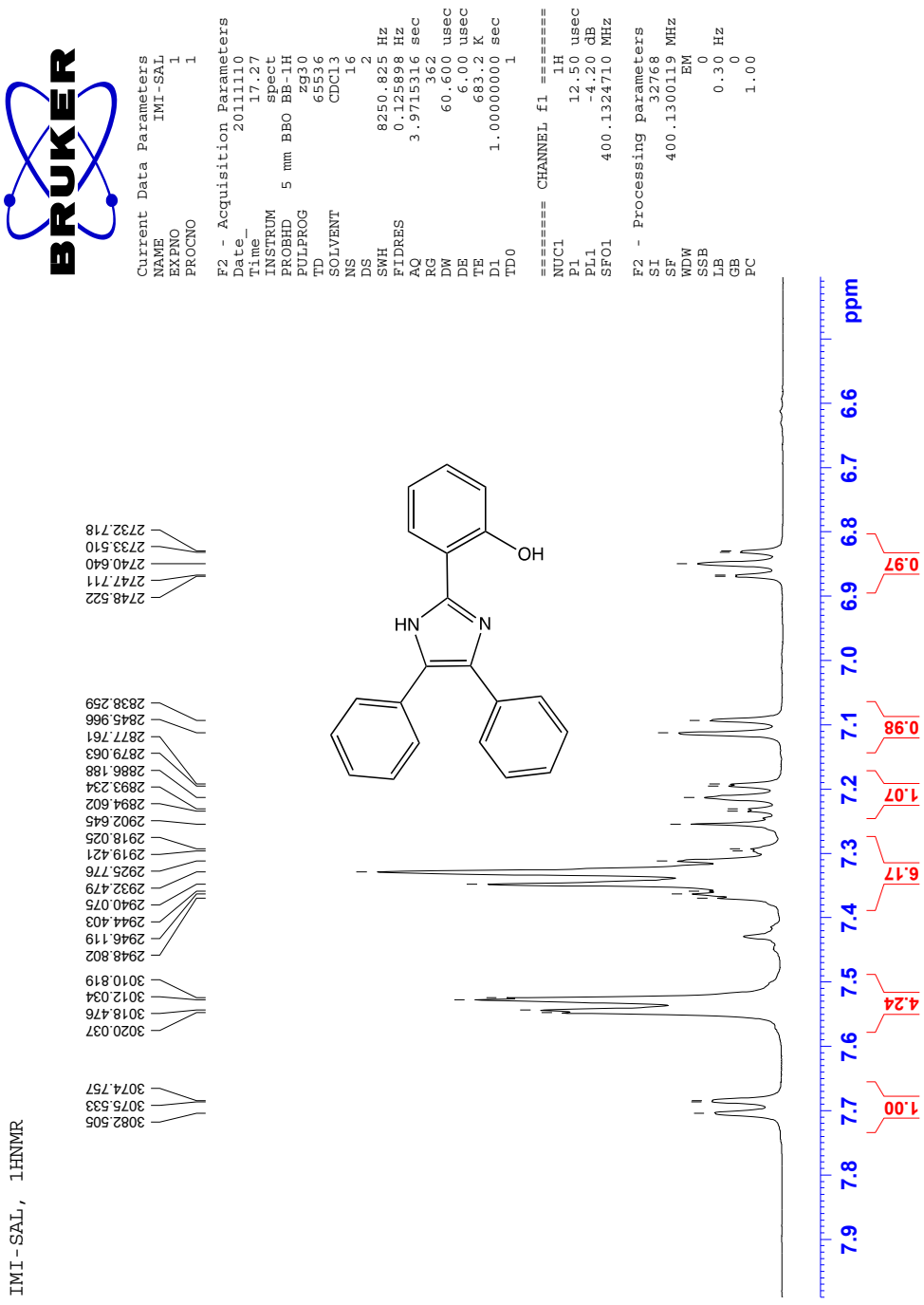
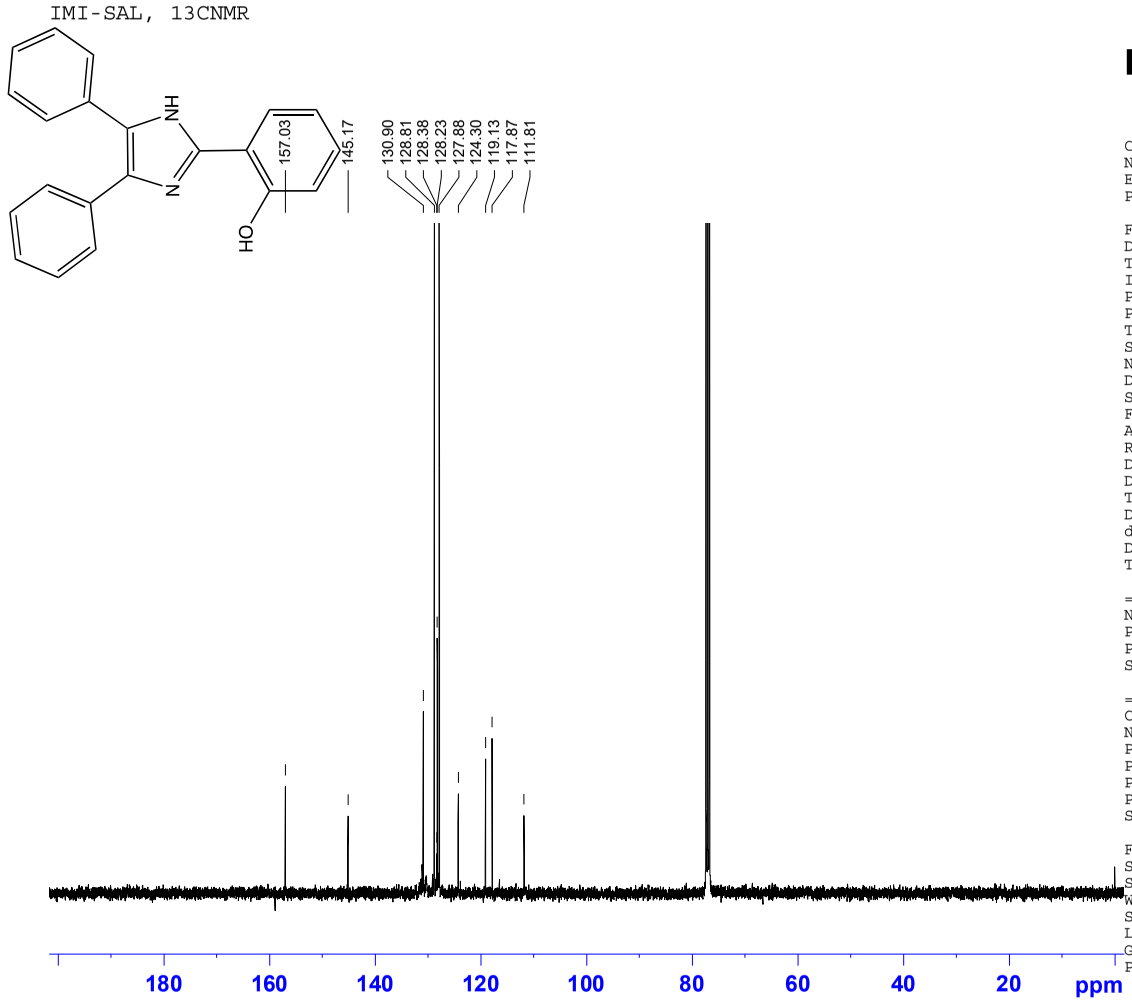


Figure S2. ^{1}H-NMR extension Compound 2.




```
Current Data Parameters
NAME                  IMI-SAL
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20111110
Time                   19.22
INSTRUM                spect
PROBHD    5 mm BBO BB-1H
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     2000
DS                        2
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631988 sec
RG                      2048
DW                   20.800 usec
DE                    6.00 usec
TE                   683.2 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                     10.20 usec
PL1                    -1.00 dB
SFO1            100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2                  90.00 usec
PL2                    -4.20 dB
PL12                   11.96 dB
PL13                   16.00 dB
SFO2            400.1316005 MHz

F2 - Processing parameters
SI                       32768
SF              100.6127690 MHz
WDW                         EM
SSB                          0
LB                      1.00 Hz
GB                           0
PC                      1.40
```

Figure S3. ^{13}C-NMR Compound 2.

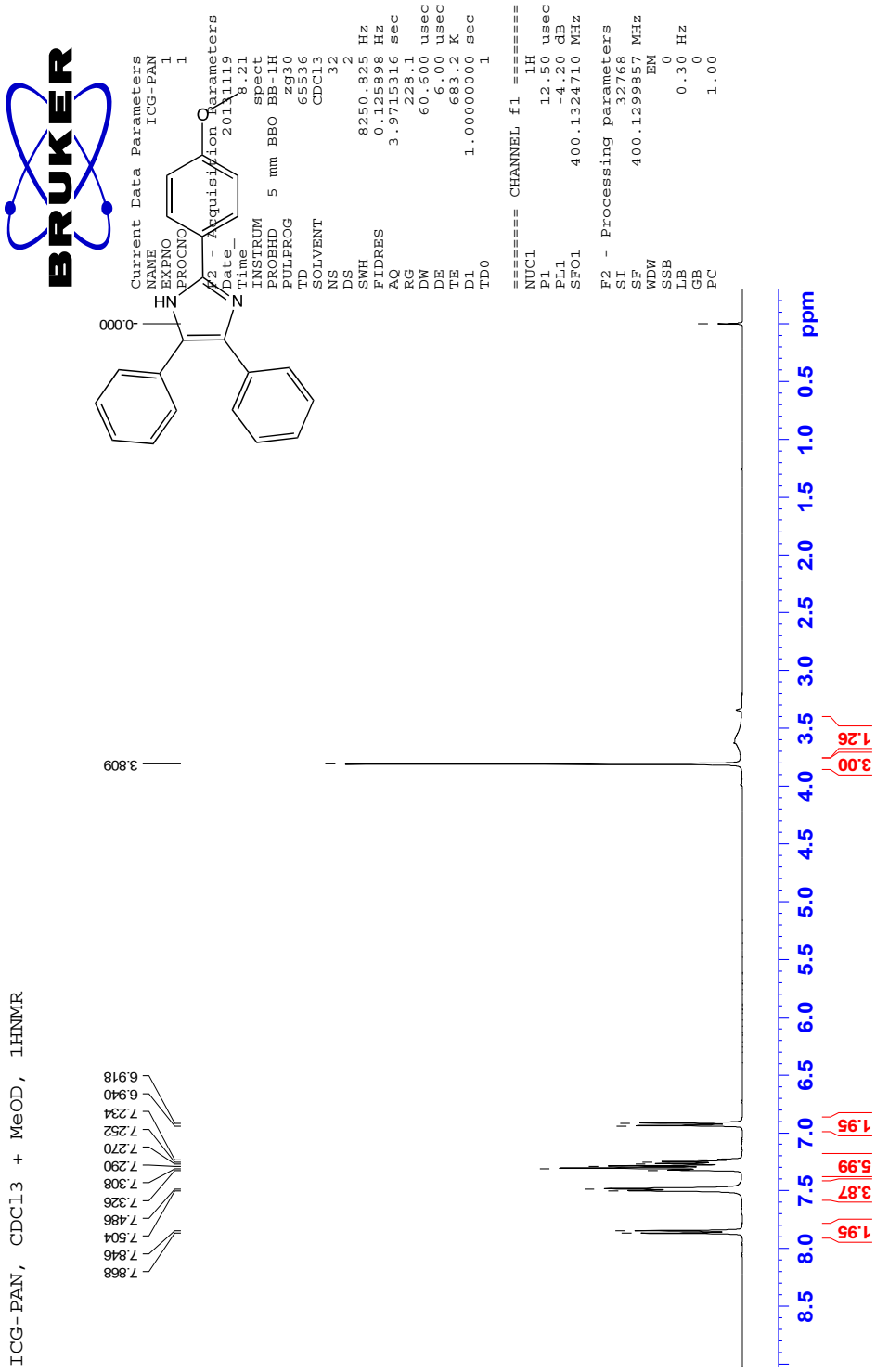
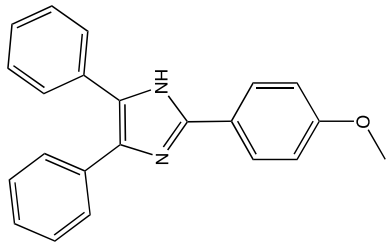
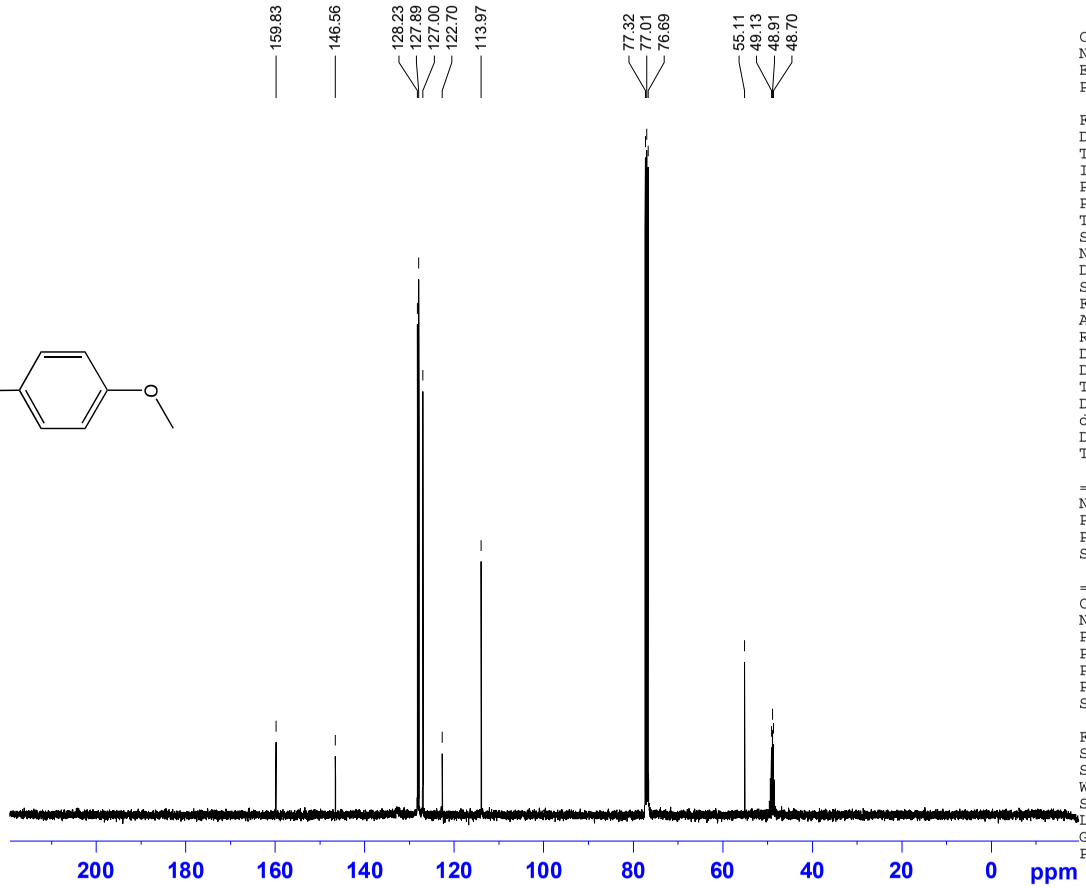


Figure S4. ^{1}H-NMR Compound 4.

ICG-PAN, 13CNMR






```
Current Data Parameters
NAME                  ICG-PAN
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20131119
Time                   9.22
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1000
DS                       2
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                  2896.3
DW                  20.800 usec
DE                   6.00 usec
TE                  683.2 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                    13C
P1                    10.20 usec
PL1                   -1.00 dB
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                  -4.20 dB
PL12                 11.96 dB
PL13                 16.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                      32768
SF            100.6127802 MHz
WDW                        EM
SSB                         0
LB                    1.00 Hz
GB                          0
PC                    1.40
```

Figure S5. ^{13}C-NMR Compound 4.

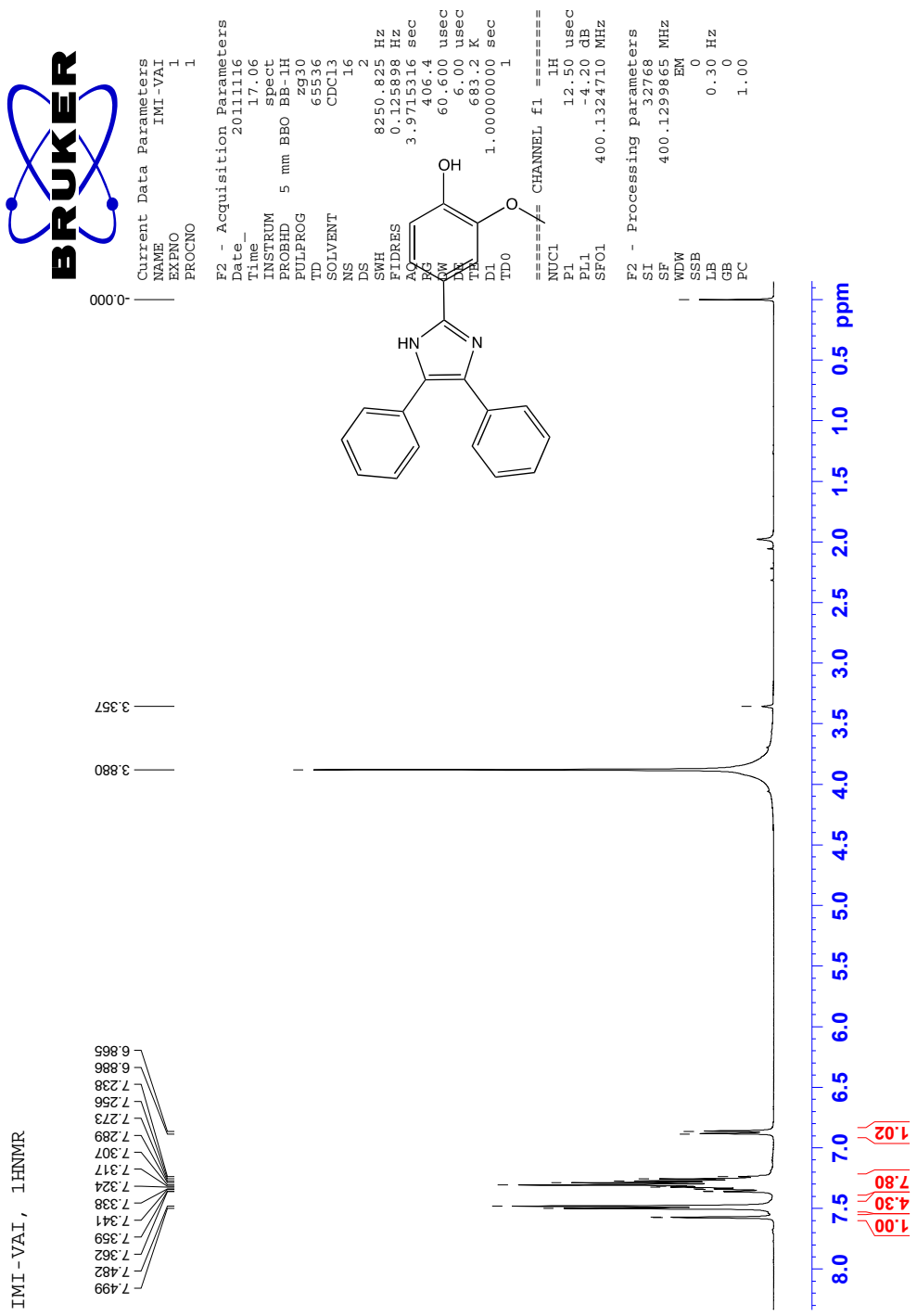


Figure S6. [1]H-NMR Compound 7.

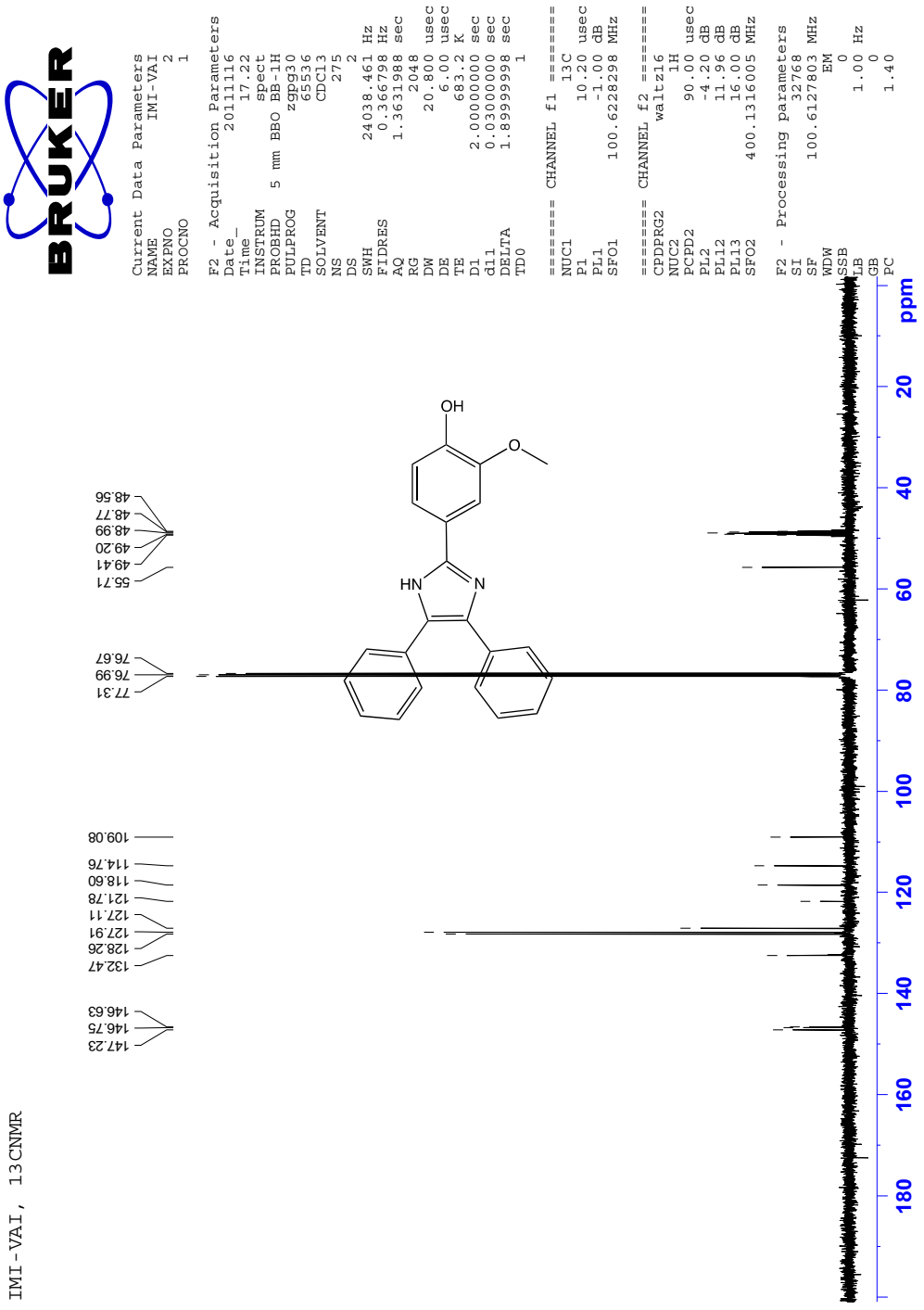
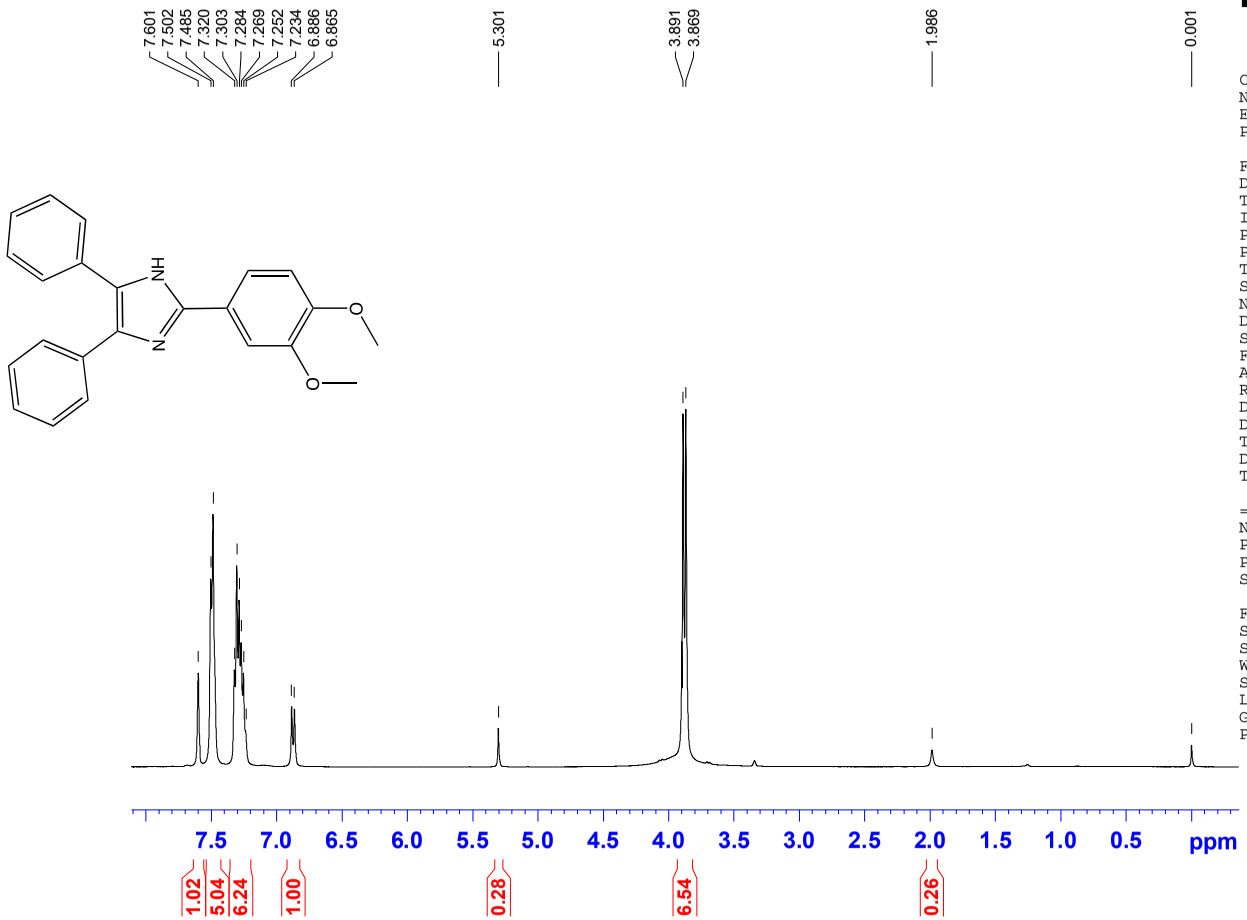


Figure S7. ^{13}C-NMR Compound 7.

ICG-DMB, CDCl3 + MeOD, 1HNMR



Current Data Parameters
NAME ICG-DMB
EXPNO 1
PROCNO 1

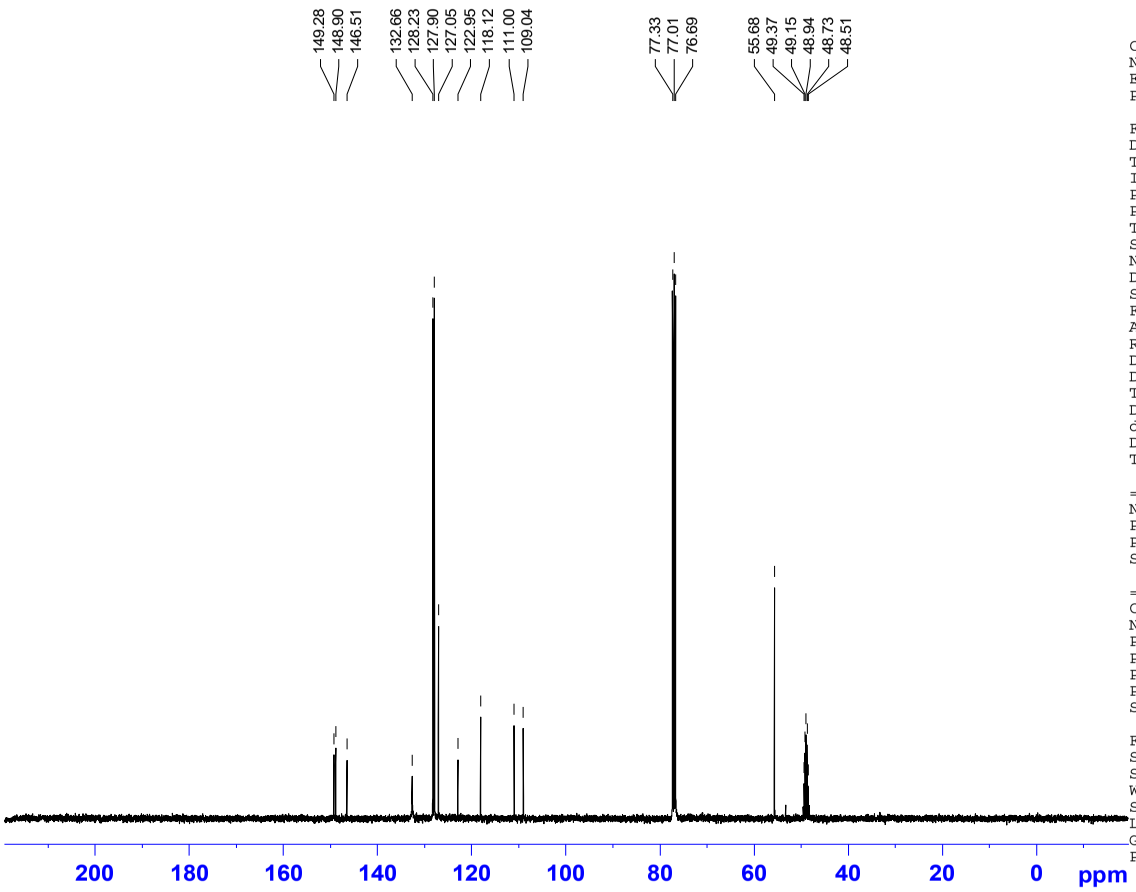
F2 - Acquisition Parameters
Date_ 20131119
Time 10.43
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8250.825 Hz
FIDRES 0.125898 Hz
AQ 3.9715316 sec
RG 161.3
DW 60.600 usec
DE 6.00 usec
TE 683.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -4.20 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1299845 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S8. ^{1}H-NMR Compound 8.

ICG-DMB, 13CNMR




```
Current Data Parameters
NAME                  ICG-DMB
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20131119
Time                  11.41
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1000
DS                        2
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                1.3631988 sec
RG                   2896.3
DW                   20.800 usec
DE                    6.00 usec
TE                   683.2 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                    13C
P1                    10.20 usec
PL1                   -1.00 dB
SFO1           100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                    1H
PCPD2                 90.00 usec
PL2                   -4.20 dB
PL12                  11.96 dB
PL13                  16.00 dB
SFO2           400.1316005 MHz

F2 - Processing parameters
SI                      32768
SF             100.6127802 MHz
WDW                        EM
SSB                         0
LB                     1.00 Hz
GB                          0
PC                     1.40
```

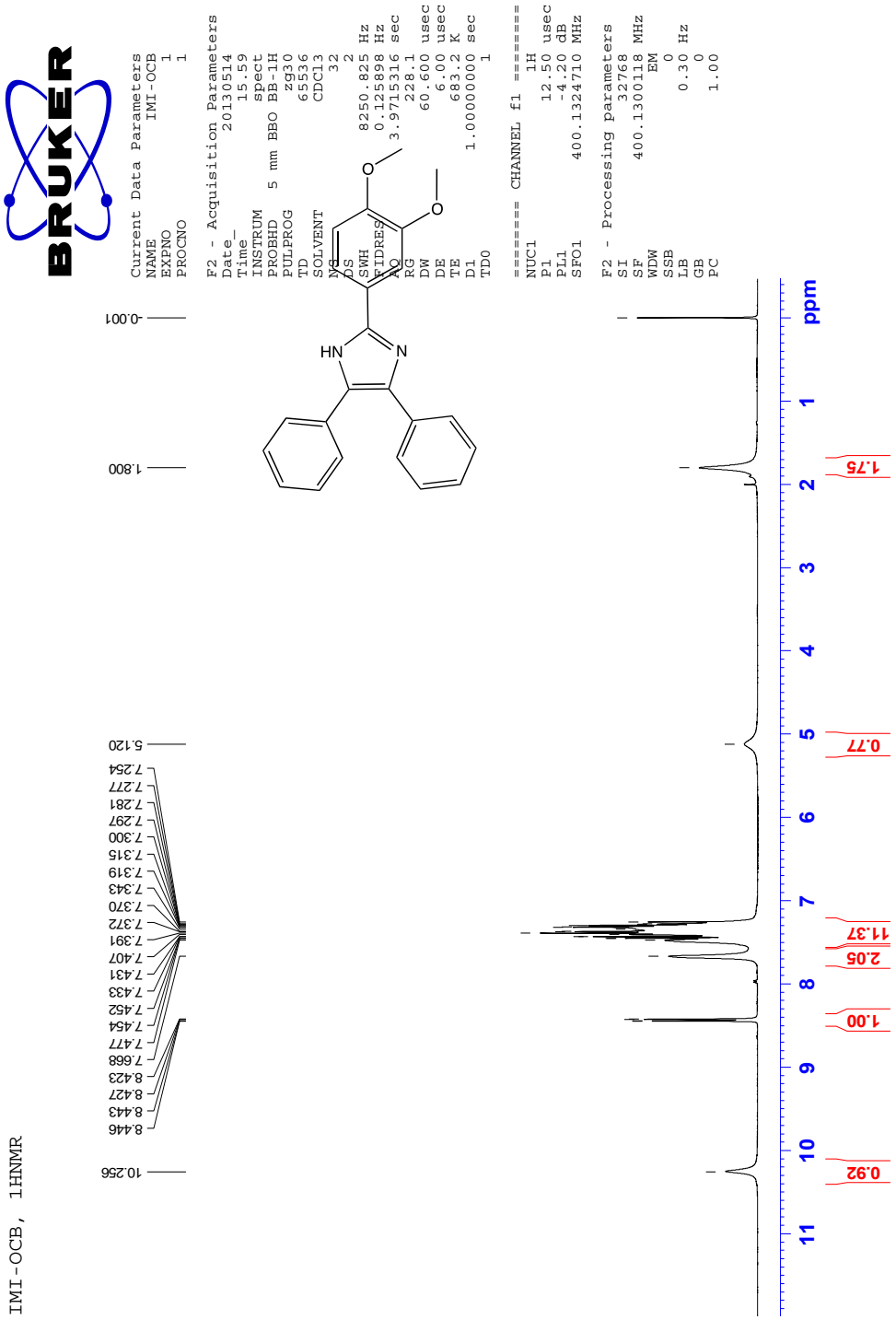


Figure S9. ^{13}C-NMR Compound 8.

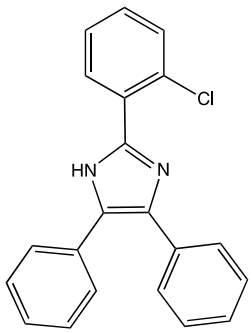
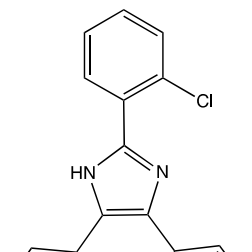


Figure S10. ^{1}H-NMR Compound 9.



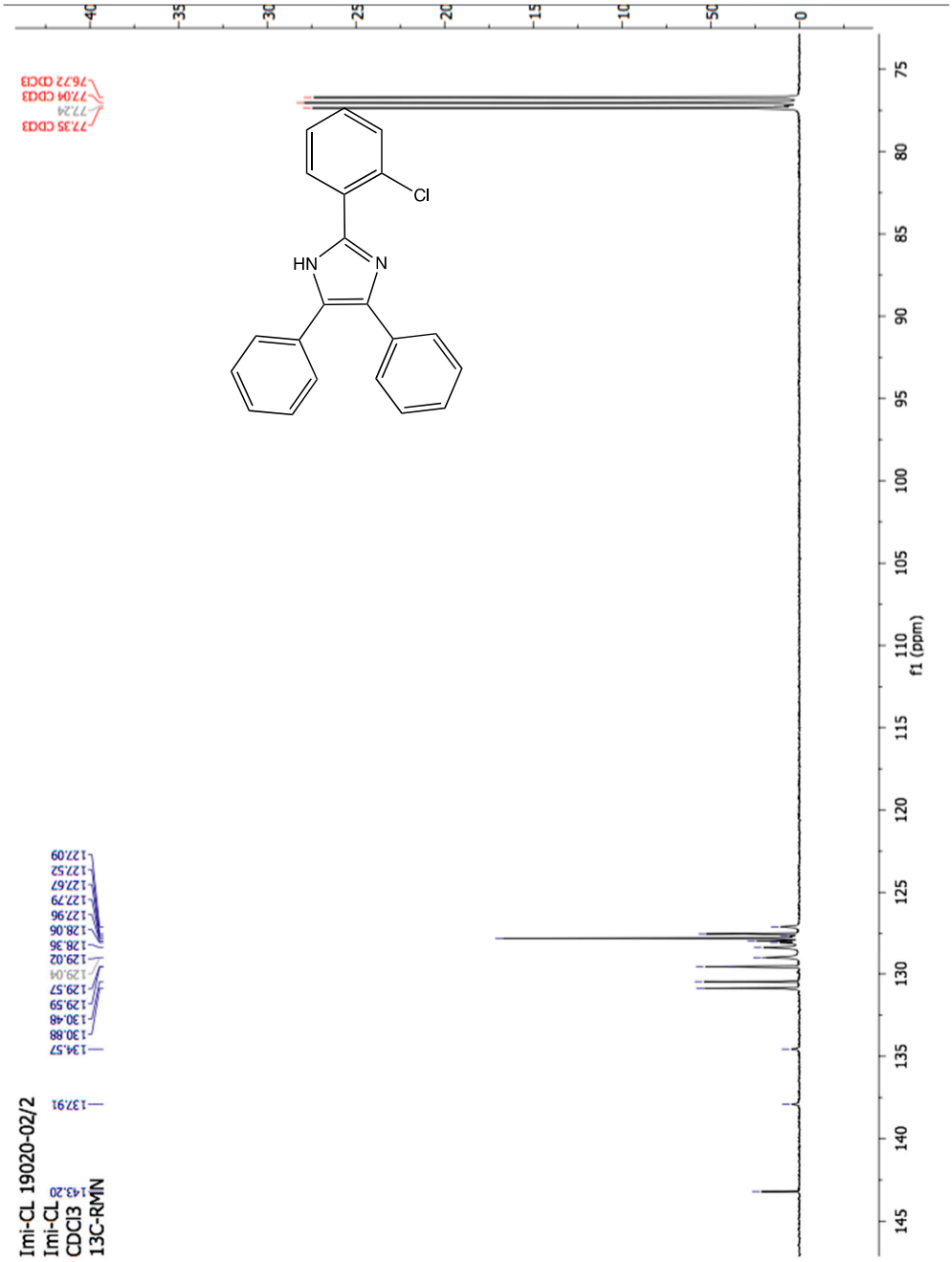
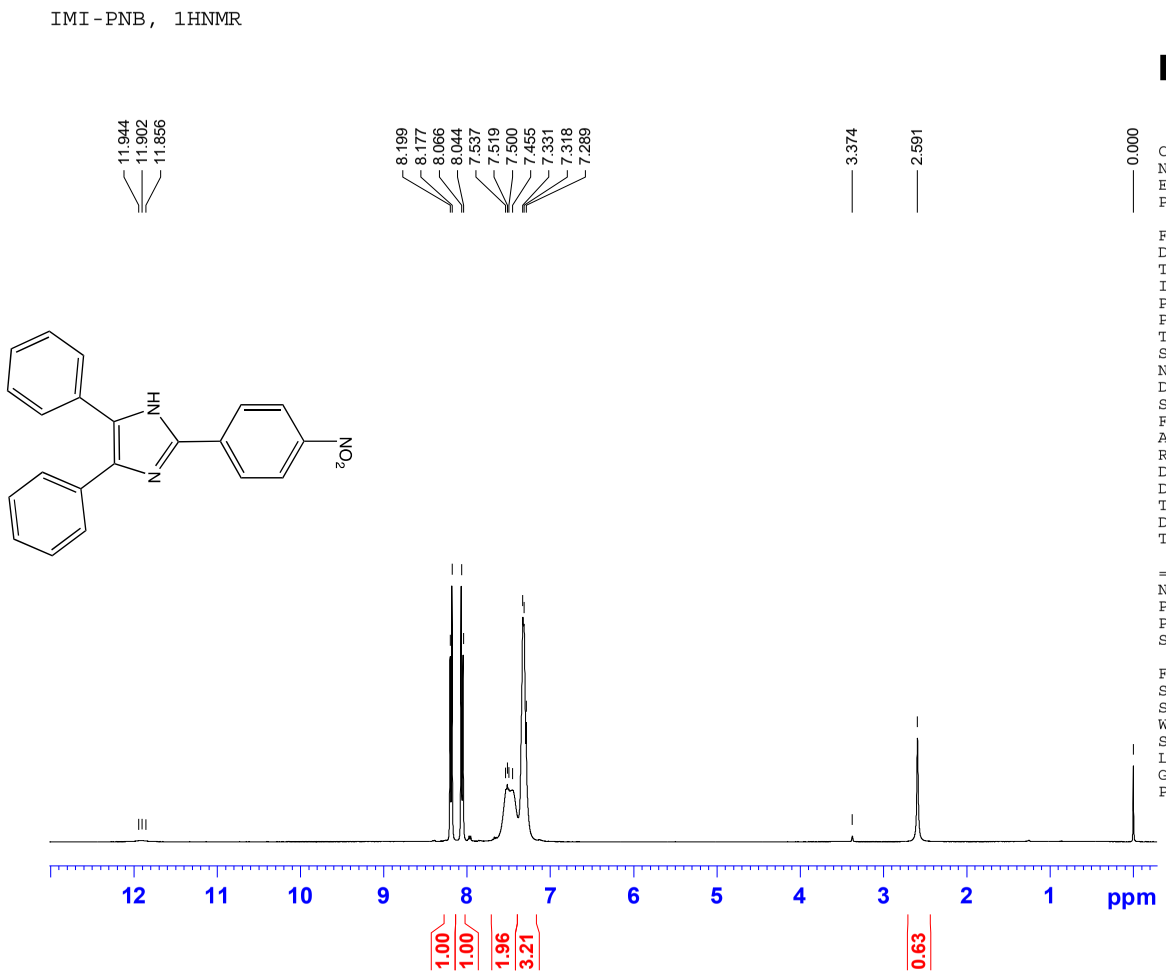


Figure S11. ^{13}C-NMR Compound 9.

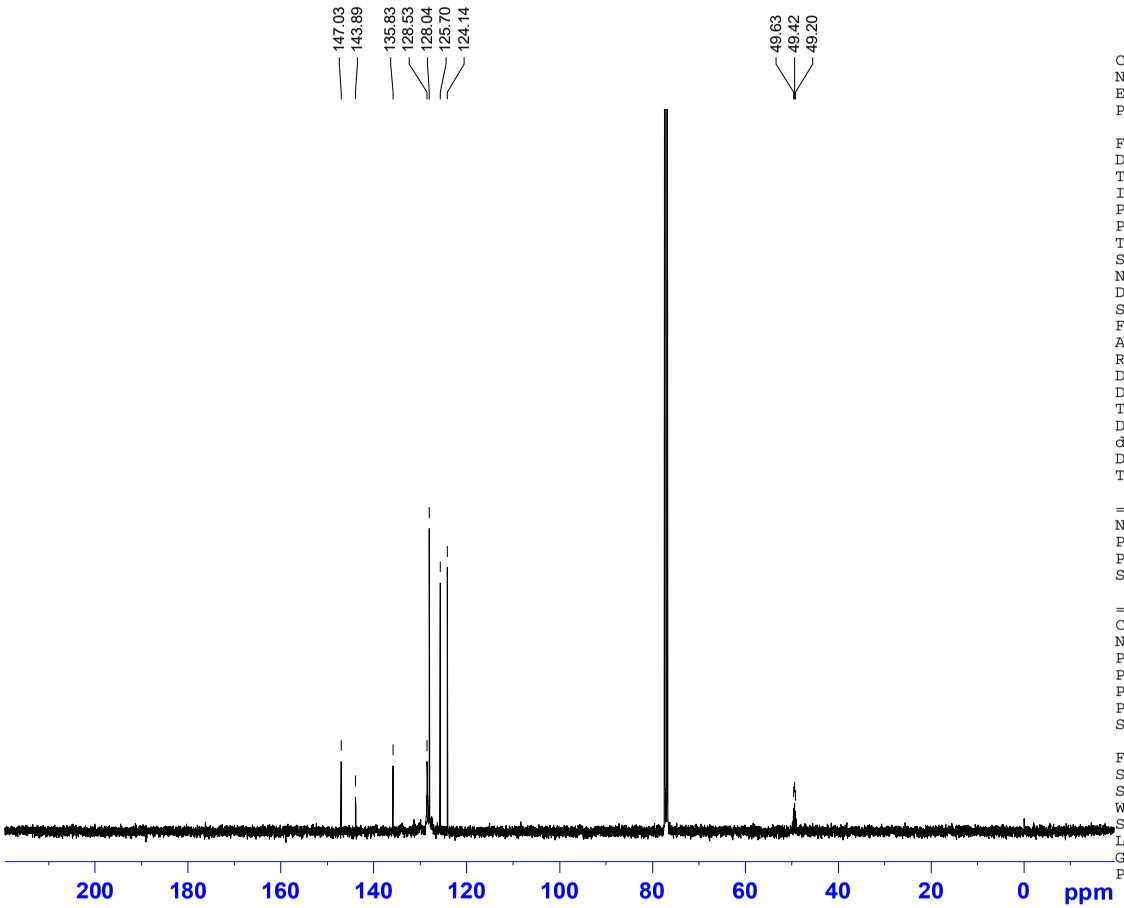
IMI-PNB, 1HNMR




```
Current Data Parameters
NAME                  IMI-PNB
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20130514
Time                  12.13
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       32
DS                        2
SWH                8250.825 Hz
FIDRES            0.125898 Hz
AQ                3.9715316 sec
RG                    228.1
DW                   60.600 usec
DE                    6.00 usec
TE                   683.2 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                   12.50 usec
PL1                  -4.20 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                    32768
SF            400.1299980 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```

Figure S12. ^{1}H-NMR Compound 11.

IMI-PNB, 13CNMR




```
Current Data Parameters
NAME                  IMI-PNB
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_                20130514
Time                    13.11
INSTRUM                 spect
PROBHD    5 mm BBO BB-1H
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                       1024
DS                          2
SWH                 24038.461 Hz
FIDRES                0.366798 Hz
AQ                    1.3631988 sec
RG                       4096
DW                      20.800 usec
DE                       6.00 usec
TE                      683.2 K
D1                  2.00000000 sec
d11                 0.03000000 sec
DELTA               1.89999998 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       13C
P1                      10.20 usec
PL1                     -1.00 dB
SFO1               100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   90.00 usec
PL2                     -4.20 dB
PL12                    11.96 dB
PL13                    16.00 dB
SFO2               400.1316005 MHz

F2 - Processing parameters
SI                         32768
SF                 100.6127690 MHz
WDW                        EM
SSB                         0
LB                       1.00 Hz
GB                          0
PC                       1.40
```

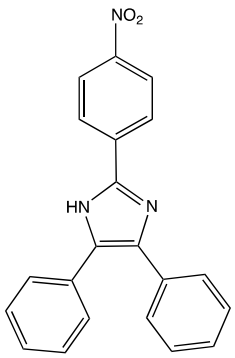


Figure S13. ^{13}C-NMR Compound 11.