

SUPPLEMENTARY INFORMATION

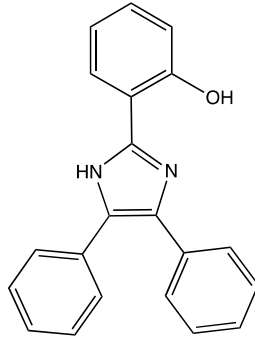
“In vitro and in silico screening of 2,4,5-trisubstituted imidazole derivatives as potential xanthine and cholinesterase inhibitors, antioxidant, and cytotoxic agents”

Representative Nuclear Magnetic Resonance Spectra

IMI - SAL, 1HNMR



6.830
6.832
6.849
6.867
6.869
7.093
7.113
7.192
7.195
7.213
7.231
7.234
7.254
7.293
7.296
7.312
7.329
7.348
7.359
7.363
7.370
7.525
7.528
7.544
7.548
7.684
7.686
7.704

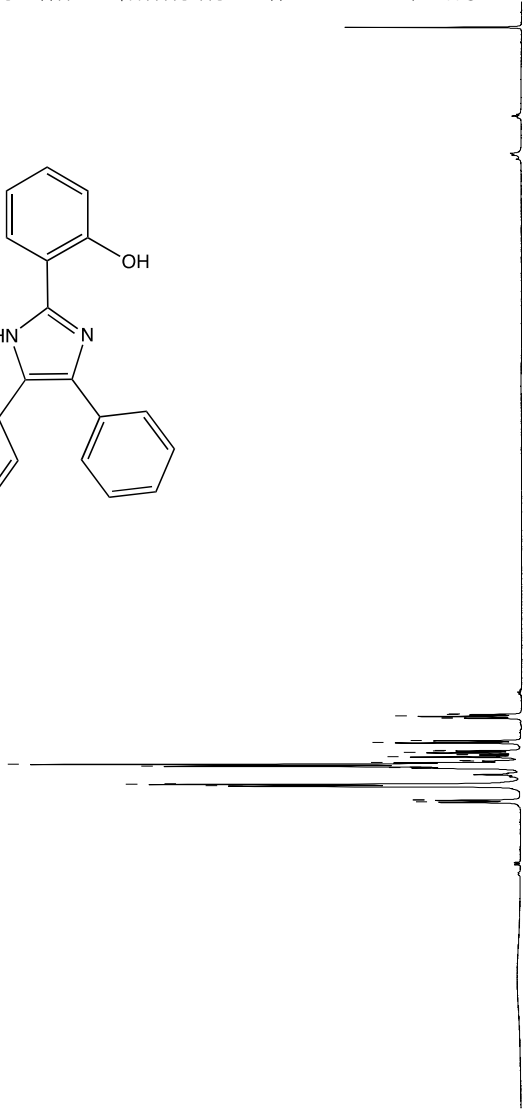


Current Data Parameters
NAME IMI-SAL
EXPNO 1
PROCNO 1

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 1.0000000 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



10 9 8 7 6 5 4 3 2 1 ppm



Current Data Parameters
NAME IMI-SAL
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 2011110
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 0.125698 Hz
AQ 3.971516 sec
RG 362
DW 60.600 usec
DE 6.00 usec
TE 683.2 K
D1 1.0000000 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

IMI-SAL, 1H NMR

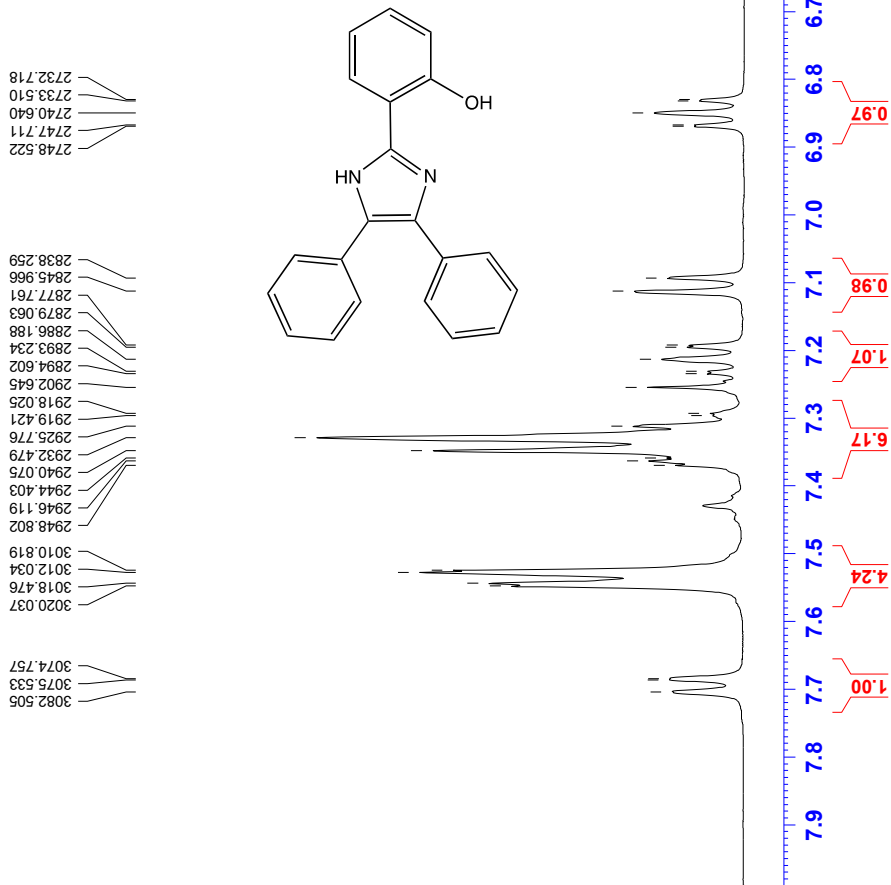
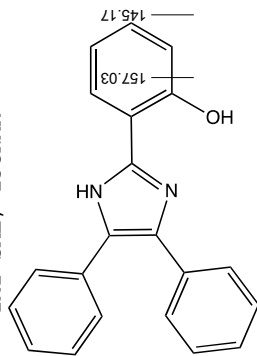


Figure S2. ¹³C-NMR extension Compound 2.



IMI - SAL, ¹³CNMR



Current Data Parameters
 NAME IMI-SAL
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 2011110
 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 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.8999998 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 10.20 usec
 PL1 -1.00 dB
 SF01 100.6282898 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -4.20 dB
 PL12 11.96 dB
 PL13 16.00 dB
 SF02 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

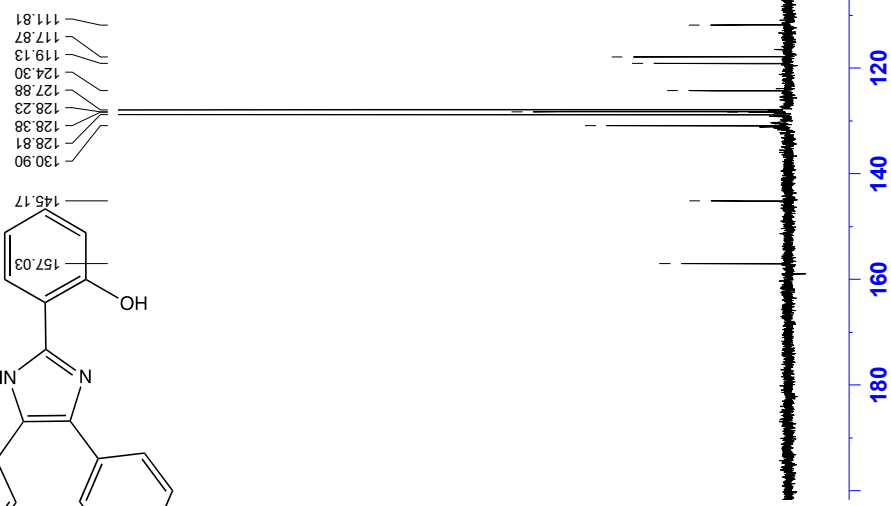
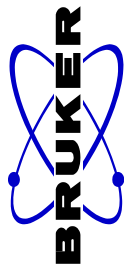


Figure S3. ^{13}C -NMR Compound 2.



ICG-PAN, CDCl3 + MeOD, 1H-NMR

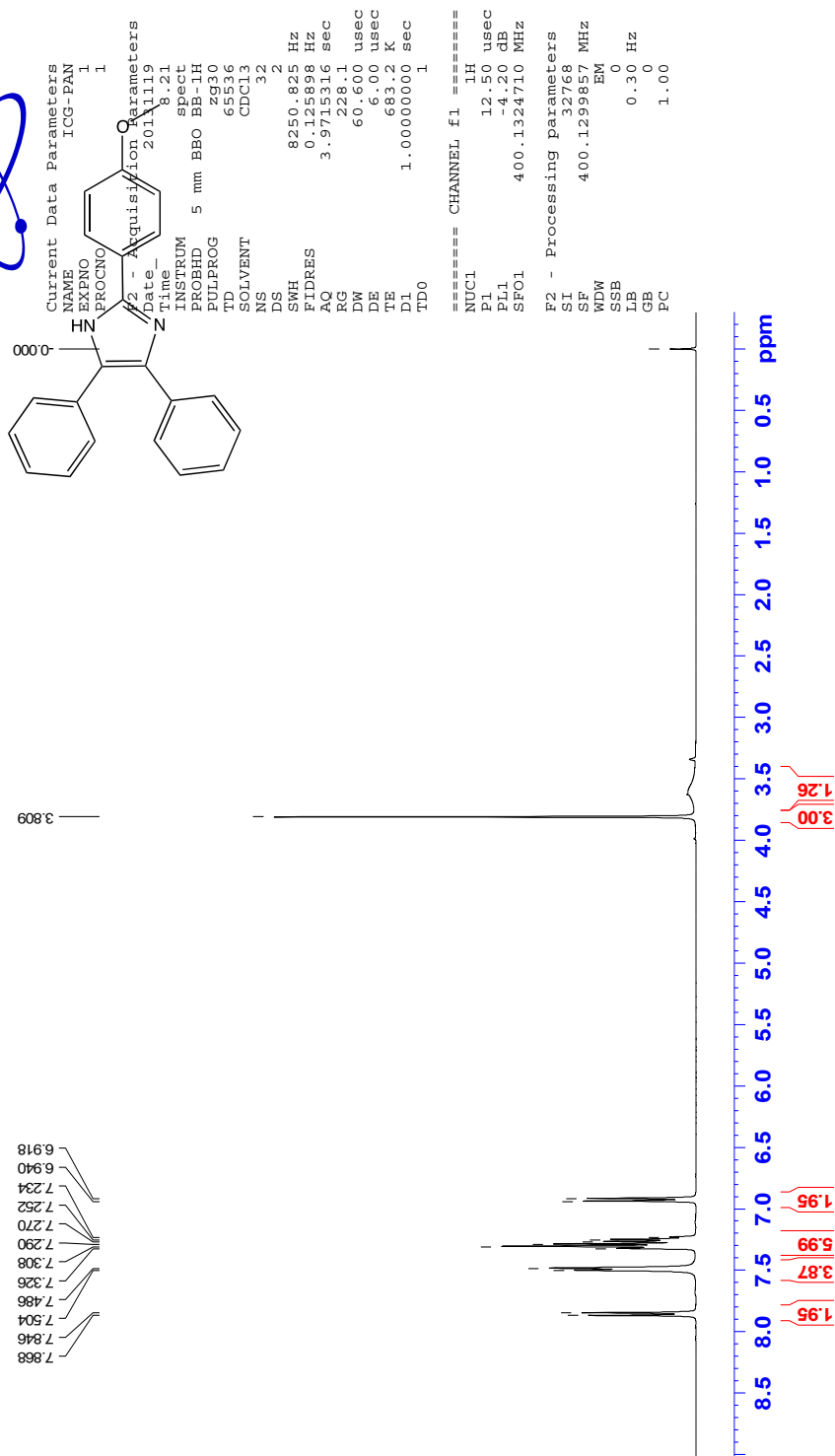


Figure S4. ¹H-NMR Compound 4.

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 1.361988 sec
 RG 2896.3
 DW 20.800 usec
 DE 6.00 usec
 TE 683.2 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.8999998 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 11.56 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

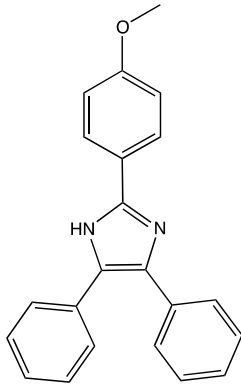
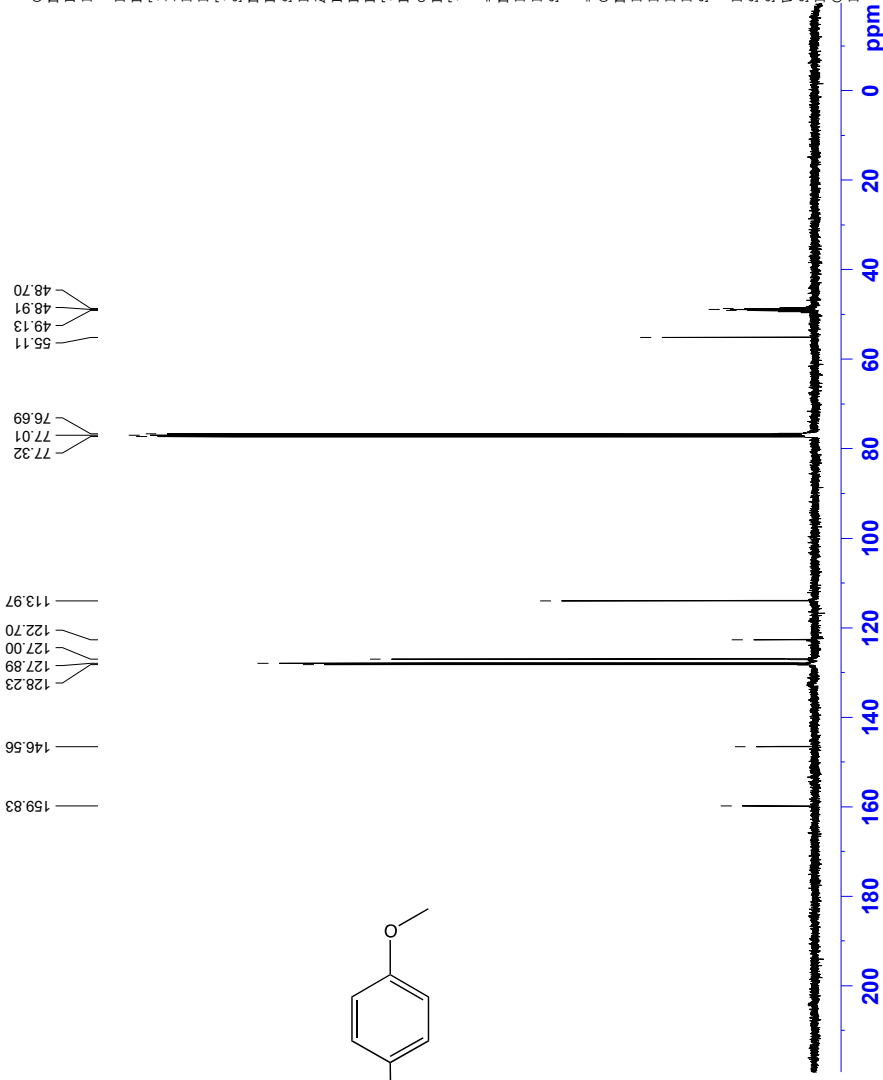


Figure S5. ^{13}C -NMR Compound 4.



IMI-VAI, 1HNMR

7.499
7.482
7.362
7.359
7.341
7.338
7.324
7.317
7.307
7.289
7.273
7.266
7.238
6.886
6.865

3.880
3.357

-0.000

Current Data Parameters
NAME IMI-VAI
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 2011116
Time_ 17.06
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 406.4
AQ 60.600 usec
RG 6.00 usec
TD 683.2 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 12.50 usec
PL1 -4.20 dB
SF01 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1299865 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

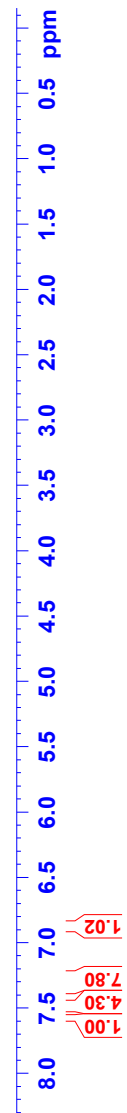
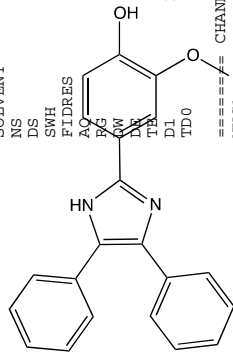


Figure S6. ¹H-NMR Compound 7.

IMI - VAI, ¹³C NMR

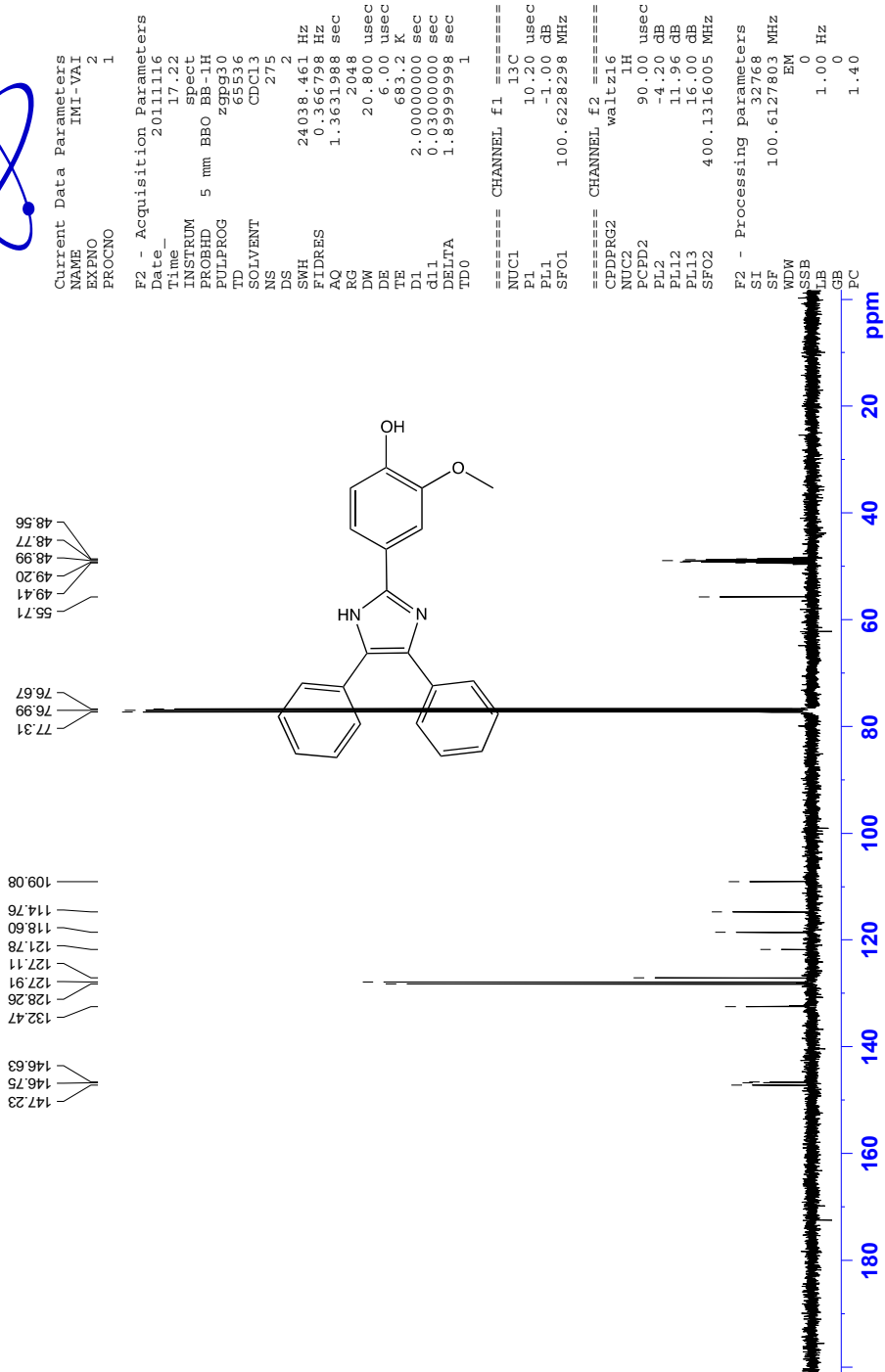


Figure S7. ¹³C-NMR Compound 7.

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

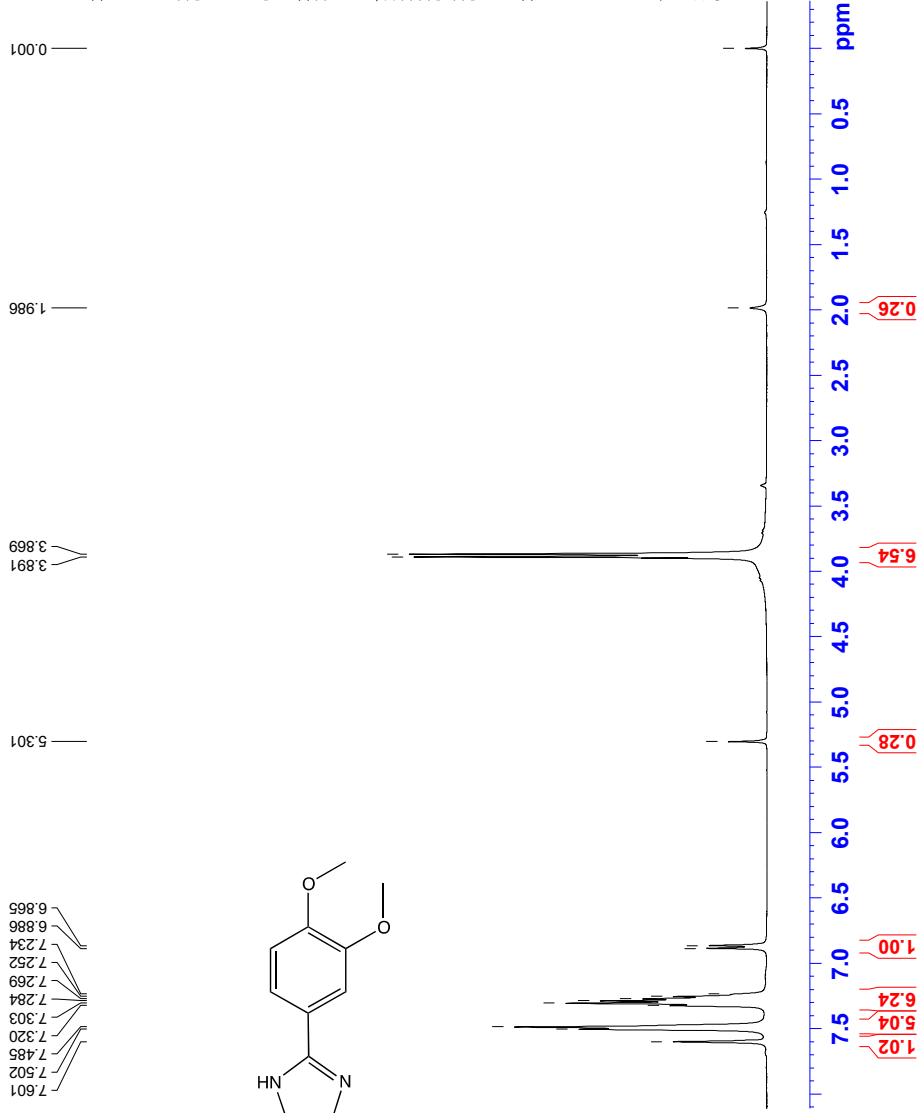


Figure S8.
¹³C-NMR
 Compound 8.



ICG-DMB, ¹³C-NMR

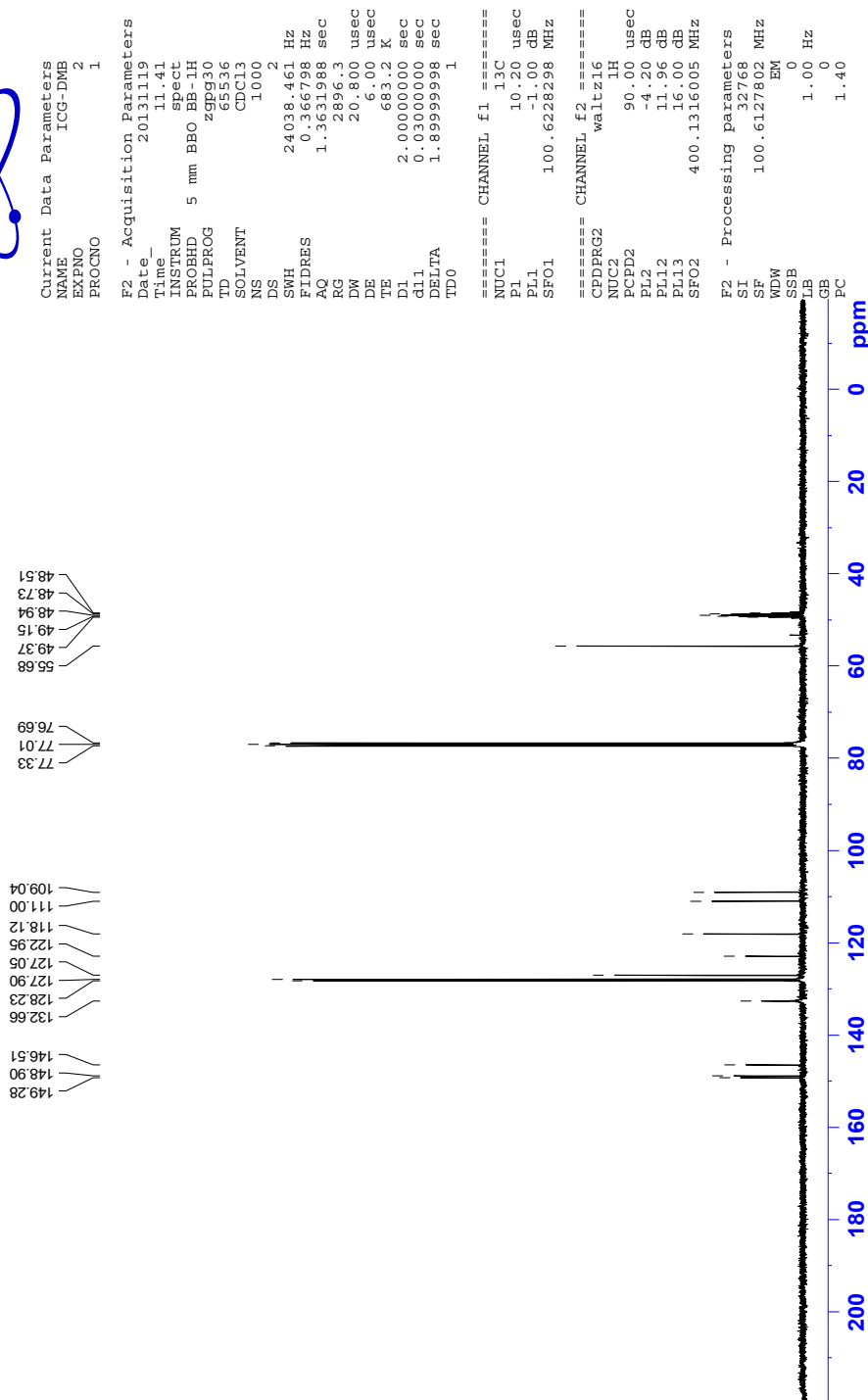
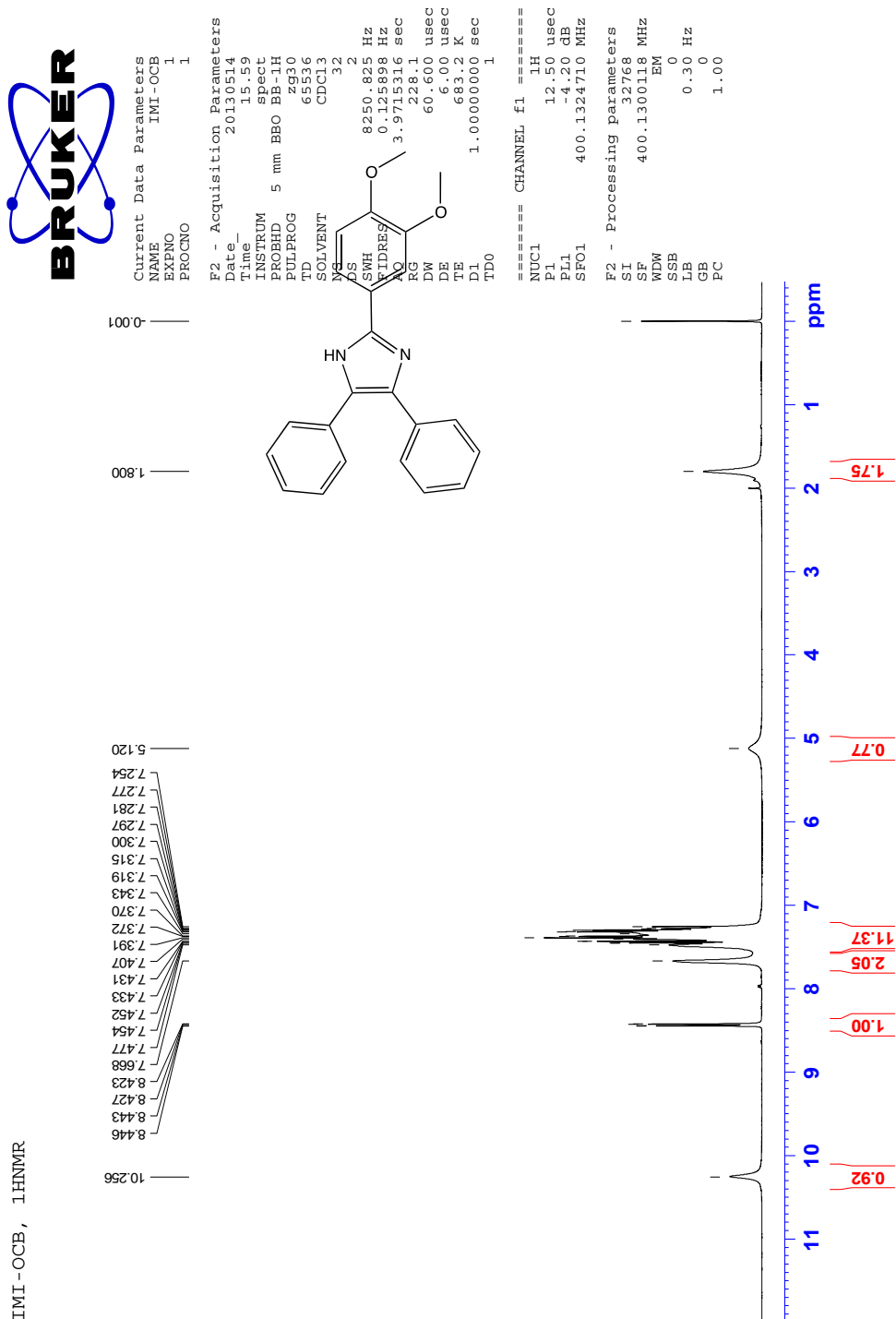


Figure S9. ¹³C-NMR Compound 8.



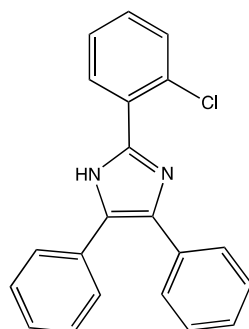
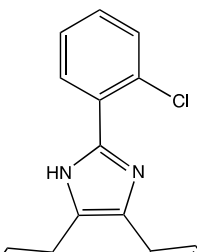
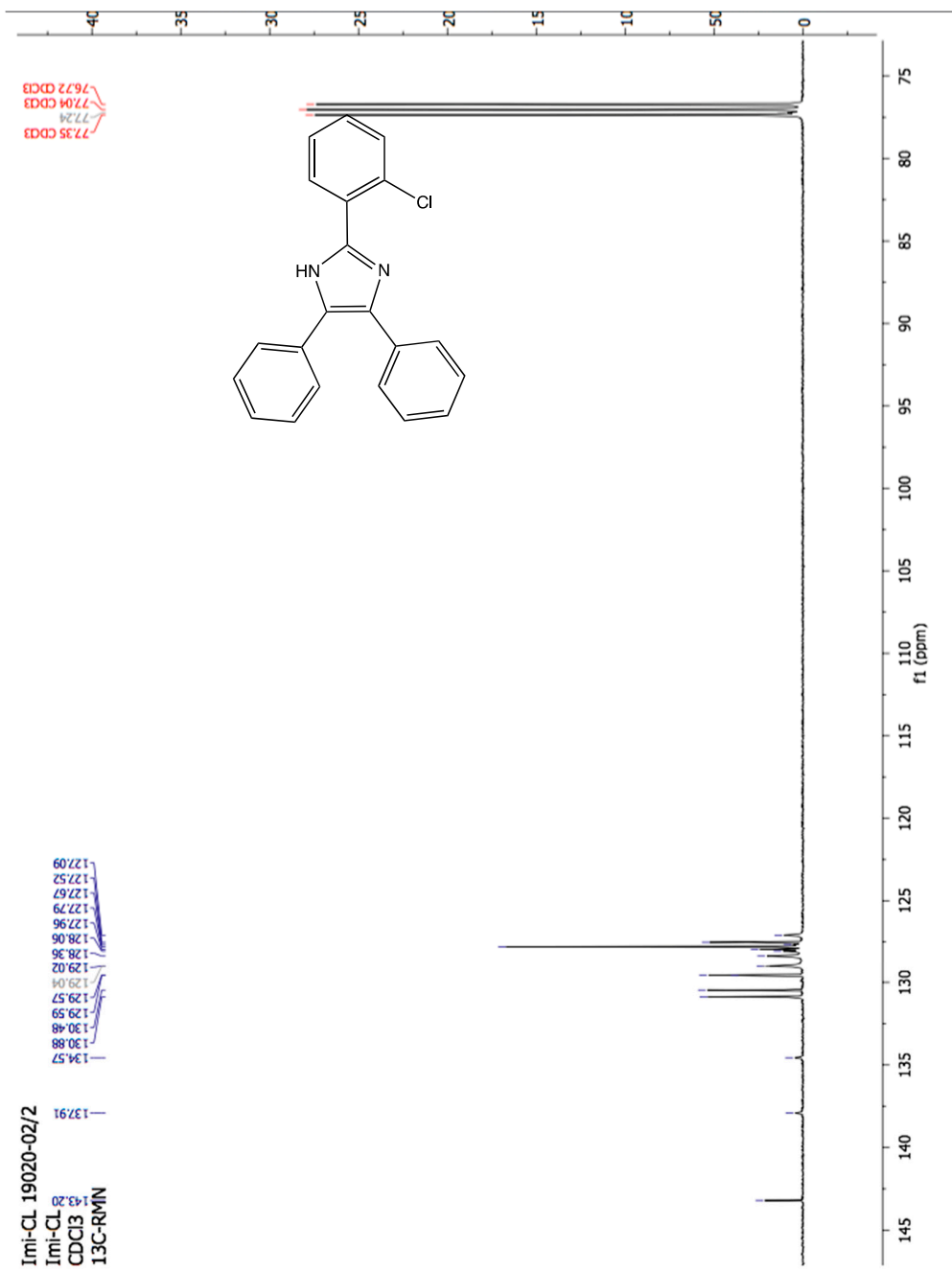


Figure S10. $^1\text{H-NMR}$ Compound 9.





¹³C-NMR Compound 9.

Figure S11.

IMI-PNB, 1H NMR



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 400.129980 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

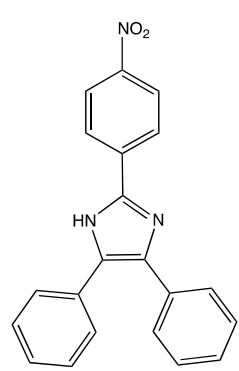
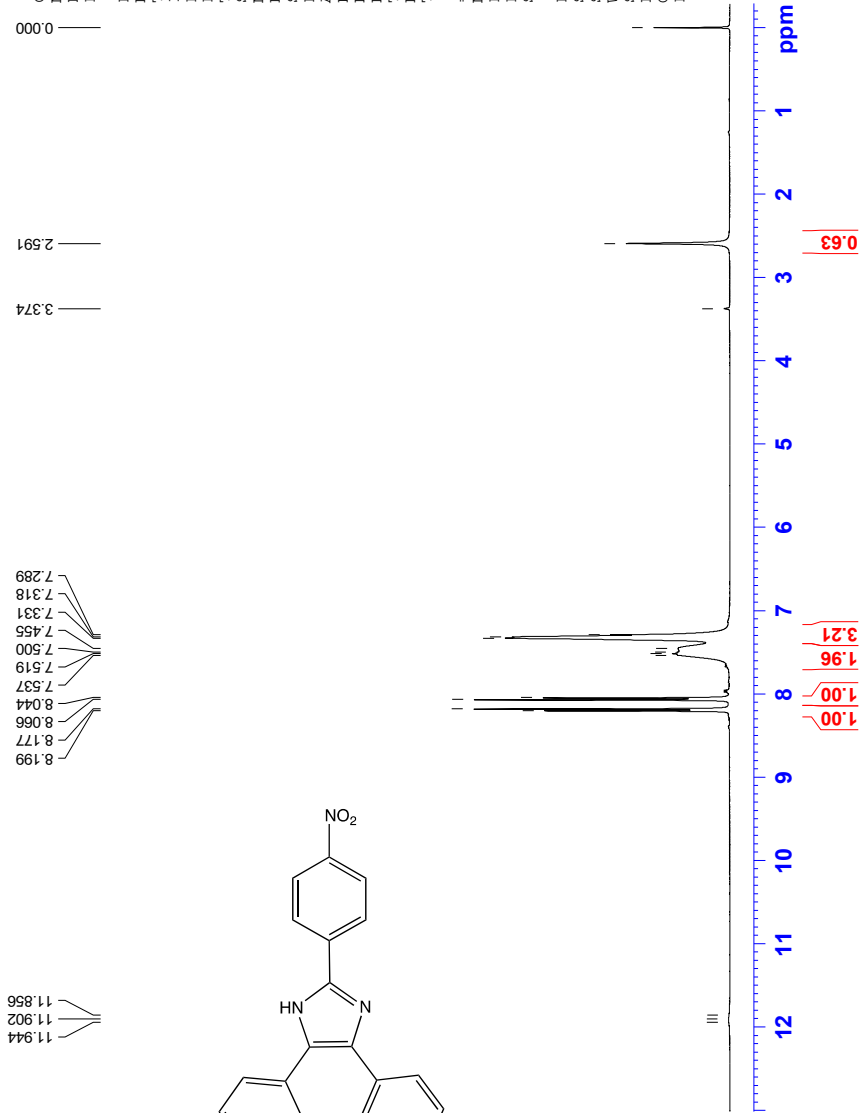
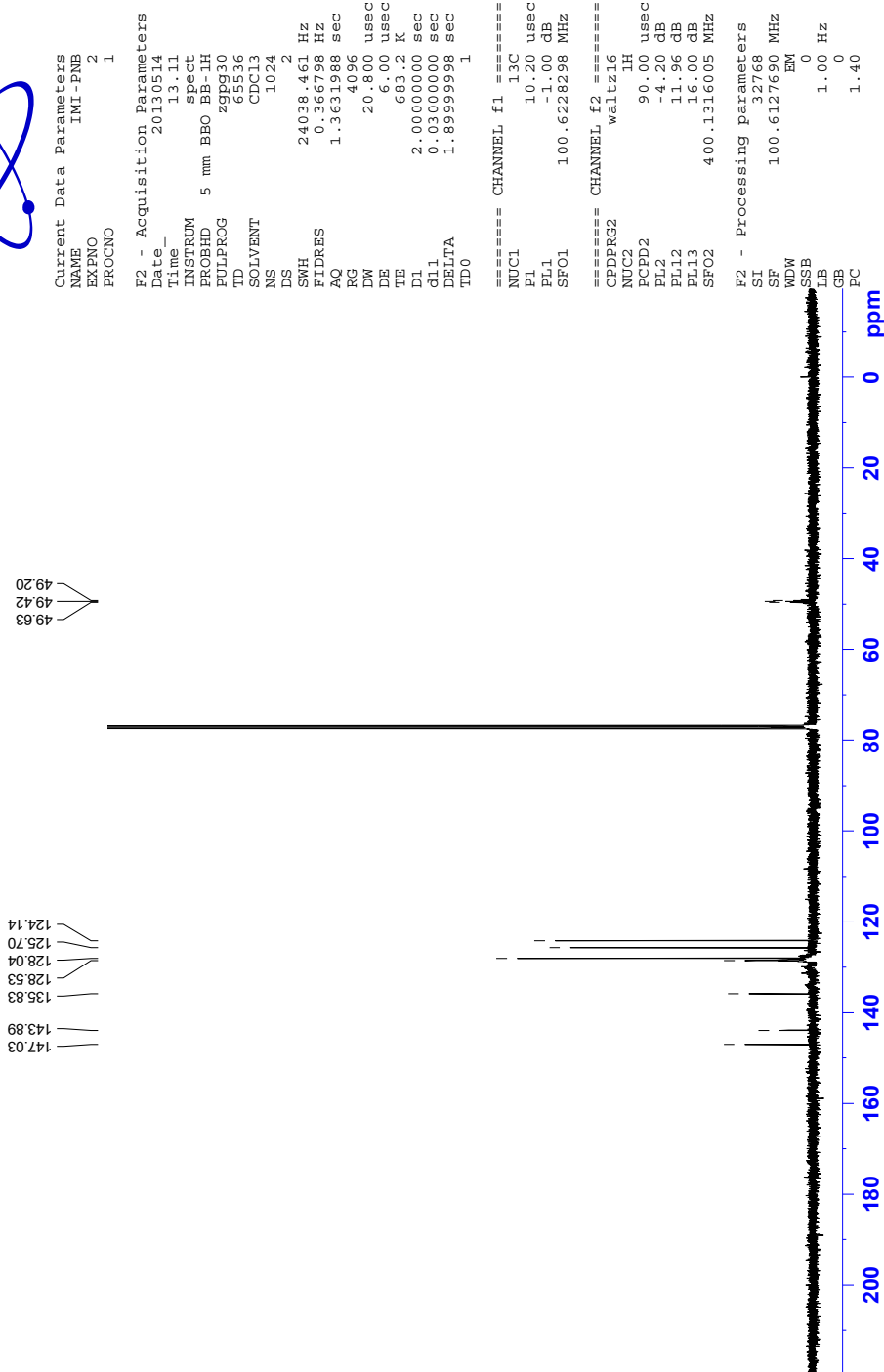


Figure S12.
¹H-NMR
 Compound 11.



IMI-PNB, ¹³CNMR



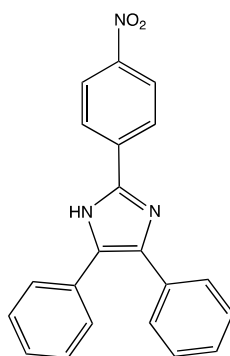


Figure S13. ¹³C-NMR Compound 11.