

Regioselective Suzuki-Miyaura Reactions of 4,7-Dichloro-*N*-methylisatin. Synthesis, Anti-HIV Activity and Modeling Study

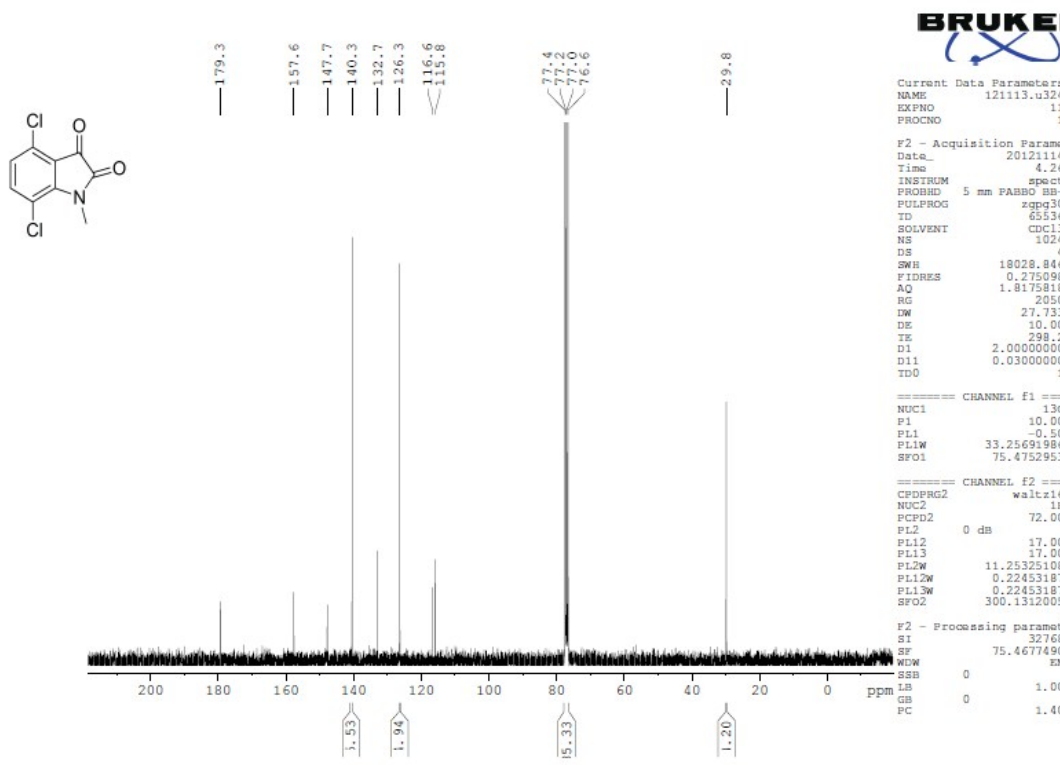
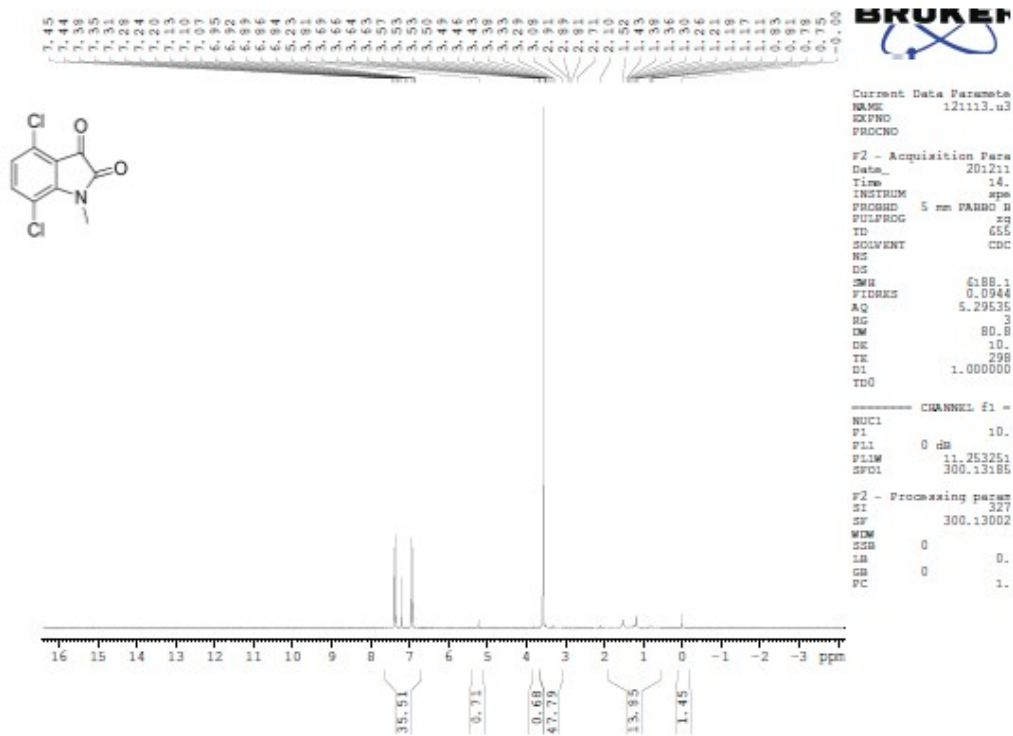
Aws M. Hamdy,^{a,b} Najim A. Al-Masoudi,^c Christophe Pannecouque,^d Qamar Rahman,^{a,e}
Alexander Villinger,^a Peter Langer*^{a,f}

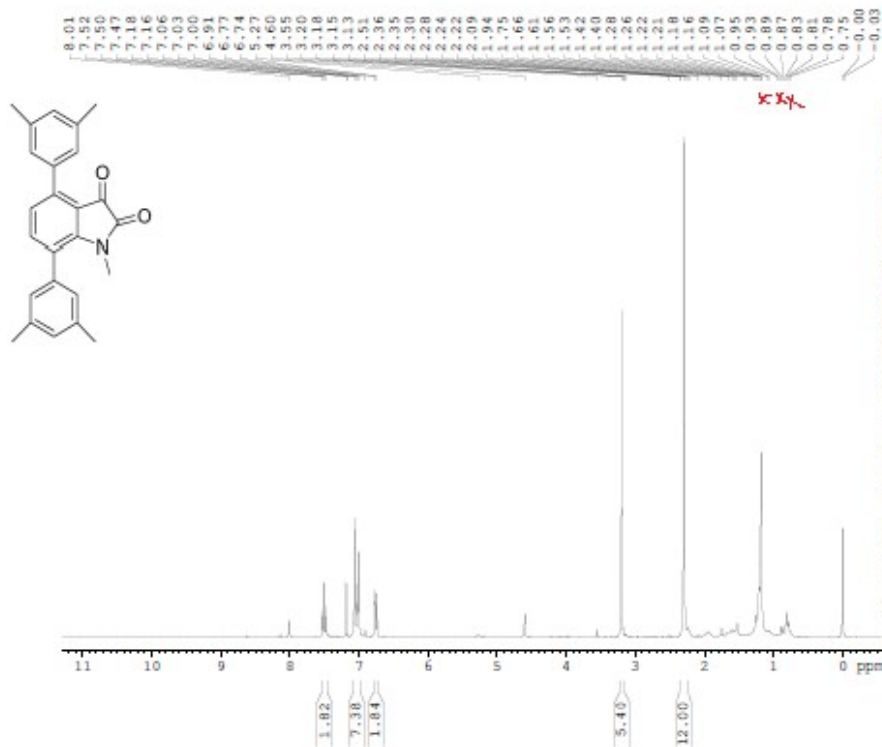
Supporting Information

Content

Copies of NMR spectra

p.2



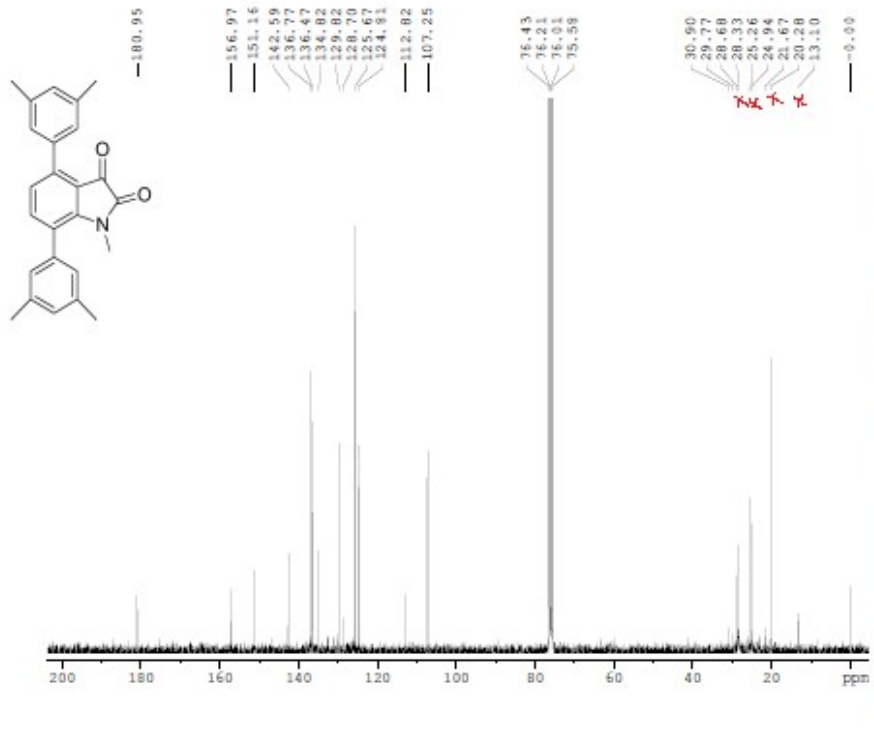


Current Data Parameters
 NAME 131212.u306
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131212
 Time 10.50
 INSTRUM spect
 PROBRD 5 mm PA100 BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.09443 Hz
 AQ 5.2953587 sec
 RG 114
 DW 80.800 usec
 DE 10.00 usec
 TE 298.2 K
 DL 1.00000000 sec
 TDO 1

CHANNEL F1
 NUC1 1H
 P1 10.00 usec
 PL1 0 dB
 PL1W 11.25325108 W
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300346 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



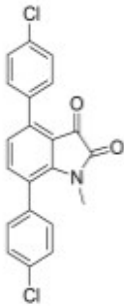
Current Data Parameters
 NAME 131212.u306
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131212
 Time 18.55
 INSTRUM spect
 PROBRD 5 mm PA100 BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 4
 DS 4
 SWH 18028.846 Hz
 FIDRES 0.275098 Hz
 AQ 1.8175818 sec
 RG 2050
 DW 27.733 usec
 DE 10.00 usec
 TE 298.2 K
 DL 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

CHANNEL F1
 NUC1 13C
 P1 10.00 usec
 PL1 -0.50 dB
 PL1W 33.25691986 W
 SFO1 75.4752953 MHz

CHANNEL F2
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 72.00 usec
 PL2 0 dB
 PL12 17.00 dB
 PL13 17.00 dB
 PL2W 11.25325108 W
 PL12W 0.22453187 W
 PL13W 0.22453187 W
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4678276 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

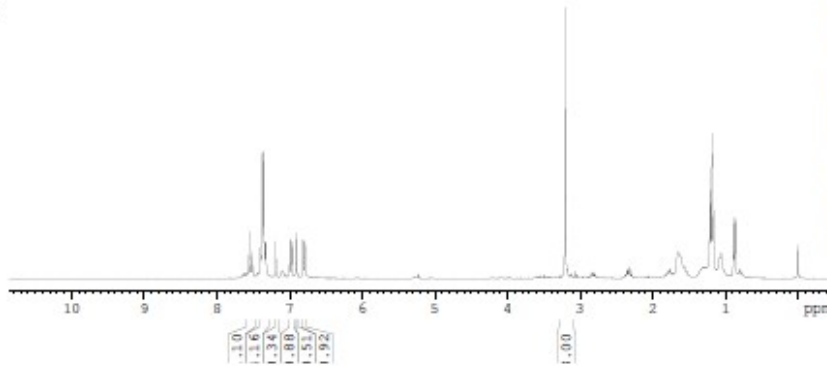


Current Data Parameters
 NAME 131126.u311
 KKFNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131126
 Time 12.50
 INSTRUM spect
 PROBRD 5 mm PARBO SB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953587 sec
 RG 90.5
 DM 80.800 usec
 DE 10.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

CHANNEL F1
 NUC1 1H
 P1 10.00 usec
 PL1 0 dB
 PL1W 11.25325108 W
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300331 MHz
 MSW 3M
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



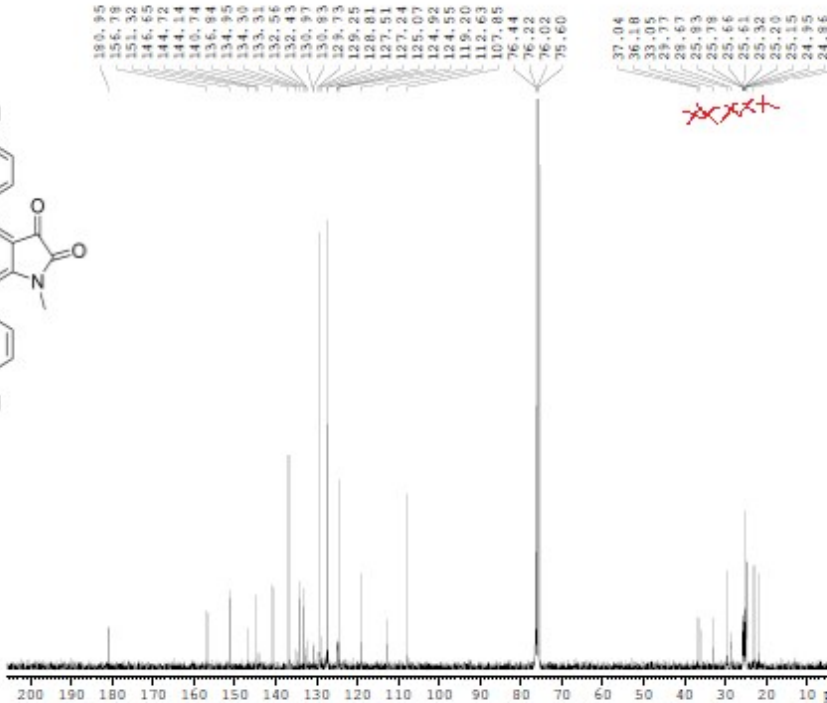
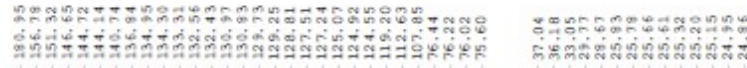
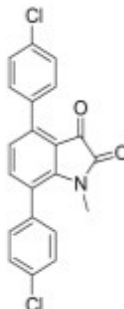
Current Data Parameters
 NAME 131126.u311
 KKFNO 11
 PROCNO 1

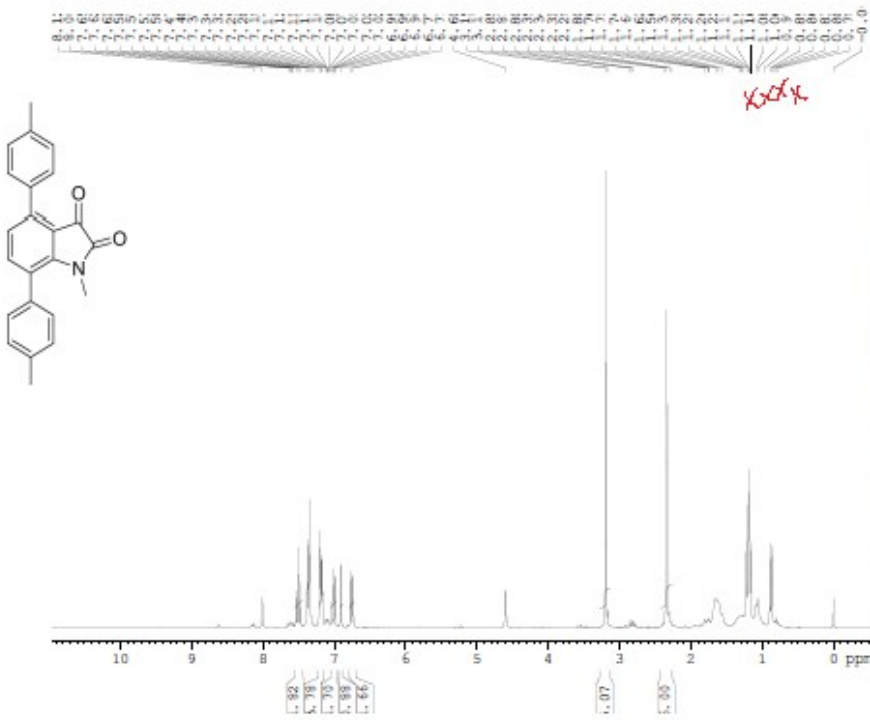
F2 - Acquisition Parameters
 Date_ 20131127
 Time 7.33
 INSTRUM spect
 PROBRD 5 mm PARBO SB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 18028.846 Hz
 FIDRES 0.275098 Hz
 AQ 1.8175818 sec
 RG 2050
 DM 27.733 usec
 DE 10.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

CHANNEL F1
 NUC1 13C
 P1 10.00 usec
 PL1 -0.50 dB
 PL1W 33.25691986 W
 SFO1 75.4752953 MHz

CHANNEL F2
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 72.00 usec
 PL2 0 dB
 PL12 17.00 dB
 PL13 17.00 dB
 PL2W 11.25325108 W
 PL12W 0.22453187 W
 PL13W 0.22453187 W
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4678276 MHz
 MSW 3M
 SSB 0
 LB 1.00 Hz
 GB 0



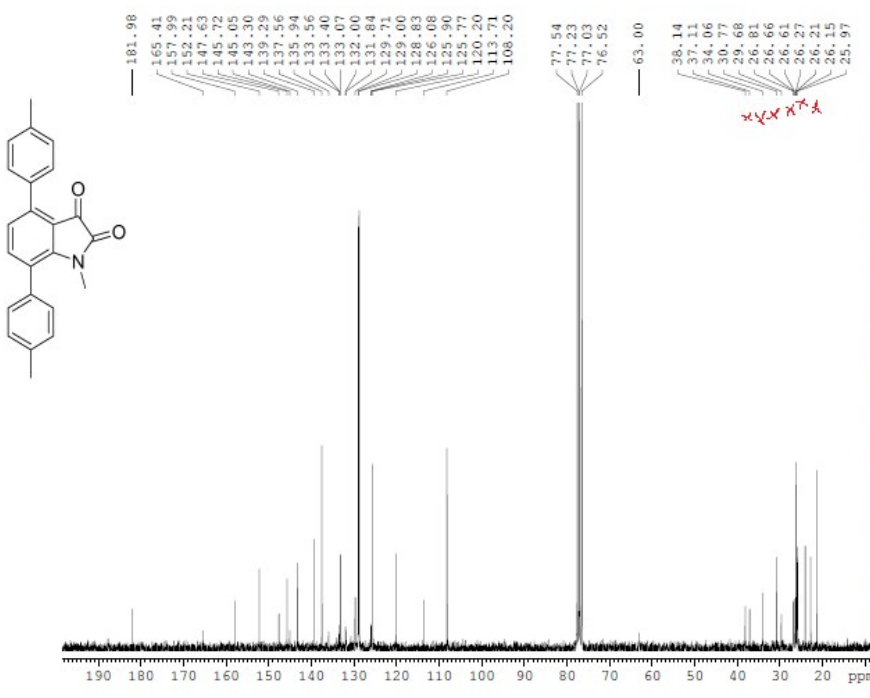


Current Data Parameters
 NAME 131216.201
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131216
 Time 10.55
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 5165.289 Hz
 FIDRES 0.078816 Hz
 AQ 6.3439350 sec
 RG 181
 DW 96.800 usec
 DE 10.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 -2.50 dB
 SFO1 250.1315447 MHz

F2 - Processing parameters
 SI 32768
 SF 250.1300193 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



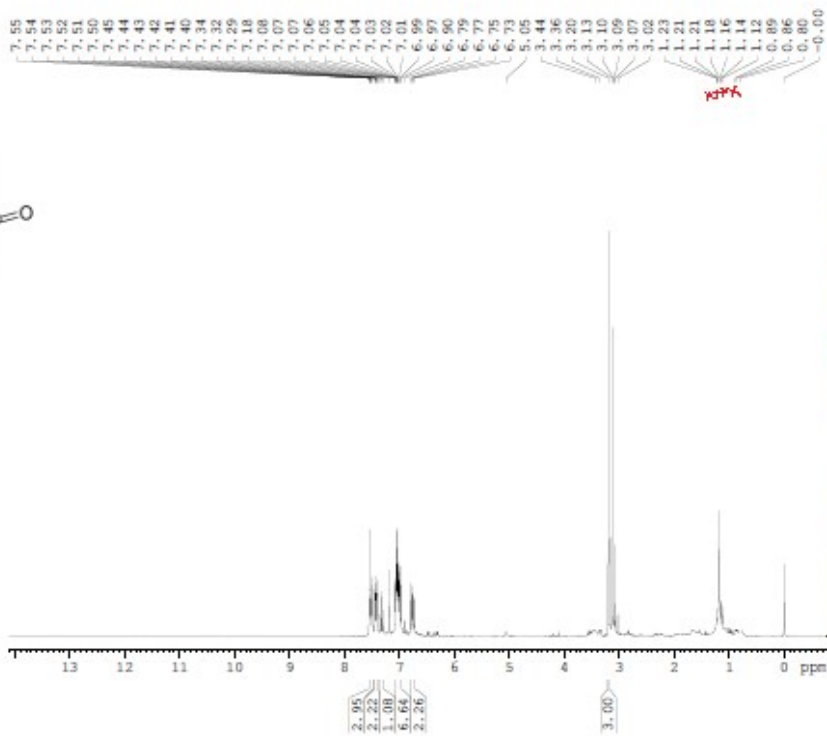
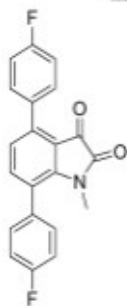
Current Data Parameters
 NAME 131216.201
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131216
 Time 12.09
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 1024
 DS 4
 SWH 15000.000 Hz
 FIDRES 0.228882 Hz
 AQ 2.1845834 sec
 RG 2050
 DW 33.333 usec
 DE 10.00 usec
 TE 298.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999999 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 -1.00 dB
 SFO1 62.9015280 MHz

==== CHANNEL f2 =====
 CDPHRG2 waltz16
 NUC2 1H
 PCPD2 70.00 usec
 PL12 15.00 dB
 PL13 15.00 dB
 PL2 -2.50 dB
 SFO2 250.1310005 MHz

F2 - Processing parameters
 SI 32768
 SF 62.8952390 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

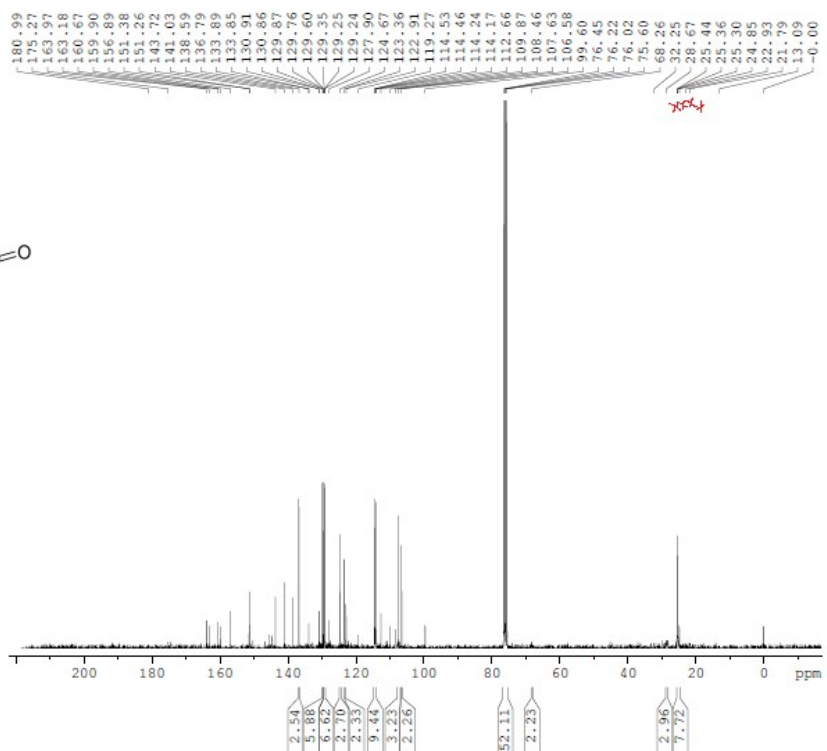
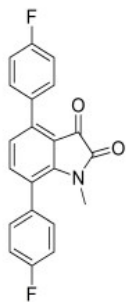


Current Data Parameter
 NAME 131010.u3
 EXPNO 1
 PROCNO 1

F2 - Acquisition Param
 Date_ 201310
 Time 10.1
 INSTRUM ape
 PROBRD 5 mm PABBO H
 PULPROG zgpg3
 TD 6553
 SOLVENT CDCl
 NS 140
 DS 18028.84
 SWH 18028.84
 FIDRES 0.27509
 AQ 1.817581
 RG 205
 DW 27.73
 DE 10.0
 TE 298.
 D1 2.0000000
 D11 0.0300000
 TD0

==== CHANNEL f1 ====
 NUC1
 P1 10.0
 PL1 0 db
 PL1W 11.2532510
 SFO1 300.13185

F2 - Processing param
 SI 327
 SF 300.13003
 MW 75.475295
 SSB 0
 LB 0.0
 GB 0
 FC 1.4



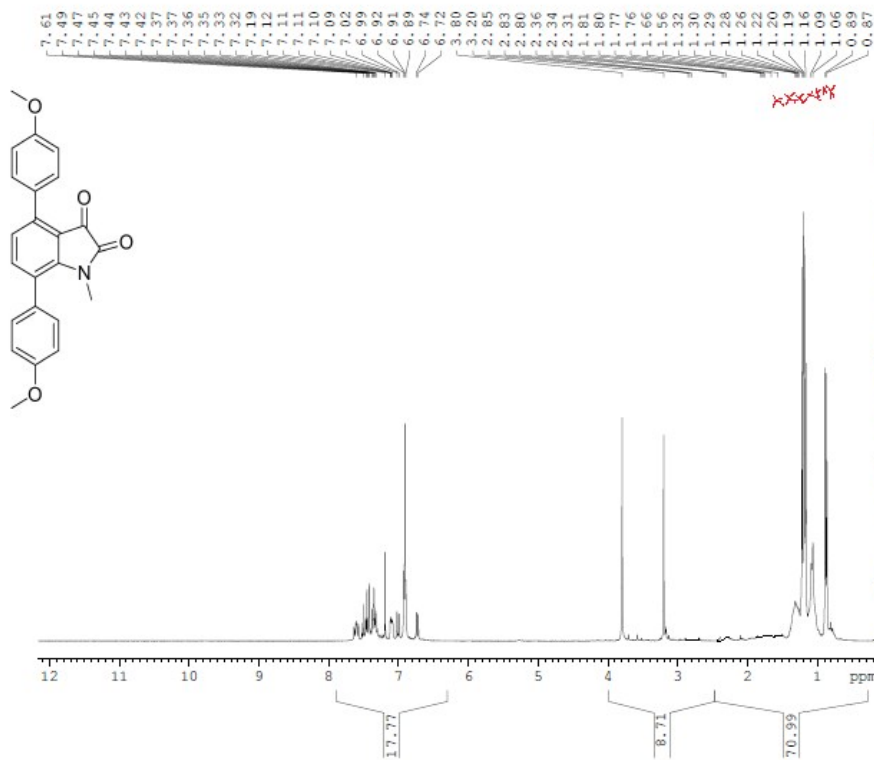
Current Data Parameter
 NAME 131010.u30
 EXPNO 1
 PROCNO 1

F2 - Acquisition Param
 Date_ 201310
 Time 10.5
 INSTRUM spec
 PROBRD 5 mm PABBO BB
 PULPROG zgpg3
 TD 6553
 SOLVENT CDCl
 NS 140
 DS 18028.84
 SWH 18028.84
 FIDRES 0.27509
 AQ 1.817581
 RG 205
 DW 27.73
 DE 10.0
 TE 298.
 D1 2.0000000
 D11 0.0300000
 TD0

==== CHANNEL f1 ====
 NUC1 13
 P1 10.0
 PL1 -0.5
 PL1W 33.2569198
 SFO1 75.475295

==== CHANNEL f2 ====
 CPDPRG2 waltz1
 NUC2 1
 PCPD2 72.0
 PL2
 PL12 0 db
 PL12 17.0
 PL13 17.0
 PL1W 11.2532510
 PL12W 0.2245318
 PL13W 0.2245318
 SFO2 300.131200

F2 - Processing param
 SI 3276
 SF 75.467827
 MW 75.475295
 SSB 0
 LB 1.0
 GB 0
 FC 1.4

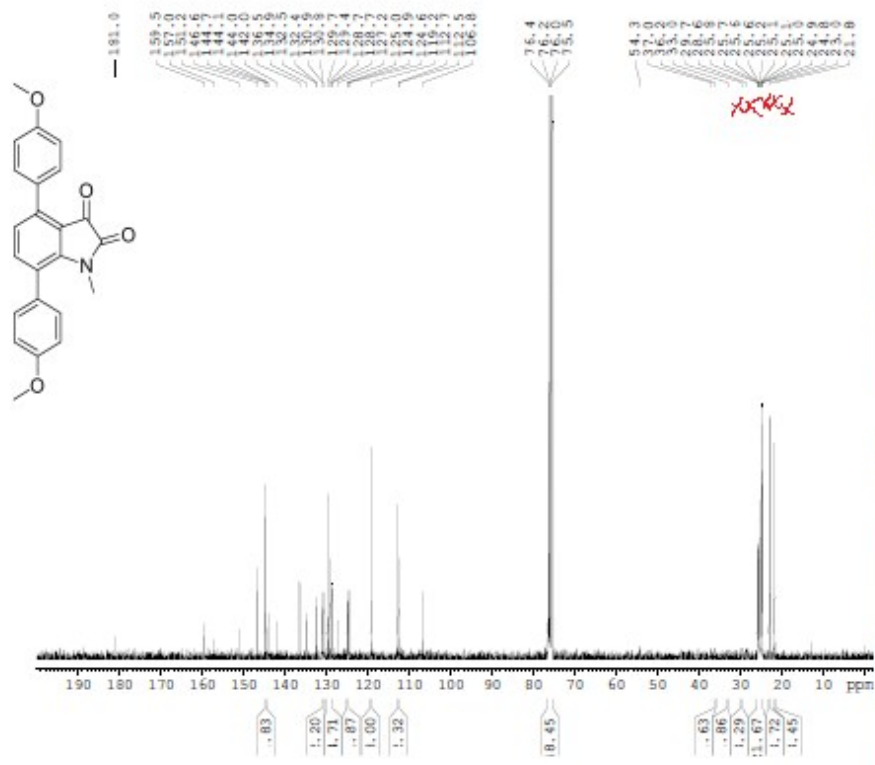


Current Data Parameters
 NAME 130926.u325
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130926
 Time 16.02
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953587 sec
 RG 50.8
 DW 80.800 usec
 DE 10.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0 dB
 PL1W 11.25325108 W
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300330 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



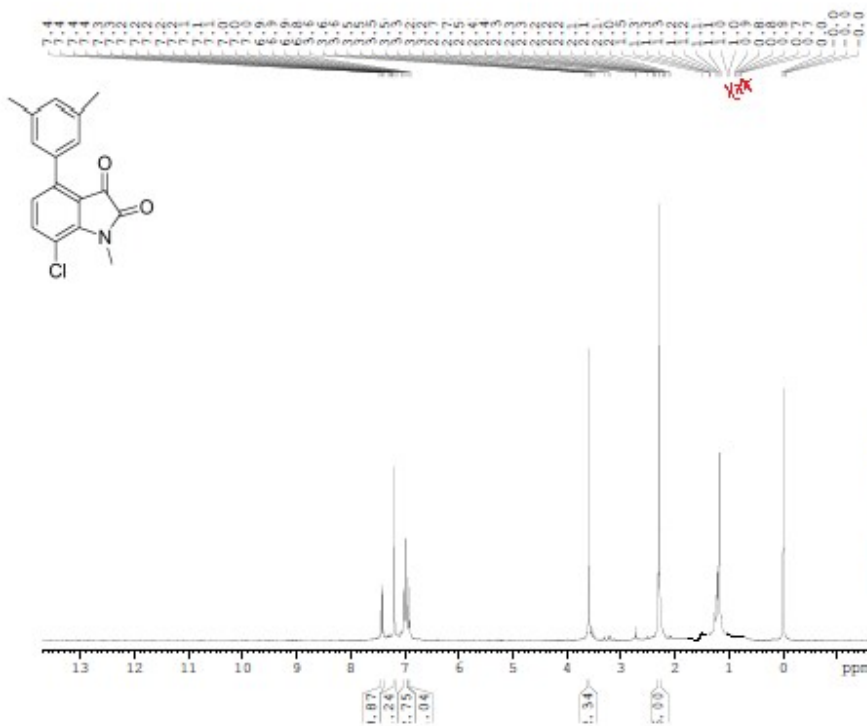
Current Data Parameters
 NAME 130926.u325
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130926
 Time 17.10
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 18028.846 Hz
 FIDRES 0.275098 Hz
 AQ 1.8175813 sec
 RG 2050
 DW 27.733 usec
 DE 10.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 -0.50 dB
 PL1W 33.25691986 W
 SFO1 75.4752953 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 FCPD2 72.00 usec
 FQ3 0 dB
 FQ12 17.00 dB
 FQ13 17.00 dB
 PL2W 11.25325108 W
 PL12W 0.22453187 W
 PL13W 0.22453187 W
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4678274 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

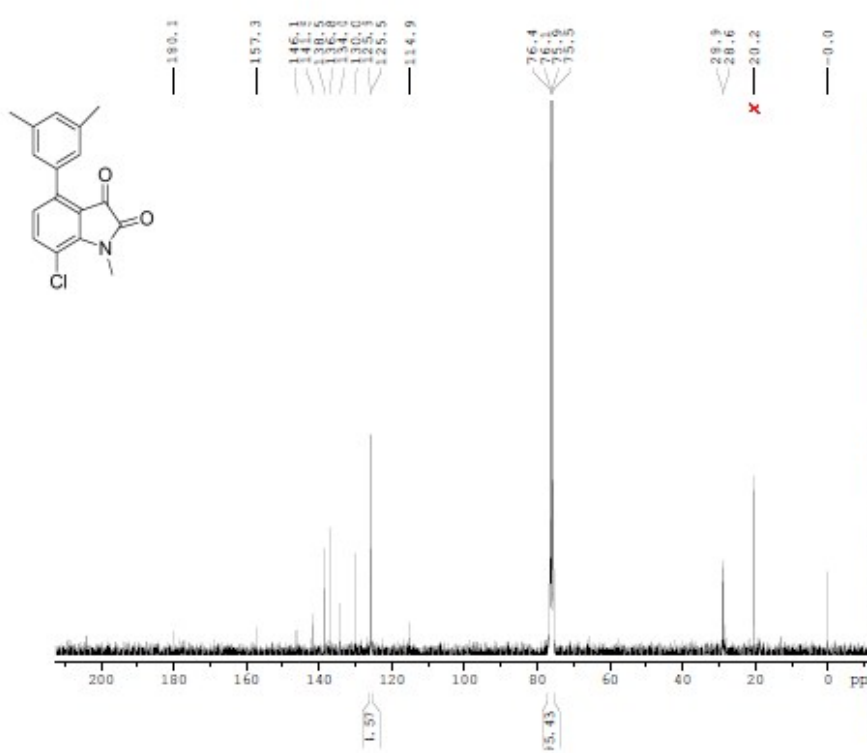


Current Data Parameters
 NAME 131108.u324
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131108
 Time 12.25
 INSTRUM spect
 PROBRD 5 mm PARBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953587 sec
 RG 287
 DM 80.800 usec
 DE 10.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 TDO 1

CHANNEL F1
 NUC1 1H
 P1 10.00 usec
 PL1 0 dB
 PL1W 11.25325108 W
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300350 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



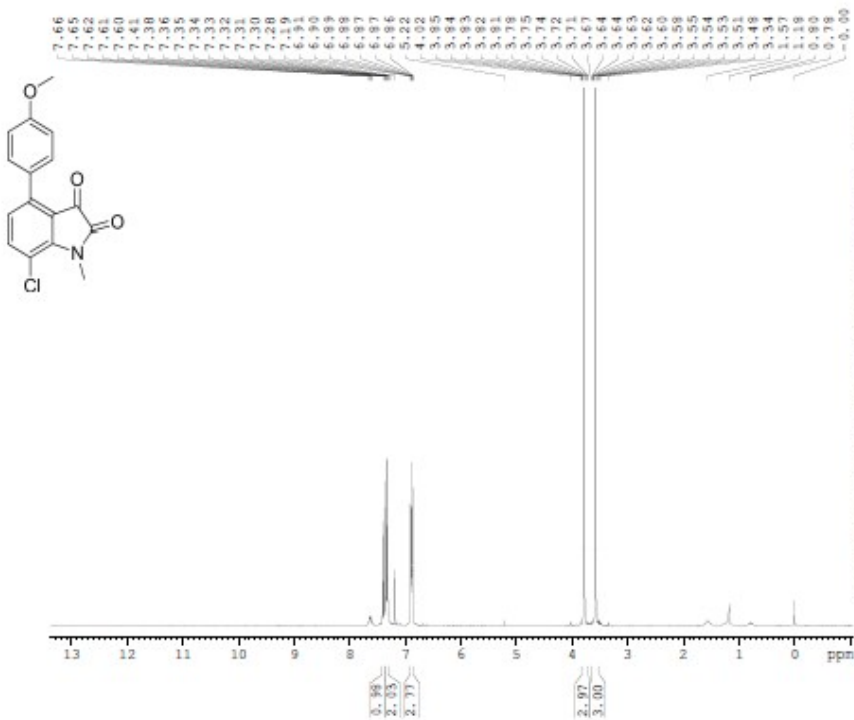
Current Data Parameters
 NAME 131108.u324
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131109
 Time 15.13
 INSTRUM spect
 PROBRD 5 mm PARBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 2048
 DS 4
 SWH 18028.846 Hz
 FIDRES 0.275098 Hz
 AQ 1.8175818 sec
 RG 2050
 DM 27.733 usec
 DE 10.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

CHANNEL F1
 NUC1 13C
 P1 10.00 usec
 PL1 -0.50 dB
 PL1W 33.25691986 W
 SFO1 75.4752953 MHz

CHANNEL F2
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 72.00 usec
 PL2 0 dB
 PL12 17.00 dB
 PL13 17.00 dB
 PL2W 11.25325108 W
 PL12W 0.22453187 W
 PL13W 0.22453187 W
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4678280 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

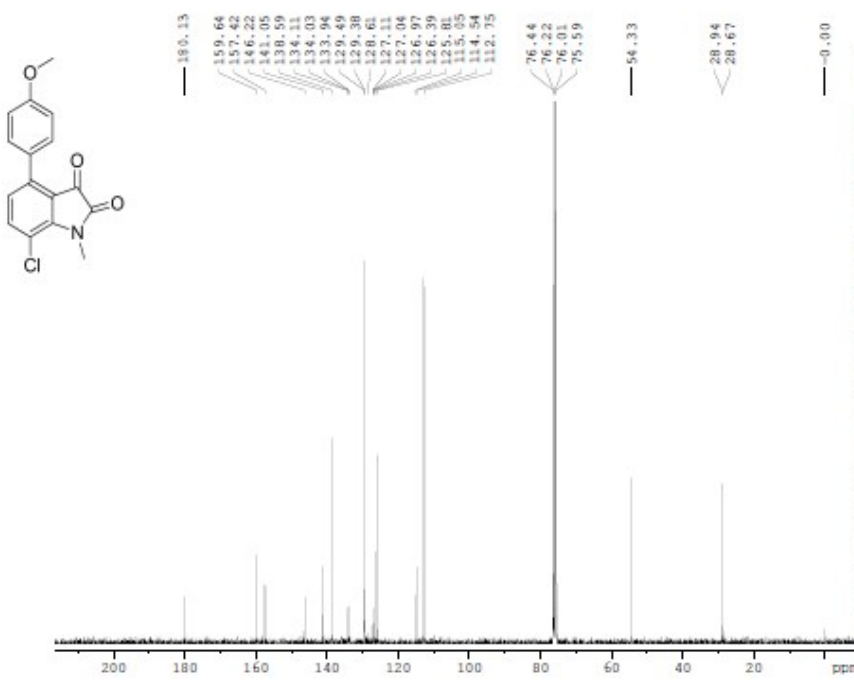


Current Data Parameters
 NAME 131108.u325
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131108
 Time 12.31
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953587 sec
 RG 101
 DM 80.800 usec
 DE 10.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 TDD 1

CHANNEL f1
 NUC1 1H
 P1 10.00 usec
 PL1 0 dB
 PL1W 11.25325108 W
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300329 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



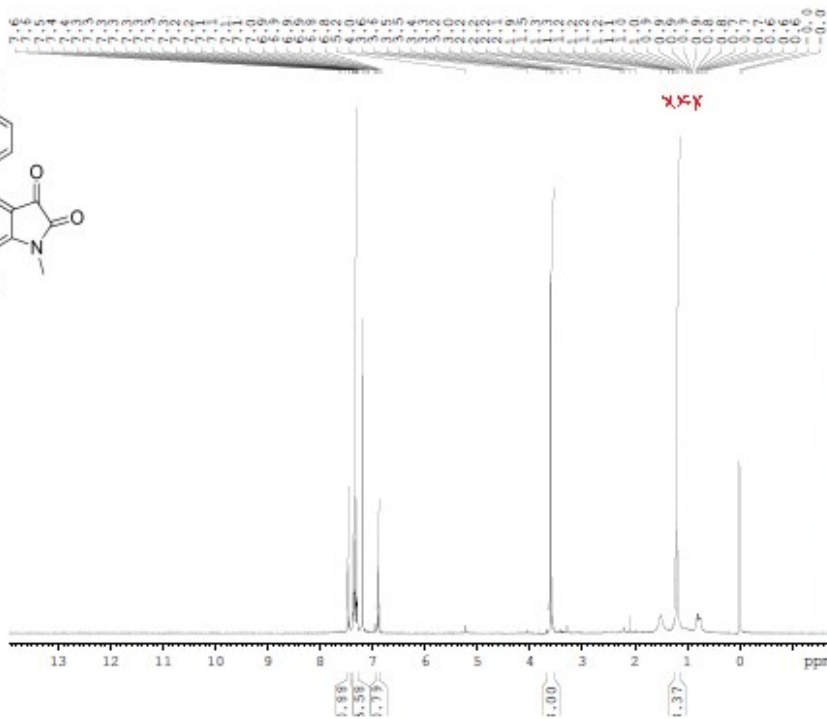
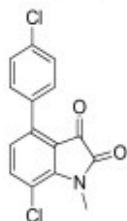
Current Data Parameters
 NAME 131108.u325
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131109
 Time 16.24
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 18028.846 Hz
 FIDRES 0.275099 Hz
 AQ 1.8175818 sec
 RG 2050
 DM 27.733 usec
 DE 10.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDD 1

CHANNEL f1
 NUC1 13C
 P1 10.00 usec
 PL1 -0.50 dB
 PL1W 33.25691986 W
 SFO1 75.4752953 MHz

CHANNEL f2
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 72.00 usec
 PL2 0 dB
 PL2 17.00 dB
 PL3 17.00 dB
 PL2W 11.25325108 W
 PL3W 0.22452187 W
 PL3W 0.22452187 W
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4676274 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

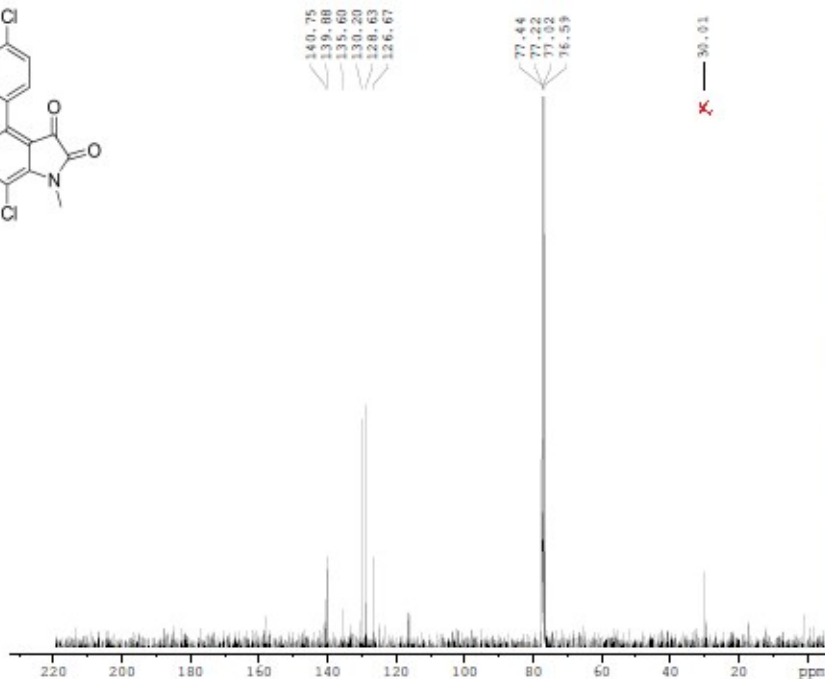
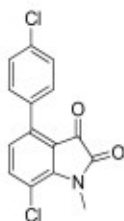


Current Data Parameters
 NAME 131107.u306
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131107
 Time 10.53
 INSTRUM spect
 PROBHD 5 mm PARHO BB-
 PULPROG zg30
 TD 65536
 SOLVENT cnc13
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953587 sec
 RG 406
 DM 80.800 usec
 DE 10.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

CHANNEL f1
 NUC1 1H
 P1 10.00 usec
 PL1 0 dB
 PL1W 11.25325108 W
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300309 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



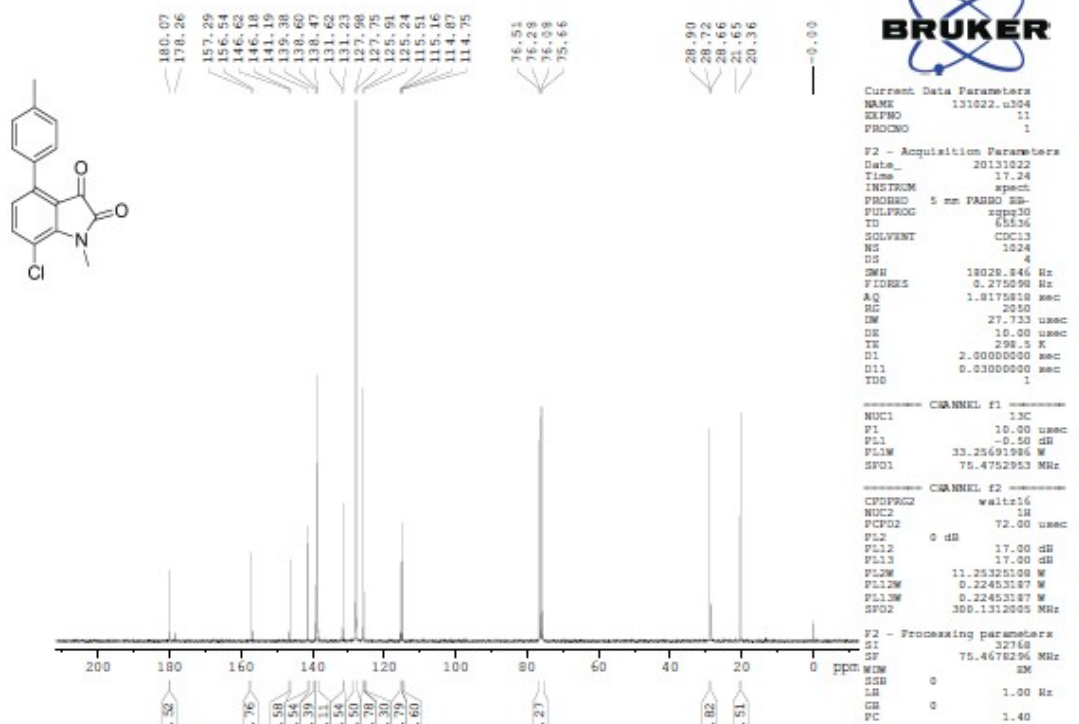
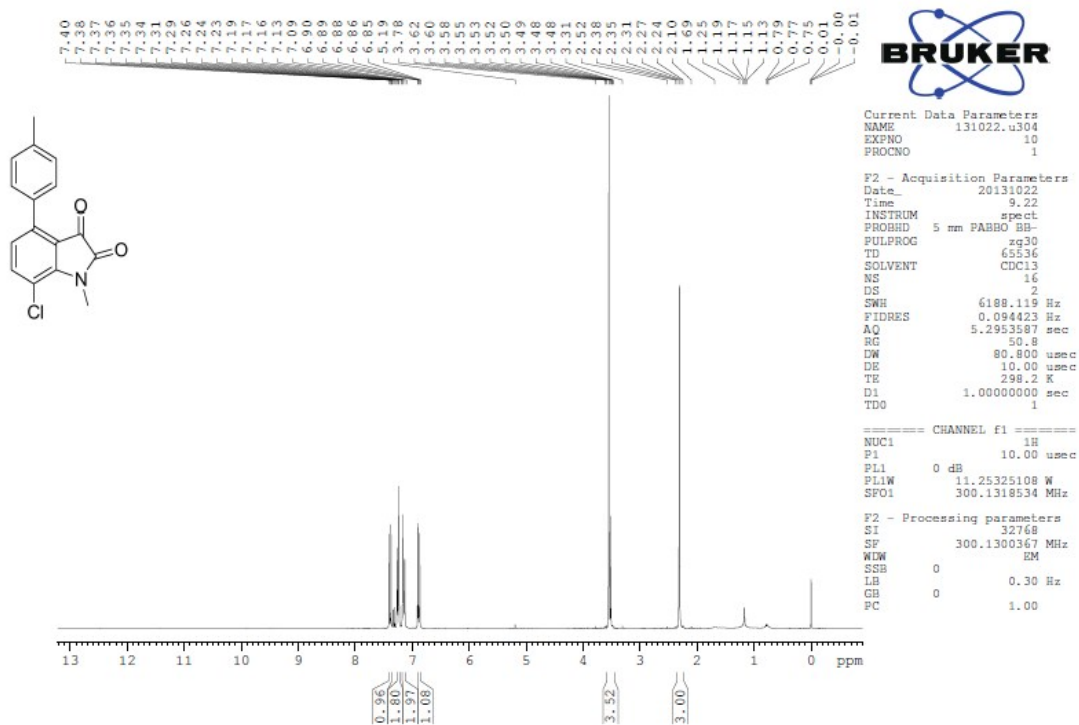
Current Data Parameters
 NAME 131107.u306
 EXPNO 12
 PROCNO 1

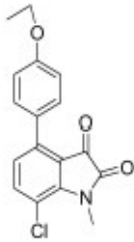
F2 - Acquisition Parameters
 Date_ 20131107
 Time 12.36
 INSTRUM spect
 PROBHD 5 mm PARHO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 1024
 DS 4
 SWH 18028.846 Hz
 FIDRES 0.275098 Hz
 AQ 1.0175818 sec
 RG 2058
 DM 21.733 usec
 DE 10.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

CHANNEL f1
 NUC1 13C
 P1 10.00 usec
 PL1 -0.50 dB
 PL1W 33.25691984 W
 SFO1 75.4752953 MHz

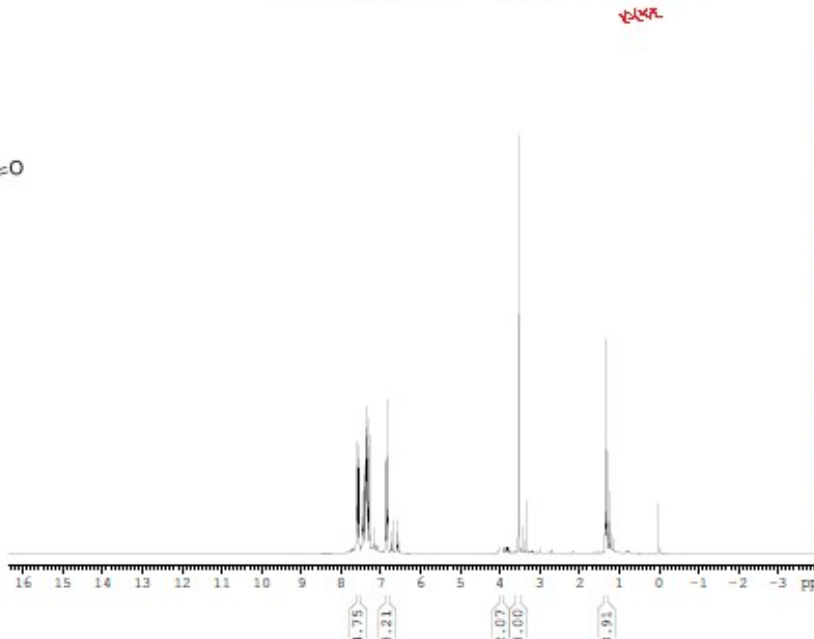
CHANNEL f2
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 72.00 usec
 PL2 0 dB
 PL12 17.00 dB
 PL13 17.00 dB
 PL2W 11.25325108 W
 PL12W 0.22453187 W
 PL13W 0.22453187 W
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40





DRUGS

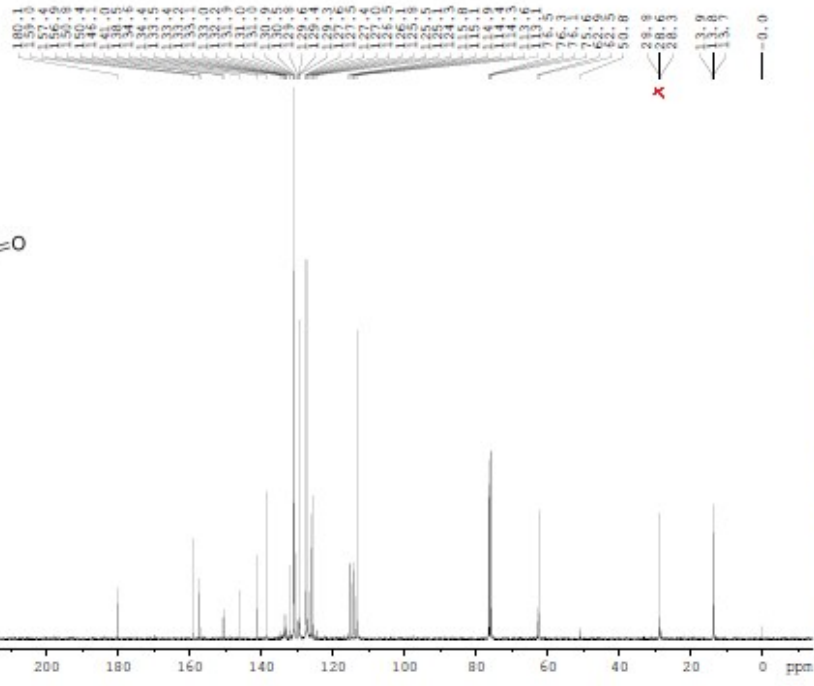
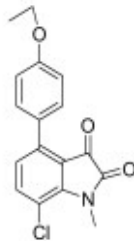


Current Data Parameters
 NAME 131021.u
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 201311
 Time 9
 INSTRUM spt
 PROBHD 5 mm FASBO 1
 PULPROG zgpg30
 TD 651
 SOLVENT CDCl3
 NS 1024
 DS 4
 SFR 6.881
 FIDRES 0.094
 AQ 5.29531
 RG 327.68
 SW 10.1
 DK 291
 TE 291
 D1 1.00000
 TDD

CHANNEL f1 -
 NUCL1 13C
 P1 10.00
 PL1 0 dB
 PLW 11.25325
 SFO1 300.13181

F2 - Processing parameters
 SI 32768
 SF 300.13000
 MWM 0
 SSR 0
 LB 0
 GB 0
 PC 1



DRUGS

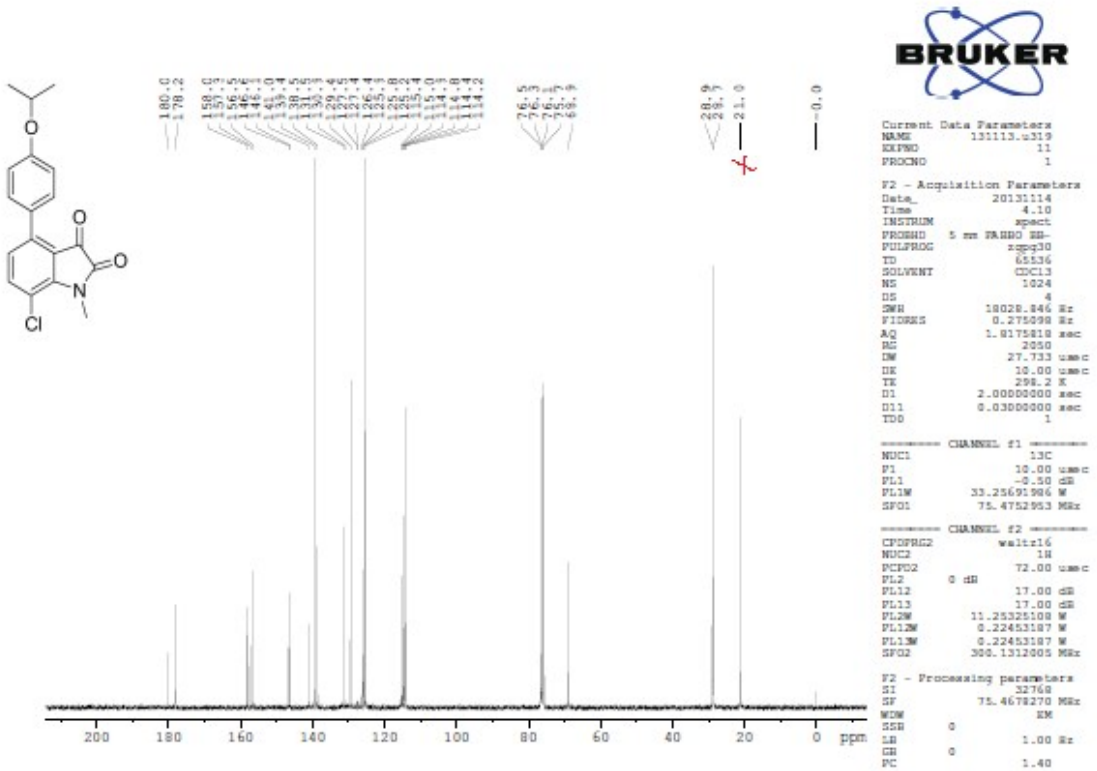
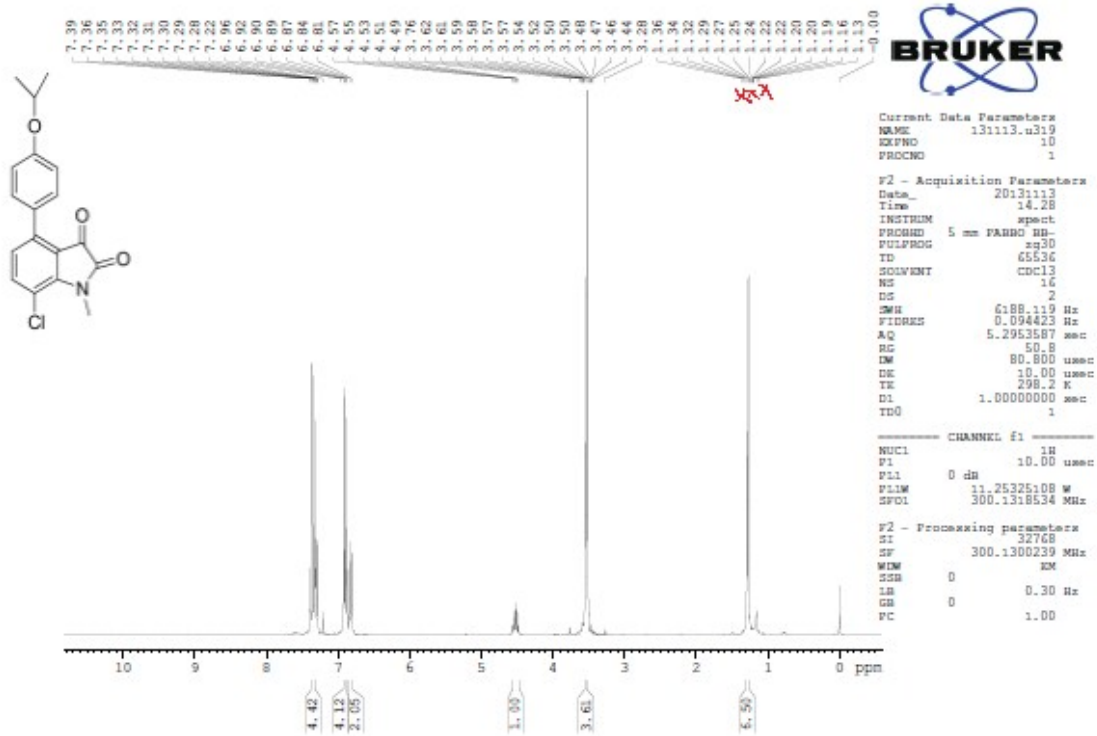
Current Data Parameters
 NAME 131021.u3
 EXPNO 1
 PROCNO 1

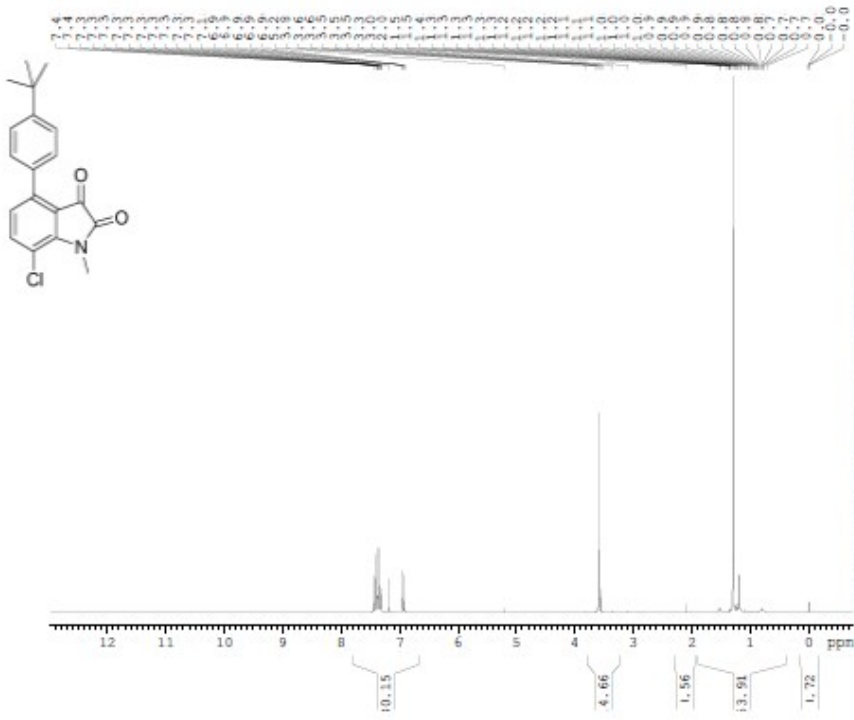
F2 - Acquisition Parameters
 Date_ 2013102
 Time 12.2
 INSTRUM spt
 PROBHD 5 mm FASBO 15
 PULPROG zgpg30
 TD 655
 SOLVENT CDCl3
 NS 1024
 DS 4
 SFR 18028.84
 FIDRES 0.27501
 AQ 1.917581
 RG 327.68
 SW 10.1
 DK 291
 TE 291
 D1 2.0000000
 D11 0.0300000
 TDD

CHANNEL f1 -
 NUCL1 13C
 P1 10.00
 PL1 0 dB
 PLW 33.2569196
 SFO1 75.475295

CHANNEL f2 -
 CPDPRG2 waltz16
 NUCL2 1H
 P2PFG2 72.0
 PL2 0 dB
 PL12 17.0
 PL13 17.0
 PLW 11.2532510
 PL12W 0.2245316
 PL13W 0.2245316
 SFO2 300.131200

F2 - Processing parameters
 SI 32768
 SF 75.467825
 MWM 0
 SSR 0
 LB 0
 GB 0
 PC 1.4



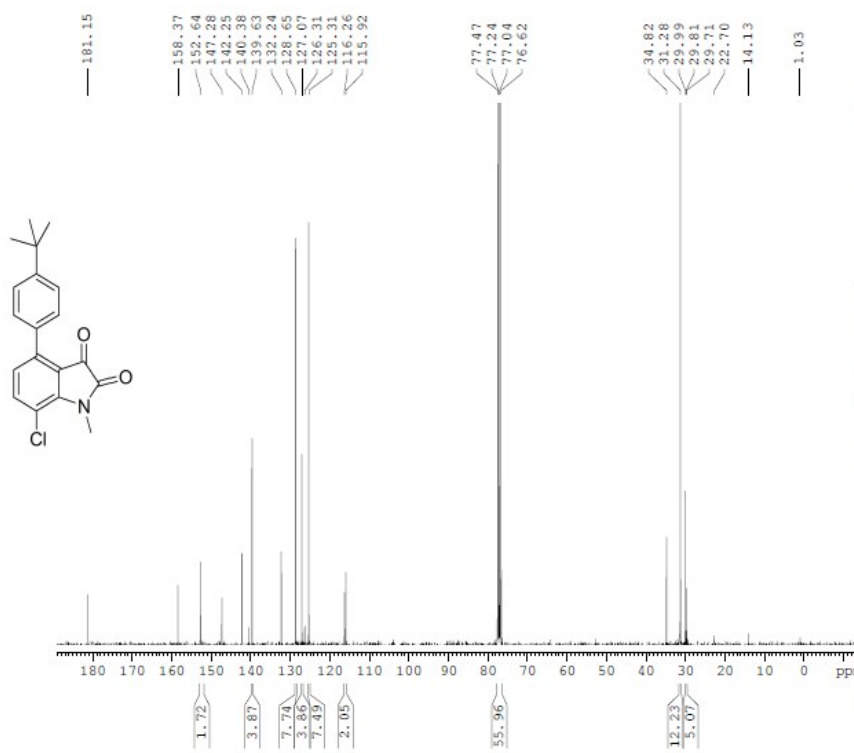


Current Data Parameters
 NAME 120427.u301
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120427
 Time 8.42
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953587 sec
 RG 90.5
 DM 80.800 usec
 DE 10.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

CHANNEL f1
 NUC1 1H
 P1 10.00 usec
 PL1 0 dB
 PL1W 11.25325108 W
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300313 MHz
 WDM KM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



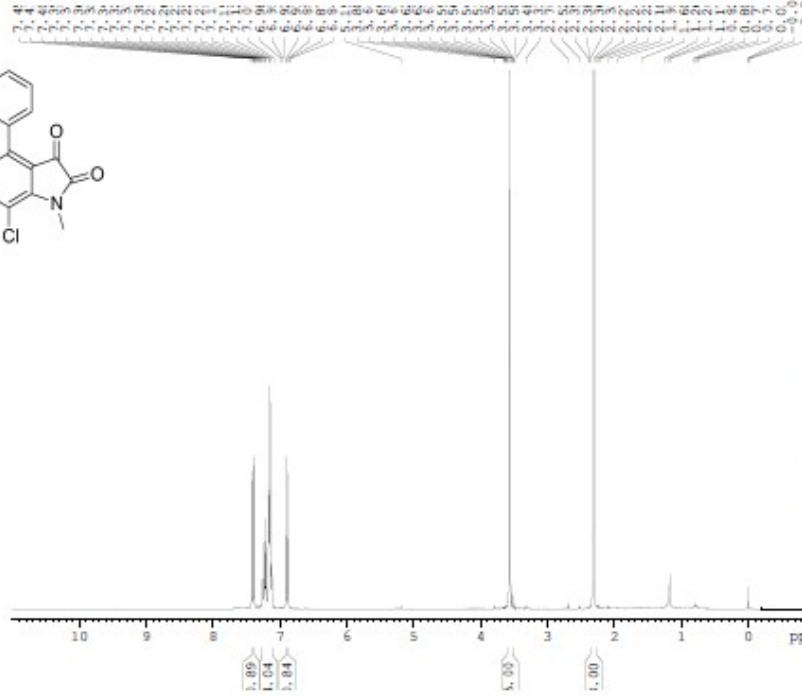
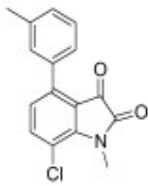
Current Data Parameters
 NAME 120427.u301
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120428
 Time 3.48
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 18028.846 Hz
 FIDRES 0.275098 Hz
 AQ 1.8175818 sec
 RG 2050
 DM 27.733 usec
 DE 10.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

CHANNEL f1
 NUC1 13C
 P1 10.00 usec
 PL1 -0.50 dB
 PL1W 33.25691986 W
 SFO1 75.4752953 MHz

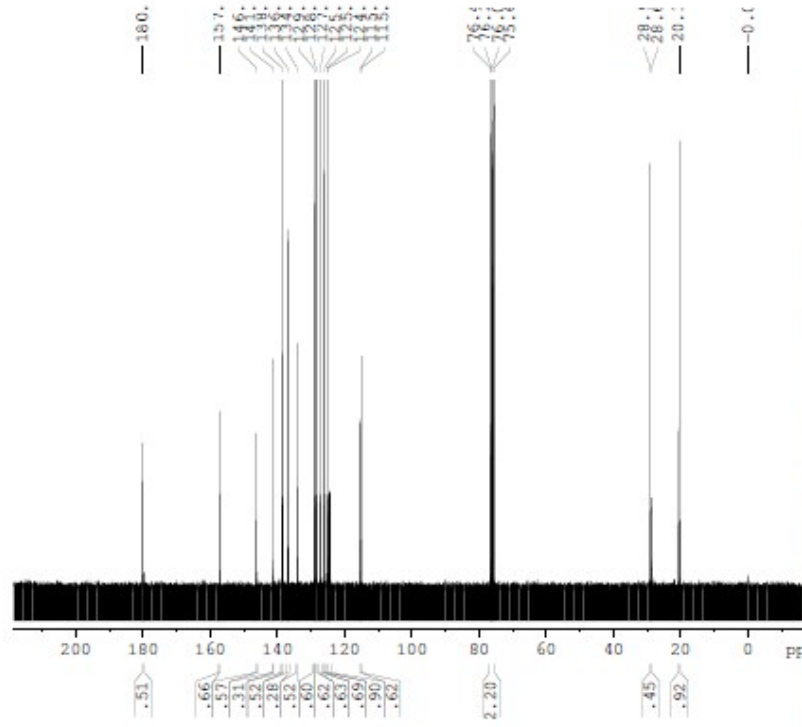
CHANNEL f2
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 72.00 usec
 PL2 0 dB
 PL12 17.00 dB
 PL13 17.00 dB
 PL2W 11.25325108 W
 PL12W 0.22453187 W
 PL13W 0.22453187 W
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 WDM KM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME 131114.u305
 EXPNO 10
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20131114
 Time 9.42
 INSTRUM spect
 PROBRD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SFR 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953587 sec
 RG 50.8
 DM 80.800 usec
 DE 10.00 usec
 TK 298.2 K
 D1 1.00000000 sec
 TDO 1

CHANNEL f1
 NUC1 1H
 P1 10.00 usec
 PL1 0 dB
 PL1W 11.25325108 W
 SFO1 300.1318534 MHz
 F2 - Processing parameters
 SI 32768
 SF 300.1300382 MHz
 WDM 0
 SSB 0 0.30 Hz
 GB 0
 PC 1.00

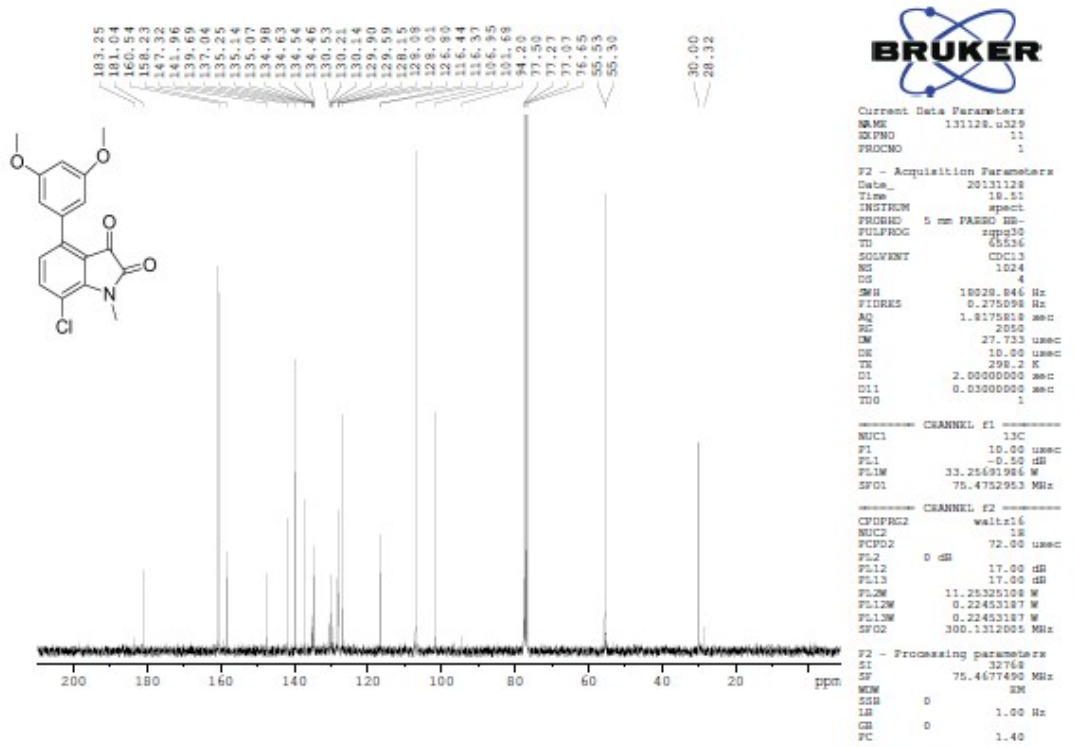
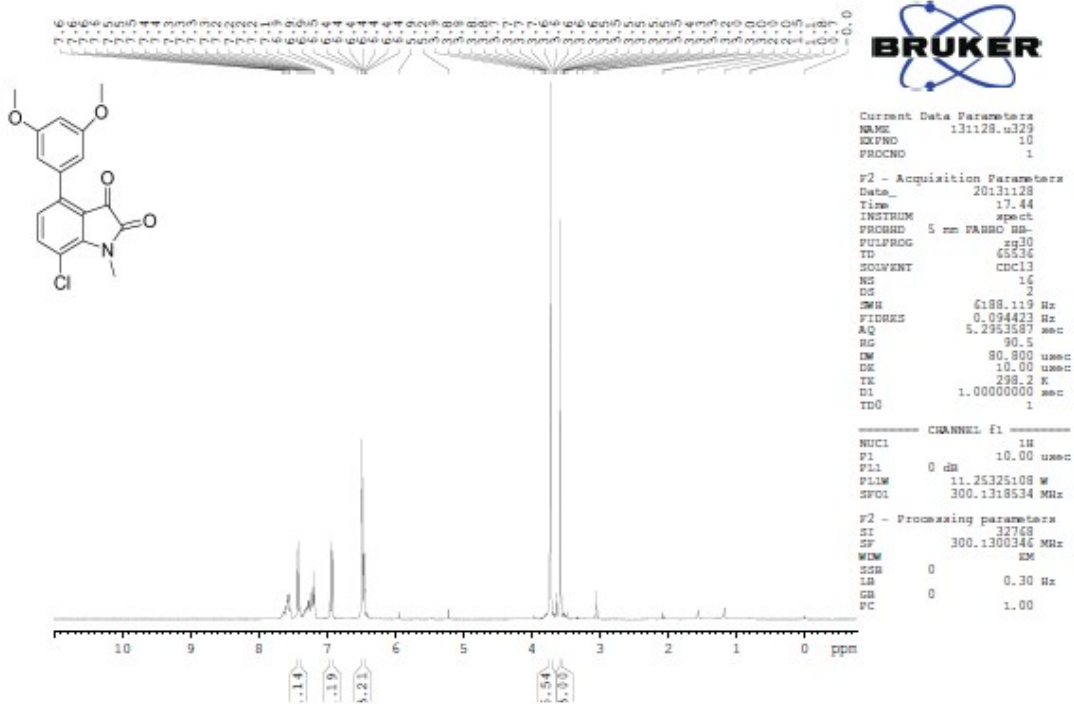


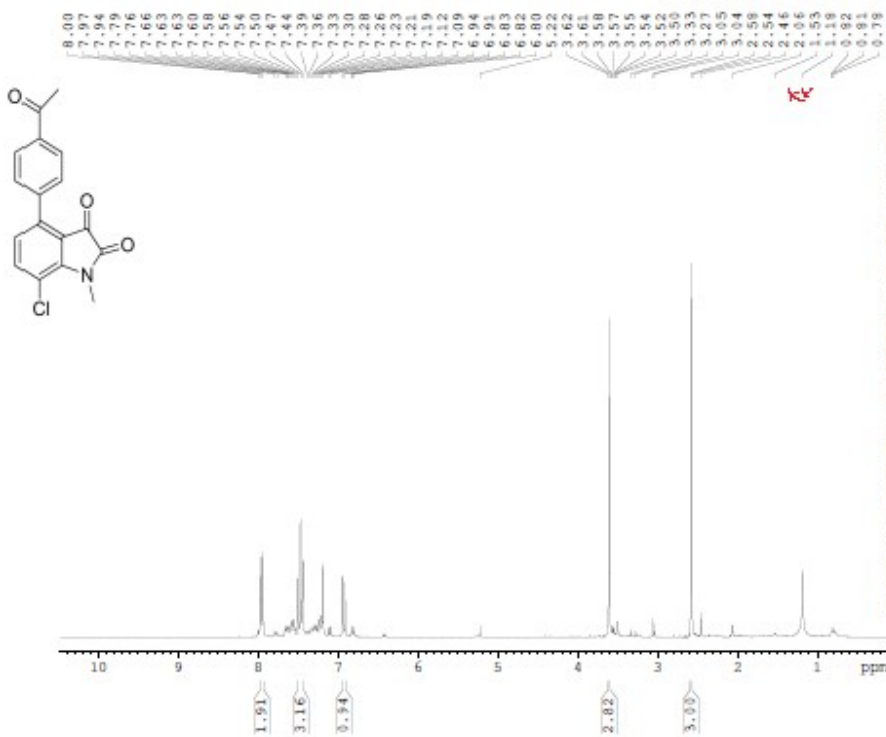
Current Data Parameters
 NAME 131114.u305
 EXPNO 11
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20131114
 Time 21.37
 INSTRUM spect
 PROBRD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SFR 18028.846 Hz
 FIDRES 0.275090 Hz
 AQ 1.8175818 sec
 RG 2050
 DM 27.733 usec
 DE 10.00 usec
 TK 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

CHANNEL f1
 NUC1 13C
 P1 10.00 usec
 PL1 -0.50 dB
 PL1W 33.25691986 W
 SFO1 75.4752953 MHz

CHANNEL f2
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 72.00 usec
 PL2 0 dB
 PL12 17.00 dB
 PL13 17.00 dB
 PL2W 11.25325108 W
 PL12W 0.22453187 W
 PL13W 0.22453187 W
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4678295 MHz
 WDM 0
 SSB 0 1.00 Hz
 GB 0
 PC 1.40



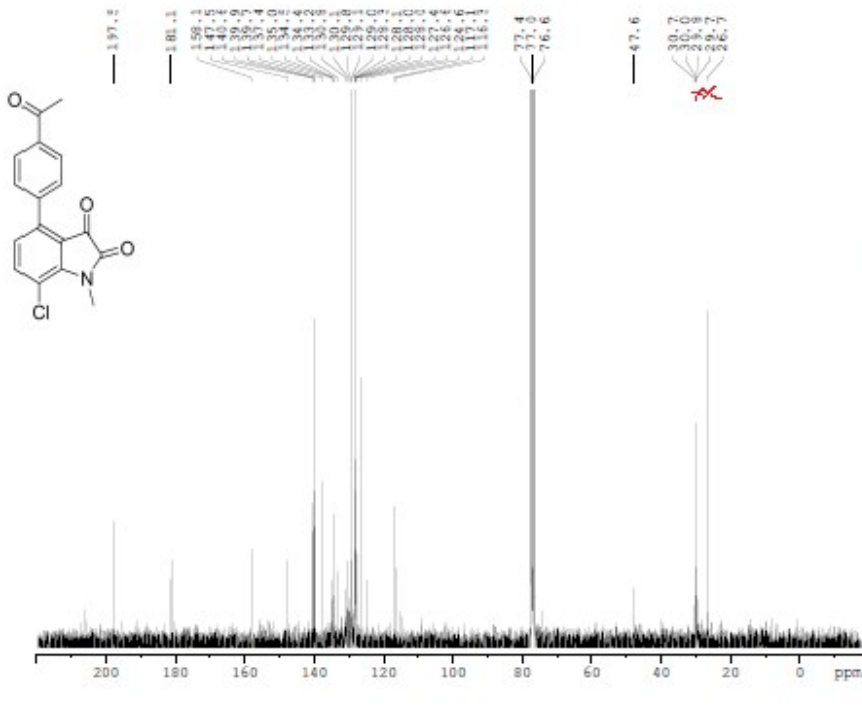


Current Data Parameters
 NAME 131120.u329
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131120
 Time 12.17
 INSTRUM spect
 PROBRD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT cdcl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953587 sec
 RG 128
 DM 80.800 usec
 DE 10.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

CHANNEL F1
 NUC1 1H
 P1 10.00 usec
 PL1 0 dB
 PL1W 11.25325108 W
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300330 MHz
 WDM 8M
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



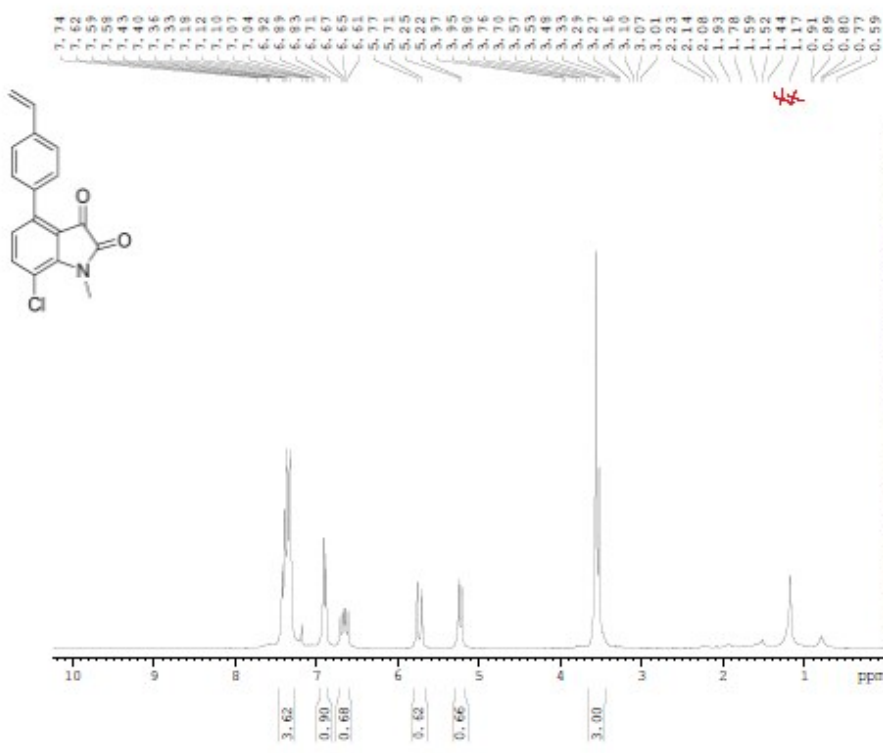
Current Data Parameters
 NAME 131120.u329
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131121
 Time 6.04
 INSTRUM spect
 PROBRD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT cdcl3
 NS 1024
 DS 4
 SWH 18028.846 Hz
 FIDRES 0.275098 Hz
 AQ 1.8175818 sec
 RG 2050
 DM 27.733 usec
 DE 10.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

CHANNEL F1
 NUC1 13C
 P1 10.00 usec
 PL1 -0.50 dB
 PL1W 33.25691986 W
 SFO1 75.4752953 MHz

CHANNEL F2
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 72.00 usec
 PL2 0 dB
 PL12 17.00 dB
 PL13 17.00 dB
 PL2W 11.25325108 W
 PL12W 0.22453187 W
 PL13W 0.22453187 W
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 WDM 8M
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

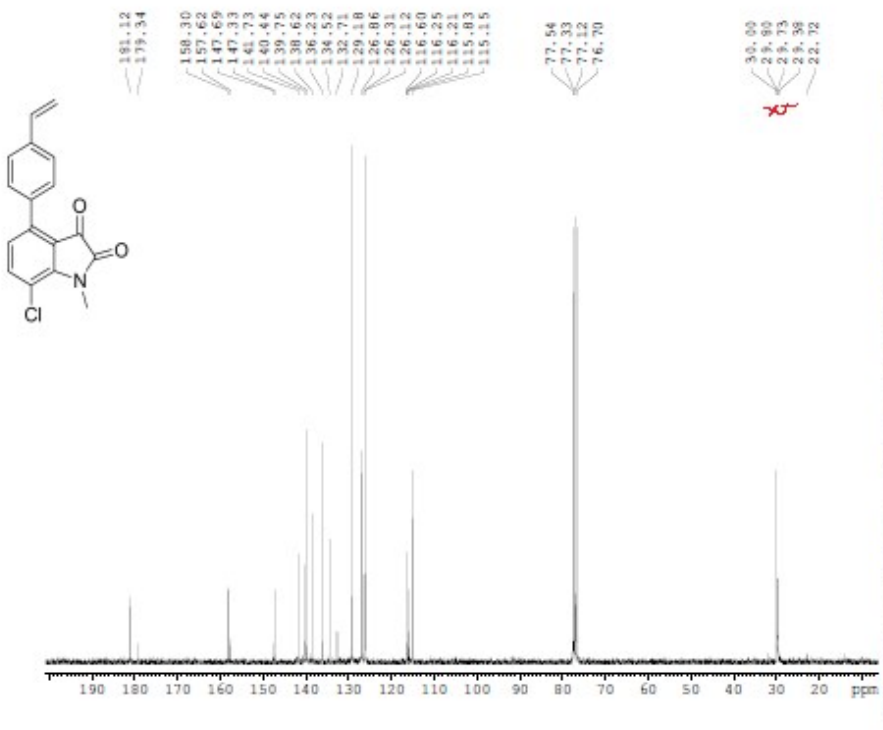


Current Data Parameters
 NAME 131128.u304
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 2013128
 Time 9.07
 INSTRUM spect
 PROBNM 5 mm FARGO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.034423 Hz
 AQ 5.2953187 sec
 RG 50.8
 ZW 80.800 usec
 DE 10.00 usec
 TK 298.2 K
 DI 1.00000000 sec
 TDD 1

CHANNEL F1
 NUC1 1H
 P1 10.00 usec
 PL1 0 dB
 PL1W 11.25325108 W
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300401 MHz
 MDW 32K
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



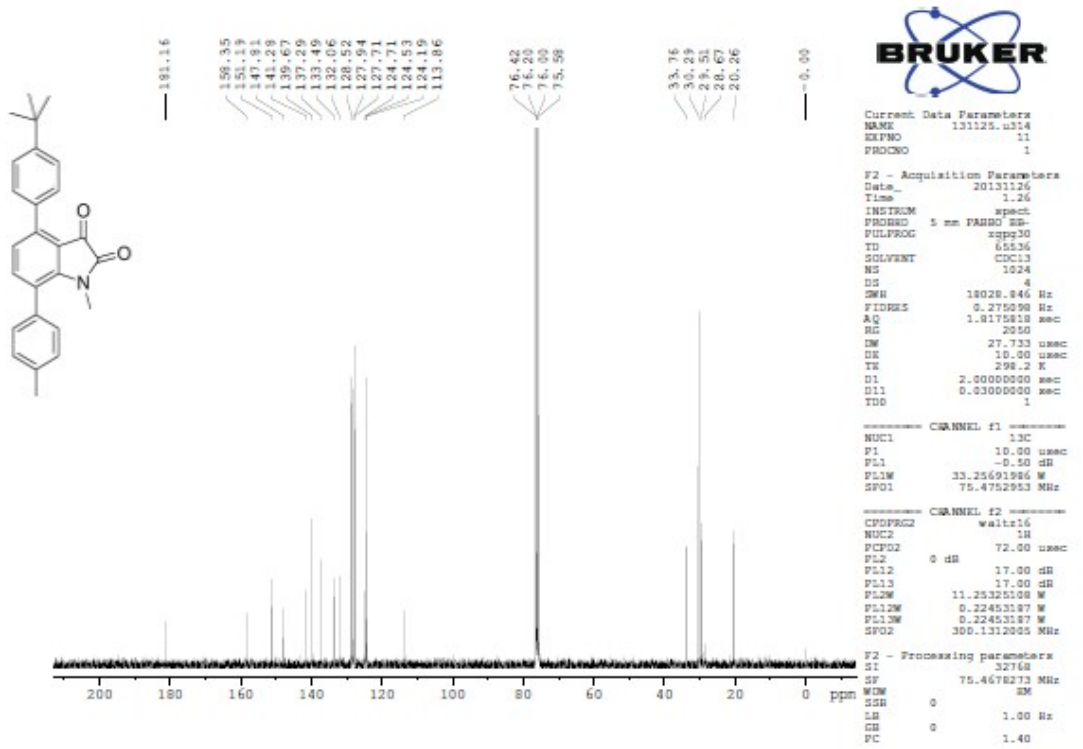
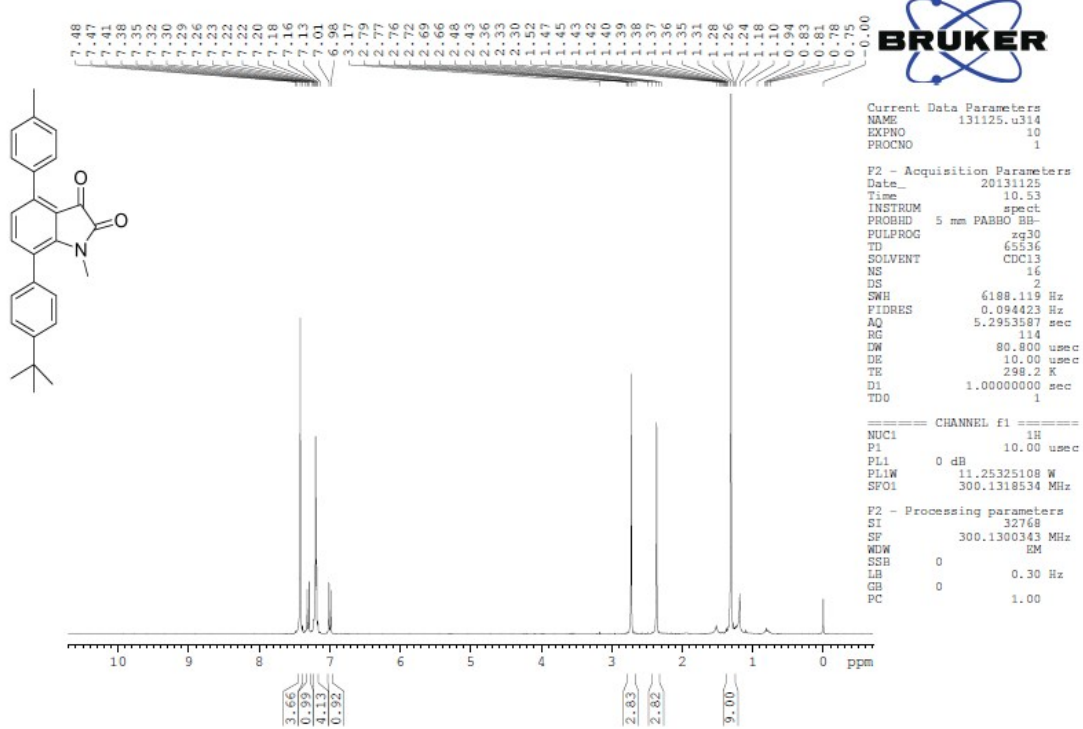
Current Data Parameters
 NAME 131128.u304
 EXPNO 12
 PROCNO 1

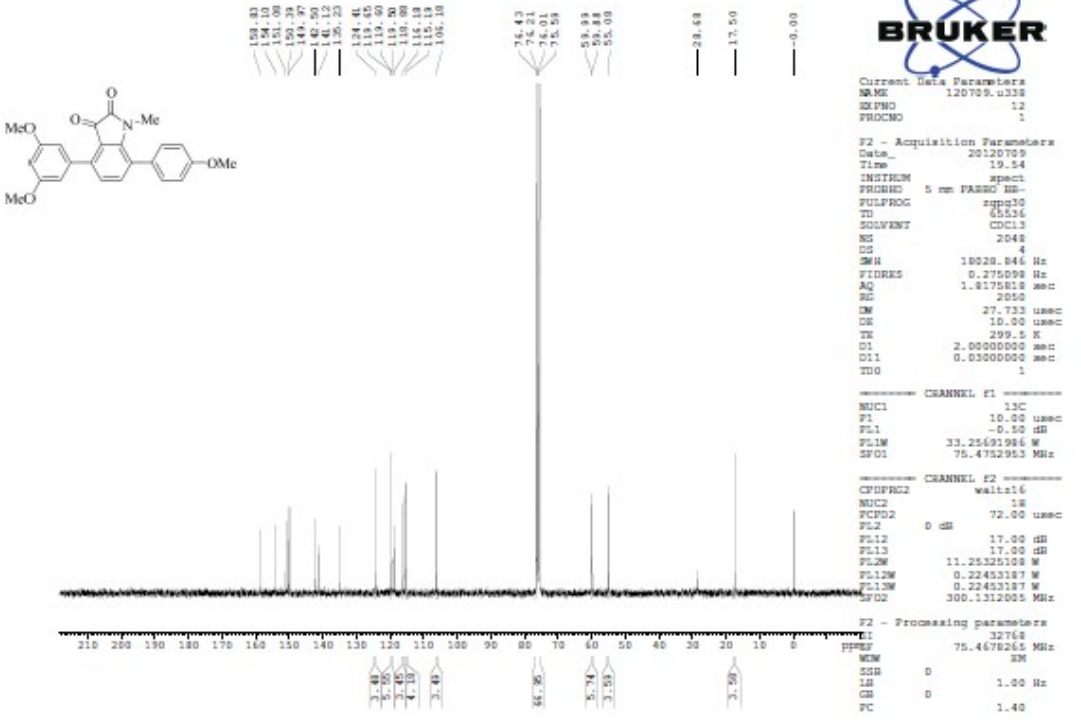
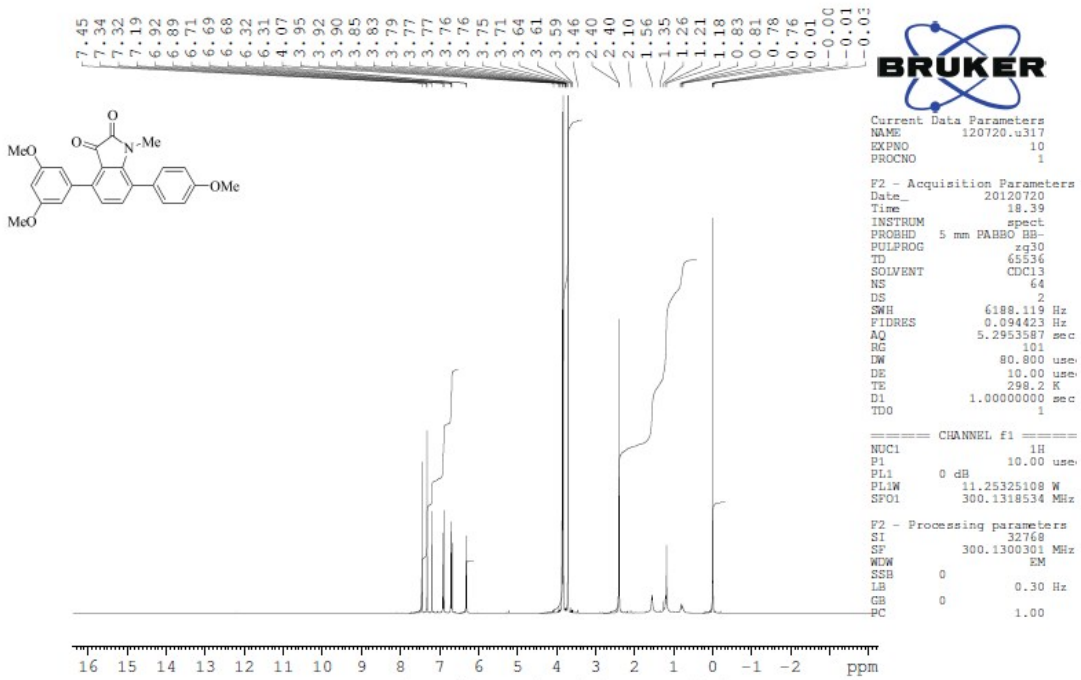
F2 - Acquisition Parameters
 Date_ 2013128
 Time 23.17
 INSTRUM spect
 PROBNM 5 mm FARGO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 10020.846 Hz
 FIDRES 0.275098 Hz
 AQ 1.8175818 sec
 RG 2050
 ZW 27.733 usec
 DE 10.00 usec
 TK 298.2 K
 DI 2.00000000 sec
 D11 0.03000000 sec
 TDD 1

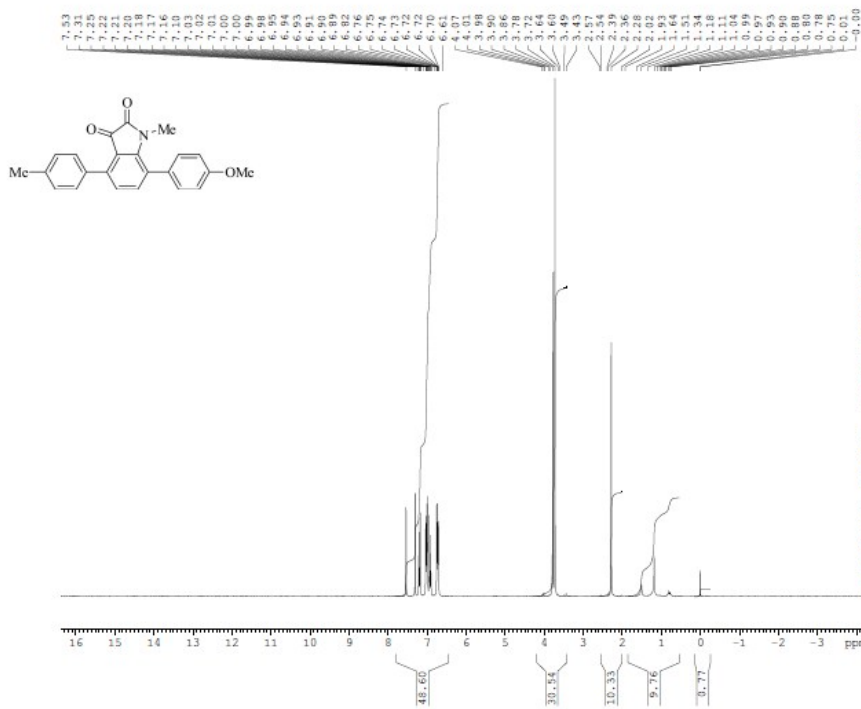
CHANNEL F1
 NUC1 13C
 P1 10.00 usec
 PL1 -0.50 dB
 PL1W 33.25692986 W
 SFO1 75.4752953 MHz

CHANNEL F2
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 72.00 usec
 PL2 0 dB
 PL12 17.00 dB
 PL13 17.00 dB
 PL1W 11.25325108 W
 PL12W 0.22453187 W
 PL13W 0.22453187 W
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 MDW 32K
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40





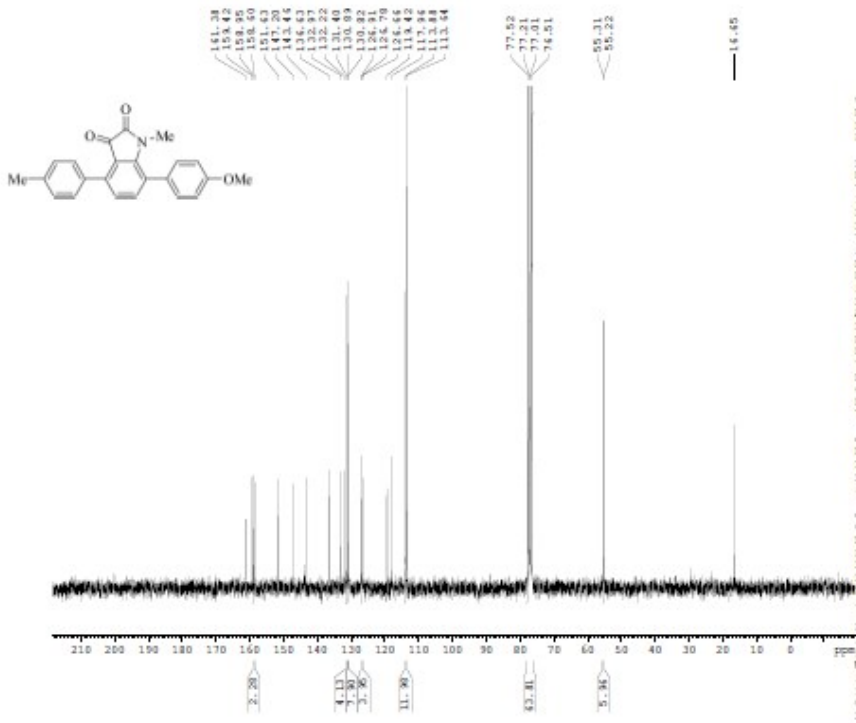


Current Data Parameters
 NAME 121219.201
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121219
 Time 8.03
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 5165.289 Hz
 FIDRES 0.078816 Hz
 AQ 6.3439350 sec
 RG 645
 DW 96.800 usec
 DE 10.00 usec
 TE 298.2 K
 D1 1.0000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.40 usec
 PL1 -3.00 dB
 SFO1 250.1315447 MHz

F2 - Processing parameters
 SI 32768
 SF 250.1300205 MHz
 WIDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME 121219.201
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121219
 Time 9.47
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1466
 DS 4
 SWH 15000.000 Hz
 FIDRES 0.228882 Hz
 AQ 2.1848334 sec
 RG 2050
 DW 33.333 usec
 DE 10.00 usec
 TE 298.2 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.89999999 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.20 usec
 PL1 0 dB
 SFO1 62.9015280 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P2 70.00 usec
 PL12 14.00 dB
 PL13 14.00 dB
 PL2 -3.00 dB
 SFO2 250.1310005 MHz

F2 - Processing parameters
 SI 32768
 SF 62.8952390 MHz
 WIDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40