

Supporting Information
for
Regioselective palladium-catalyzed ring-opening reactions of
C1-substituted oxabicyclo[2,2,1]hepta-2,5-diene-2,3-
dicarboxylates

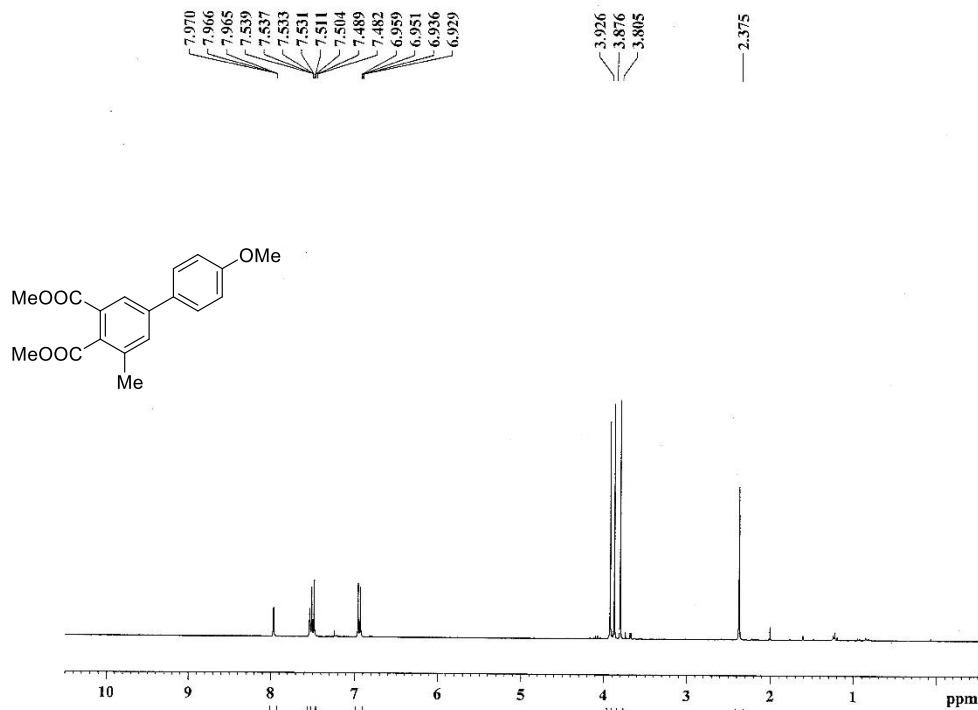
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Email: William Tam - wtam@uoguelph.ca

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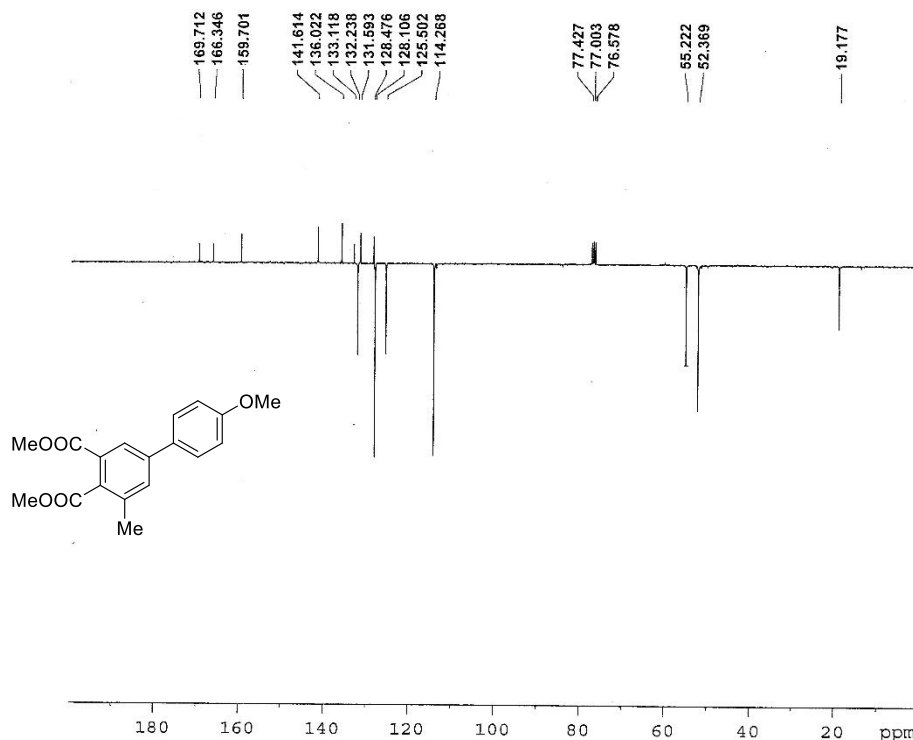
Copies of ^1H and ^{13}C NMR spectra for compounds 3a–l

300 MHz ¹H NMR spectrum of **3a** in CDCl₃

NAME MAR-II-26-1
EXPNO 1
PROCNO 1
Date_ 20100328
Time 16.06
INSTRUM av300
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl₃
NS 8
DS 0
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 35.9
DW 104.400 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 ¹H
P1 13.50 usec
PL1 0.00 dB
PL1W 10.29873466 W
SFO1 300.1317168 MHz
SI 32768
SF 300.1300124 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

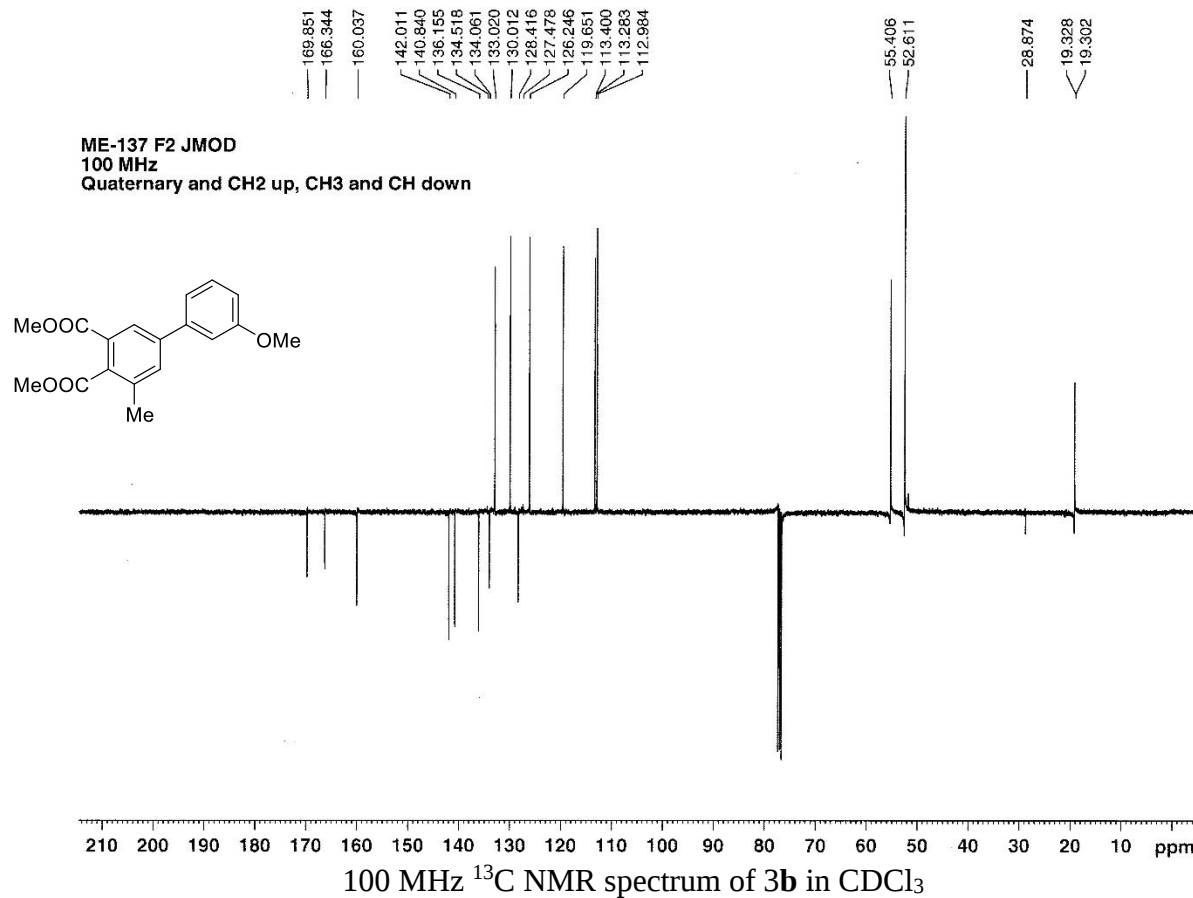
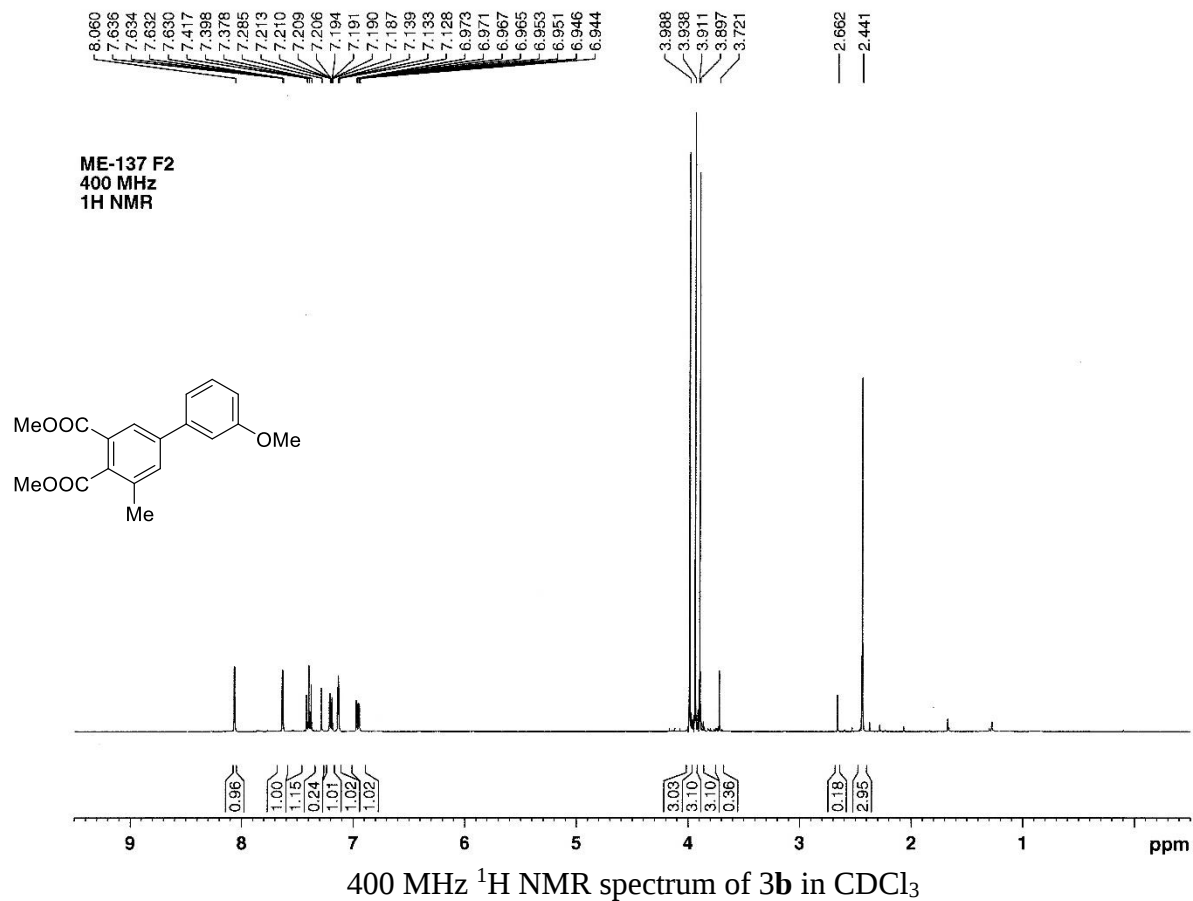
MAR-II-26-1 in CDCl₃
CH2 and C up, CH3 and CH down

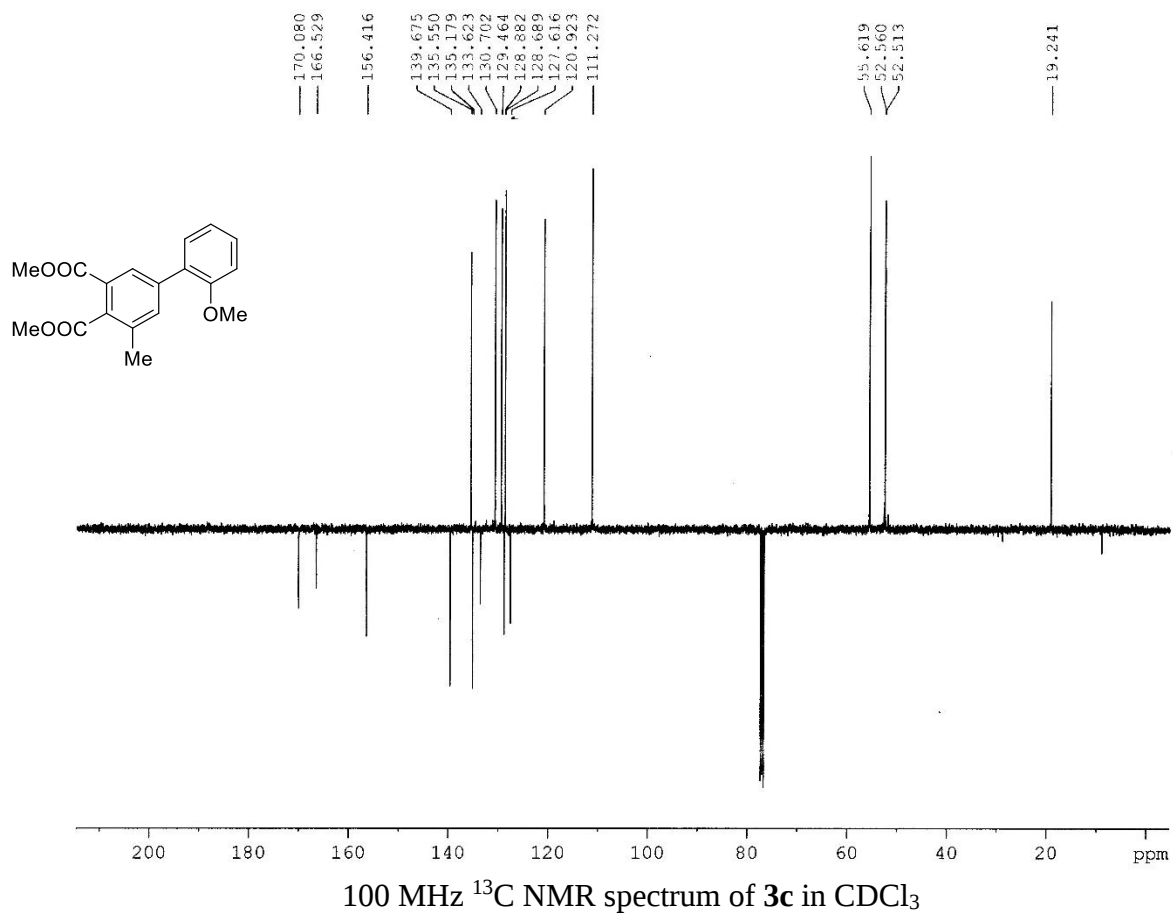
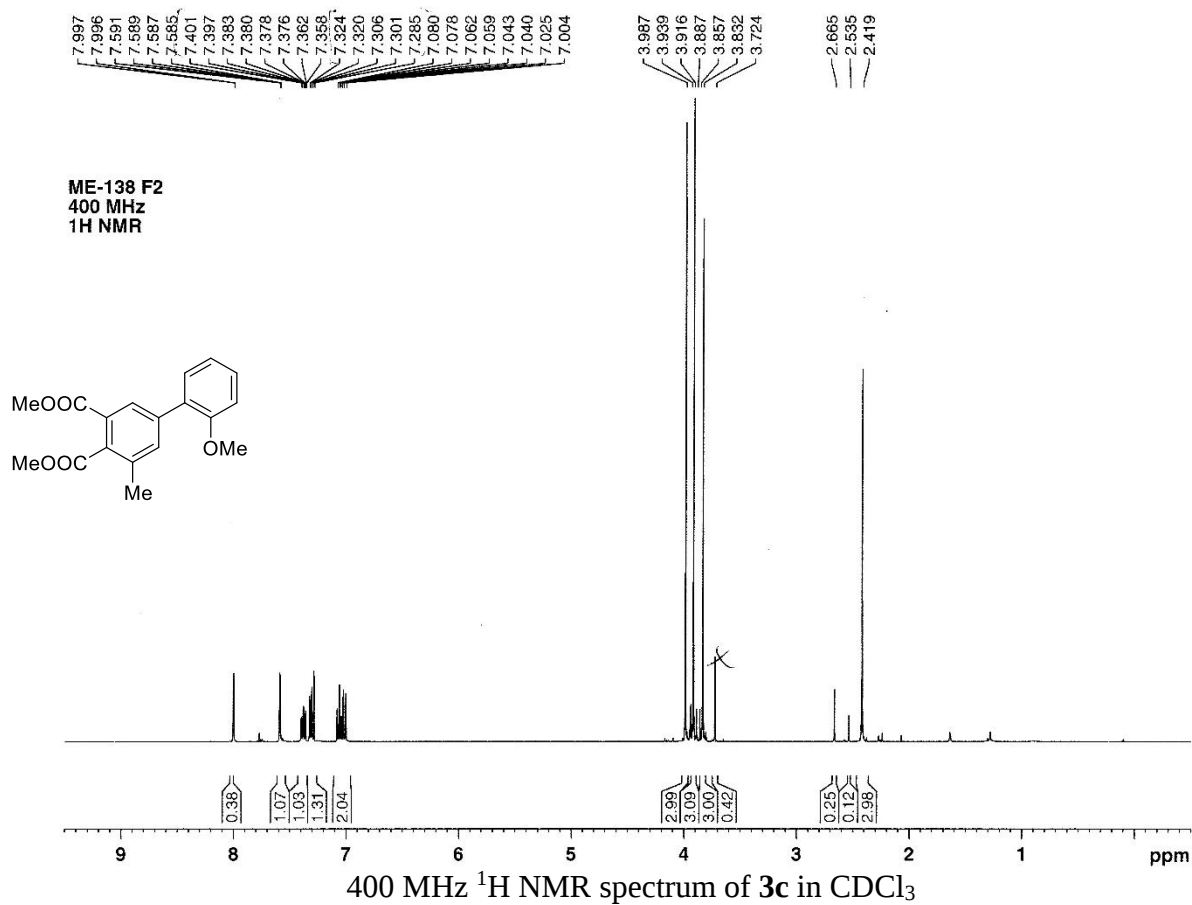
75 MHz ¹³C NMR spectrum of **3a** in CDCl₃

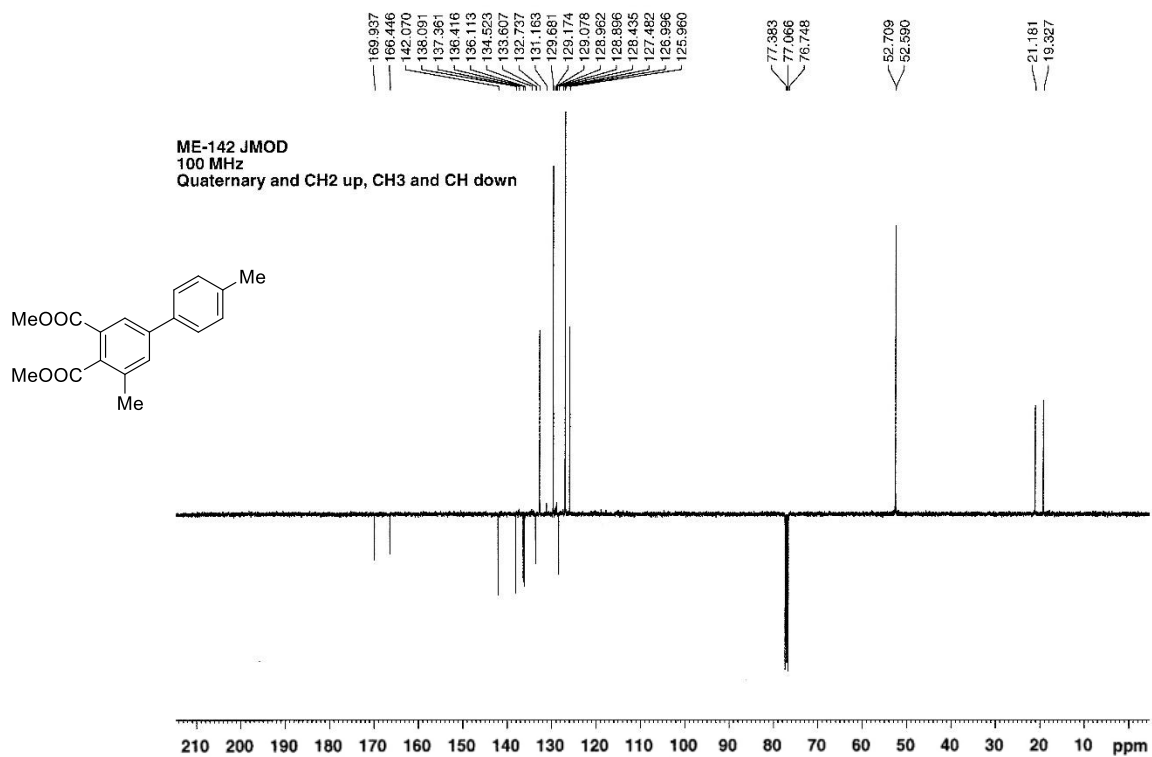
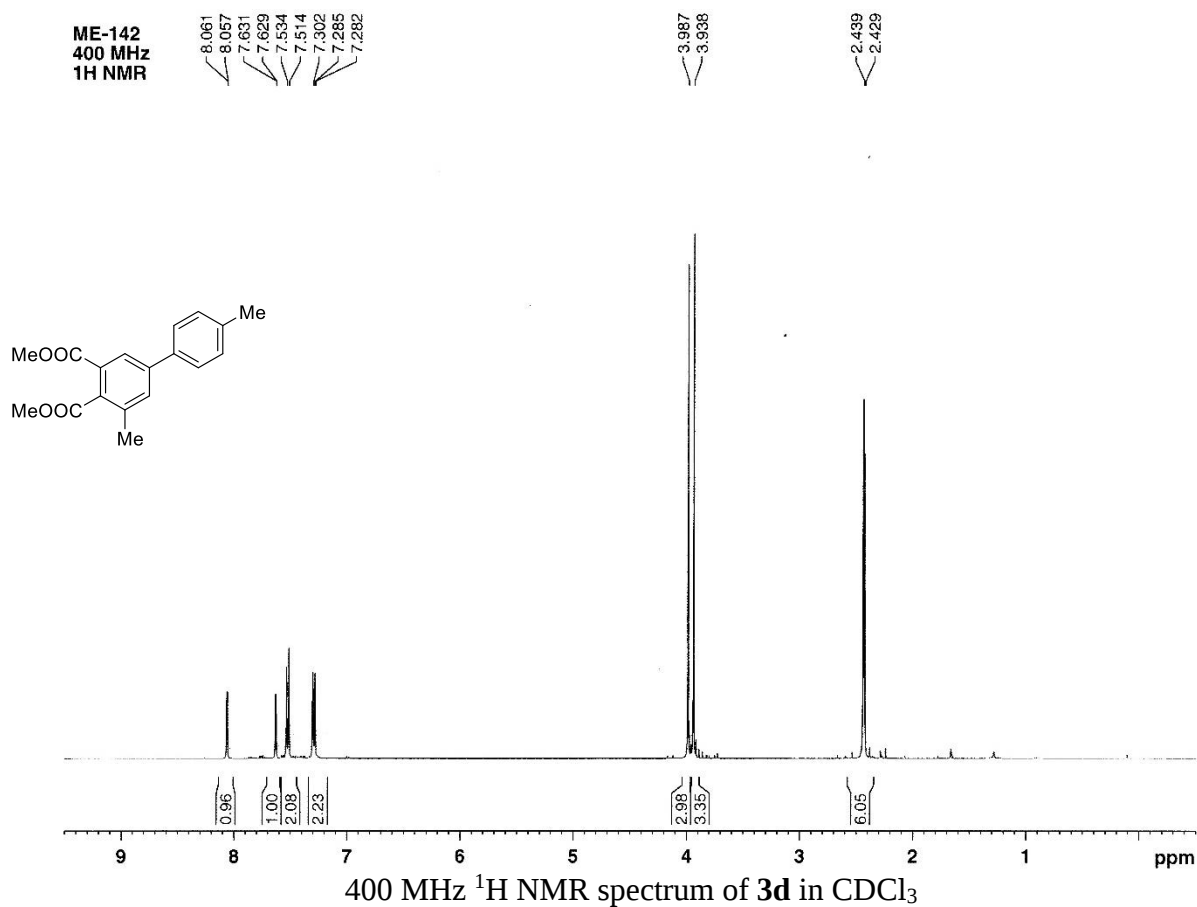
NAME MAR-II-26-1
EXPNO 2
PROCNO 1
Date_ 20100328
Time 15.46
INSTRUM av300
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT CDCl₃
NS 200
DS 0
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 23170.5
DW 27.800 usec
DE 6.00 usec
TE 299.8 K
CNST2 145.0000000
CNST11 1.0000000
D1 6.00000000 sec
D20 0.00689655 sec
TD0 1

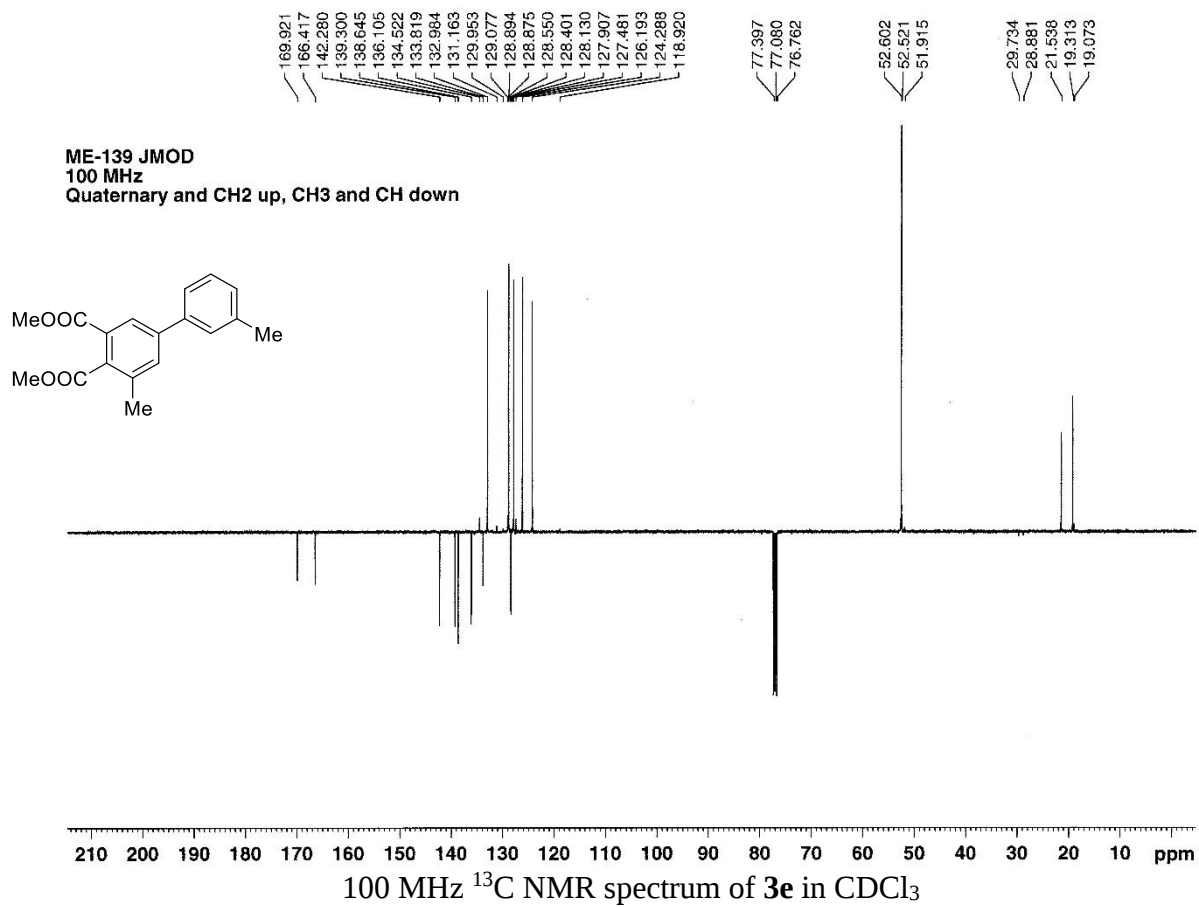
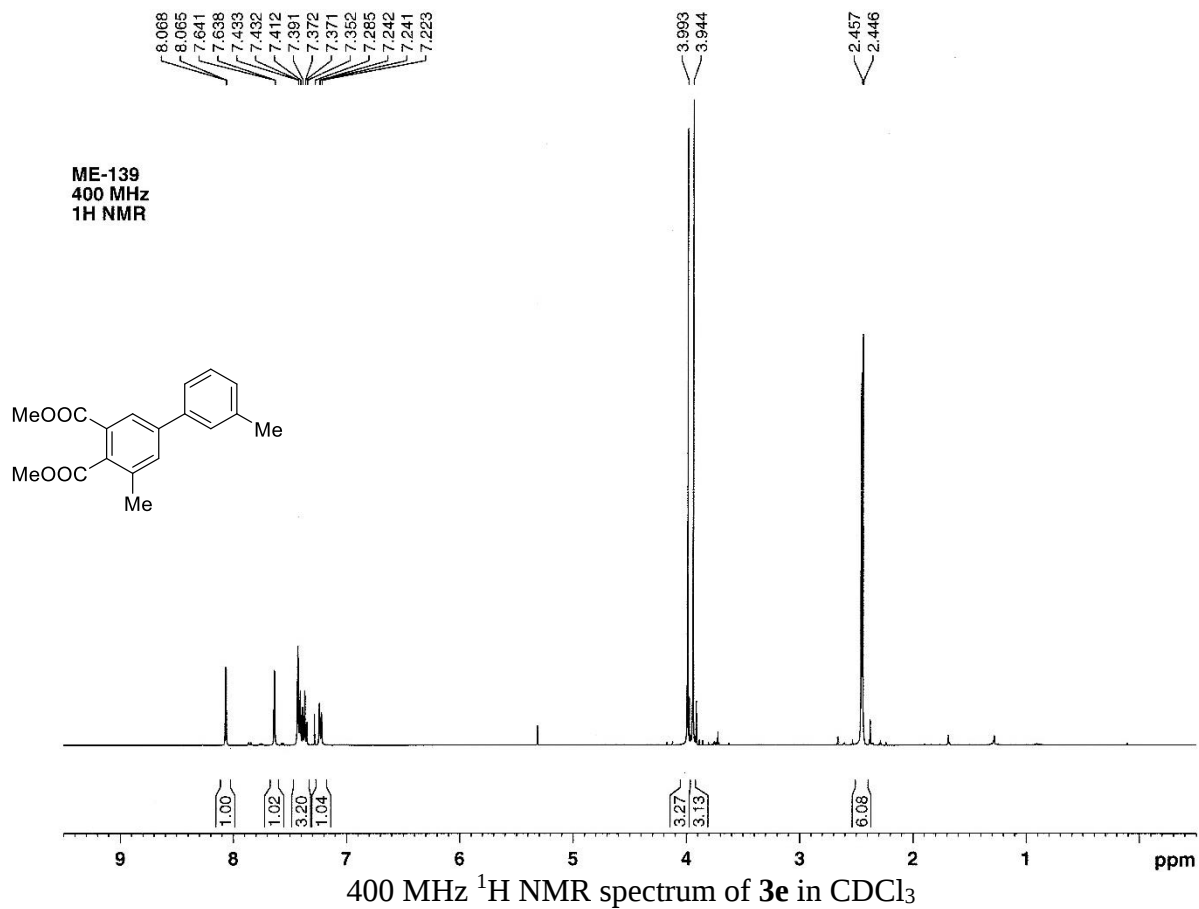
===== CHANNEL f1 =====
NUC1 ¹³C
P1 9.00 usec
P2 18.00 usec
PL1 -2.00 dB
PL1W 48.96718216 W
SFO1 75.4752953 MHz

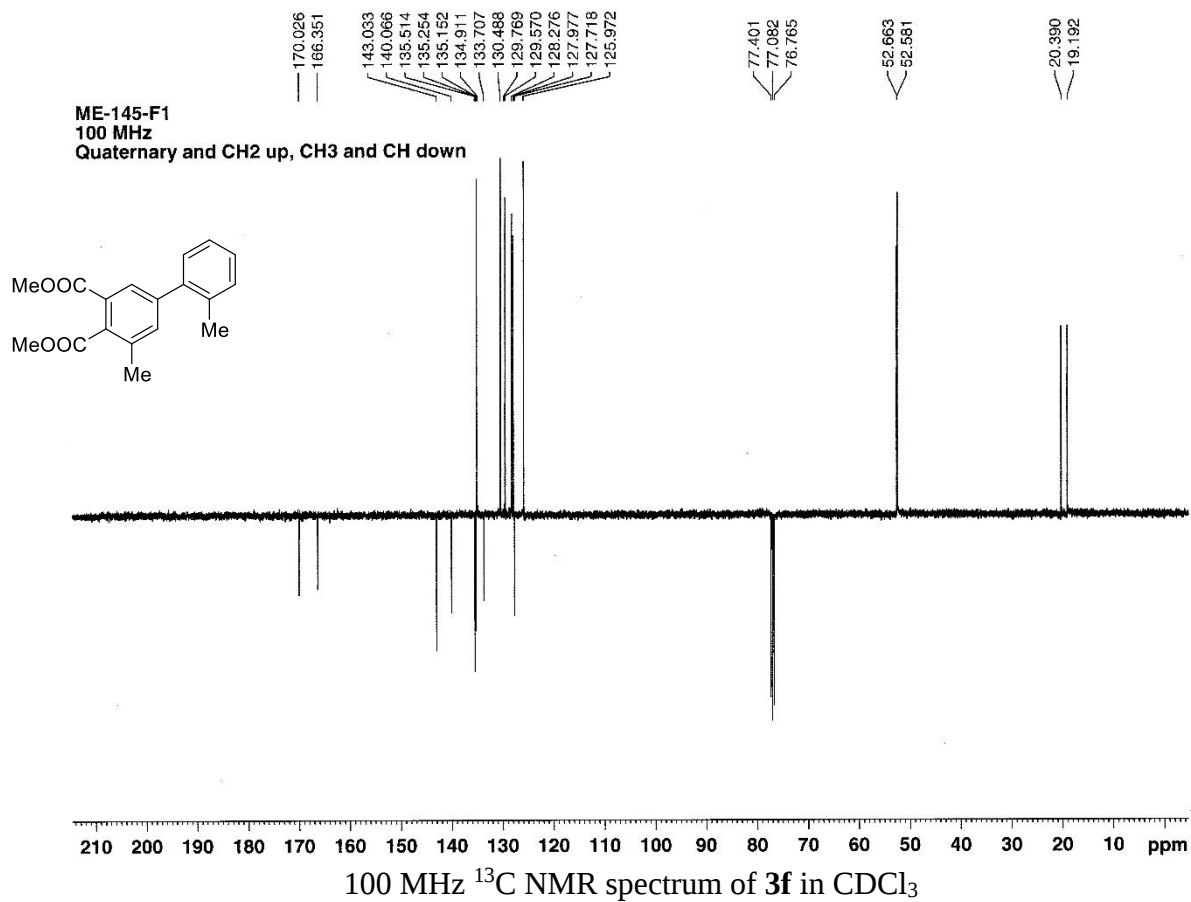
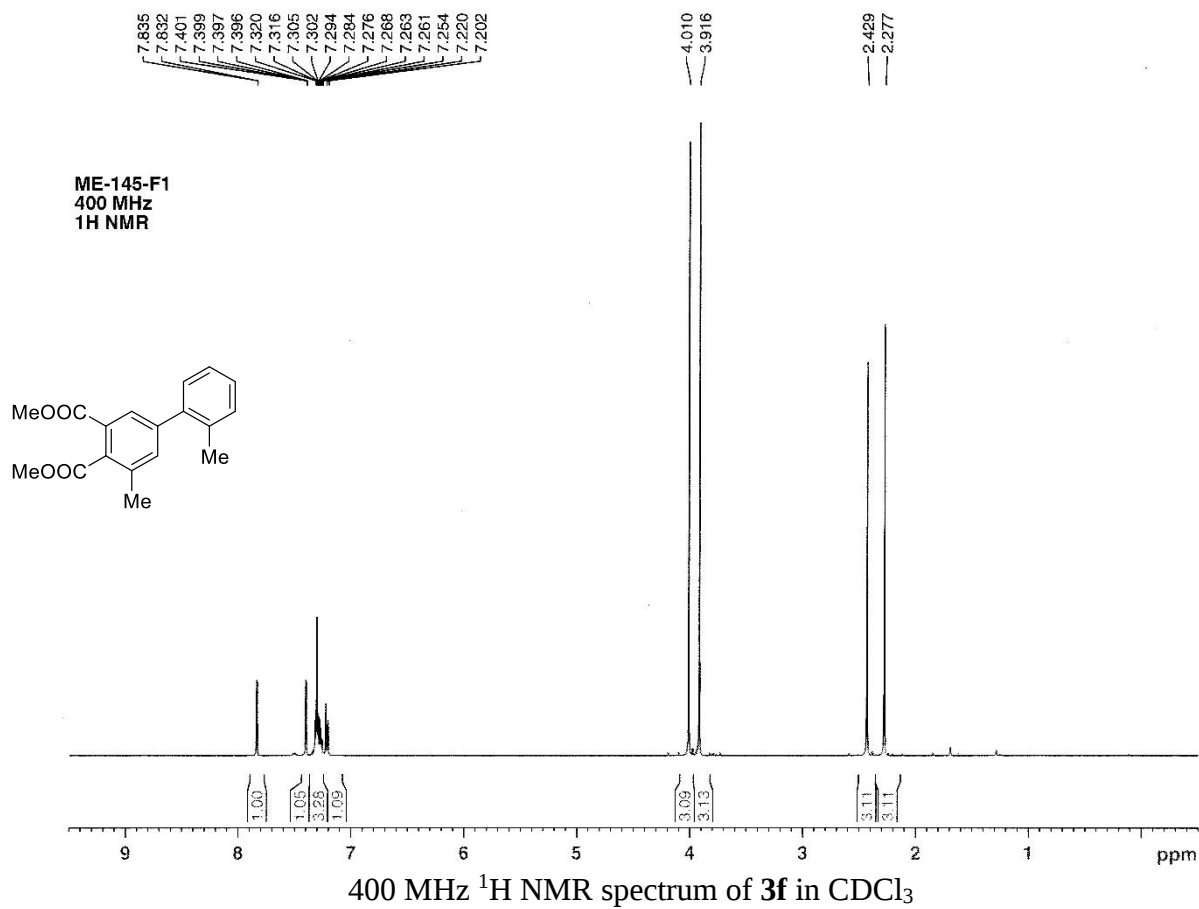
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 ¹H
PCPD2 70.00 usec
PL2 0.00 dB
PL12 14.30 dB
PL2W 10.29873466 W
PL12W 0.38263425 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677568 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50

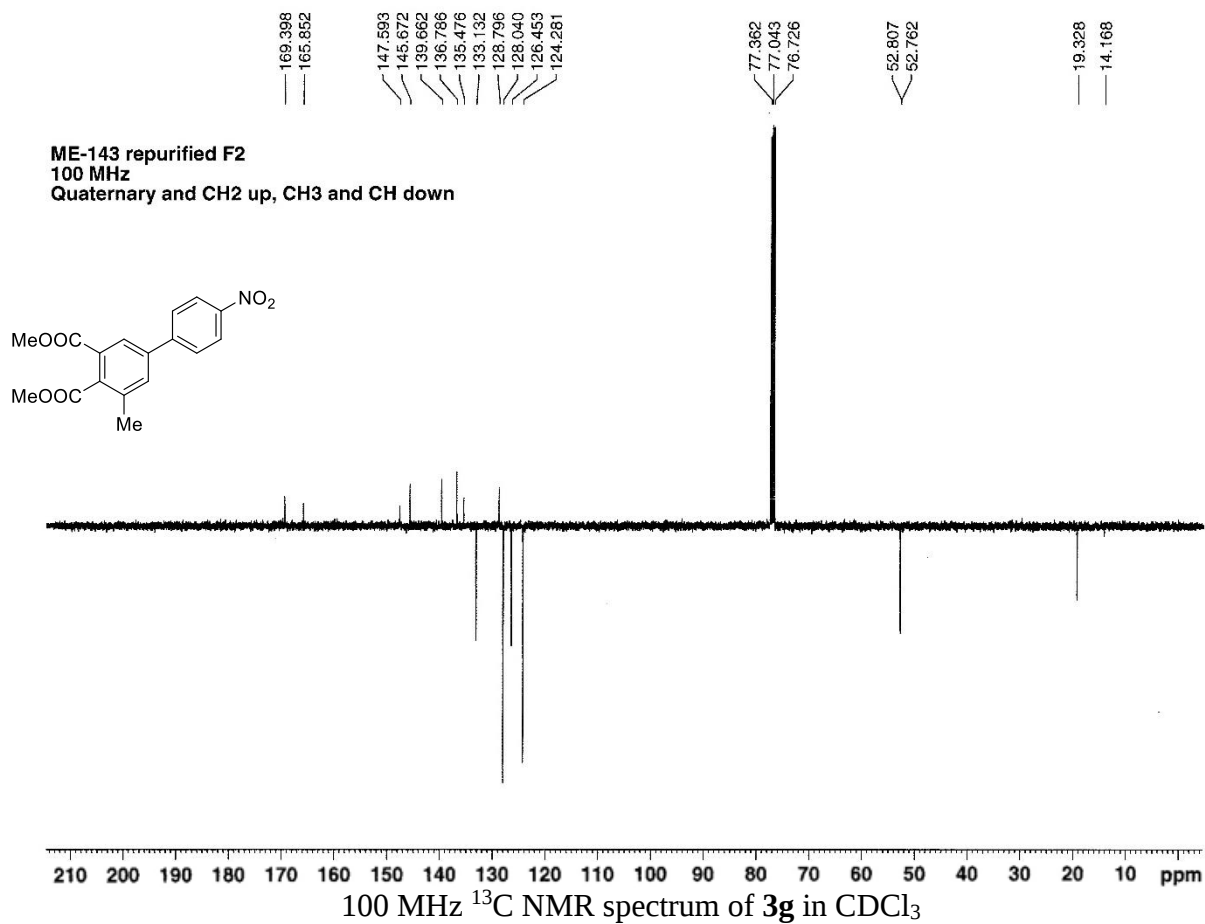
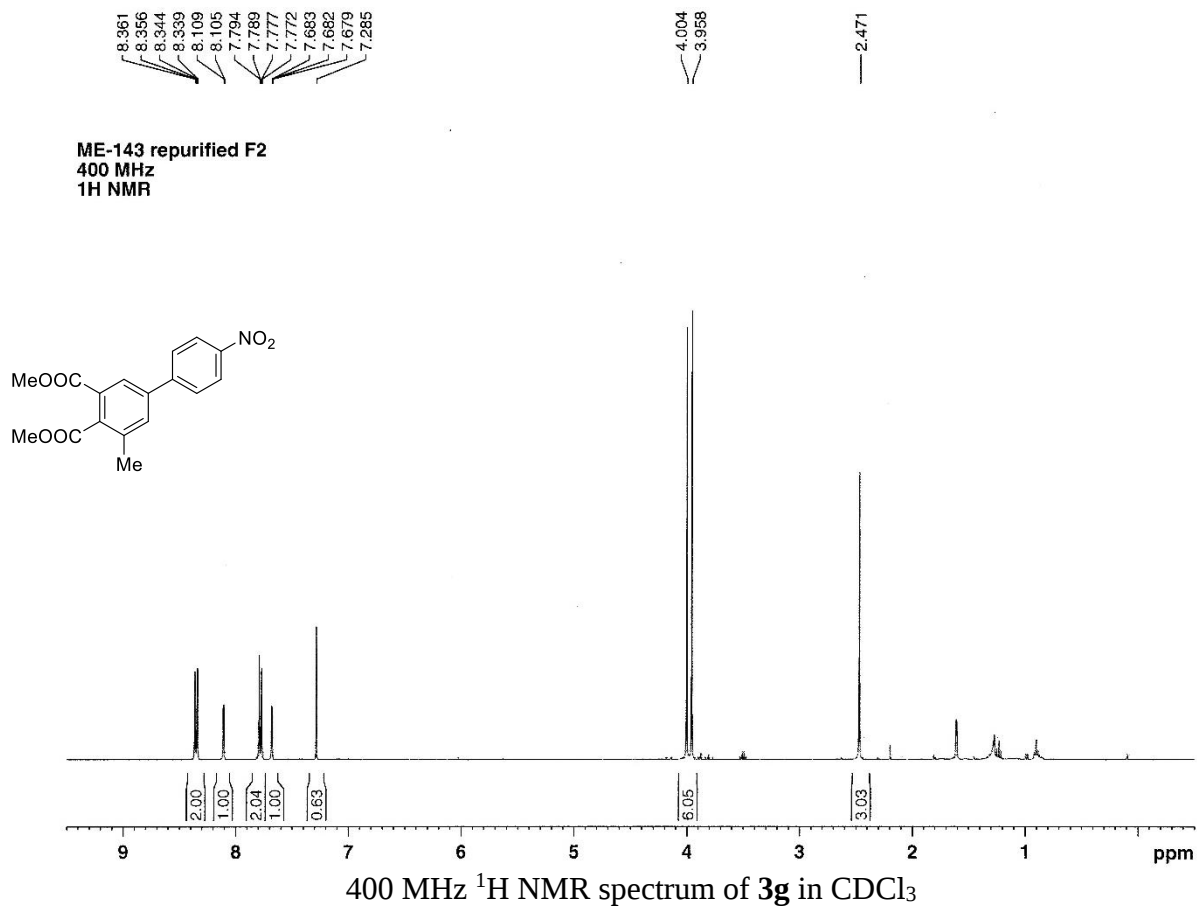


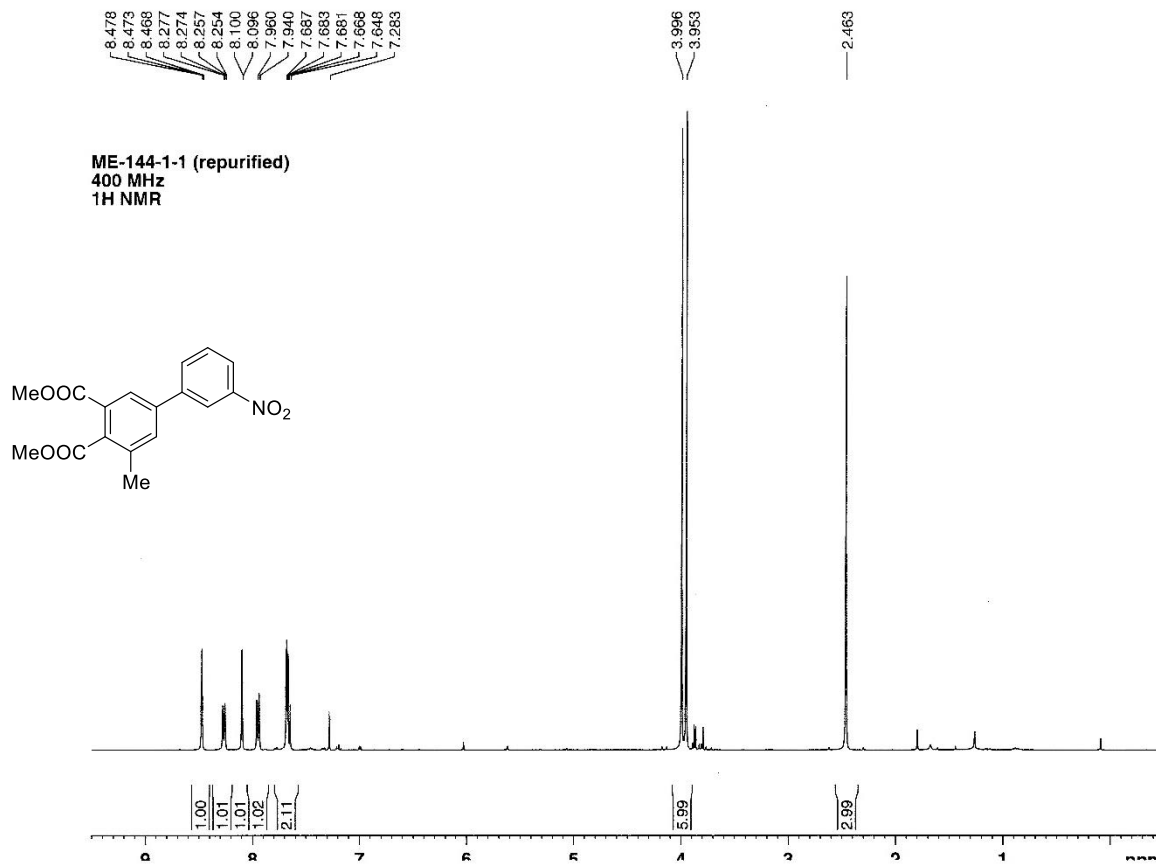
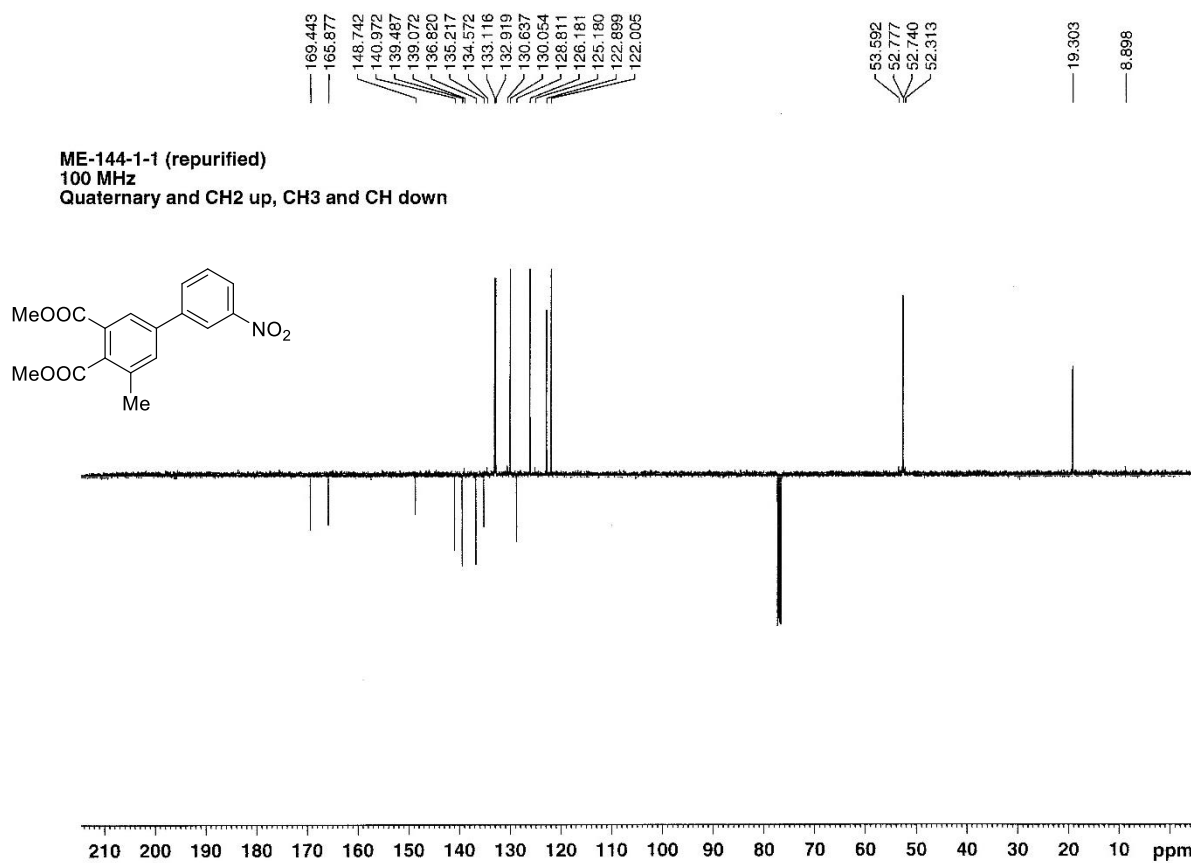


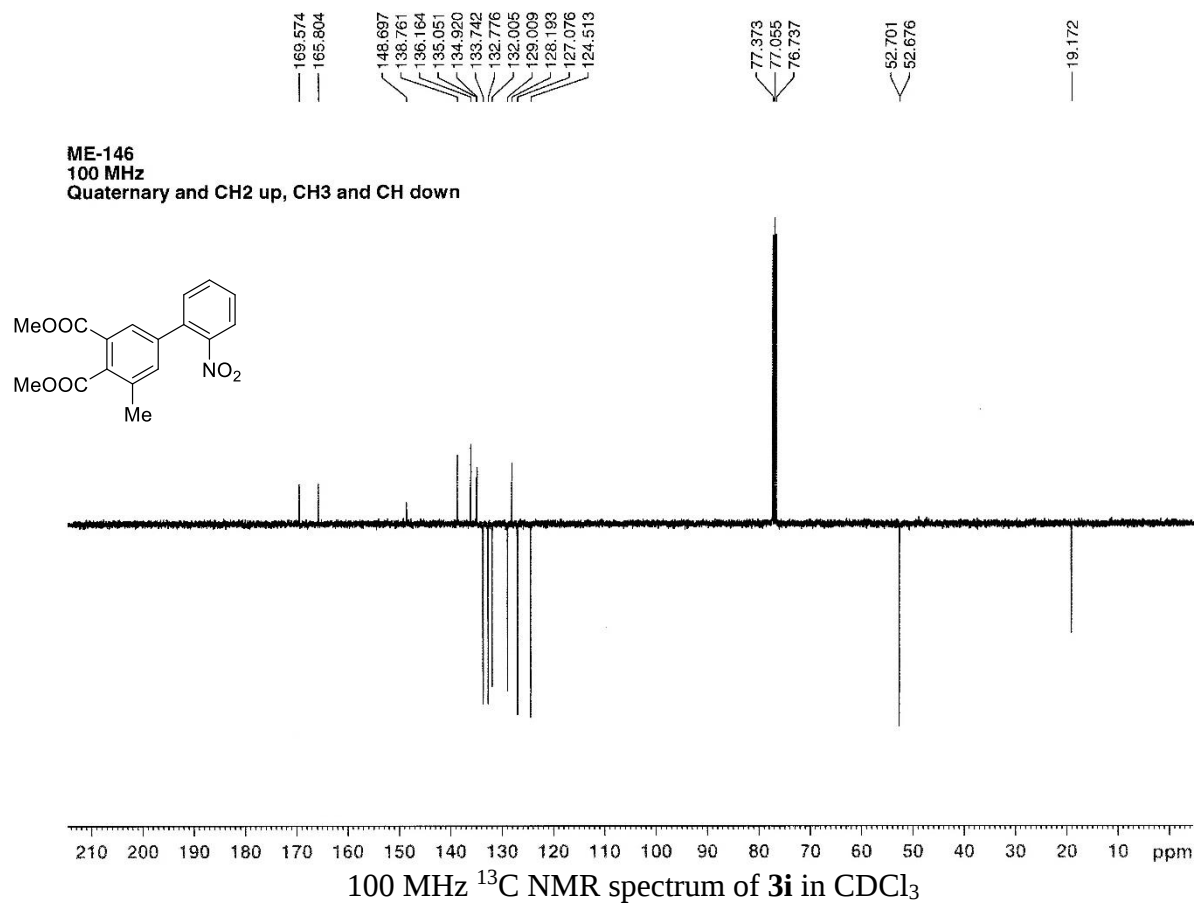
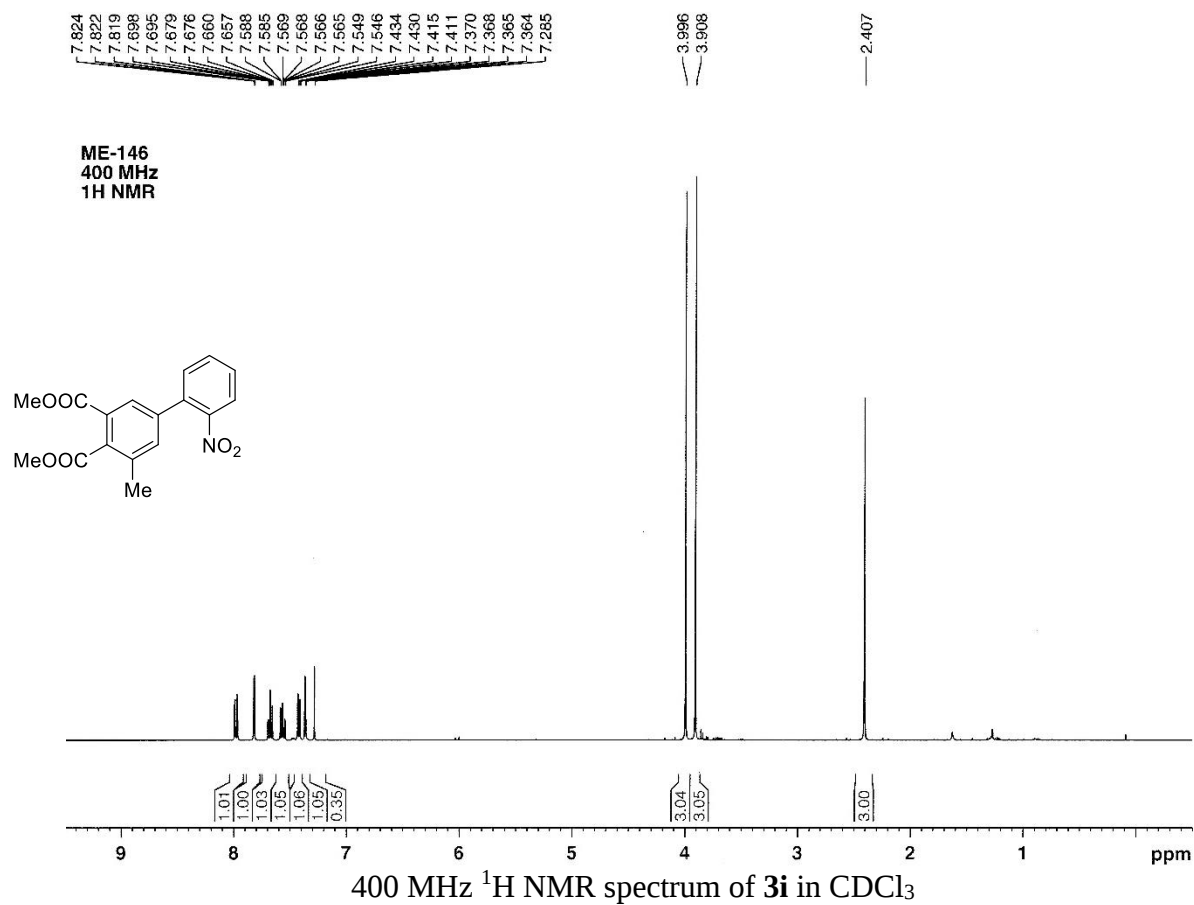


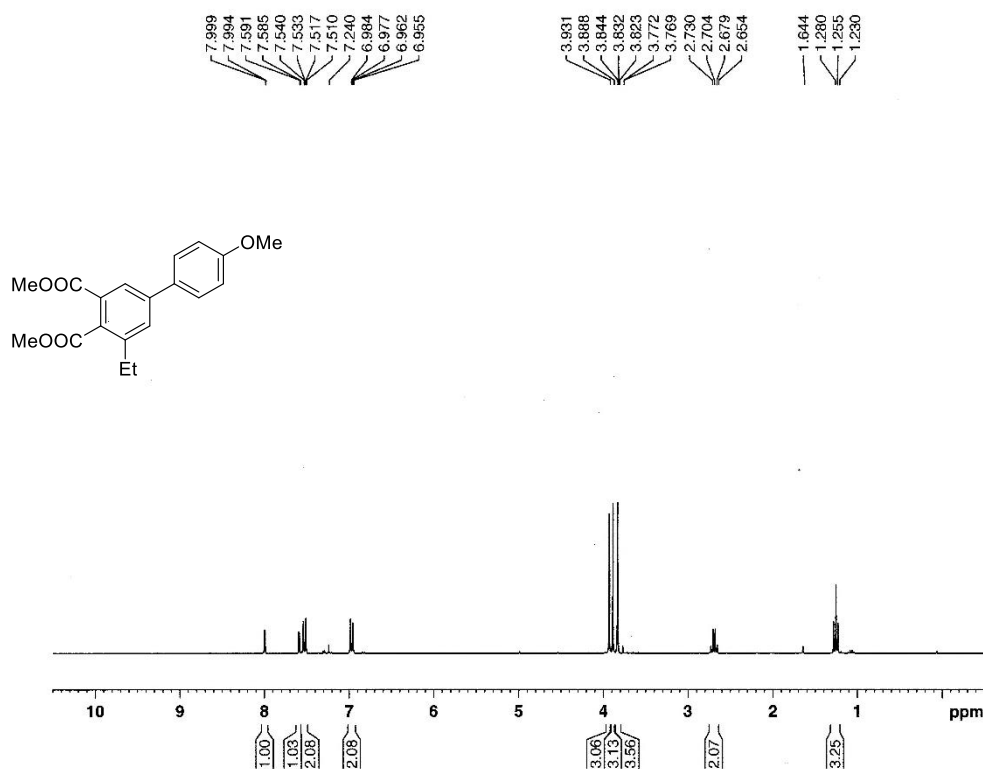






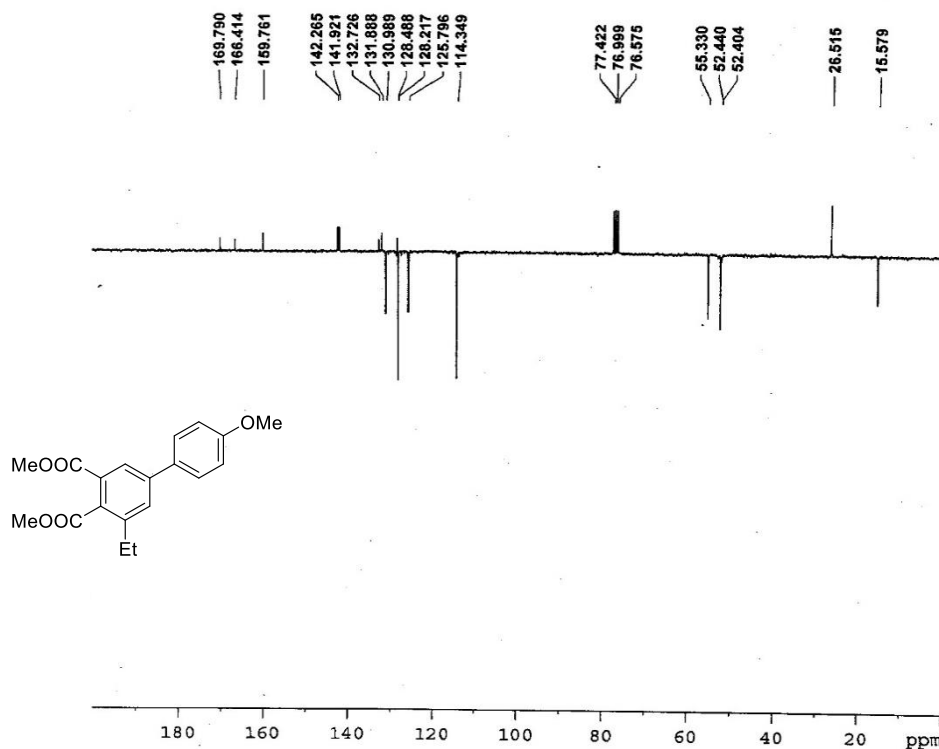
400 MHz ¹H NMR spectrum of **3h** in CDCl₃100 MHz ¹³C NMR spectrum of **3h** in CDCl₃



MAR-II-27-1 in CDCl₃
 Ethyl derivative ring open

 300 MHz ¹H NMR spectrum of **3j** in CDCl₃

NAME MAR-II-27-1
 EXPNO 1
 PROCNO 1
 Date 20100404
 Time 18.30
 INSTRUM av300
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT CDCl₃
 NS 8
 DS 0
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 90.5
 DW 104.400 usec
 DE 6.00 usec
 TE 299.4 K
 D1 1.00000000 sec
 TD0 1

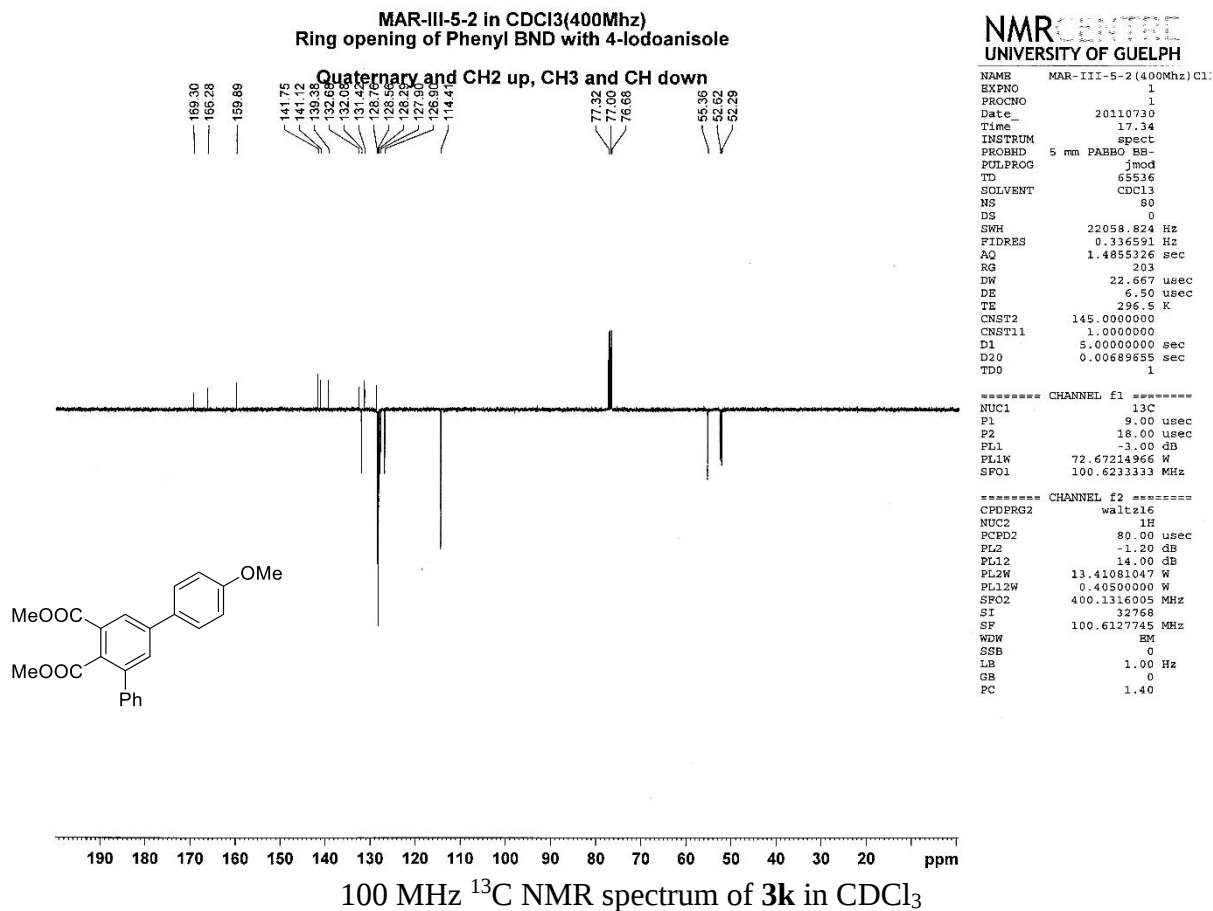
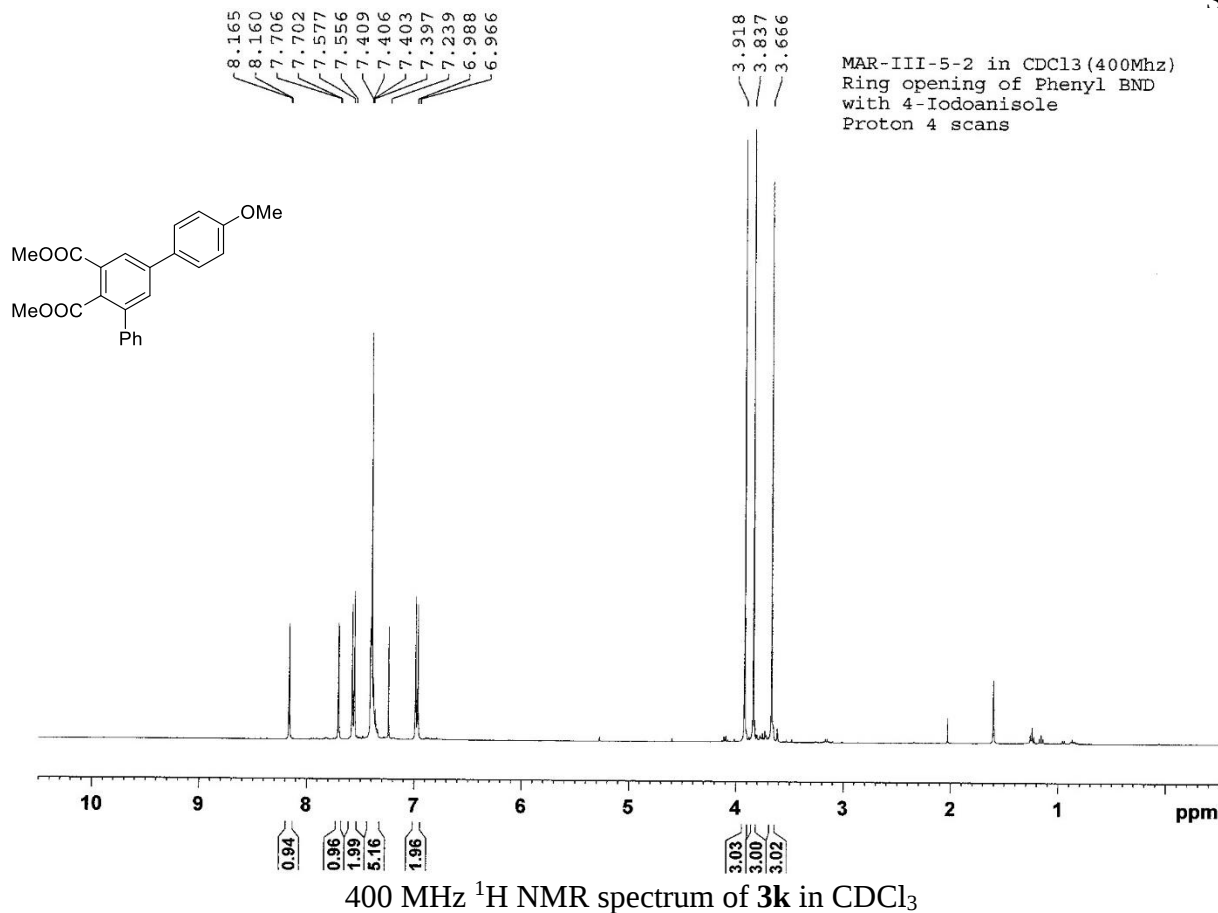
===== CHANNEL f1 =====
 NUC1 1H
 P1 13.50 usec
 PL1 0.00 dB
 PL1W 10.29873466 W
 SFO1 300.1317168 MHz
 SI 32768
 SF 300.1300121 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

MAR-II-27-1 in CDCl₃
 Ethyl substituent
 CH2 and C up, CH3 and CH down.

 100 MHz ¹³C NMR spectrum of **3j** in CDCl₃

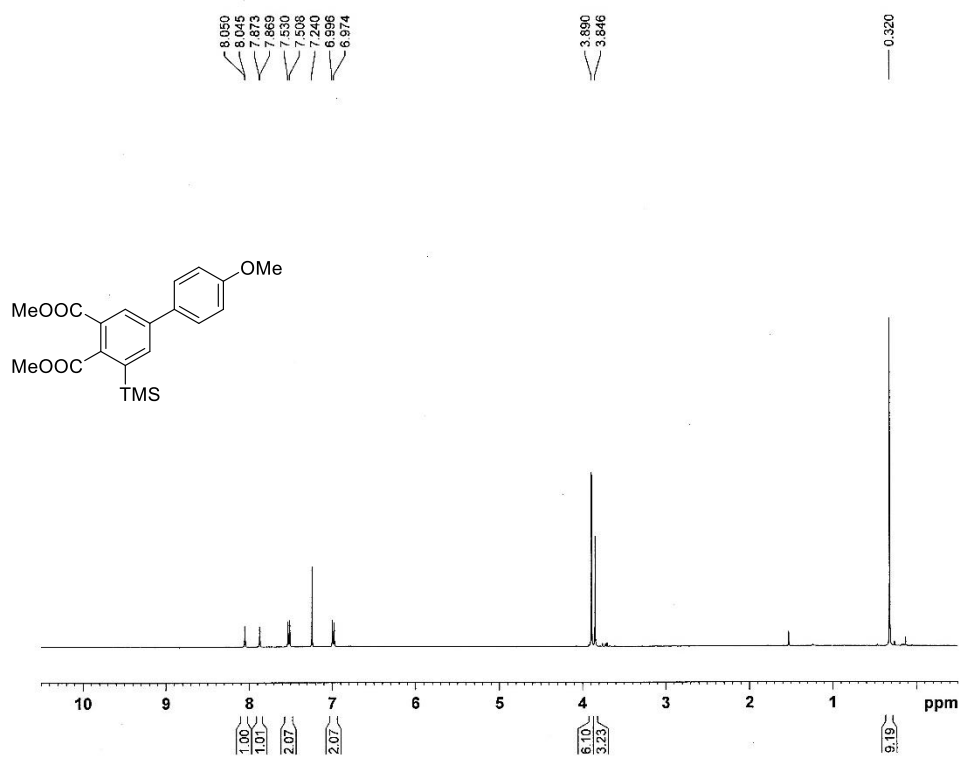
NAME MAR-II-27-1
 EXPNO 2
 PROCNO 1
 Date 20100404
 Time 18.00
 INSTRUM av300
 PROBHD 5 mm PABBO BB-
 PULPROG jmod
 TD 65536
 SOLVENT CDCl₃
 NS 200
 DS 0
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 23170.5
 DW 27.800 usec
 DE 6.00 usec
 TE 301.2 K
 CNST2 145.8000000
 CNST11 1.8000000
 D1 6.00000000 sec
 D20 0.00689655 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.00 usec
 P2 18.00 usec
 PL1 -2.00 dB
 PL1W 48.96718216 W
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 70.00 usec
 PL2 0.00 dB
 PL12 14.30 dB
 PL12W 10.29873466 W
 PL12W 0.38263425 W
 SFO2 300.1312005 MHz
 SI 32768
 SF 75.4677523 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 0.50



MAR-III-2-1 in CDCl₃(400Mhz)
Repeat



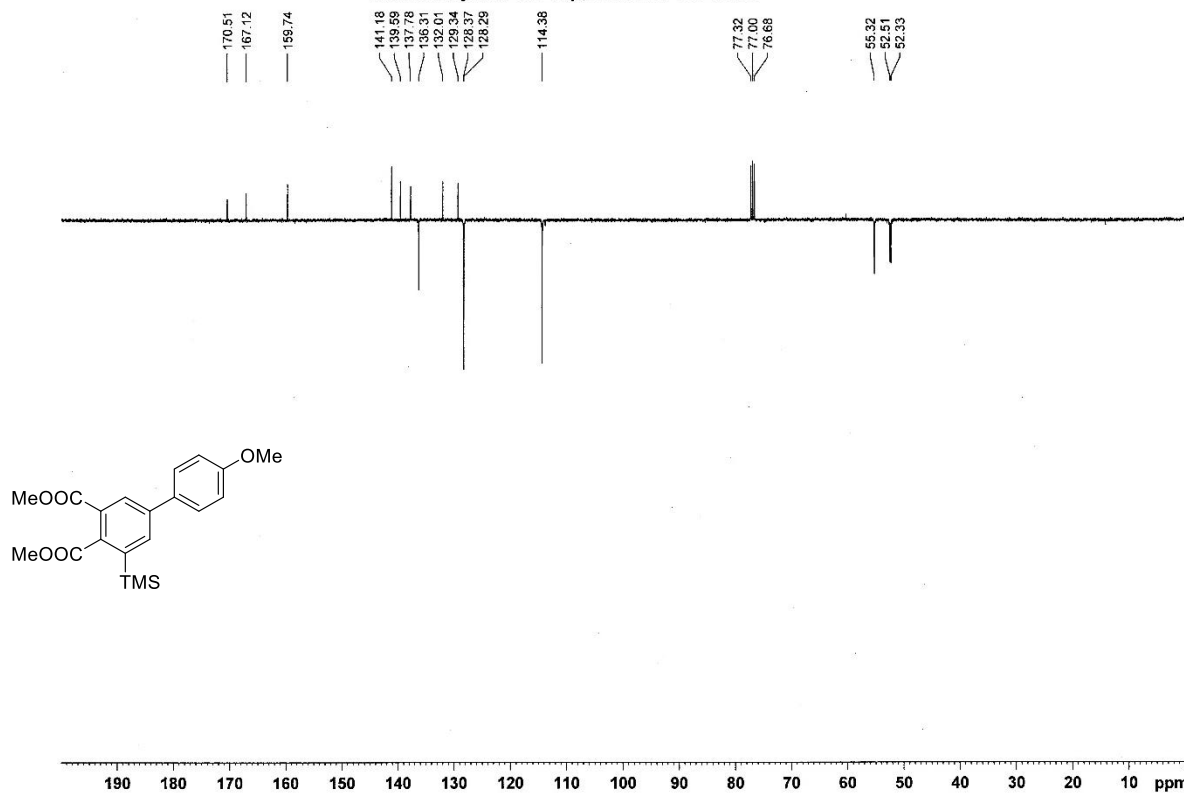
400 MHz ¹H NMR spectrum of **3I** in CDCl₃

NMR
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NAME MAR-III-2-1(400Mhz)1H
EXPNO 1
PROCNO 1
Date 20111008
Time 13.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl₃
NS 4
DS 0
SWH 5597.015 Hz
FIDRES 0.170807 Hz
AQ 2.9273248 sec
RG 203
DW 89.333 usec
DE 6.50 usec
TE 295.1 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 1H
P1 14.00 usec
PL1 -1.20 dB
PL1W 13.41081047 W
SF01 400.1324710 MHz
SI 32768
SF 400.1300176 MHz
NDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

MAR-III-2-1 in CDCl₃
Ring opng of TMS NBD with 4-Iodoanisole
Quaternary and CH₂ up, CH₃ and CH down



100 MHz ¹³C NMR spectrum of **3I** in CDCl₃

NMR
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