

Supporting Information

A Single Pot Synthesis of Atovaquone: An Antiparasitic Drug of Choice

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Swapnil Kore and Ashok Kumar**

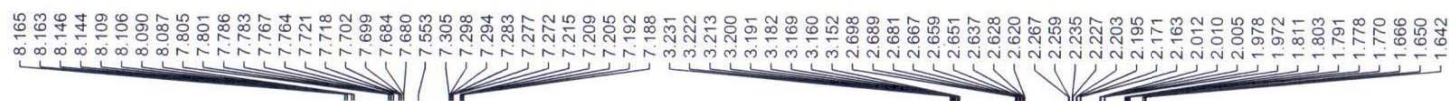
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ATO/ATO/9197 1H (Structure No. 1)



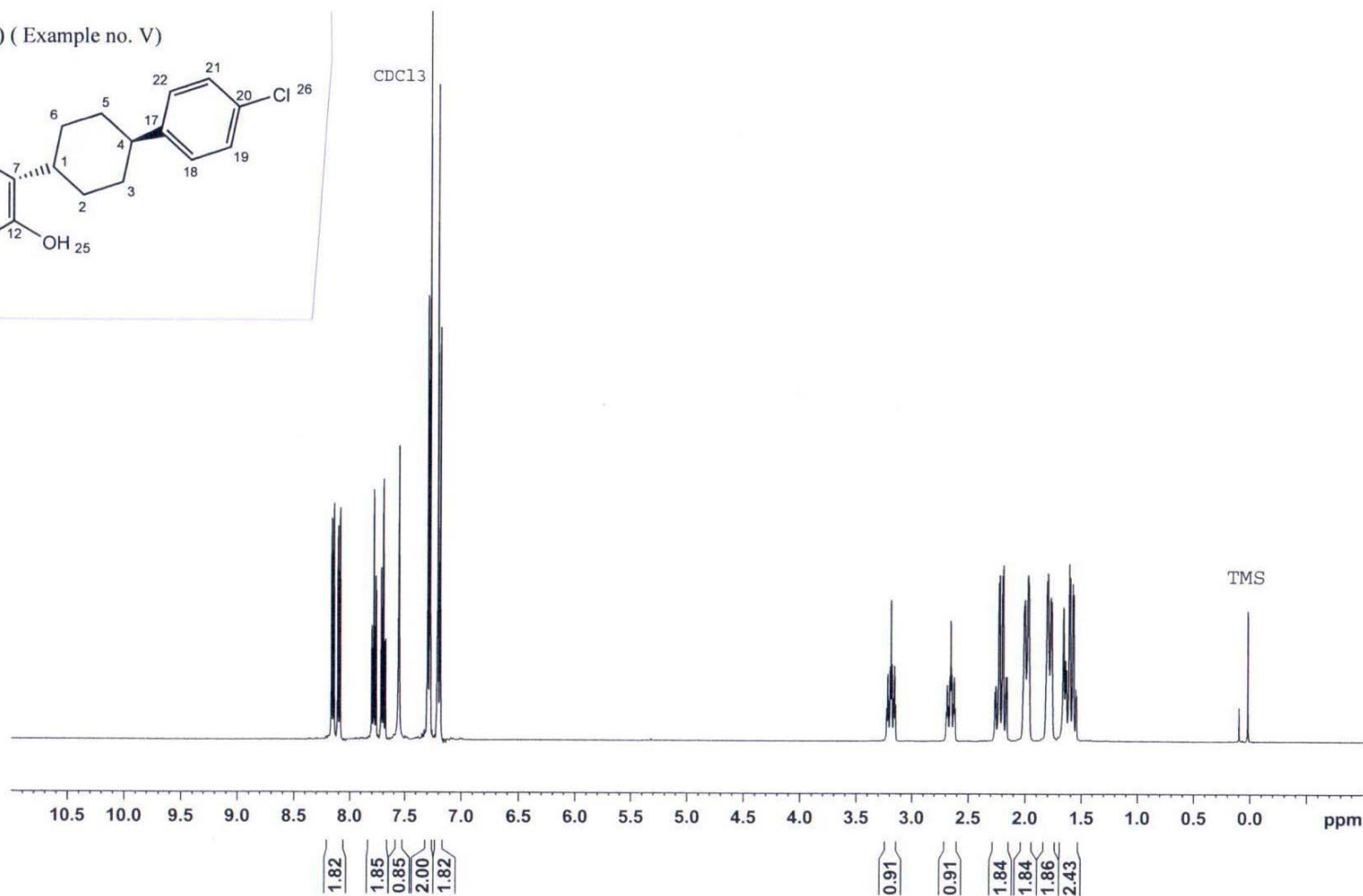
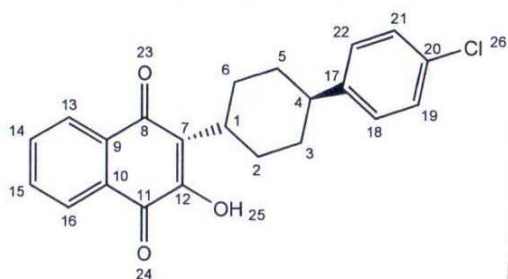
Current Data Parameters
 NAME Mar21-2013
 EXPNO 8
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130321
 Time 13.29
 INSTRUM AV400
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 4
 SWH 9980.040 Hz
 FIDRES 0.152283 Hz
 AQ 3.2834036 sec
 RG 128
 DW 50.100 usec
 DE 6.00 usec
 TE 300.0 K
 D1 3.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.15 usec
 PL1 0.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

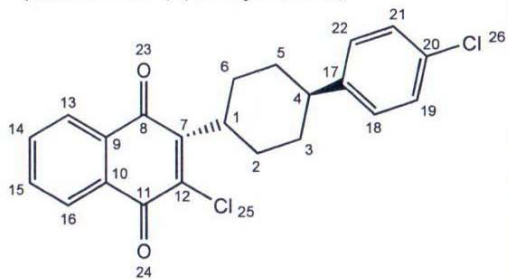
(Structure no. 1) (Example no. V)



ATO/Cl-ATO/8091 1H (Structure No. 4)

8.163 8.160 8.156 8.146 8.141 8.124 8.119 8.109 8.105 8.102 7.800 7.796 7.782 7.777 7.771 7.765 7.759 7.752 7.748 7.734 7.730 7.309 7.303 7.303 7.299 7.287 7.282 7.276 7.220 7.214 7.197 7.193 3.408 3.399 3.391 3.377 3.369 3.360 3.347 3.338 3.330 3.244 2.736 2.728 2.714 2.706 2.697 2.683 2.675 2.667 2.412 2.403 2.380 2.371 2.348 2.340 2.316 2.308 2.054 2.049 2.022 2.015 1.851 1.843 1.831 1.817 1.810 1.665 1.645 1.636 1.613

(Structure no. 4) (Example no. IV)



CDC13

Current Data Parameters
NAME Mar21-2013
EXPNO 19
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130321
Time 18.00
INSTRUM AV400
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 4
SWH 9980.040 Hz
FIDRES 0.152283 Hz
AQ 3.2834036 sec
RG 90.5
DW 50.100 usec
DE 6.00 usec
TE 300.0 K
D1 3.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 12.15 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 5.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -0.500 ppm
F2 -200.06 Hz
PPMCM 0.52500 ppm/cm
HZCM 210.06825 Hz/cm

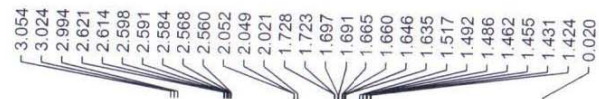
TMS

10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

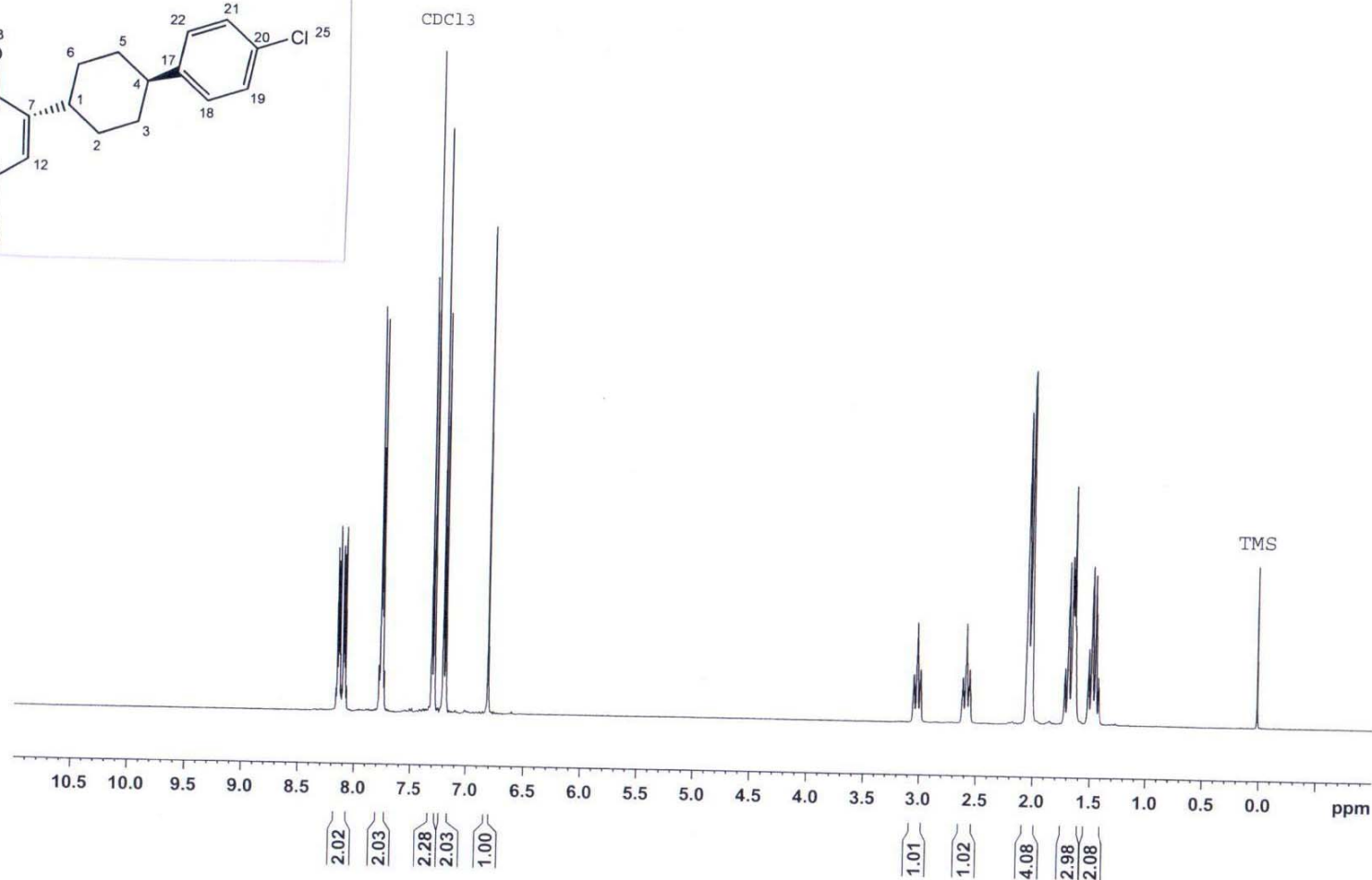
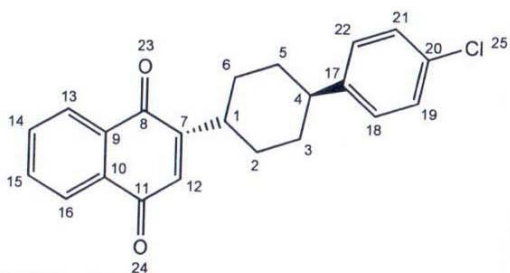
1.99 2.02 2.13 2.00

1.00 1.00 2.02 2.03 2.03 2.05

ATO/CPCN/7155 1H (Structure No. 6)



(Structure no. 6) (Example no. I)



Current Data Parameters
NAME Mar21-2013
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130321
Time 12.39
INSTRUM AV400
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 4
SWH 9980.040 Hz
FIDRES 0.152283 Hz
AQ 3.2834036 sec
RG 161.3
DW 50.100 usec
DE 6.00 usec
TE 300.0 K
D1 3.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 12.15 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 6.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -0.500 ppm
F2 -200.06 Hz
PPMCM 0.52500 ppm/cm
HZCM 210.06825 Hz/cm

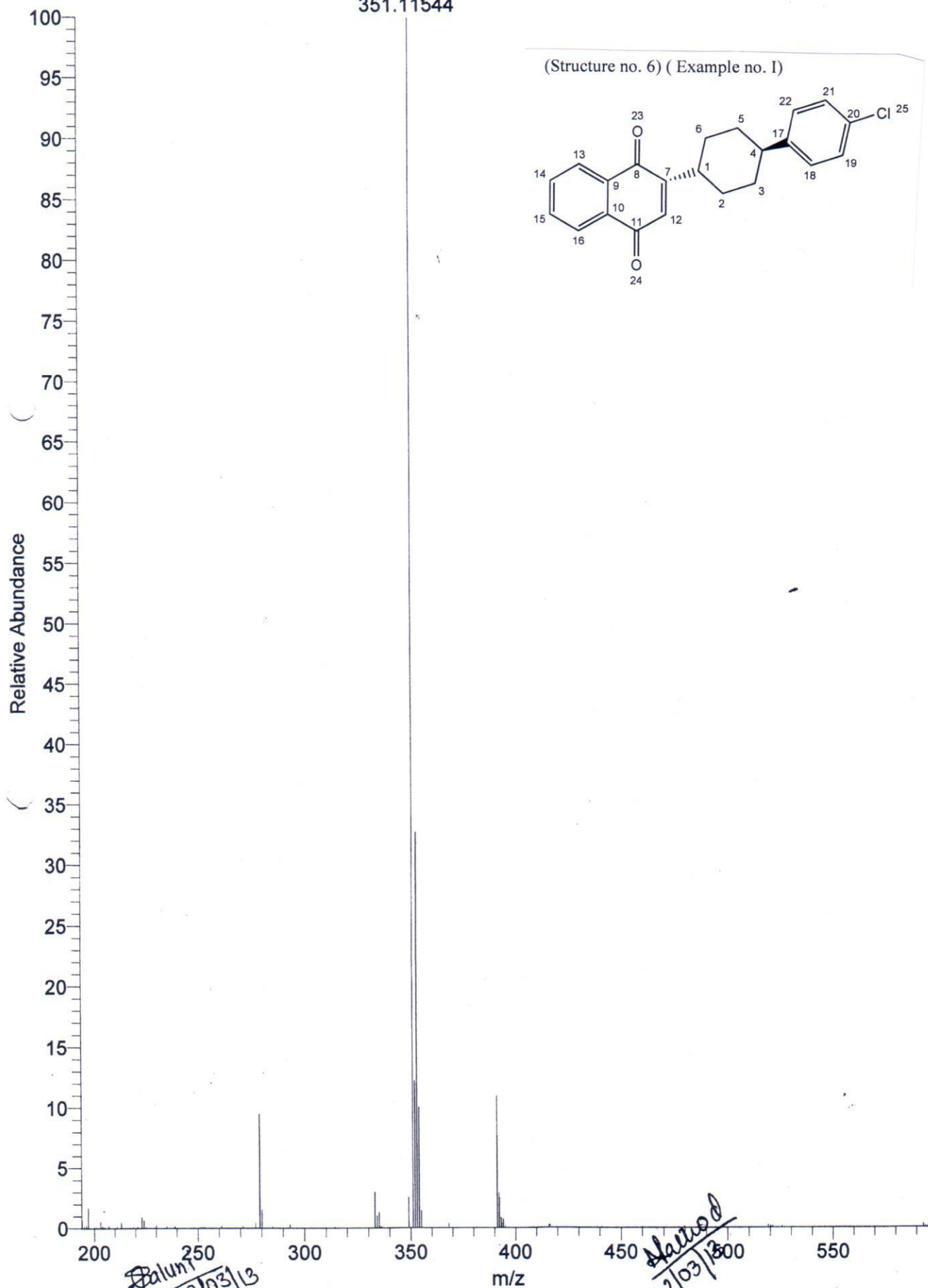
Details for HRMS Measurements

Mass Analyzer Instrument	Thermo Q-Exactive Orbitrap
MS Ionization Method	
Sheath gas flow rate	30
Auxiliary gas flow rate	10
Spray Voltage(kV)	4.0
Capillary Temp(°C)	320
S-lens RF Level	55
Heater Temperature(°C)	350
Sample Preparation	200 ppm in Water: Acetonitrile (50:50)

130313_06 #27 RT: 0.22 AV: 1 SB: 75 0.00-0.16 , 2.54-3.00 NL: 5.11E7

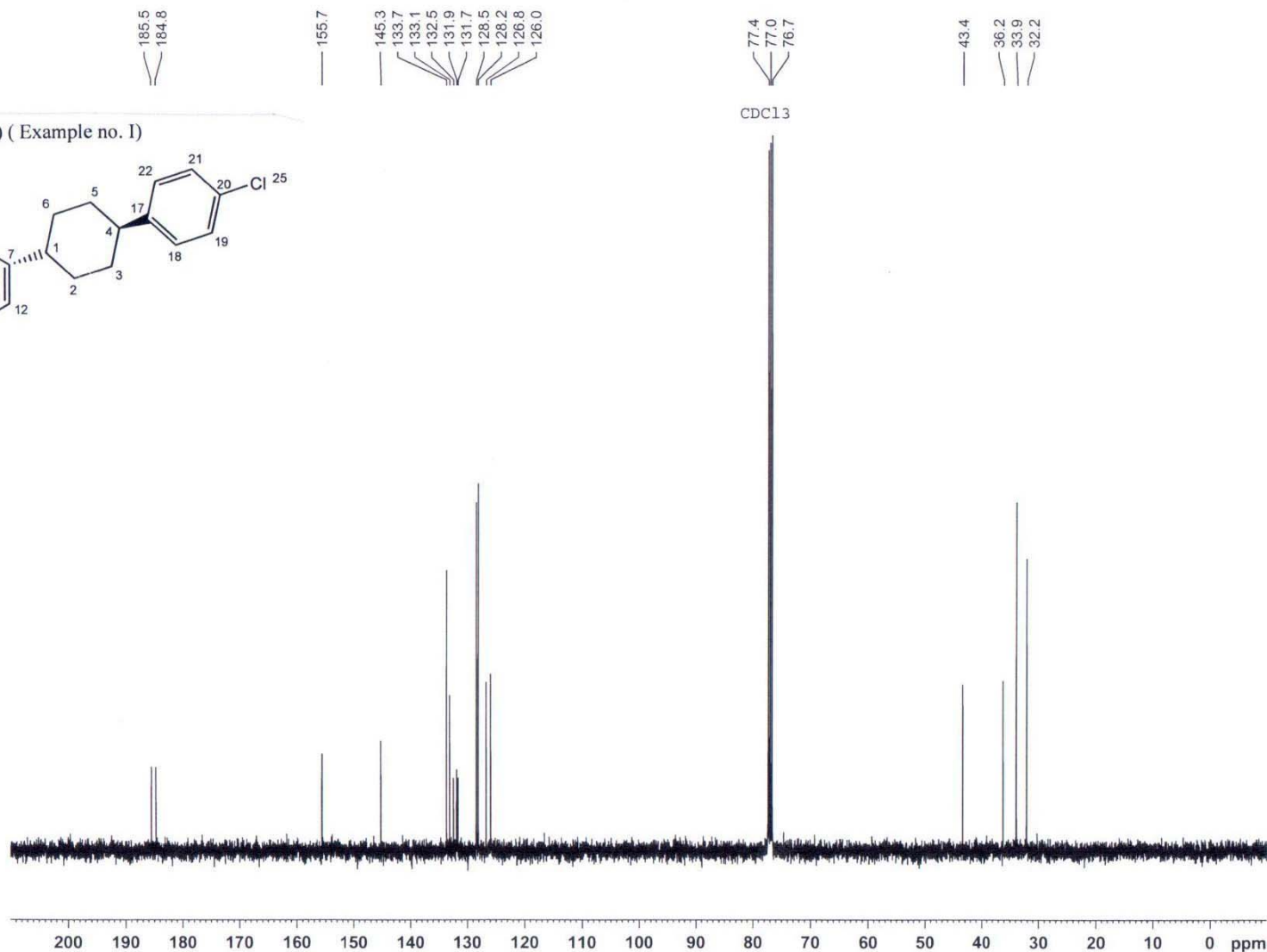
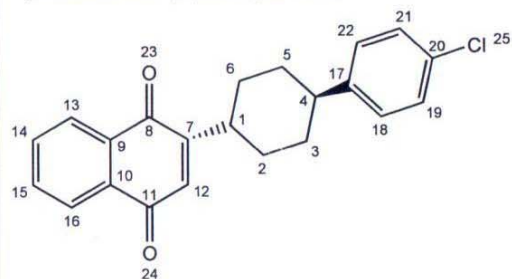
T: FTMS + p APCI corona Full ms [66.70-1000.00]

351.11544



ATO/CPCN/7155 13C (Structure No. 6)

(Structure no. 6) (Example no. 1)



Current Data Parameters
NAME Mar23-2013
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130323
Time 16.10
INSTRUM AV400
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 16384
DW 20.850 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

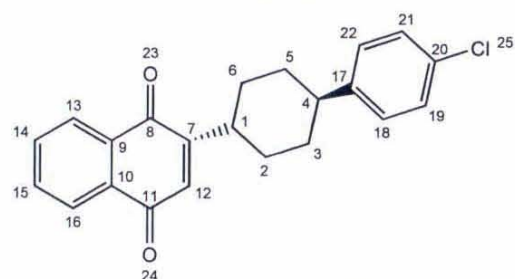
===== CHANNEL f1 =====
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 16.48 dB
PL13 17.00 dB
SFO2 400.1316005 MHz

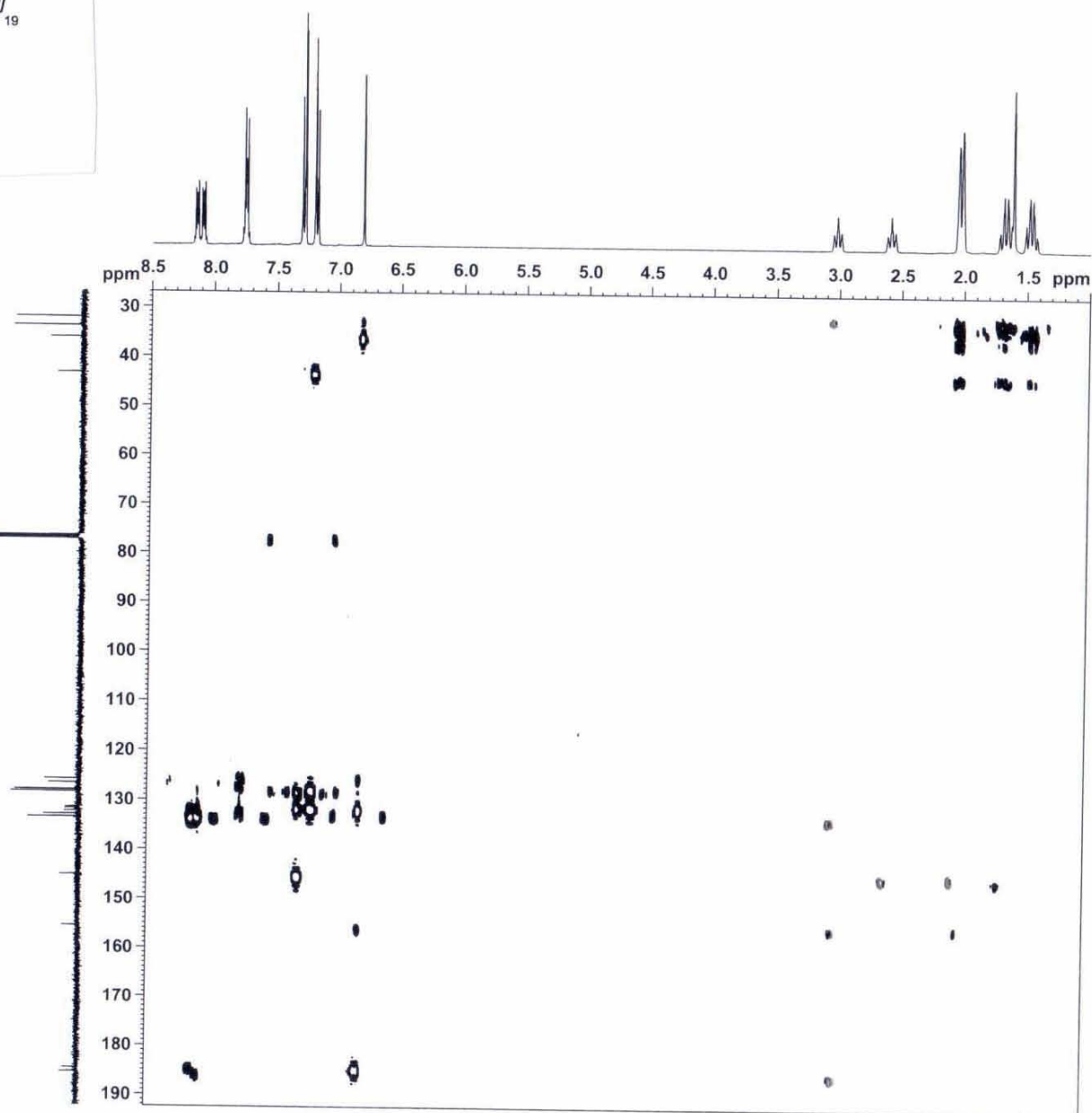
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
F1P 215.000 ppm
F1 21631.75 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 11.00000 ppm/cm
HZCM 1106.74048 Hz/cm

(Structure no. 6) (Example no. I)



ATO/CPCN/7155 1H (Structure No. 6)



Current Data Parameters
NAME Mar29-2013
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130329
Time_ 14.37
INSTRUM AV400
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 4
SWH 9980.040 Hz
FIDRES 0.152283 Hz
AQ 3.2834036 sec
RG 228.1
DW 50.100 usec
DE 6.00 usec
TE 300.0 K
D1 3.00000000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 12.15 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00