

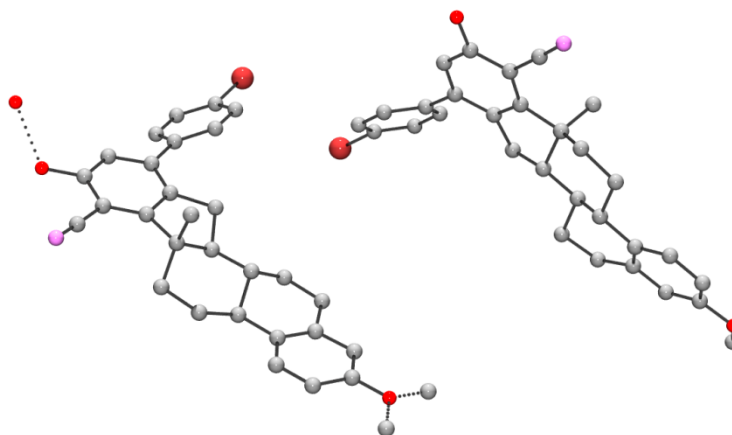
RSC Advances
Supplementary Information

Synthesis, photophysical and anticancer study of D-ring extended estrone analogues

Hardesh K. Maurya,^a Mohammad Hasanain,^b Ch Pavan Kumar,^c Prema G. Vasudeva,^d Jayanta Sarkar,^b M. Chandrasekharam^c and Atul Gupta^{*a}

1. Supplementary Figure 1:

(a)



(b)

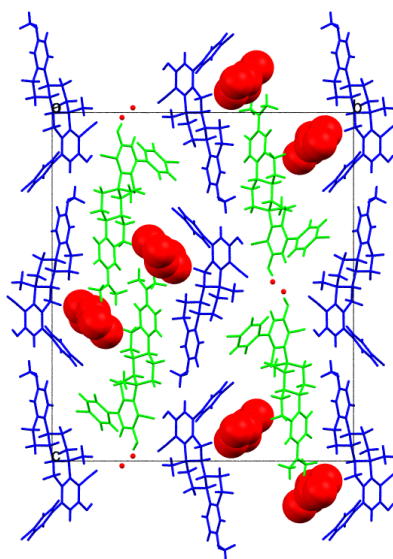


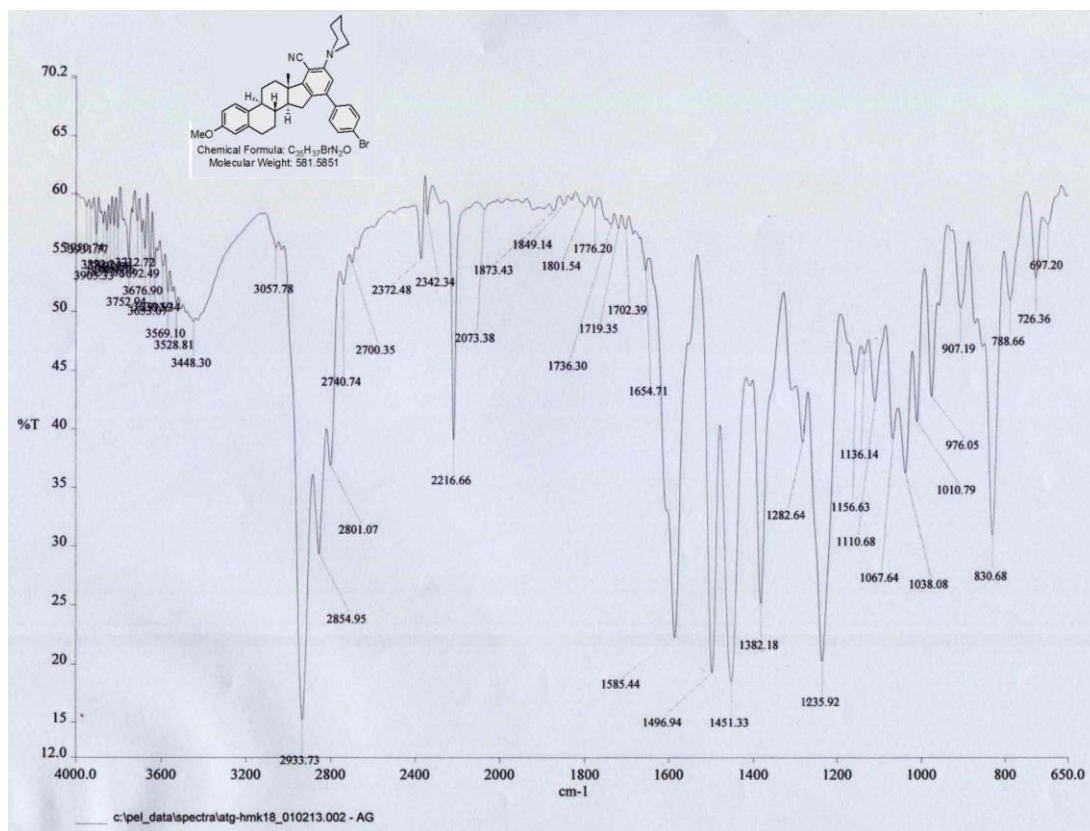
Figure S1. (a) A view of the asymmetric unit of **8** in crystals. Hydrogen atoms are not shown for clarity. Bonds to the disordered methyl groups in OMe moiety and a hydrogen bond to the co-crystallized water molecule are shown in dotted lines. (b) Packing of molecules in the crystals of **8** when viewed down the crystallographic a-axis. The two independent molecules are shown in

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different colors (Mol-1 in green, Mol-2 in Blue). Disordered water molecules (shown as bigger balls in red color) form a continuous channel and not connected to the steroidal molecules though hydrogen bonds. The ordered water molecule which is hydrogen bonded to the hydroxyl group of molecule-1 in the asymmetric unit, is shown as smaller balls in red color.

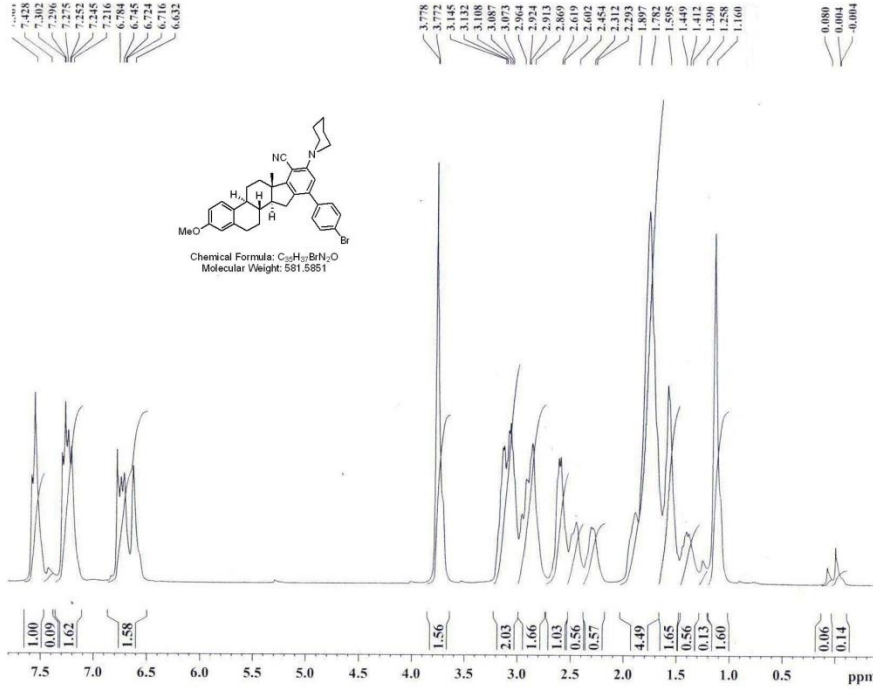
2. Scanned copy of Spectra

(+)(6bS,8aS,13aS,13bS)-12-(4-bromophenyl)-4-methoxy-8a-methyl-10-(piperidin-1-yl)-2,6b,7,8,8a,13,13a,13b-octahydro-1H-indeno[2,1-a]phenanthrene-9-carbonitrile (**7a**).



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CIMAP-PROTON
PROJECT NO.: NWP-09



Current Data Parameters
NAME atghmk18.p
EXPNO 1
PROCNO 1

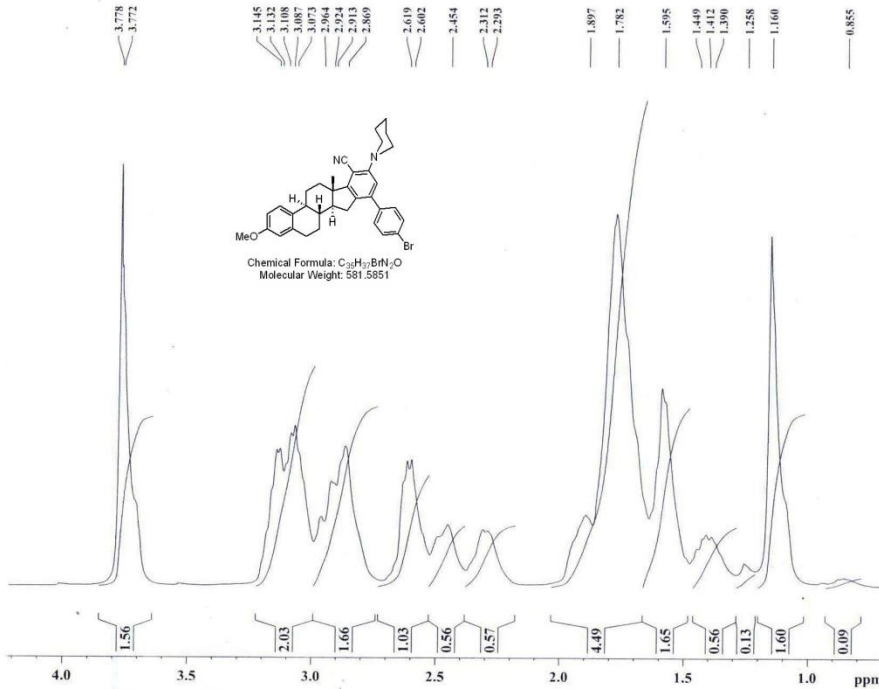
F2 - Acquisition Parameters
Date_ 20121001
Time 18.05
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 96
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 114
DW 81.000 usec
DE 6.00 usec
TE 297.7 K
D1 1.00000000 sec
TD0 1

CHANNEL f1

NUC1 1H
PI 6.65 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300132 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

CIMAP-PROTON
PROJECT NO.: NWP-09



Current Data Parameters
NAME atghmk18.p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121001
Time 18.05
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 96
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
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DW 81.000 usec
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TE 297.7 K
D1 1.00000000 sec
TD0 1

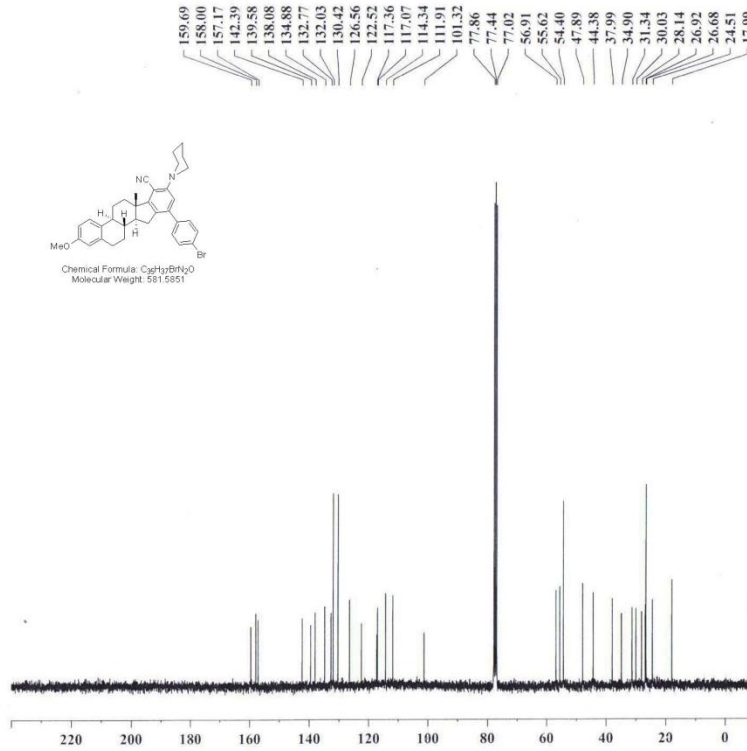
CHANNEL f1

NUC1 1H
PI 6.65 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300132 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

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CIMAP-CARBON
PROJECT NO.: MLP-04



Current Data Parameters
NAME atghmk18.p
EXPNO 9
PROCNO 1

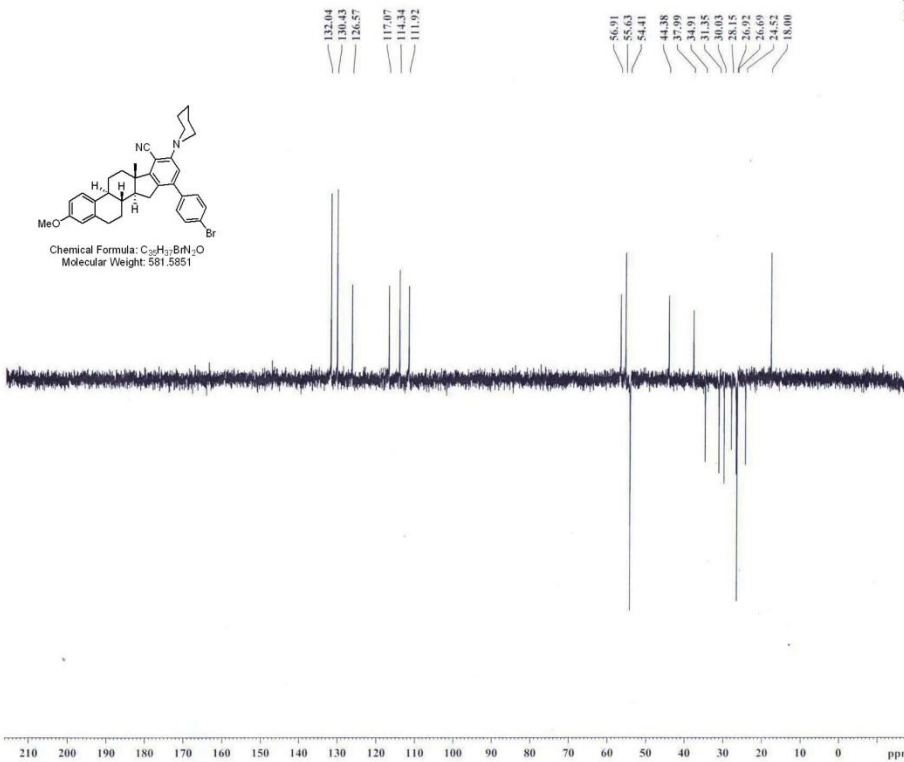
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Date_ 20121004
Time 10.12
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1509
DS 4
SWH 21097.047 Hz
FIDRES 0.321915 Hz
AQ 1.5532532 sec
RG 32768
DW 23.700 usec
DE 6.00 usec
TE 298.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

CHANNEL f1
NUC1 13C
P1 12.50 usec
PL1 -6.00 dB
SFO1 75.4752950 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 25.35 dB
PL13 29.61 dB
SFO2 300.1312000 MHz

F2 - Processing parameters
SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

CIMAP-DEPT 135
PROJECT NO.: ILP-13



Current Data Parameters
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EXPNO 3
PROCNO 1

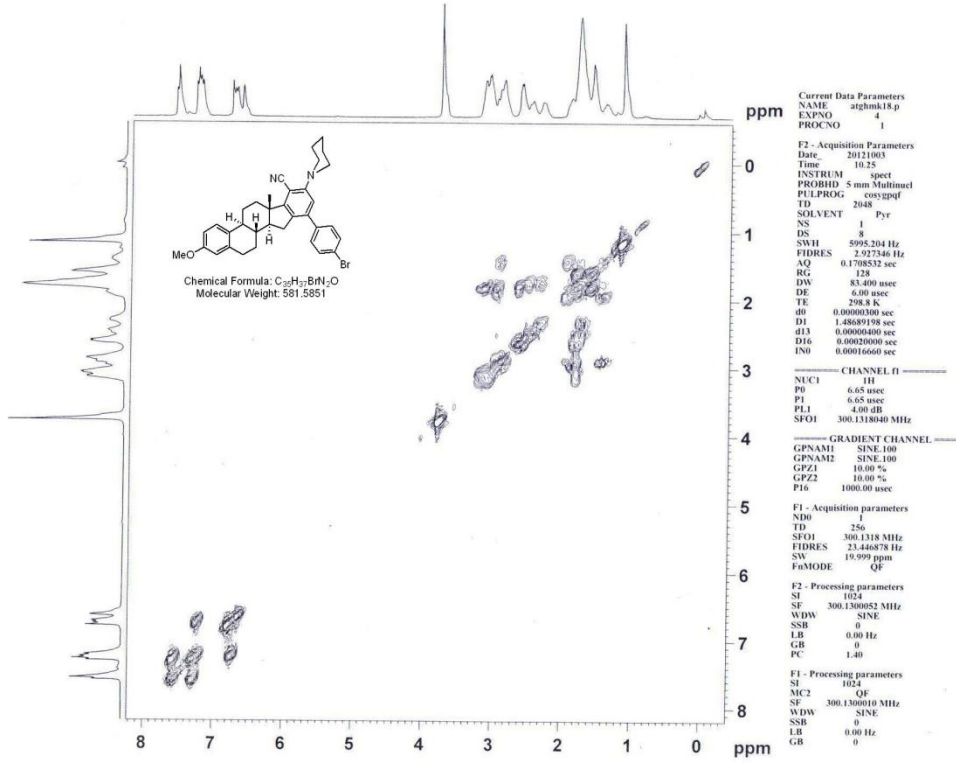
F2 - Acquisition Parameters
Date_ 20121003
Time 10.94
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 561
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 6.00 usec
TE 299.0 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.0034828 sec
d12 0.00002000 sec
DELTA 0.00001592 sec
TD0 1

CHANNEL f1
NUC1 13C
P1 12.50 usec
PL1 25.00 usec
PL1 -6.00 dB
SFO1 75.4752950 MHz

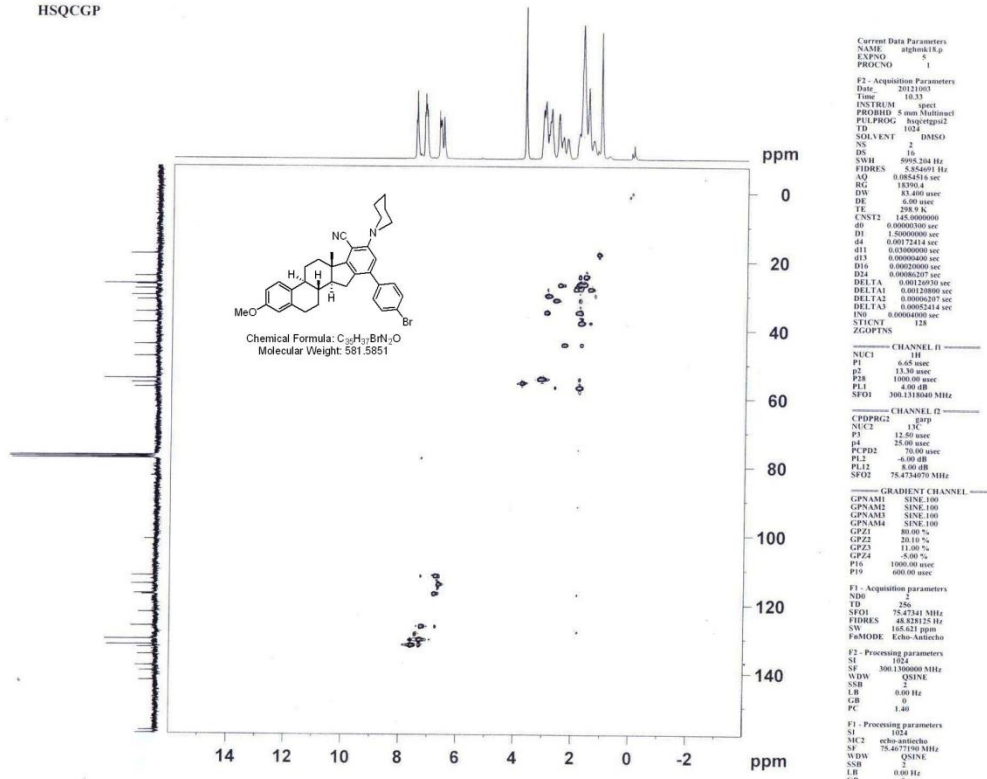
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
P3 6.65 usec
P4 13.30 usec
PCPD2 80.00 usec
PL2 4.00 dB
PL12 25.61 dB
SFO2 300.1312000 MHz

F2 - Processing parameters
SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

COSY

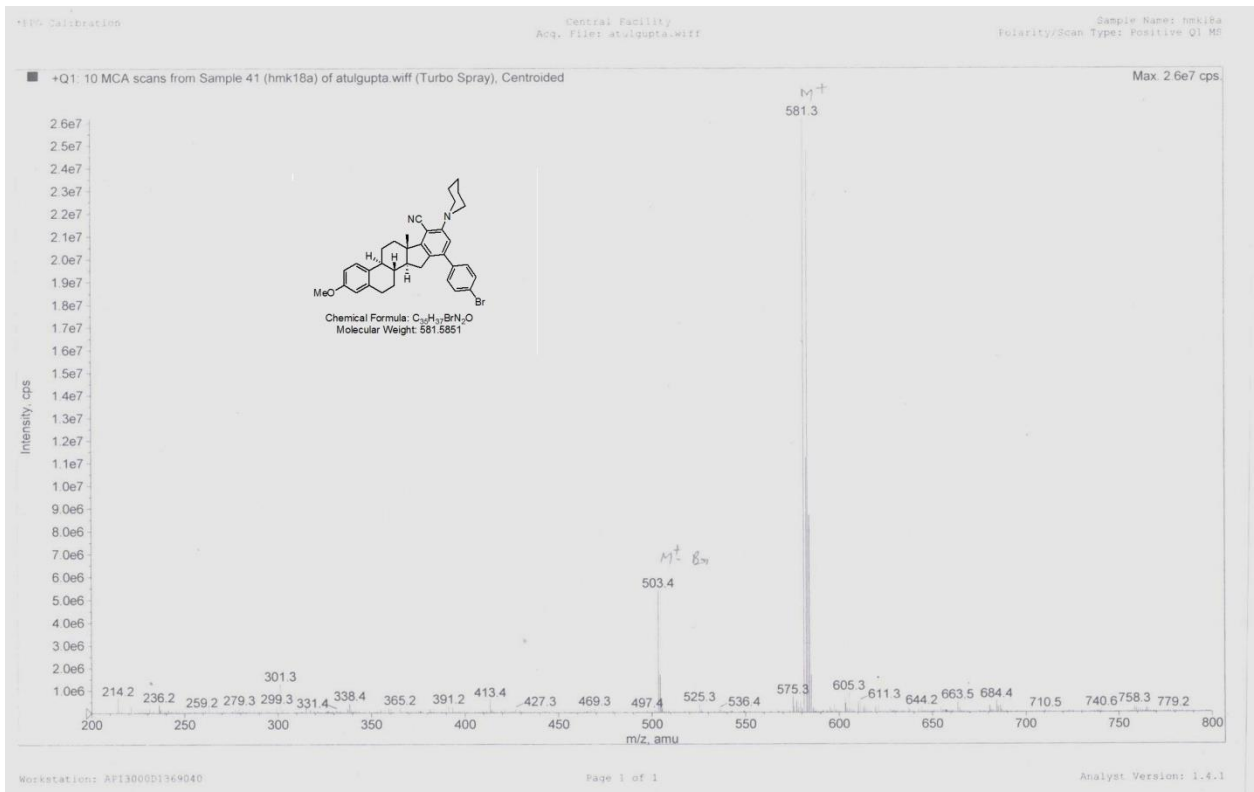
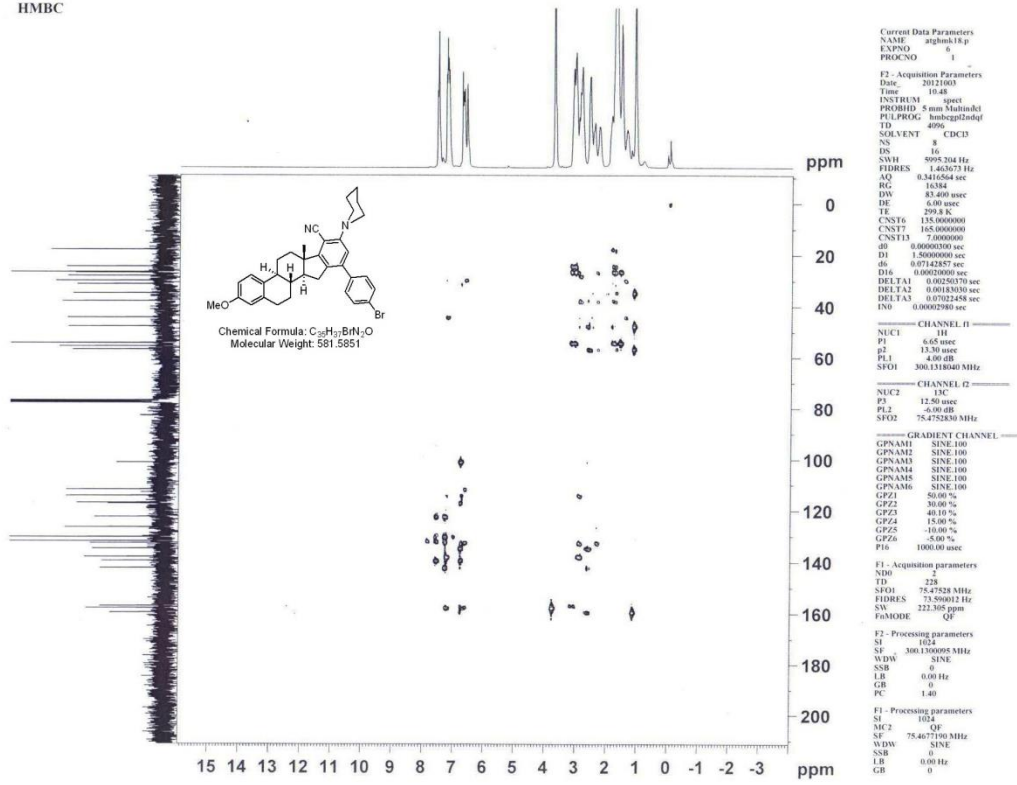


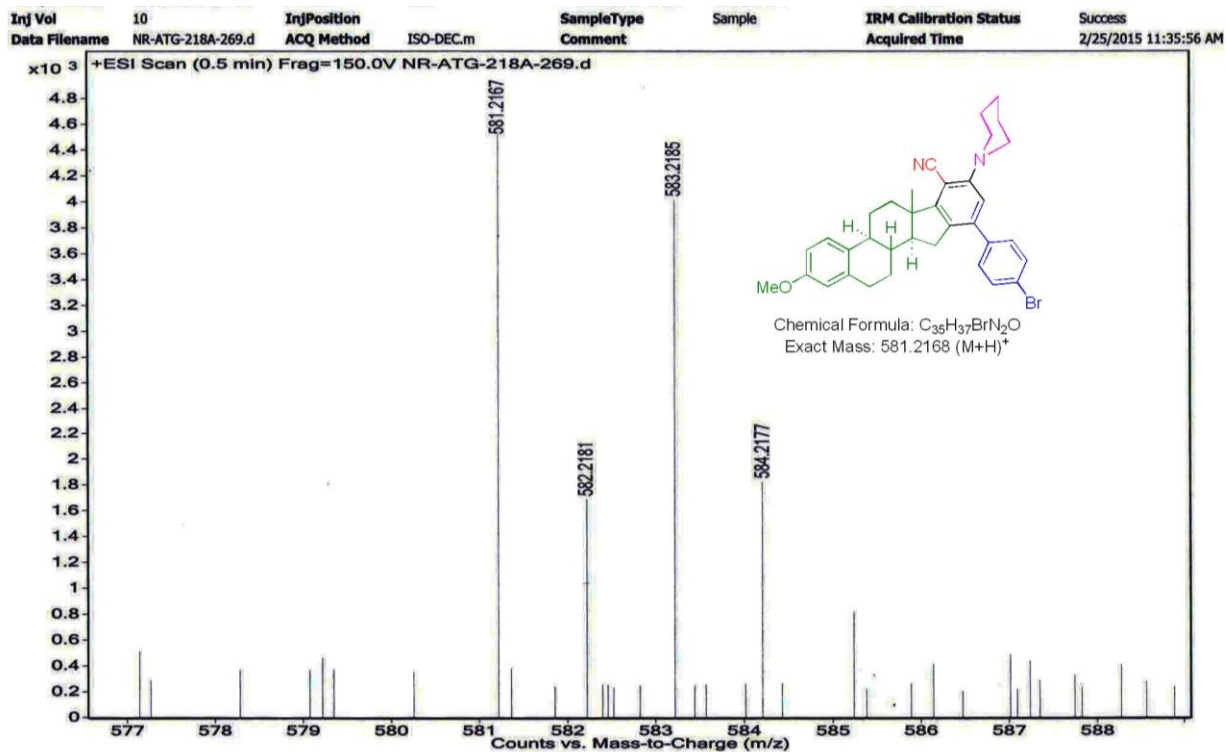
HSQC



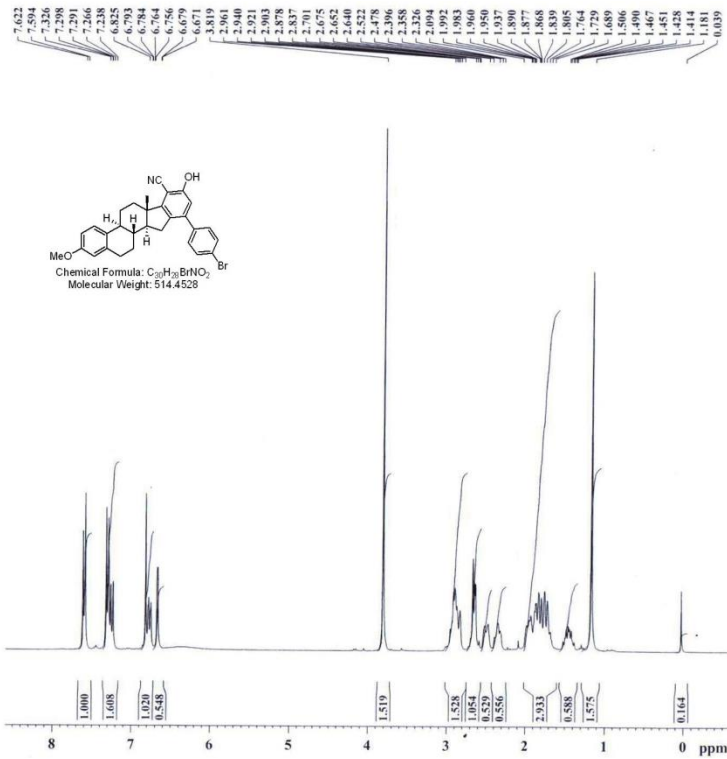
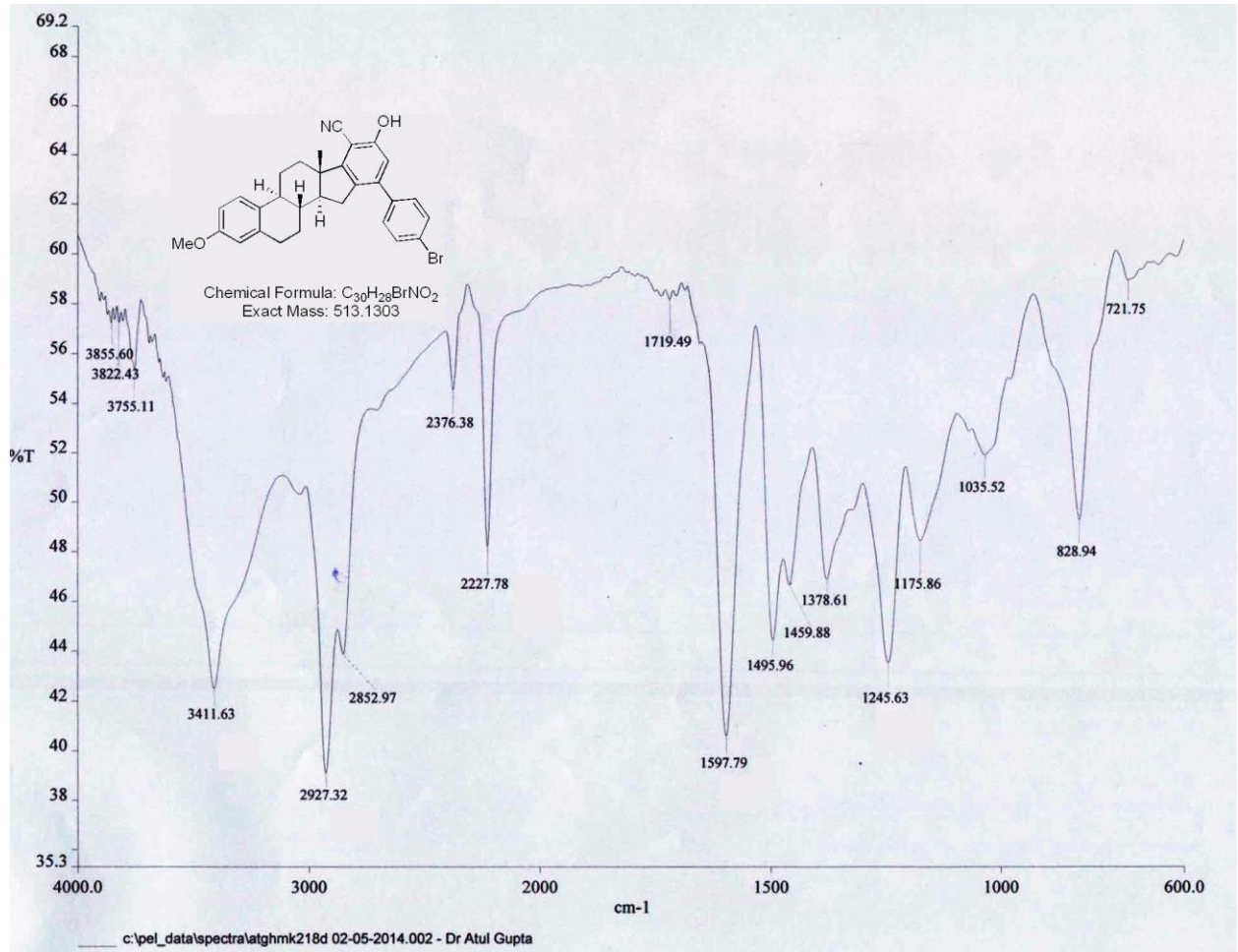
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HMBC





(+)(6bS,8aS,13aS,13bS)-12-(4-bromophenyl)-10-hydroxy-4-methoxy-8a-methyl-2,6b,7,8,8a,13,13a,13b-octahydro-1H-indeno[2,1-a]phenanthrene-9-carbonitrile (**8a**)



CIMAP PROTON
PROJECT NO.: mlp-02

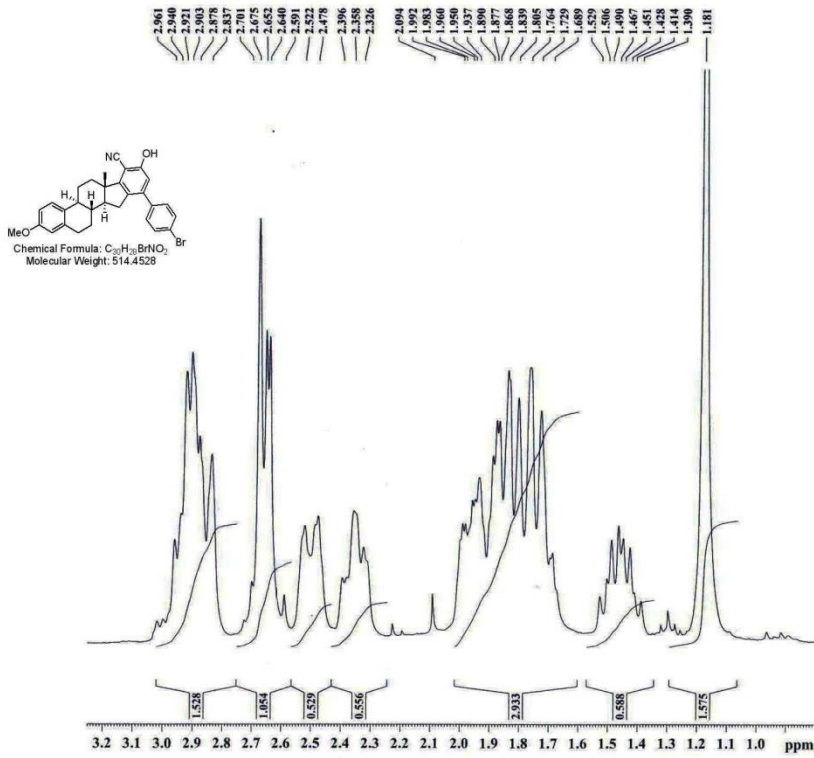
Current Data Parameters
NAME atghmk218d.p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140603
Time 11.38
INSTRUM spect
PROBHD 5 mm Multinuel
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 203.2
DW 55.600 usec
DE 6.00 usec
TE 300.7 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 7.15 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299972 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

RSC Advances



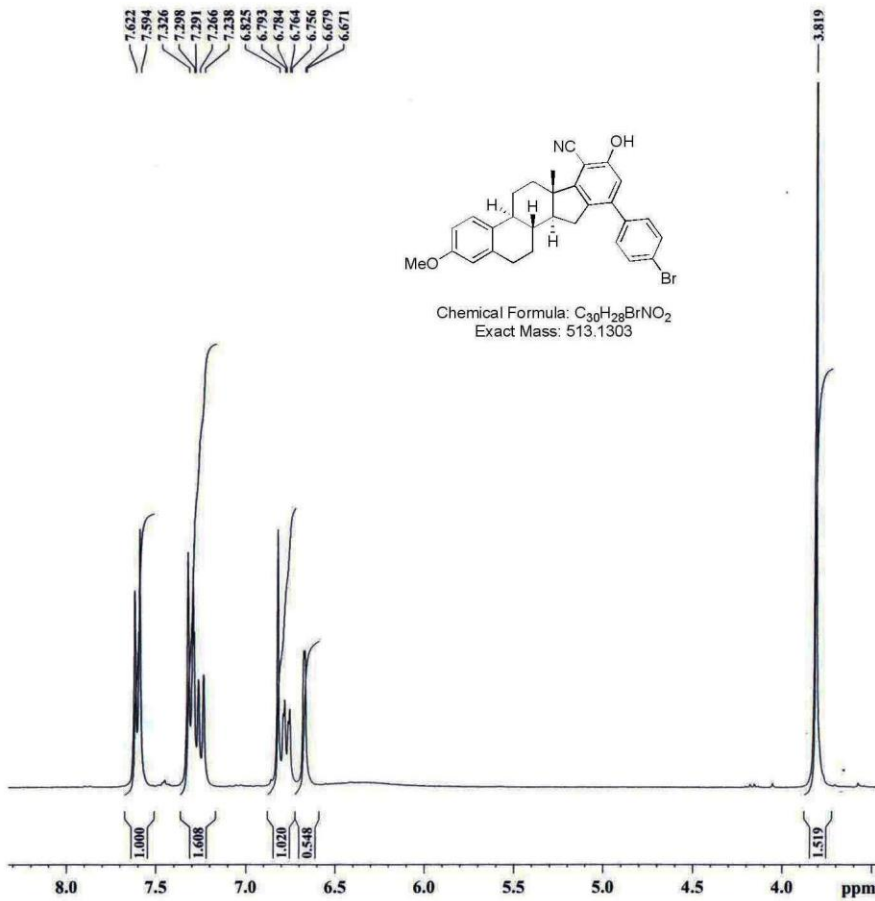
CIMAP PROTON
PROJECT NO.: mlp-02

Current Data Parameters
NAME atghmk218d.p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date 20140603
Time 11.38
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 203.2
DW 55.600 usec
DE 6.00 usec
TE 300.7 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 7.15 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299972 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40



CIMAP PROTON
PROJECT NO.: mlp-02

Current Data Parameters
NAME atghmk218d.p
EXPNO 1
PROCNO 1

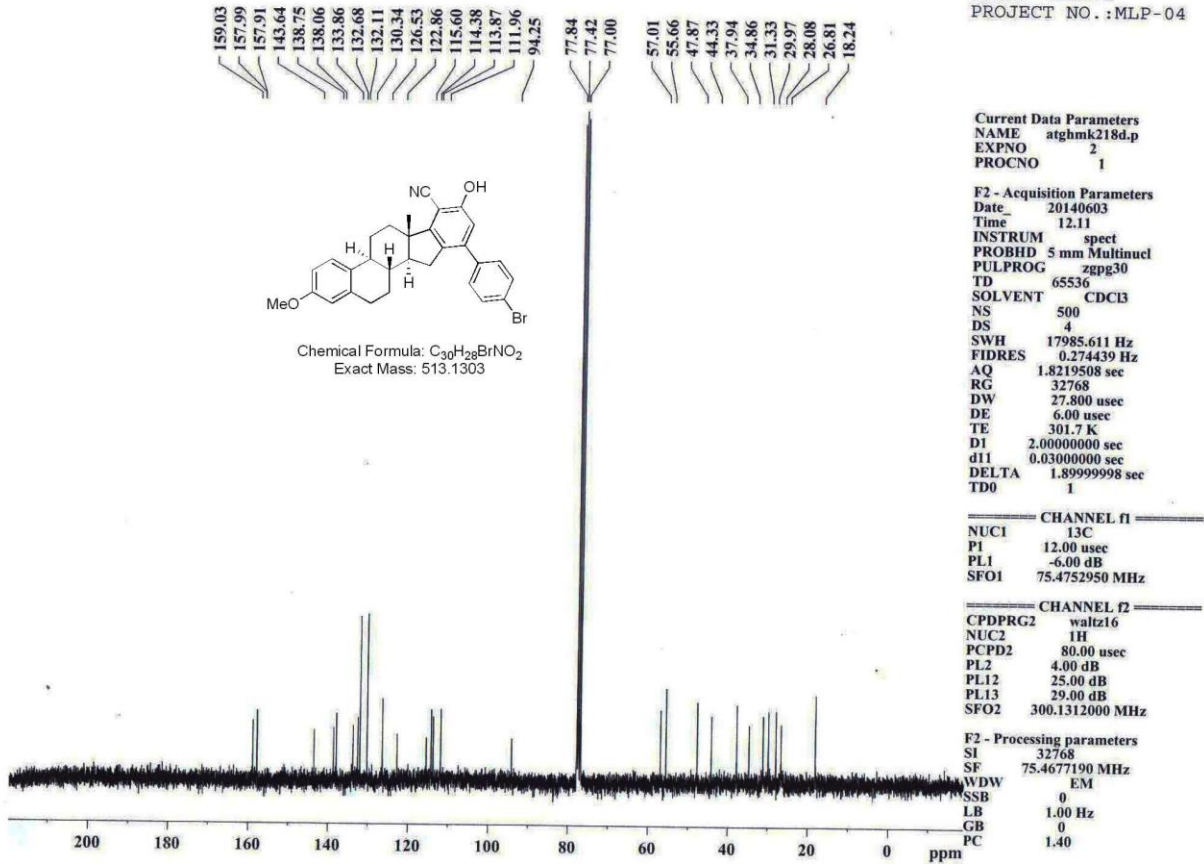
F2 - Acquisition Parameters
Date 20140603
Time 11.38
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 203.2
DW 55.600 usec
DE 6.00 usec
TE 300.7 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 7.15 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

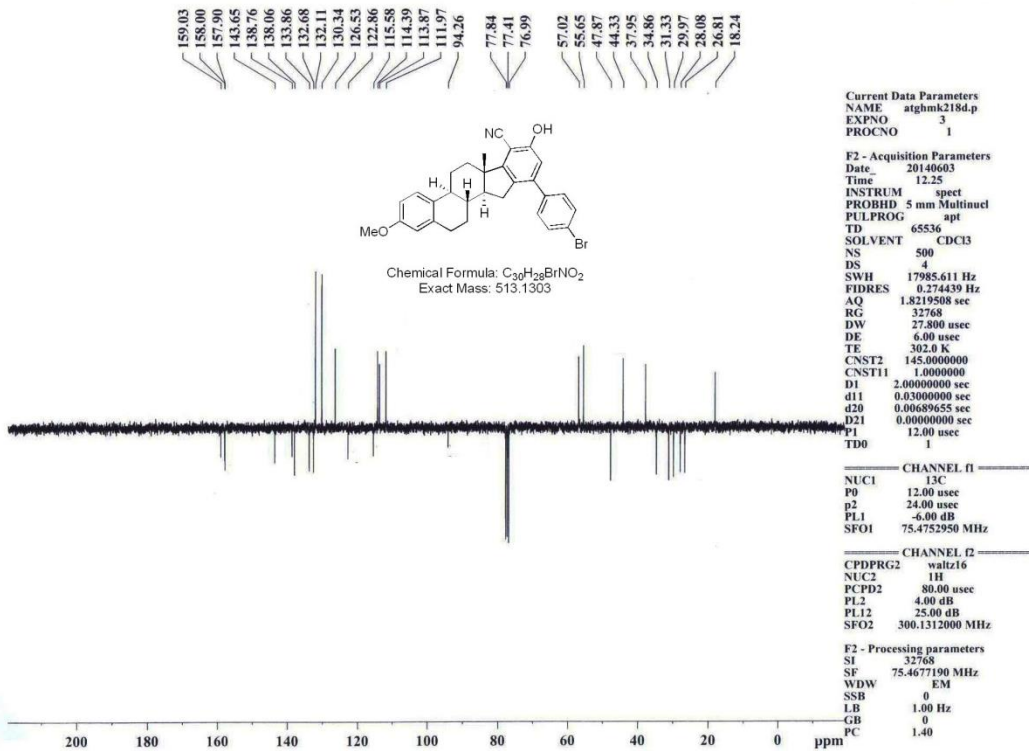
F2 - Processing parameters
SI 32768
SF 300.1299972 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

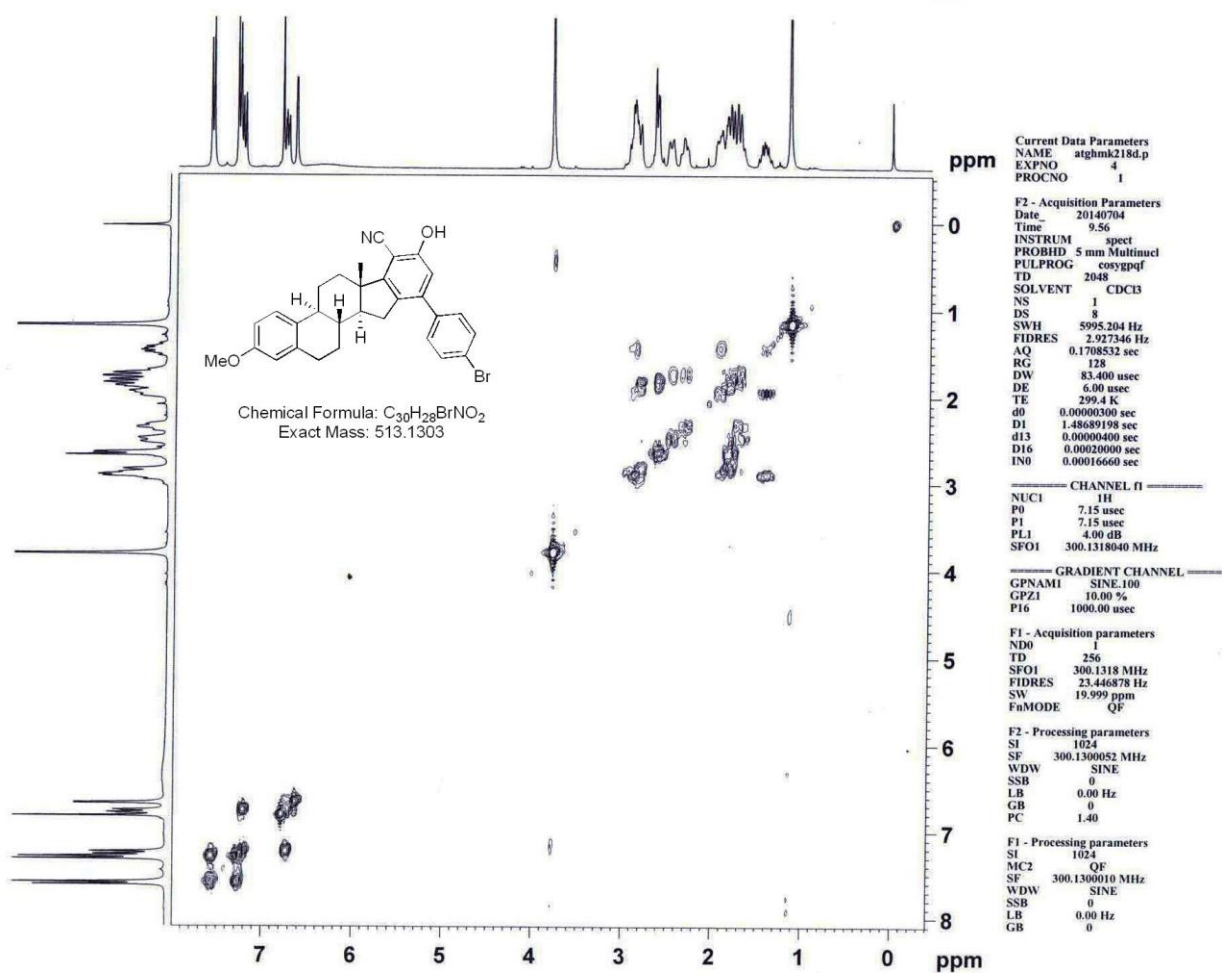
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CIMAP-CARBON
PROJECT NO. : MLP-04



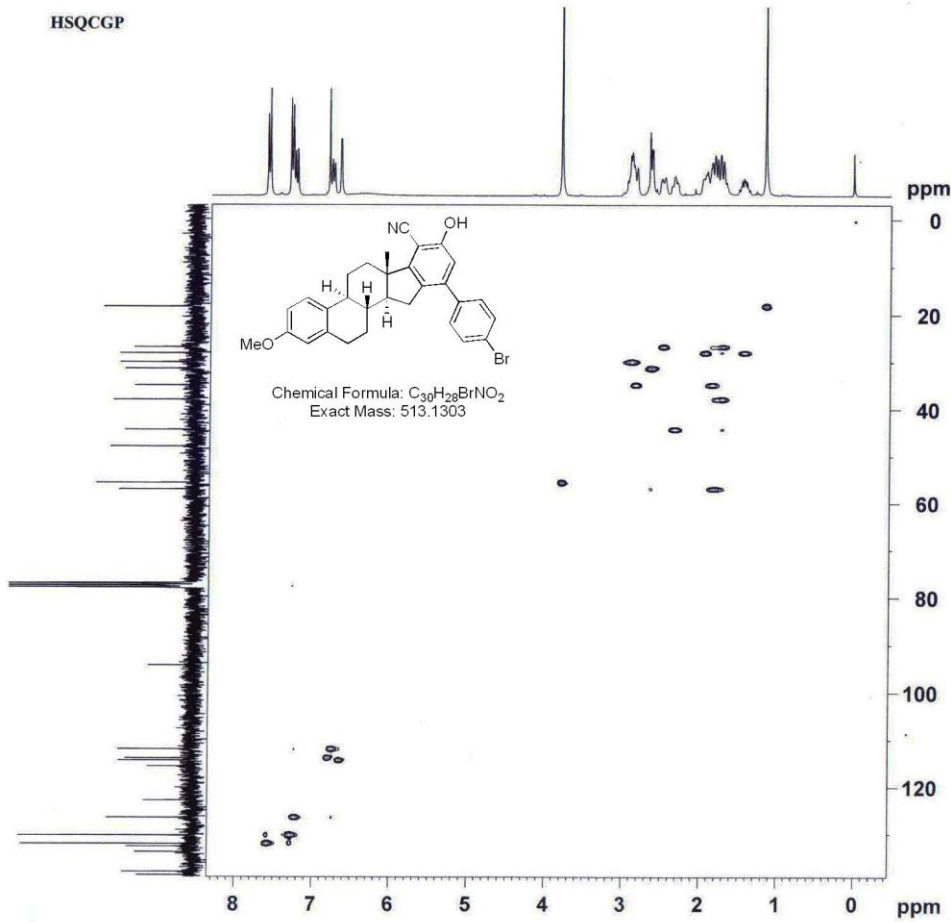
APT: X, XH2 positiv





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HSQC/GP



Current Data Parameters
NAME stghmk218d.p
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140704
Time 10:04
INSTRUM spect
PROBHD 5 mm Multinuc
PULPROG hzgpgprg2
TD 1024
SOLVENT DMSO
NS 2
DS 16
SWH 5995.204 Hz
FIDRES 5.854691 Hz
AQ 0.0685416 sec
RG 18390.4
DW 83.480 usec
DE 6.00 usec
TE 299.6 K
CNST2 145.000000
d0 0.00000000 sec
D1 1.50000000 sec
d4 0.00172414 sec
d11 0.03000000 sec
d13 0.00000000 sec
D16 0.00020000 sec
D24 0.00006207 sec
DELTA 0.00127030 sec
DELTA1 0.00120809 sec
DELTA2 0.00006397 sec
DELTA3 0.00052414 sec
IN0 0.00004000 sec
STICNT 128
ZGPGNS

CHANNEL f1
NUC1 1H
P1 7.15 usec
P2 14.30 usec
P28 1900.00 usec
PL1 4.90 dB
SFO1 300.131040 MHz

CHANNEL f2
CPDPRG2 EPT
NUC2 13C
P3 12.00 usec
P4 24.00 usec
PCPD2 70.00 usec
PL2 -6.00 dB
PL12 9.32 dB
SFO2 75.4734070 MHz

GRADIENT CHANNEL
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPNAM4 SINE.100
GPZ1 80.00 %
GPZ2 20.10 %
GPZ3 11.00 %
GPZ4 5.00 %
P16 1000.00 usec
P19 600.00 usec

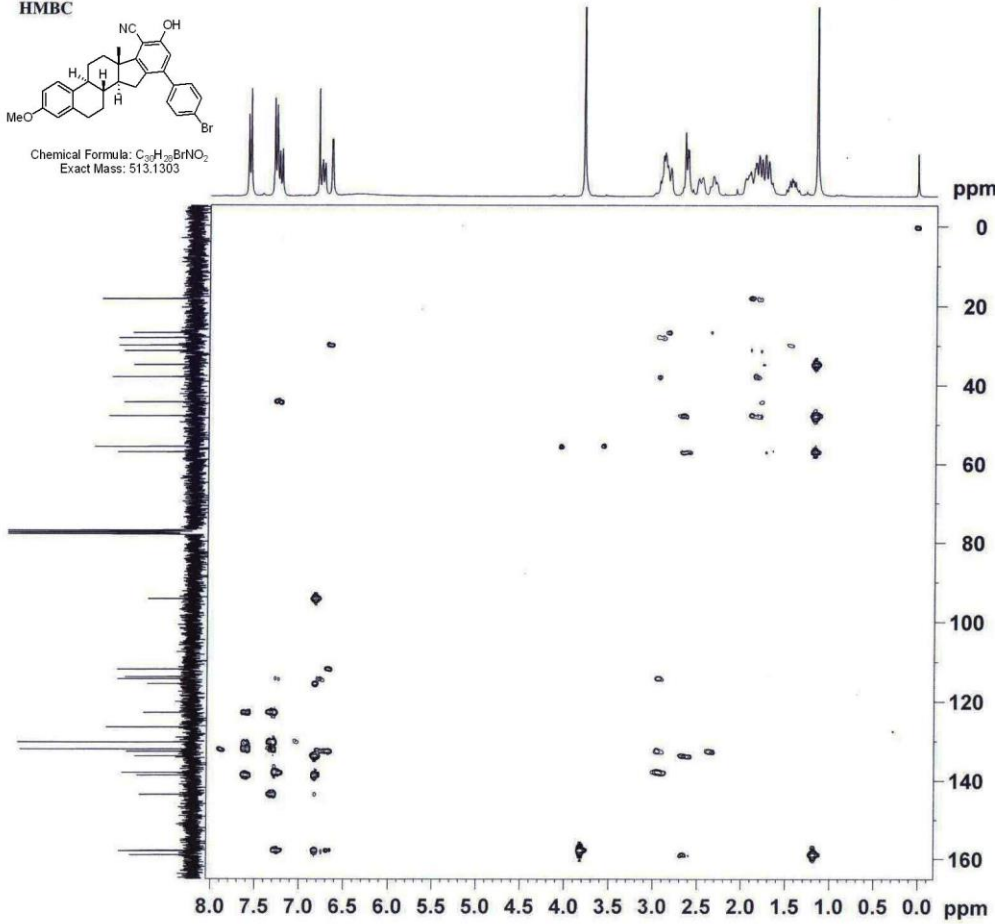
F1 - Acquisition parameters
ND0 2
TD 256
SFO1 75.47341 MHz
FIDRES 48.828125 Hz
SW 165.621 ppm
F2MODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 300.1300000 MHz
WDW QSI
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 75.4677150 MHz
WDW QSI
SSB 2
LB 0.00 Hz
GB 0

RSC Advances

HMBC



Current Data Parameters
NAME aigmk118d.p
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140704
Time 10:19
INSTRUM spect
PROBHD 5 mm Multinuc
PULPROG hmcpgp2dqf
TD 4096
SOLVENT CDCl3
NS 8
DS 16
SWH 8995.204 Hz
FIDRES 1.463673 Hz
AQ 0.341564 sec
RG 16384
DW 83.400 usec
DE 6.00 usec
TE 300.4 K
CNST6 135.0000000
CNST7 165.0000000
CNST13 7.0000000
d0 0.00000300 sec
D1 1.50000000 sec
d6 0.07142857 sec
D16 0.00020000 sec
DELTA1 0.00250370 sec
DELTA2 0.00183030 sec
DELTA3 0.07022458 sec
IN0 0.00002980 sec

CHANNEL f1
NUC1 1H
P1 7.15 usec
P2 14.30 usec
PL1 4.00 dB
SFO1 300.1318640 MHz

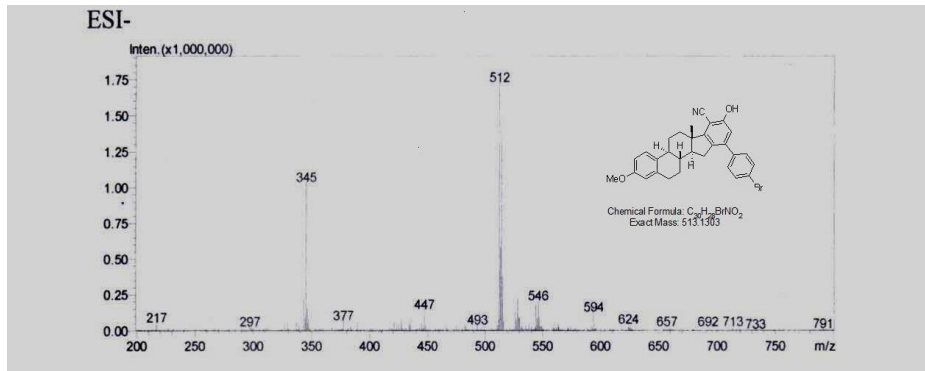
CHANNEL f2
NUC2 13C
P3 12.00 usec
PL2 -6.00 dB
SFO2 75.4752830 MHz

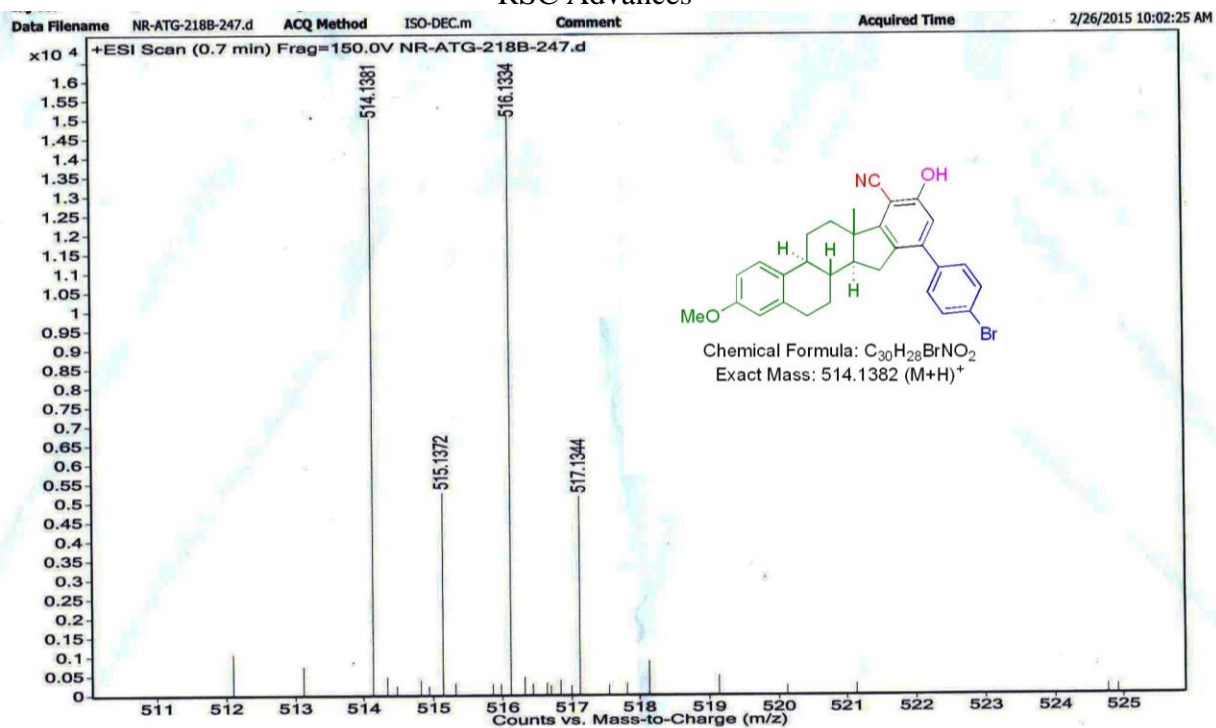
GRADIENT CHANNEL
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPNAM4 SINE.100
GPNAM5 SINE.100
GPNAM6 SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
GPZ4 15.00 %
GPZ5 -10.00 %
GPZ6 -5.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ND0 2
TD 256
SFO1 75.47528 MHz
FIDRES 65.541107 Hz
SW 222.305 ppm
F0MODE QF

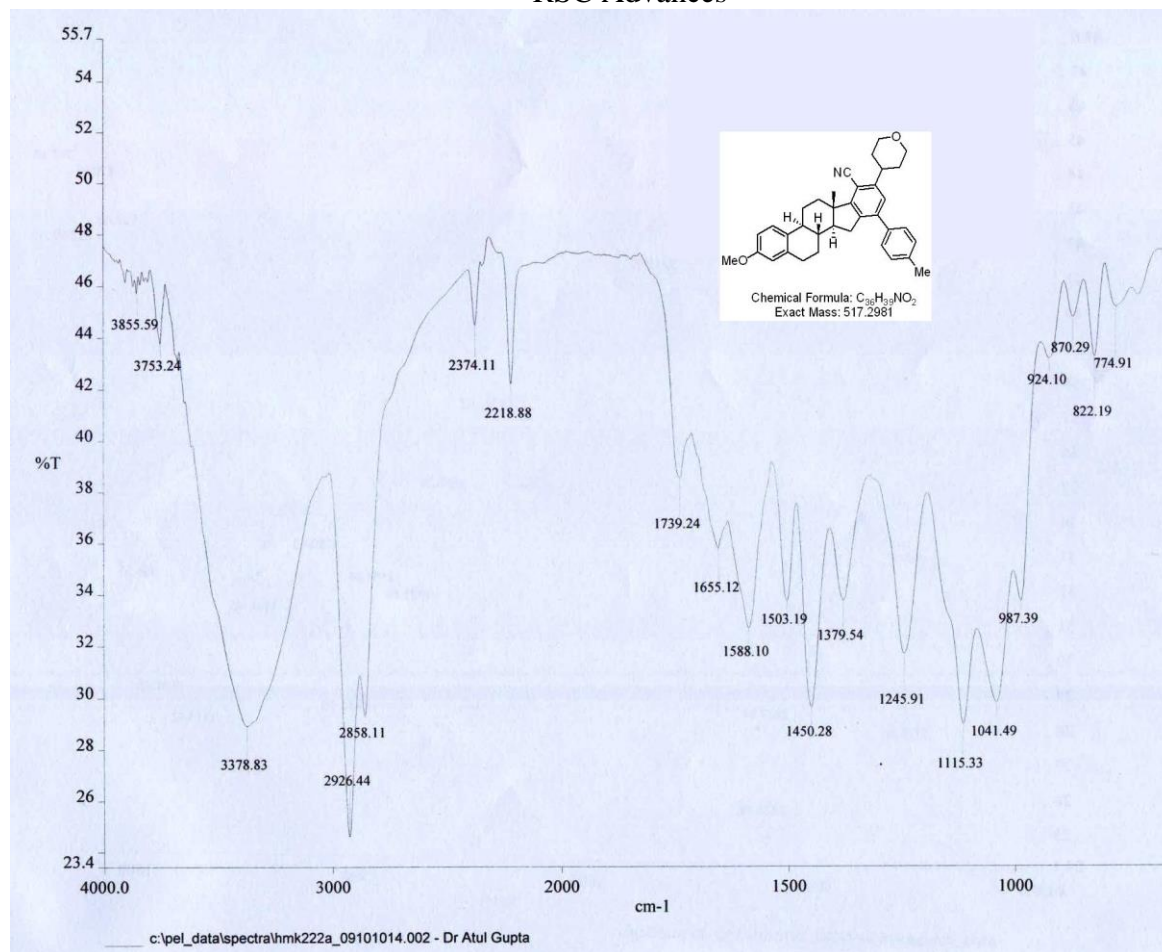
F2 - Processing parameters
SI 1024
SF 300.1299920 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 75.4677190 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

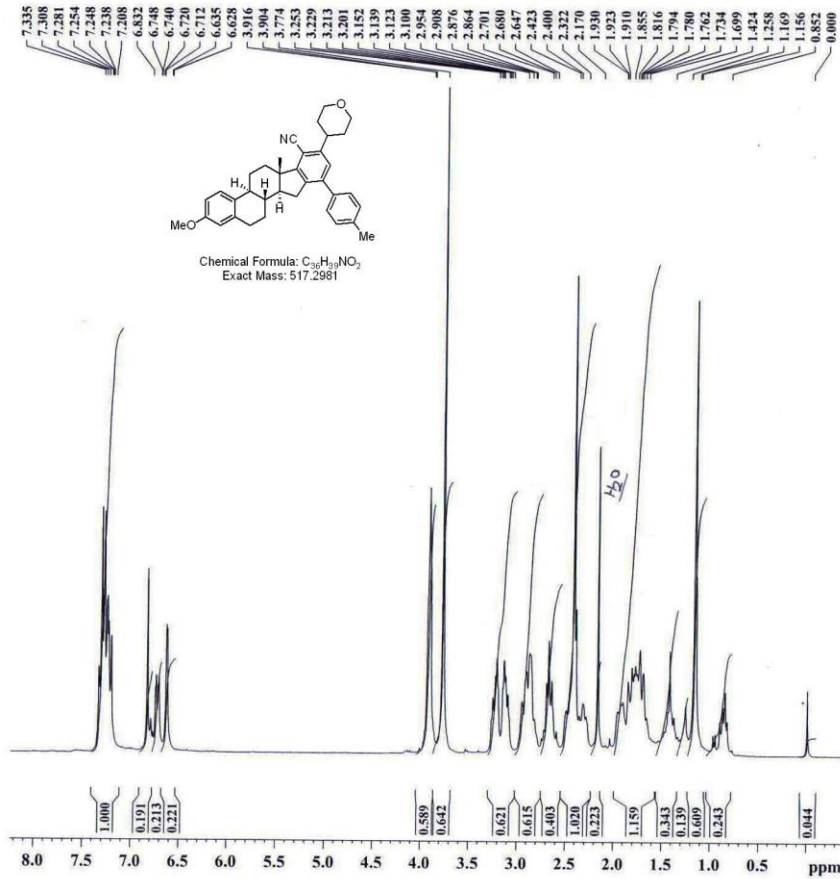




(+)(6*b*S,8*a*S,13*a*S,13*b*S)-4-methoxy-8*a*-methyl-10-morpholino-12-*p*-tolyl-2,6*b*,7,8,8*a*,13,13*a*,13*b*-octahydro-1*H*-indeno[2,1-*a*]phenanthrene-9-carbonitrile (**7b**)



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CIMAP PROTON
PROJECT NO.: mlp-02

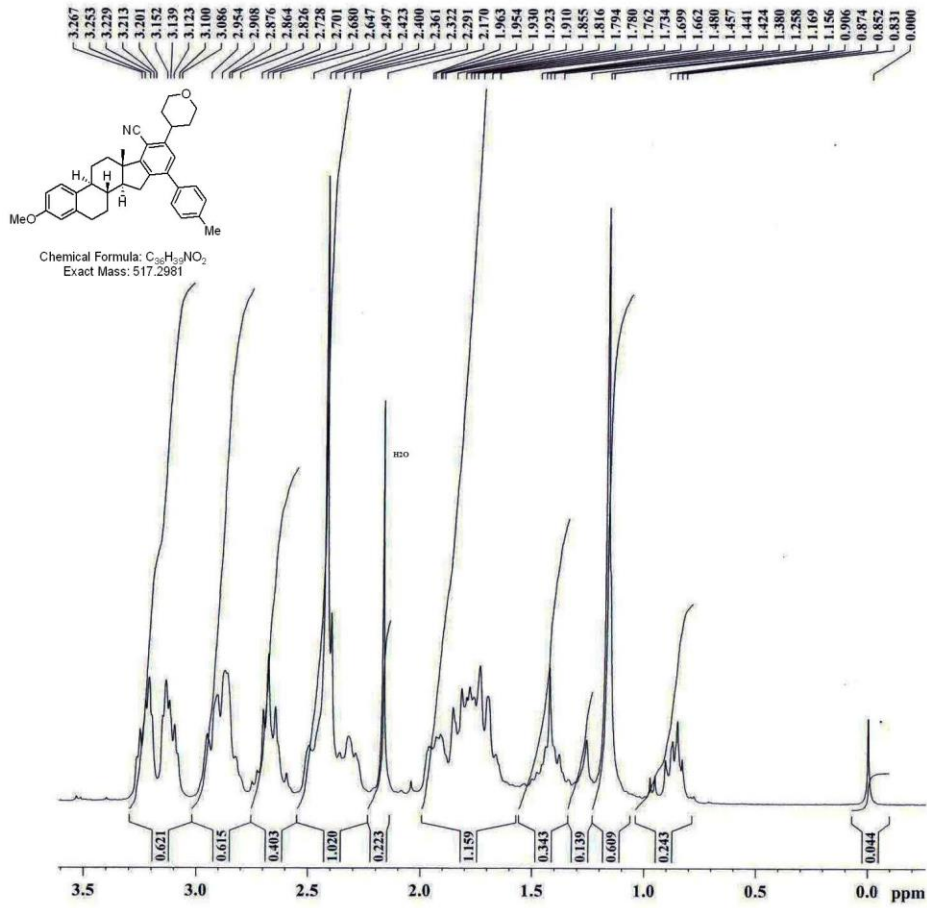
Current Data Parameters
NAME atghmk222a.p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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Time 10.16
INSTRUM spect
PROBHD 5 mm Multinuc1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 30
DS 2
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 128
DW 55.600 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 7.15 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

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CIMAP PROTON
PROJECT NO.: mlp-02

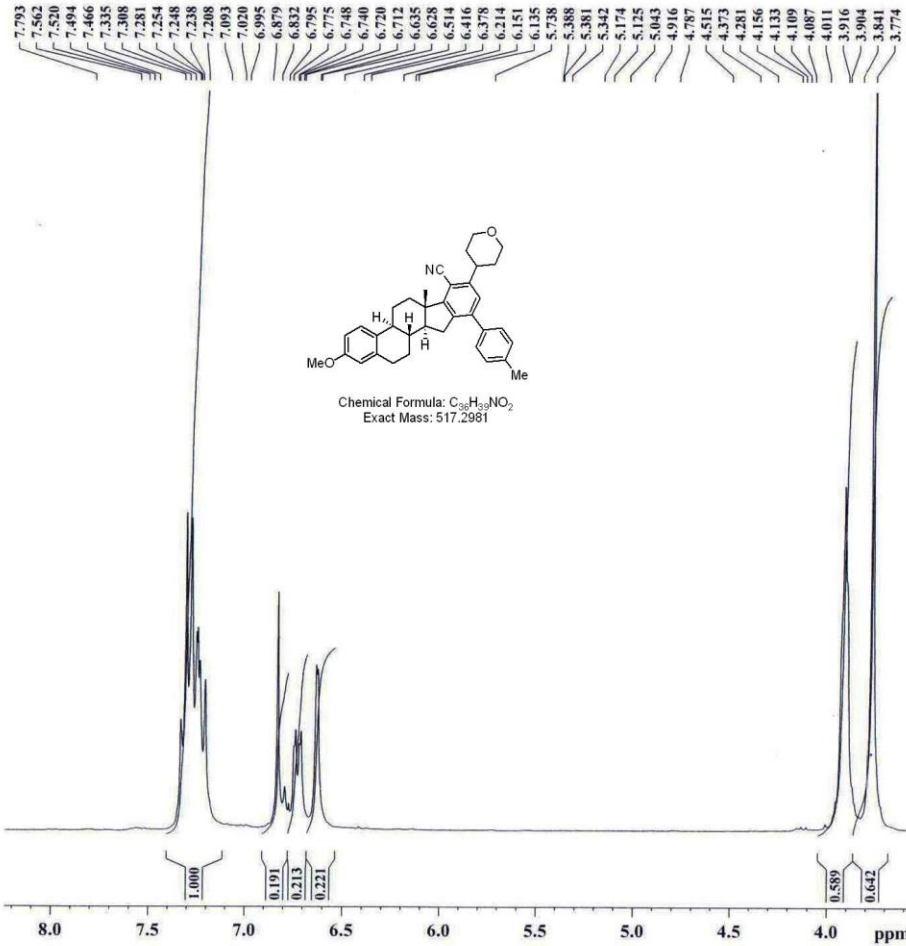
Current Data Parameters
NAME atghmk222a.p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date 20140702
Time 10.16
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 30
DS 2
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 128
DW 55.600 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 7.15 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

RSC Advances



CIMAP PROTON
PROJECT NO.: mlp-02

Current Data Parameters
NAME atghmk222a.p
EXPNO 1
PROCNO 1

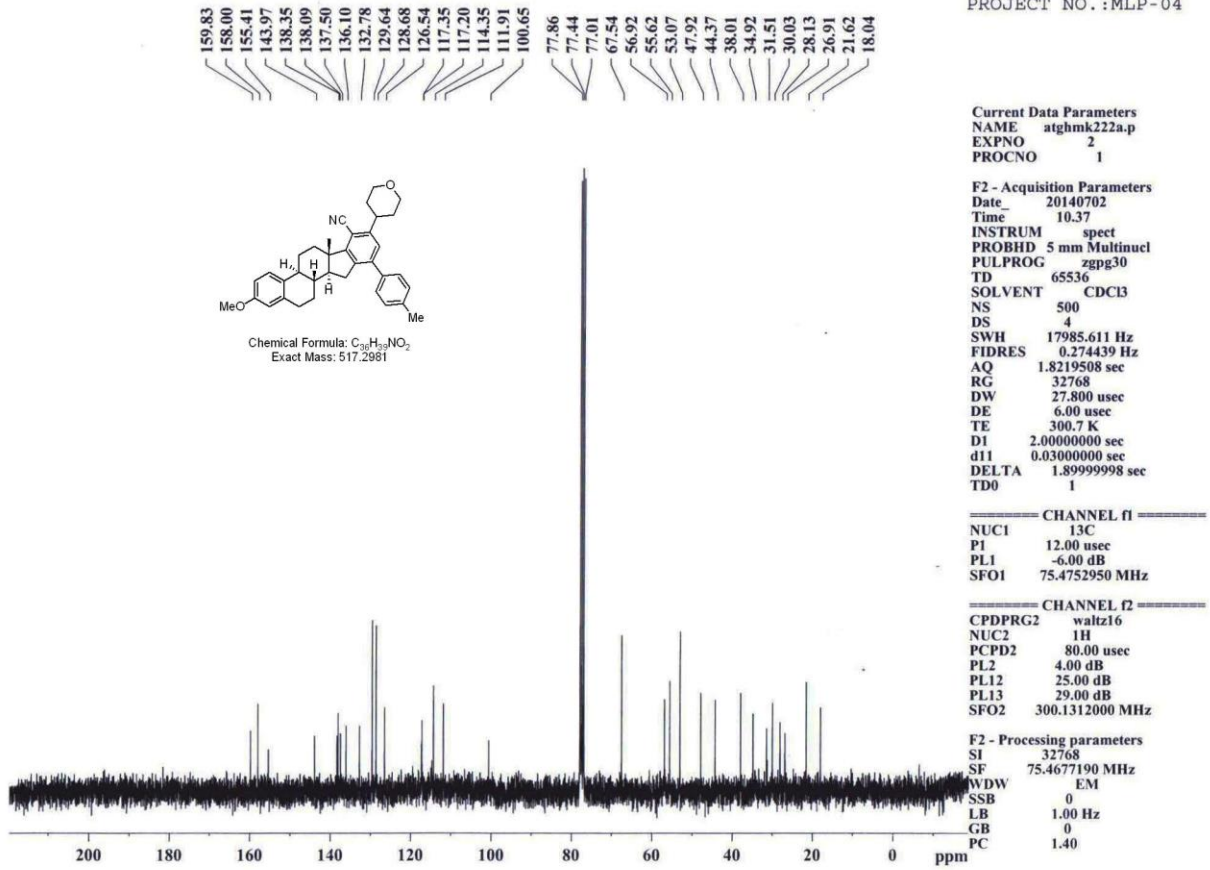
F2 - Acquisition Parameters
Date_ 20140702
Time 10.16
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 30
DS 2
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 128
DW 55.600 usec
DE 6.00 usec
TE 300.0 K
D1 1.0000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 7.15 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

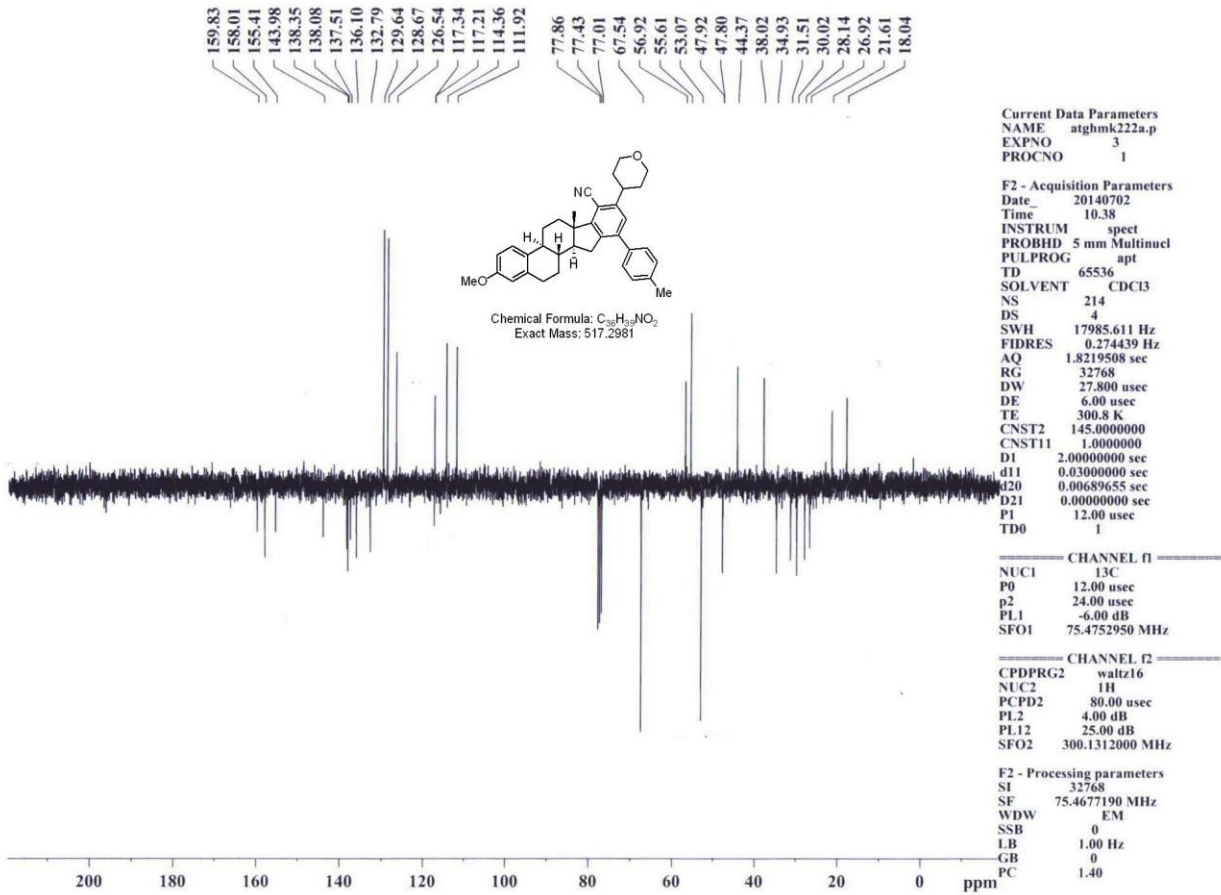
RSC Advances

CIMAP-CARBON
PROJECT NO.: MLP-04



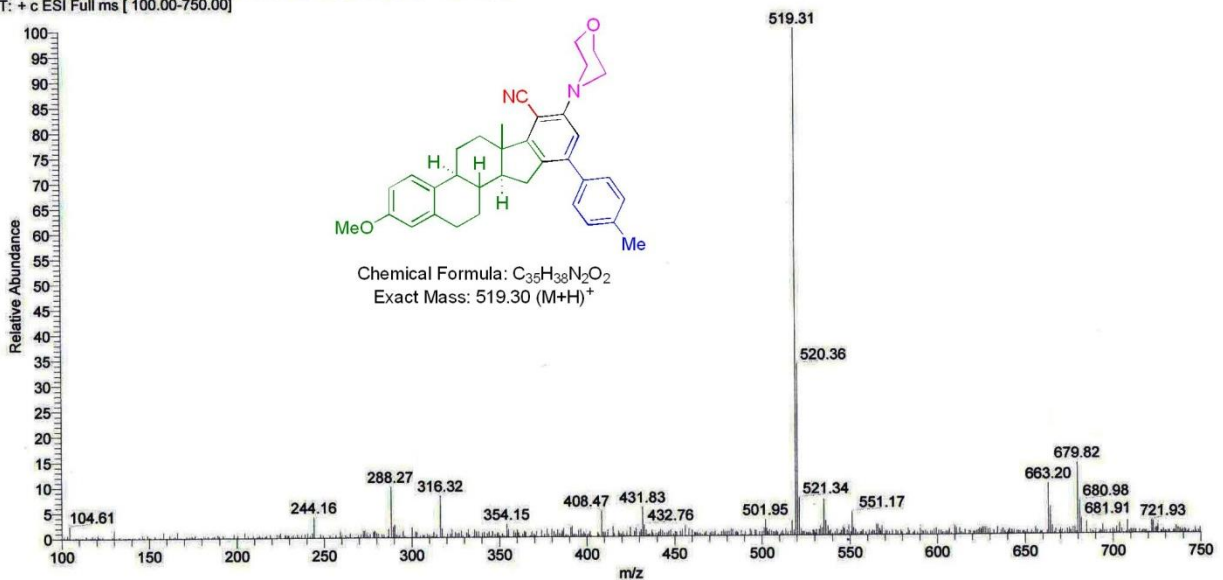
RSC Advances

APT: X, XH2 positi

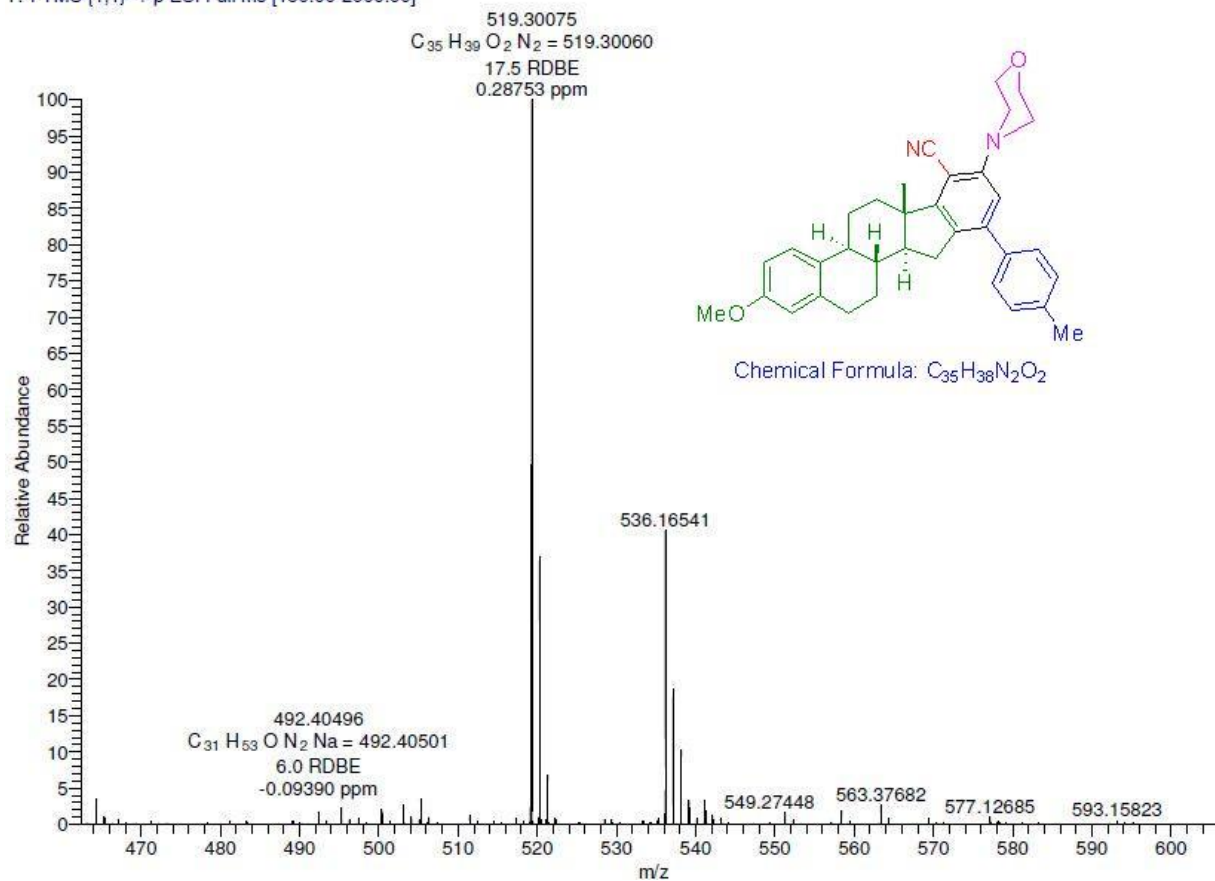


Sample ID: NR-ATG-222A
Acquisition Date: 02/03/15 12:19:02

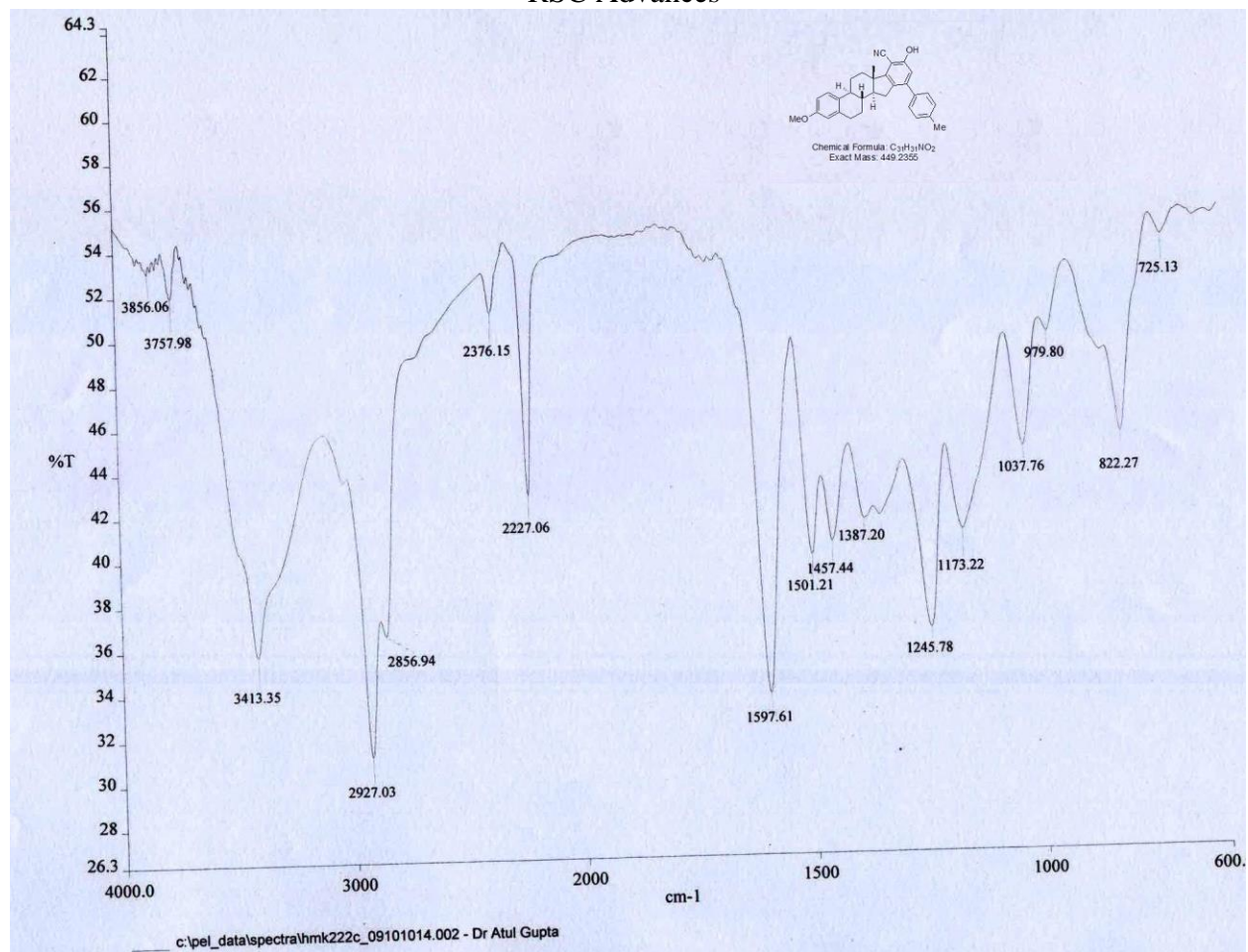
15I03FEB001 #24-56 RT: 0.30-0.69 AV: 33 SB: 2 0.01, 0.01 NL: 1.07E7
T: + c ESI Full ms [100.00-750.00]



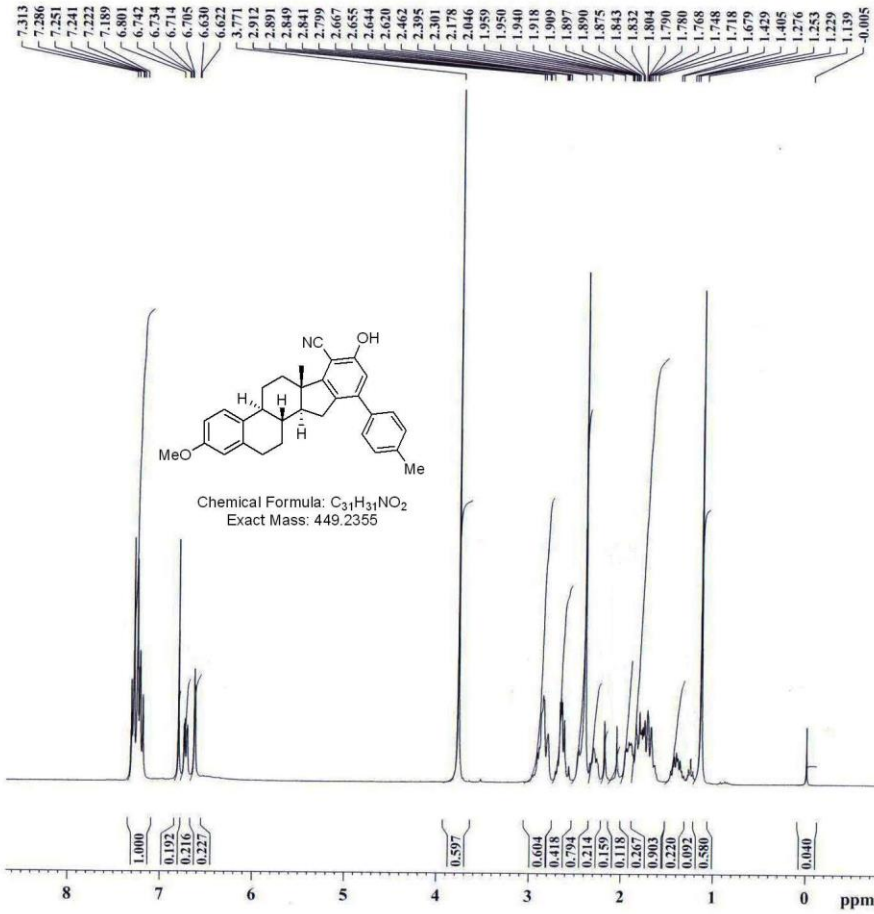
ION TRAP LCQ ADVANTAGE MAX
THERMO ELECTRON CORPORATION

MCS-7B #4-19 RT: 0.02-0.13 AV: 16 NL: 6.48E6
T: FTMS {1,1} + p ESI Full ms [150.00-2000.00]

(+)(6*S*,8*aS*,13*aS*,13*bS*)-10-hydroxy-4-methoxy-8*a*-methyl-12-*p*-tolyl-2,6*b*,7,8,8*a*,13,13*a*,13*b*-octahydro-1*H*-indeno[2,1-*a*]phenanthrene-9-carbonitrile (8*b*)



RSC Advances



CIMAP PROTON
PROJECT NO.: mlp-02

Current Data Parameters
NAME atghmk222c.p
EXPNO 1
PROCNO 1

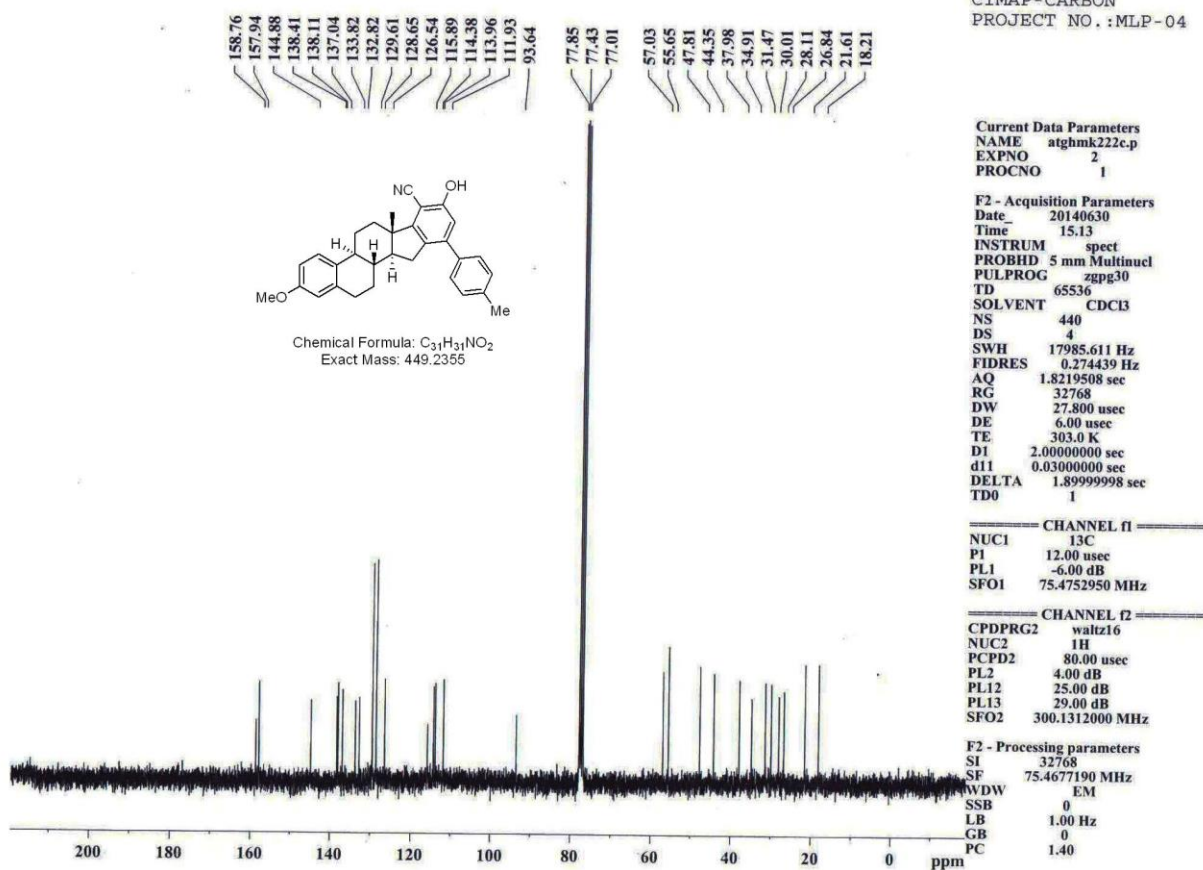
F2 - Acquisition Parameters
Date 20140630
Time 15.00
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 28
DS 2
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 181
DW 55.600 usec
DE 6.00 usec
TE 302.5 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 7.15 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300117 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

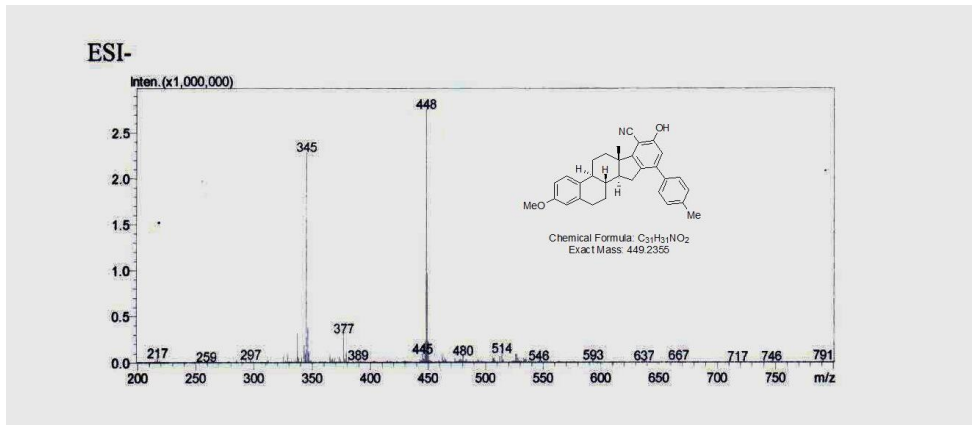
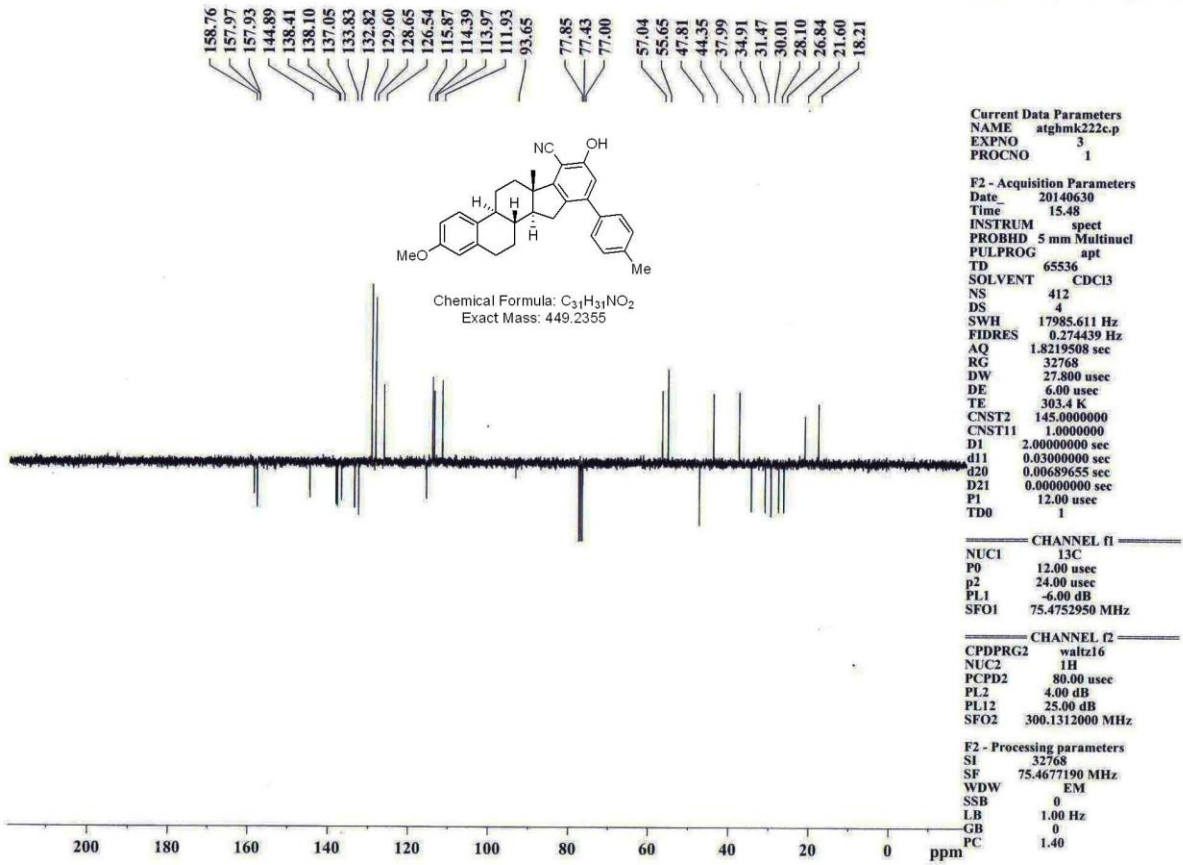
RSC Advances

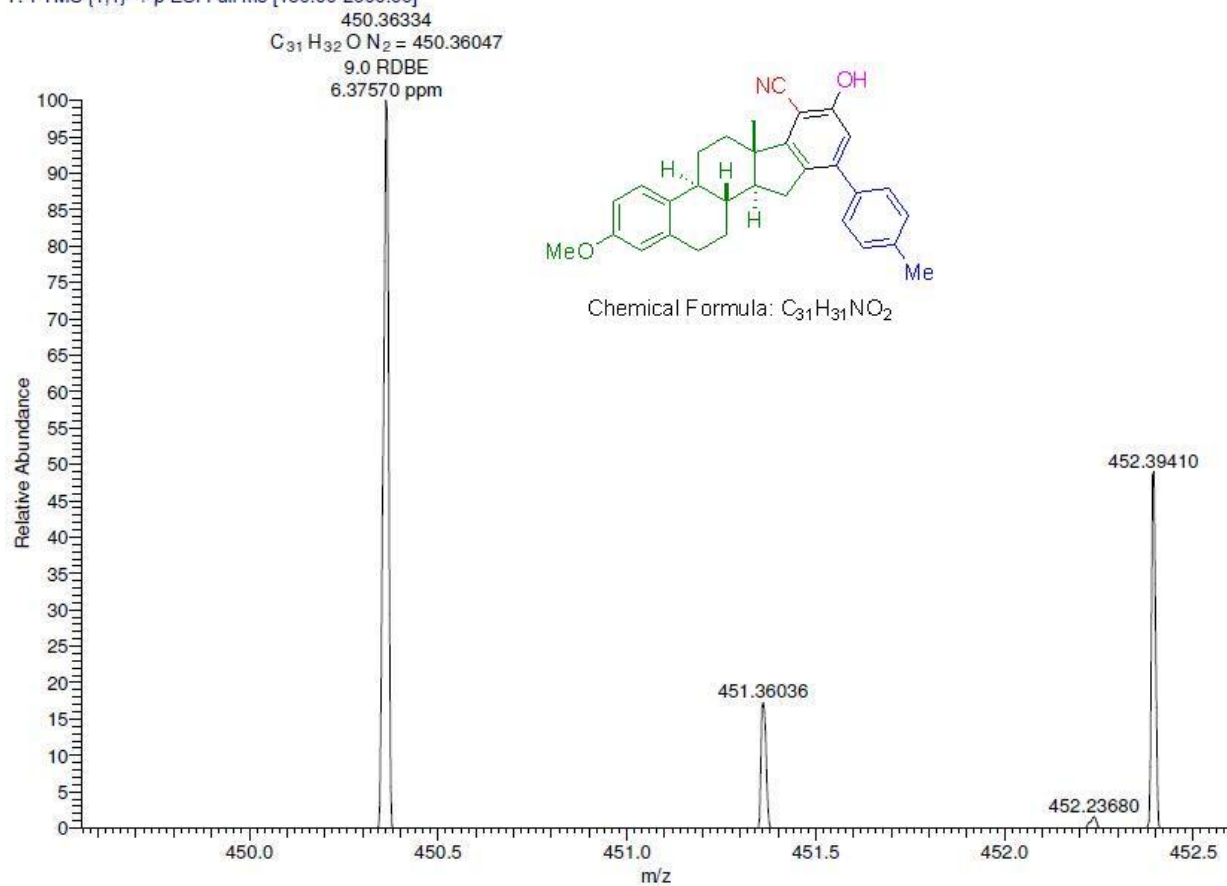
CIMAP-CARBON
PROJECT NO. :MLP-04



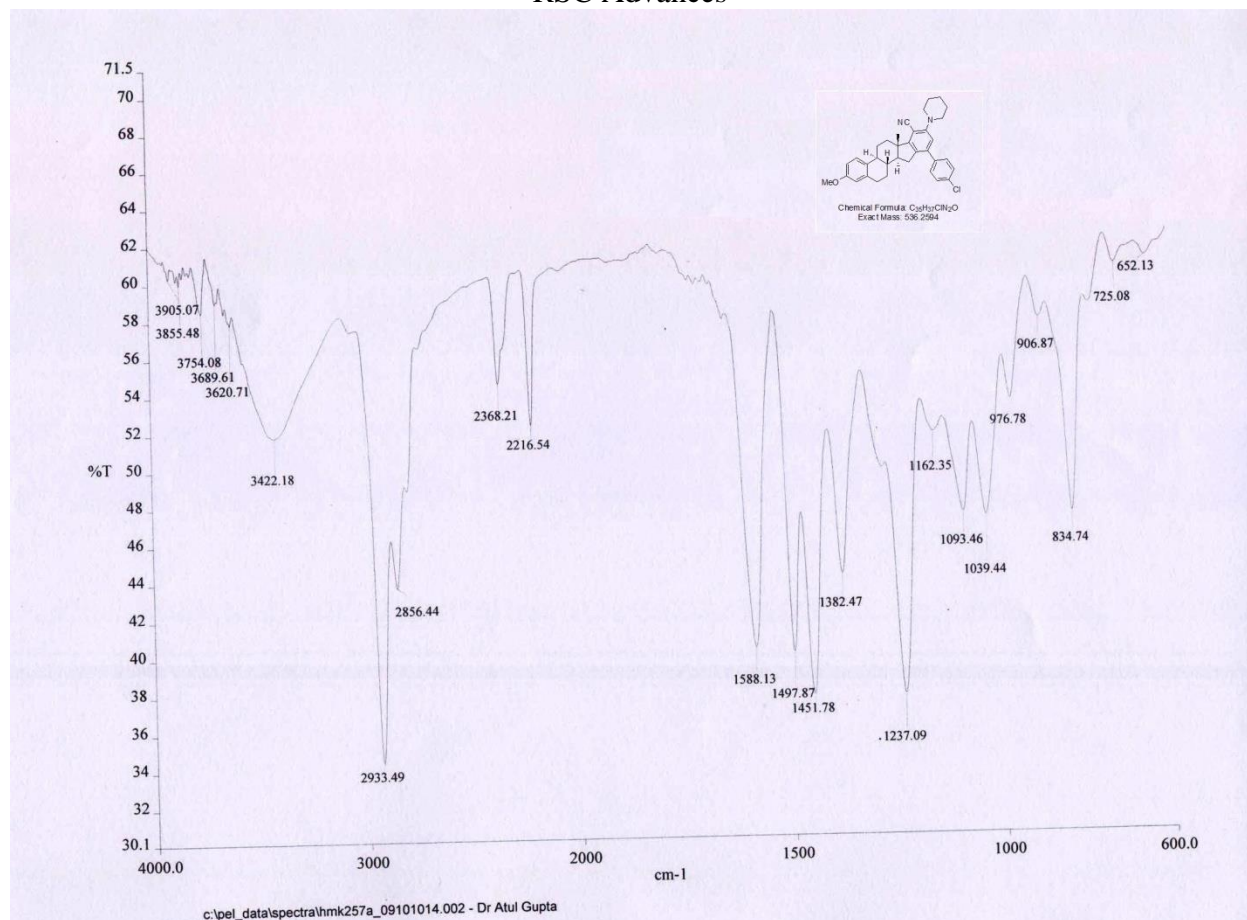
RSC Advances

APT: X, XH2 positiv

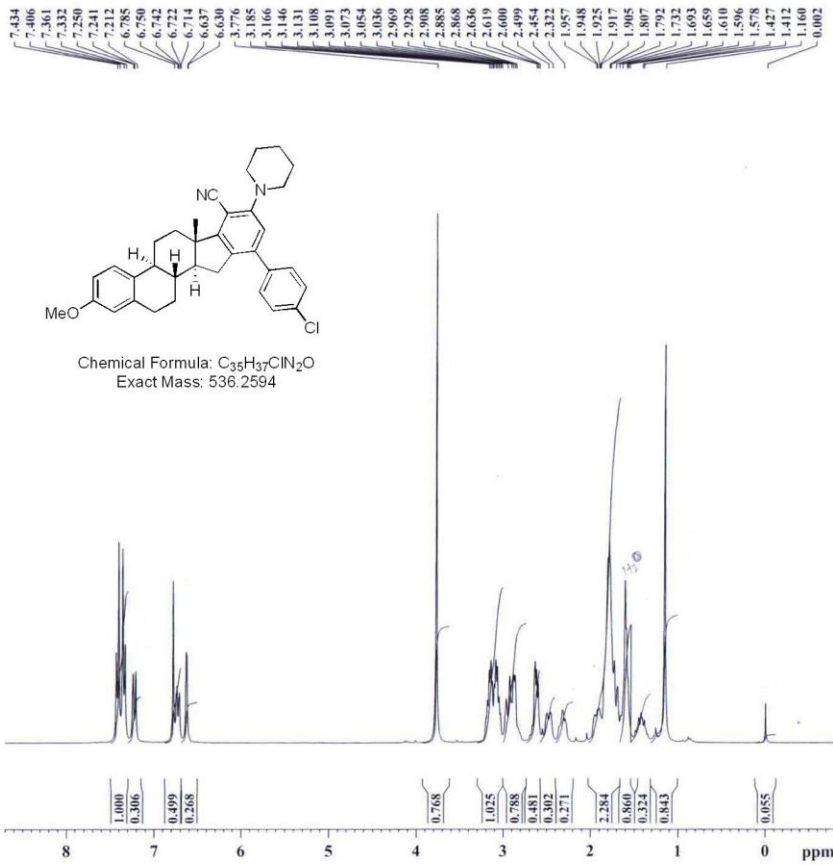


MCS-8B #4-19 RT: 0.02-0.13 AV: 16 NL: 3.98E4
T: FTMS {1,1} + p ESI Full ms [150.00-2000.00]

(+)(6*S*,8*aS*,13*aS*,13*bS*)-12-(4-chlorophenyl)-4-methoxy-8*a*-methyl-10-(piperidin-1-yl)-2,6*b*,7,8,8*a*,13,13*a*,13*b*-octahydro-1*H*-indeno[2,1-*a*]phenanthrene-9-carbonitrile (**7c**)



RSC Advances



CIMAP PROTON
PROJECT NO.: mlp-02

Current Data Parameters
NAME atghmk257a.p
EXPNO 1
PROCNO 1

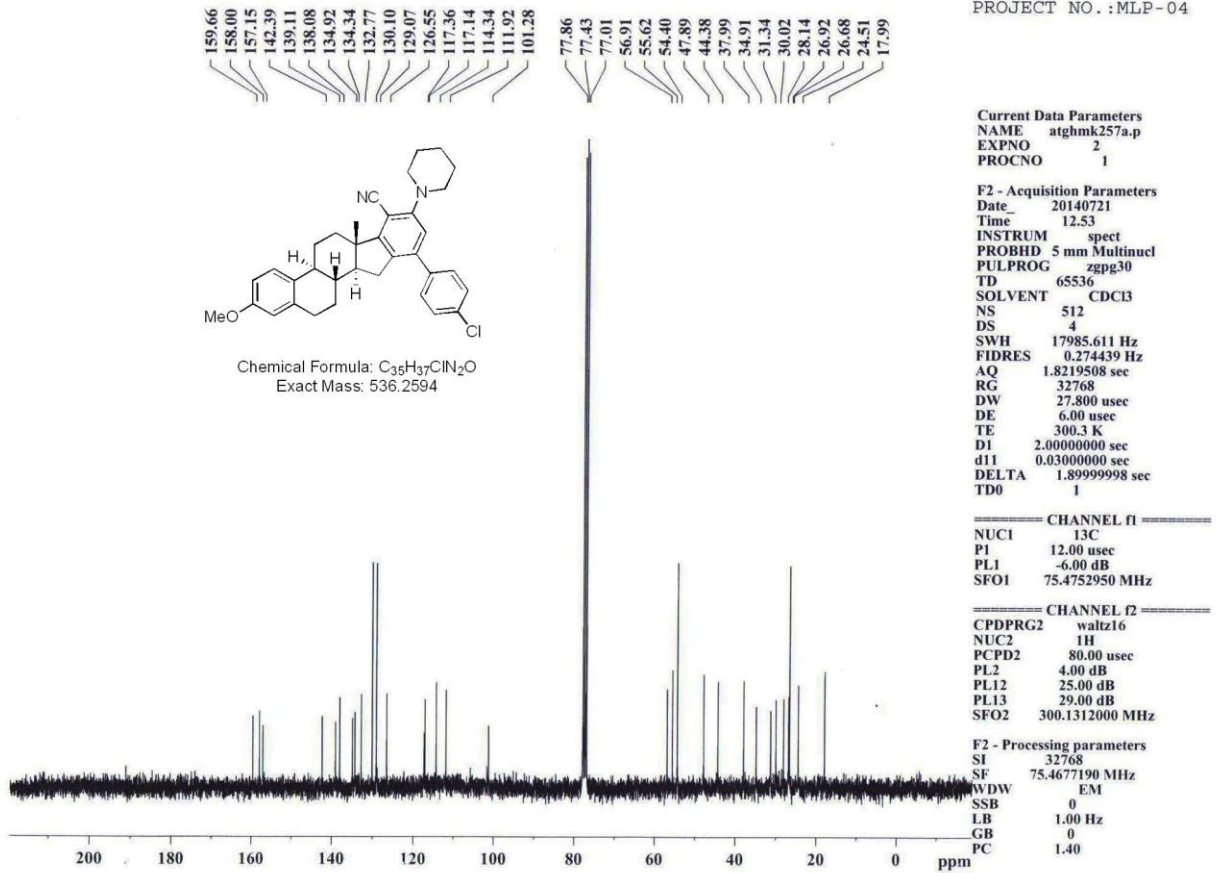
F2 - Acquisition Parameters
Date_ 20140721
Time 12.25
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 28
DS 2
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 128
DW 55.600 usec
DE 6.00 usec
TE 299.6 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 7.15 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

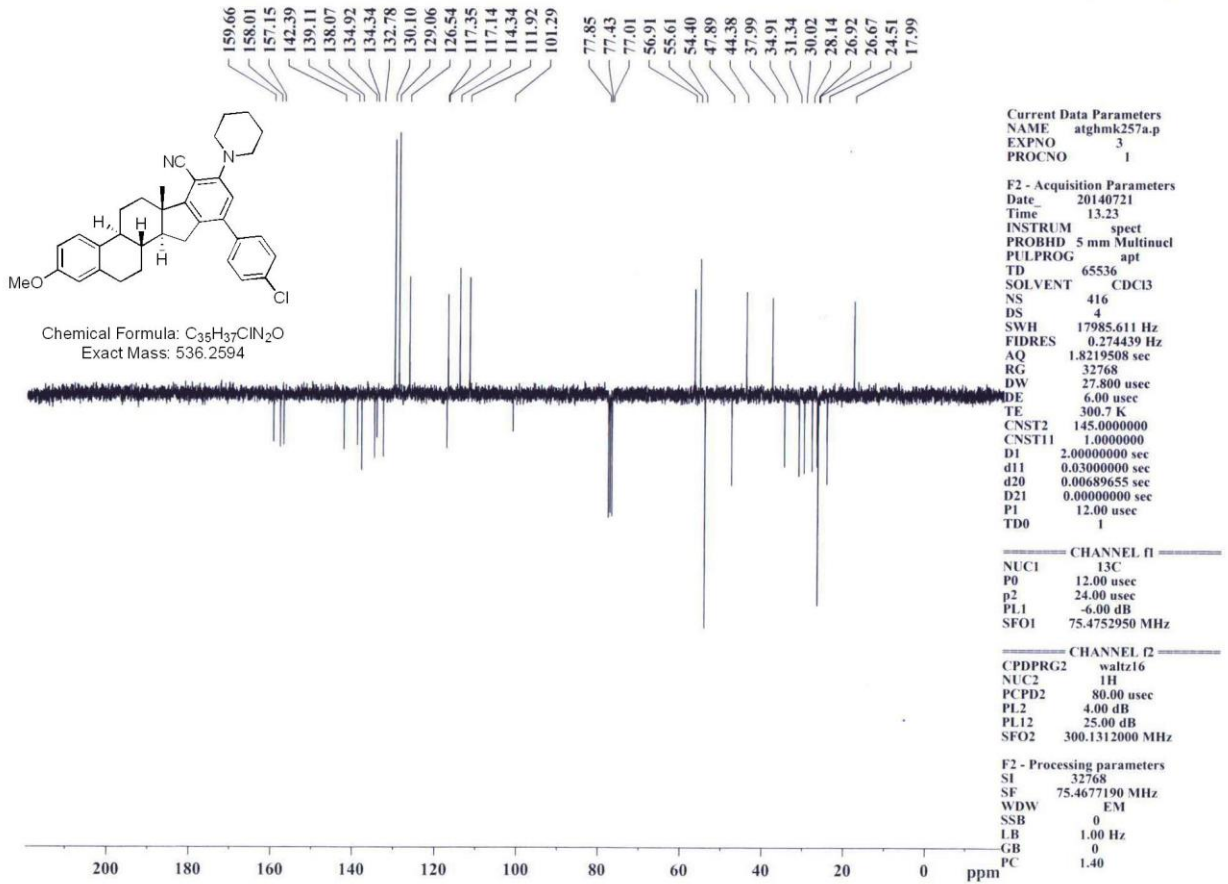
RSC Advances

CIMAP-CARBON
PROJECT NO. :MLP-04



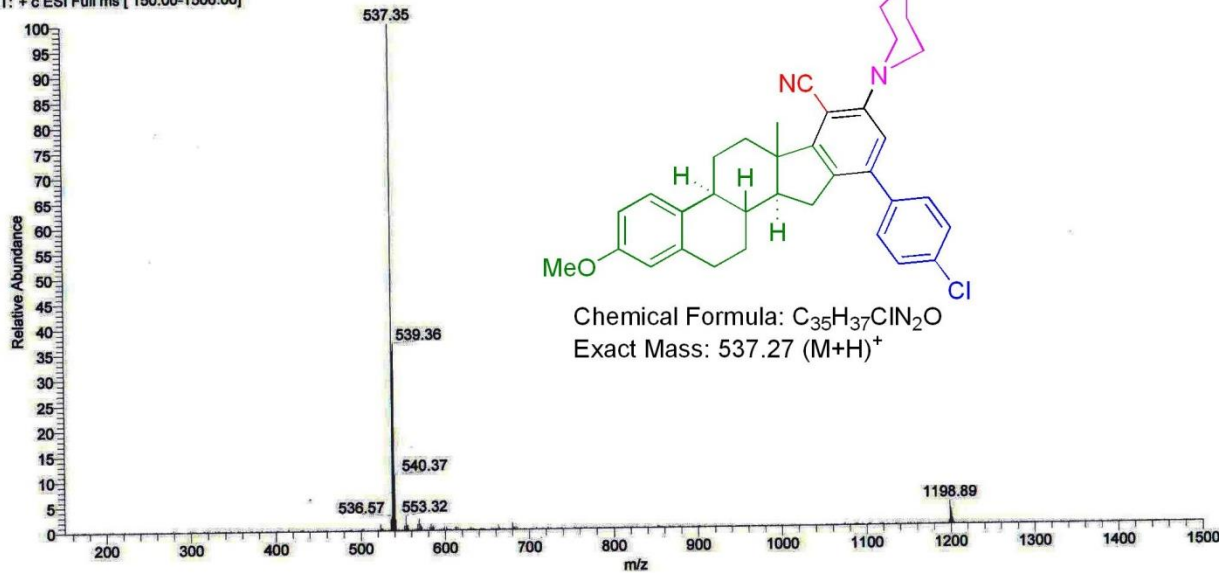
RSC Advances

APT: X, XH2 positiv

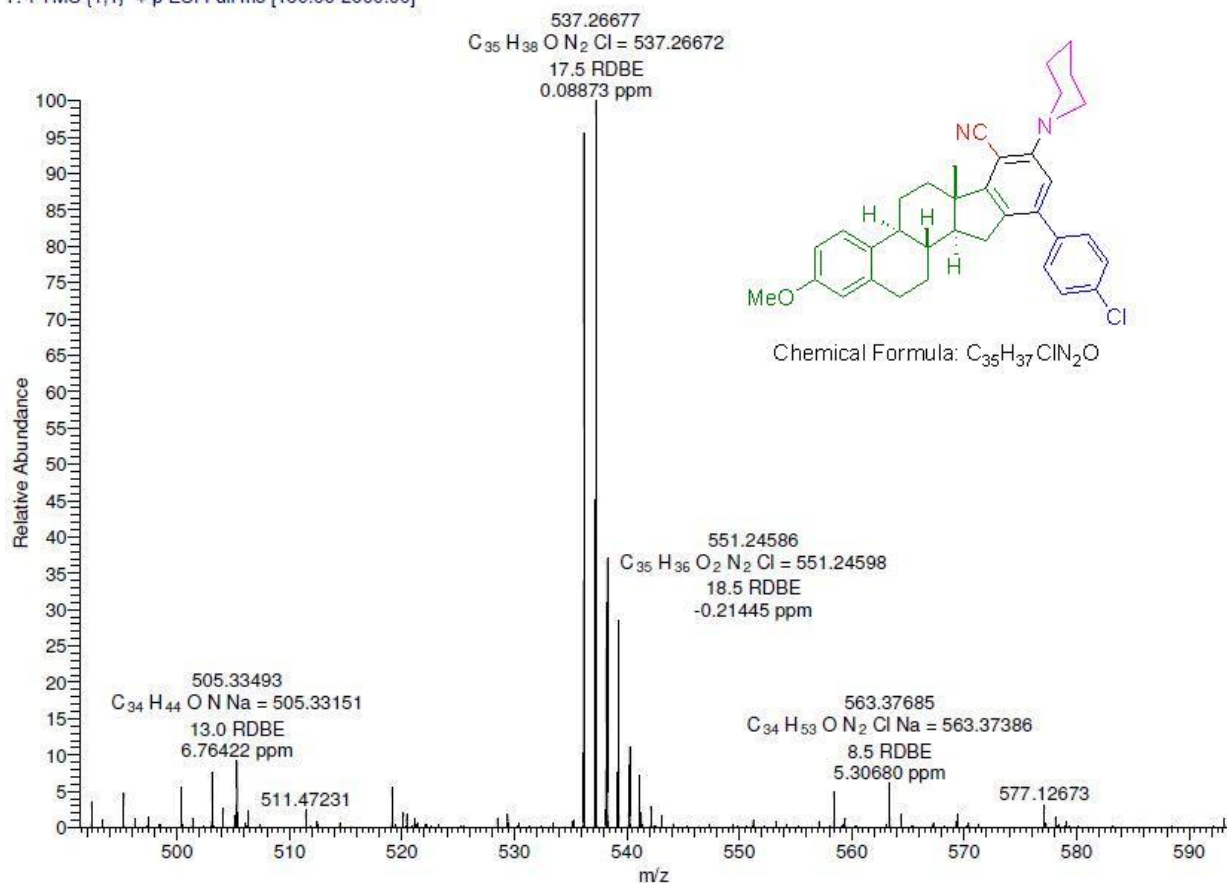


Sample ID: NR-ATG-257A
Acquisition Date: 02/23/15 13:52:26

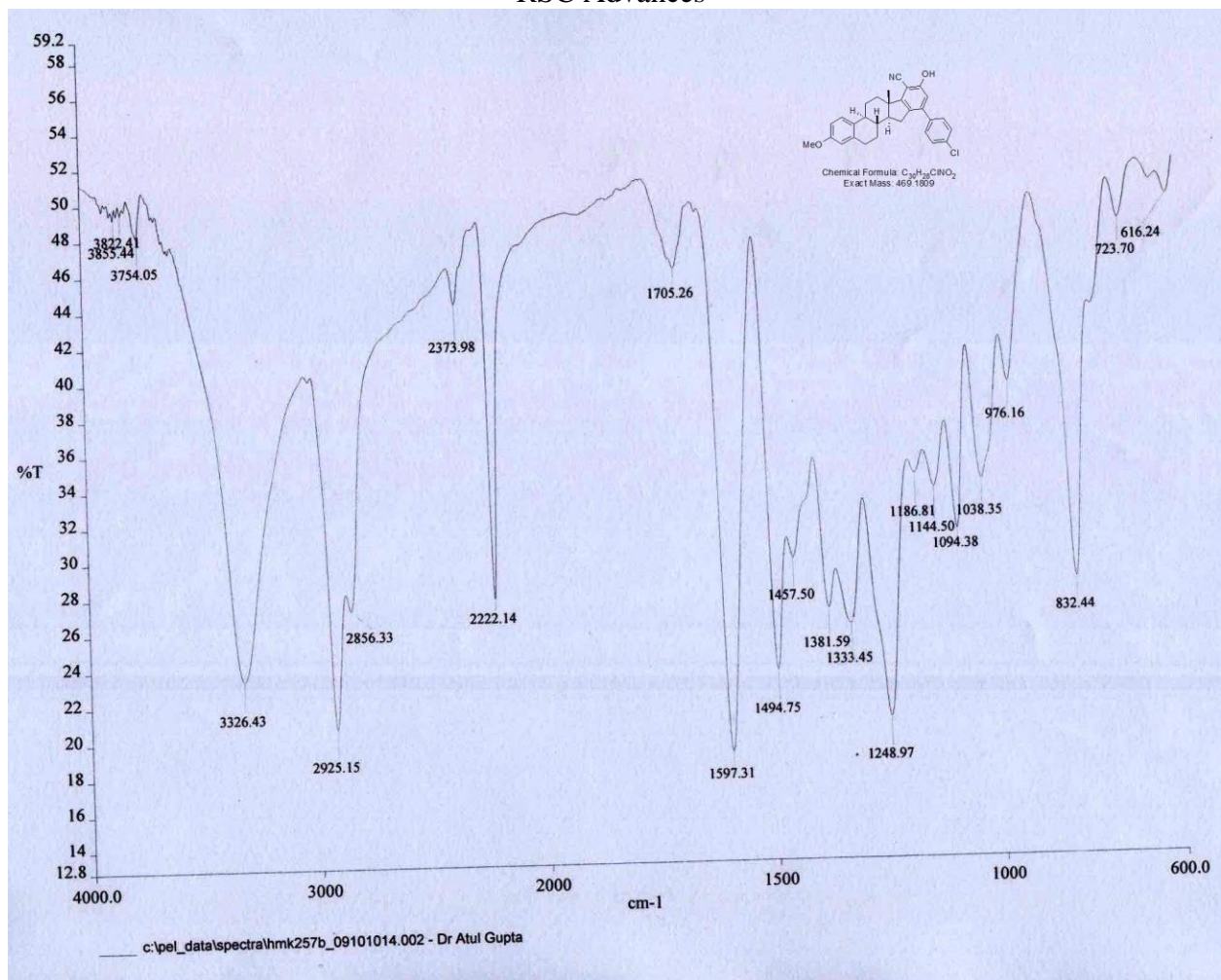
15I23FEB51 #15-35 RT: 0.31-0.70 AV: 21 SB: 2 0.01, 0.01 NL: 2.47E7
T: + c ESI Full ms [150.00-1500.00]



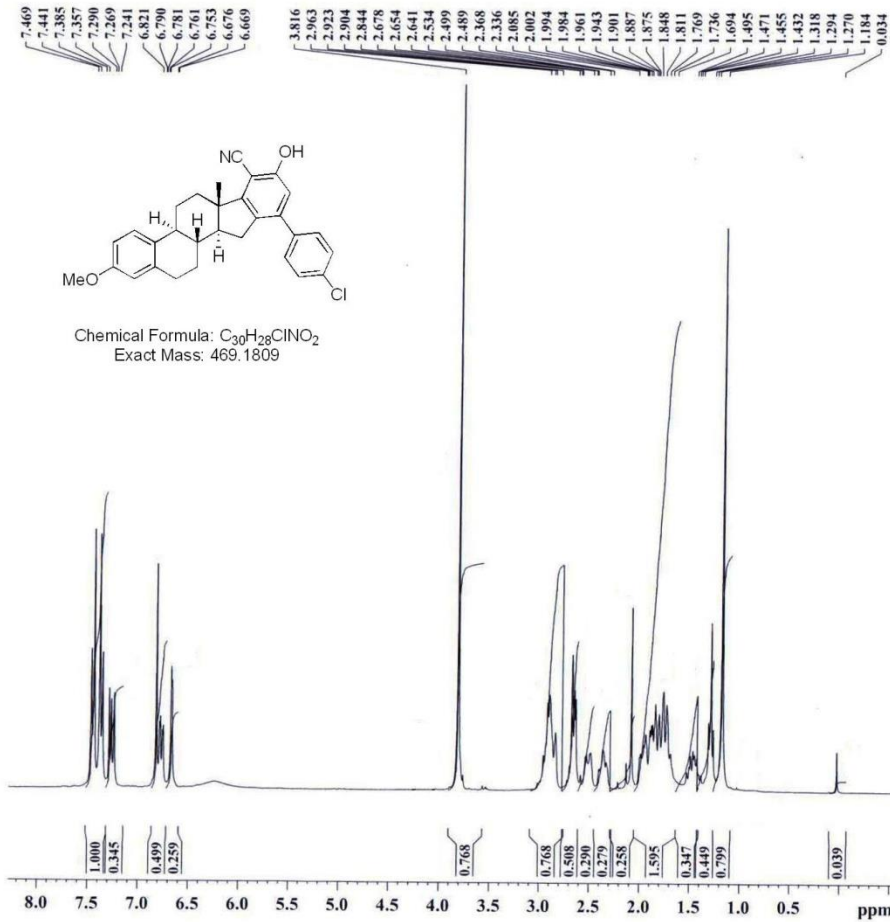
ION TRAP LCQ ADVANTAGE MAX
THERMO ELECTRON CORPORATION

MCS-7C #4-19 RT: 0.02-0.13 AV: 16 NL: 3.45E6
T: FTMS (1,1) + p ESI Full ms [150.00-2000.00]

(+)(6*S*,8*aS*,13*aS*,13*bS*)-12-(4-chlorophenyl)-10-hydroxy-4-methoxy-8*a*-methyl-2,6*b*,7,8,8*a*,13,13*a*,13*b*-octahydro-1*H*-indeno[2,1-*a*]phenanthrene-9-carbonitrile (**8c**)



RSC Advances



CIMAP PROTON
PROJECT NO.: mlp-02

Current Data Parameters
NAME atghmk257b.p
EXPNO 1
PROCNO 1

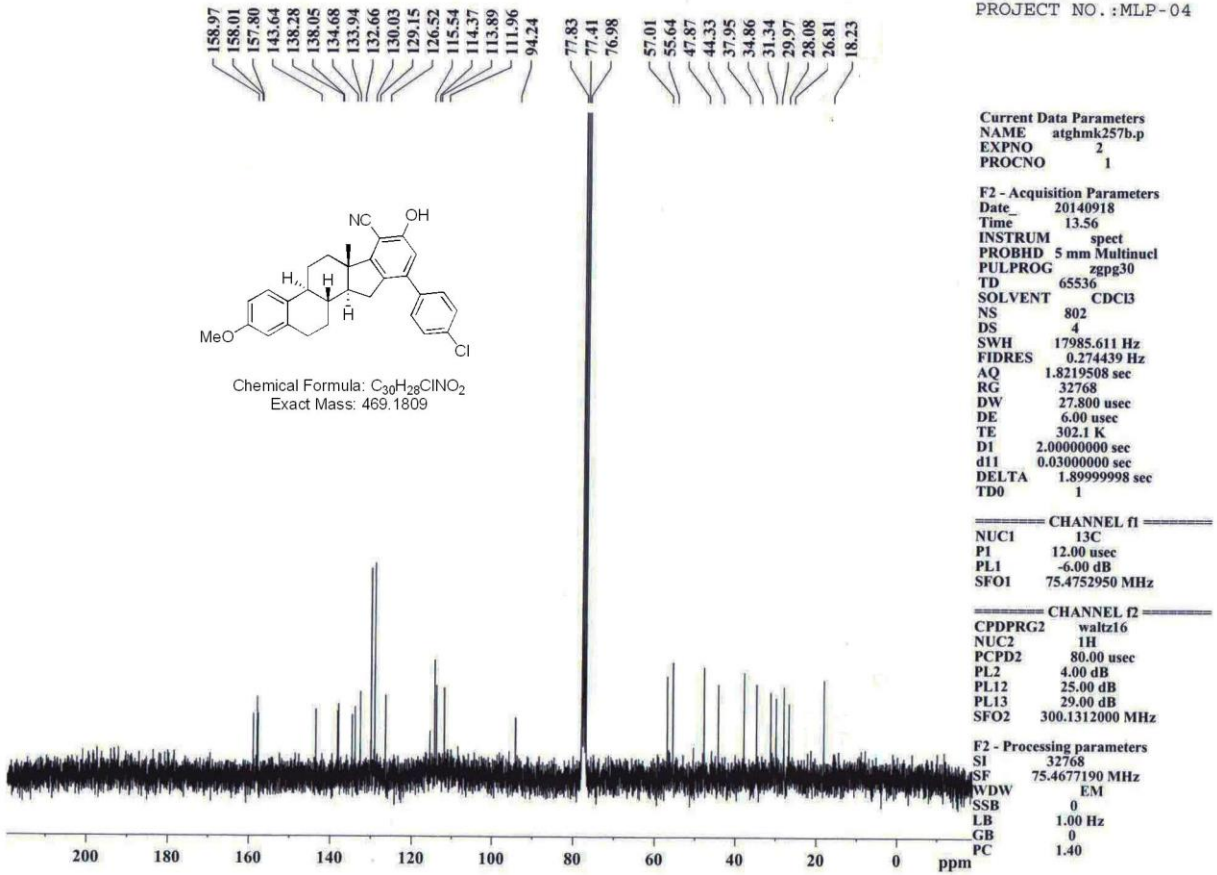
F2 - Acquisition Parameters
Date_ 20140918
Time 13.35
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 17
DS 2
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 256
DW 55.600 usec
DE 6.00 usec
TE 301.7 K
D1 1.00000000 sec
TD0 1

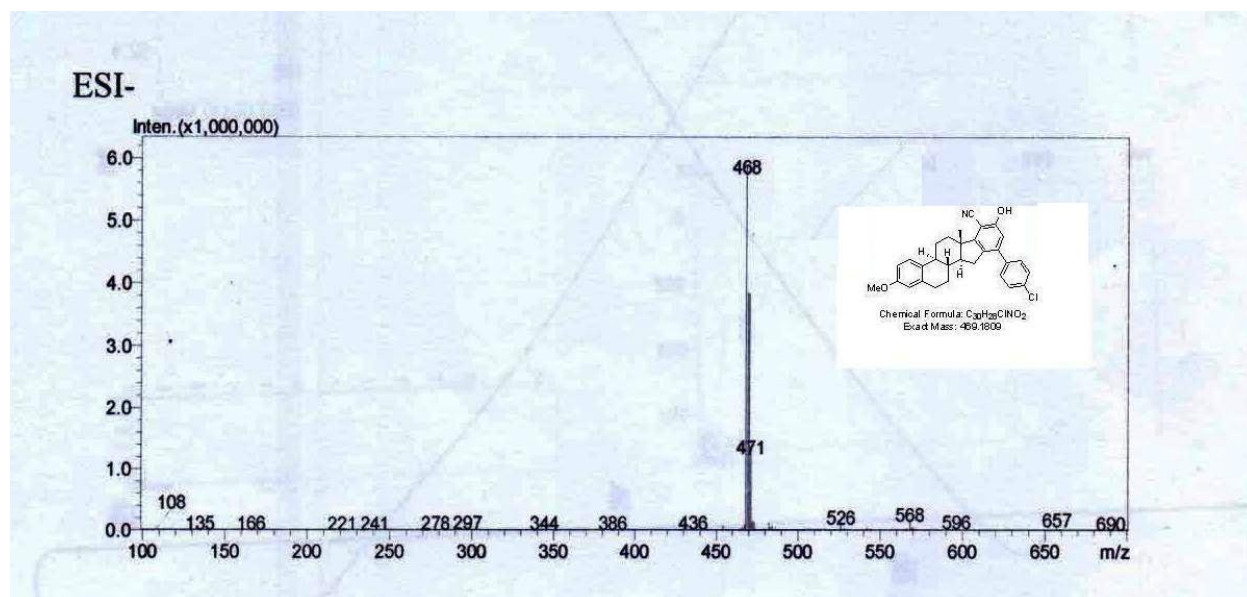
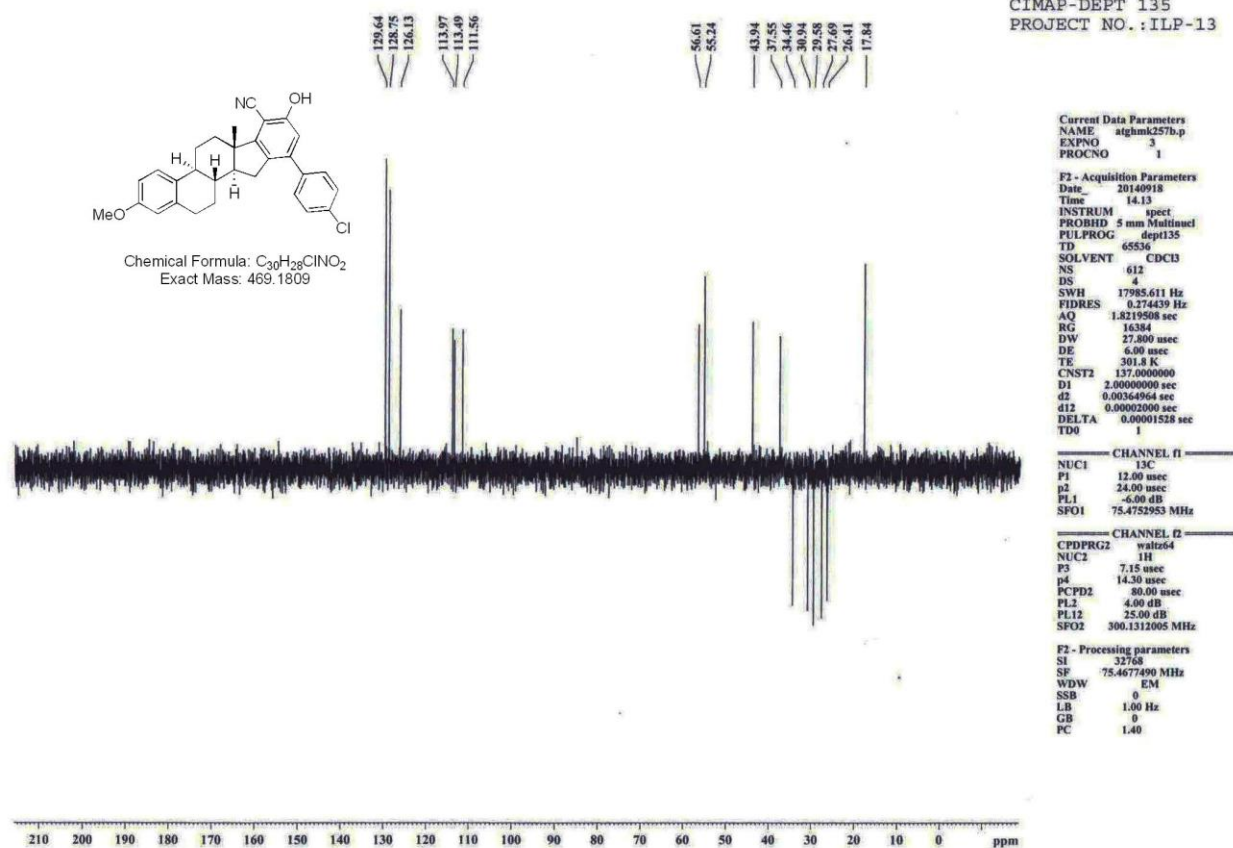
===== CHANNEL f1 =====
NUC1 1H
P1 7.15 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299972 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

RSC Advances

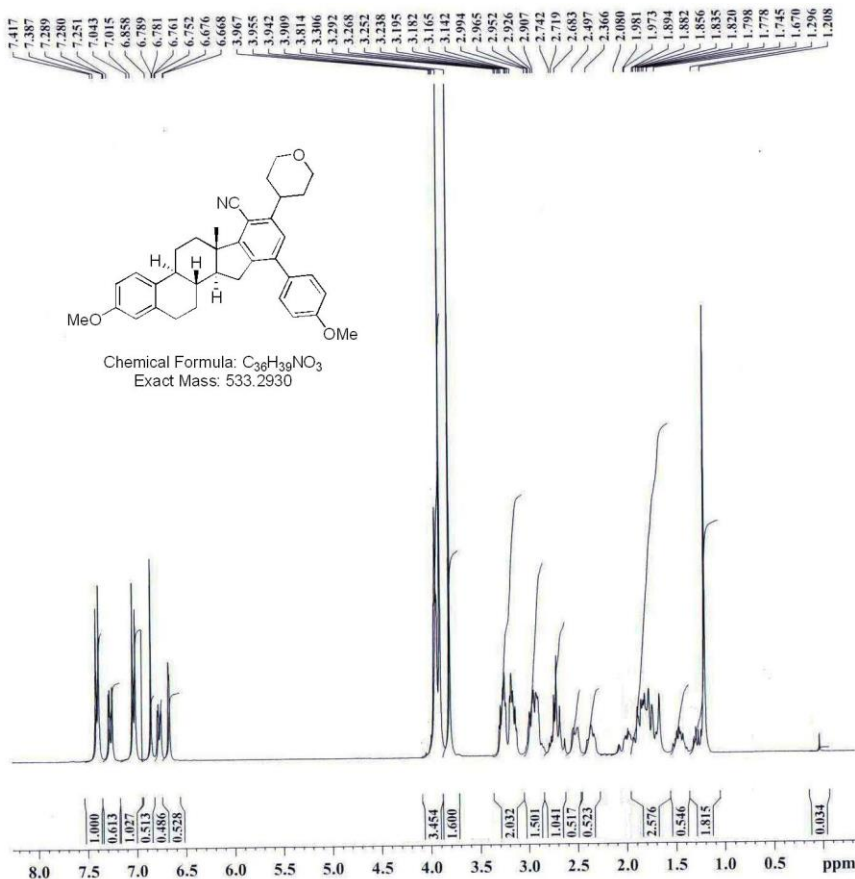
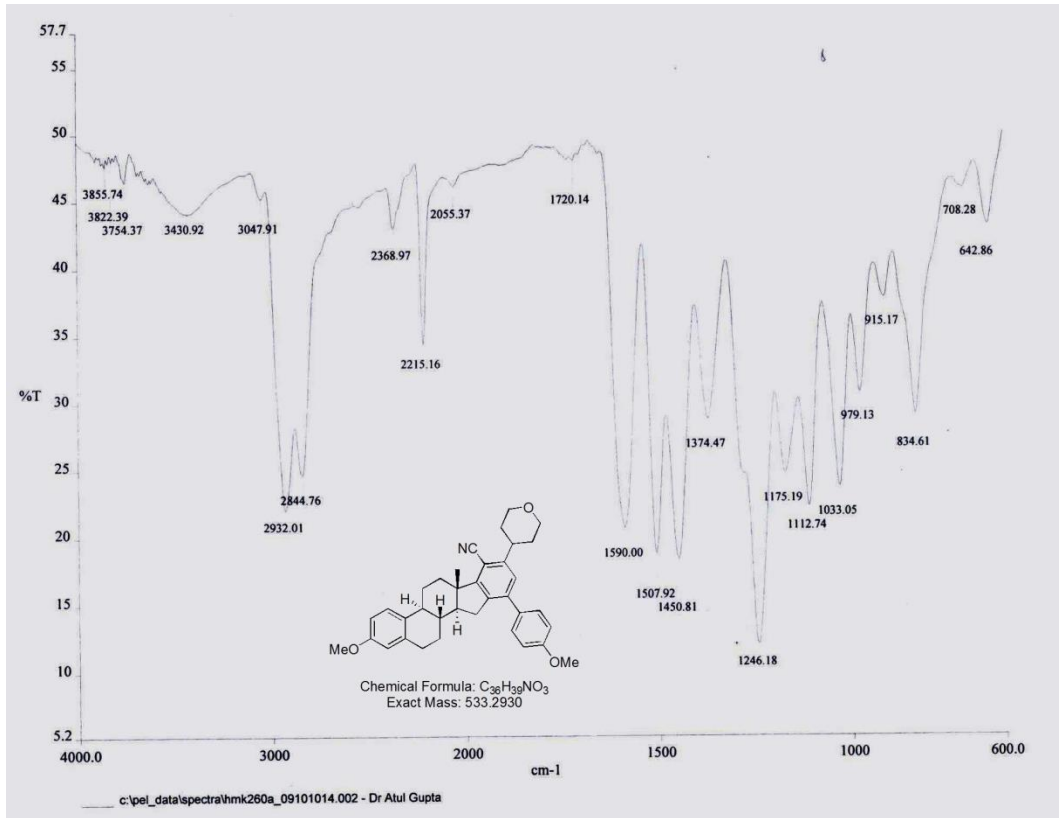
CIMAP-CARBON
PROJECT NO.: MLP-04





(+)(6bS,8aS,13aS,13bS)-4-methoxy-12-(4-methoxyphenyl)-8a-methyl-10-morpholino-2,6b,7,8,8a,13,13a,13b-octahydro-1H-indeno[2,1-a]phenanthrene-9-carbonitrile (**7d**)

RSC Advances



CIMAP PROTON
PROJECT NO.: mlp-02

Current Data Parameters
NAME atghmk260a.p
EXPNO 1
PROCNO 1

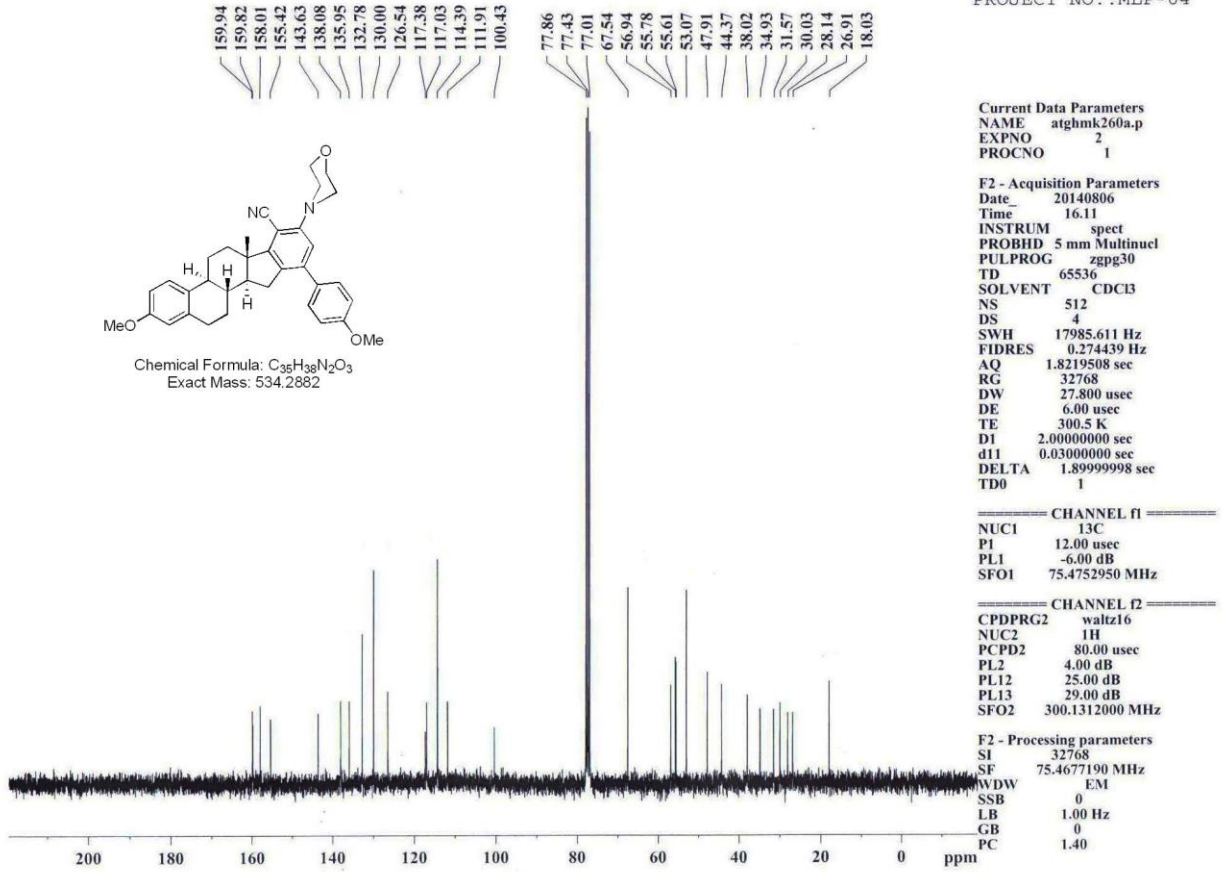
F2 - Acquisition Parameters
Date 20140806
Time 15.45
INSTRUM spect
PROBHD 5 mm Multinuel
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 2
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 128
DW 55.600 usec
DE 6.00 usec
TE 299.8 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 7.15 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299972 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

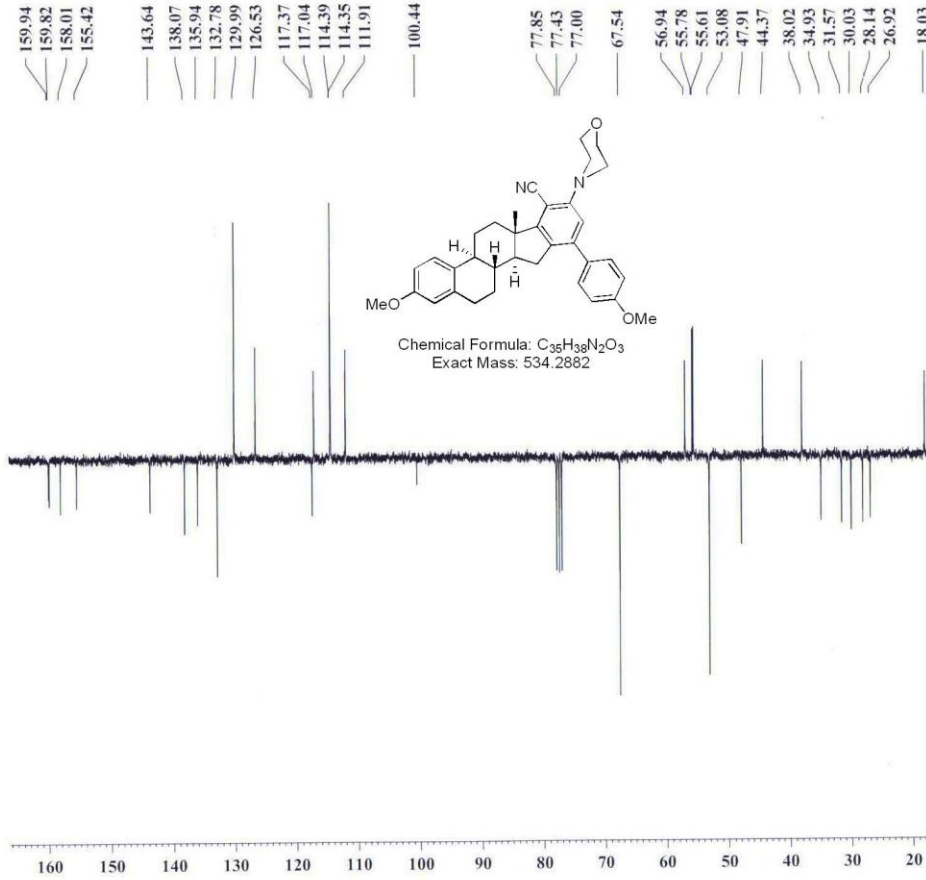
RSC Advances

CIMAP-CARBON
PROJECT NO.: MLP-04



RSC Advances

APT: X, XH2 positiv



Current Data Parameters
NAME atghmk260a.p
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140806
Time 17.13
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG apt
TD 65536
SOLVENT CDCl3
NS 826
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 300.6 K
CNST2 145.000000
CNST11 1.0000000
D1 2.00000000 sec
d11 0.03000000 sec
d20 0.00689655 sec
D21 0.00000000 sec
P1 12.00 usec
TD0 1

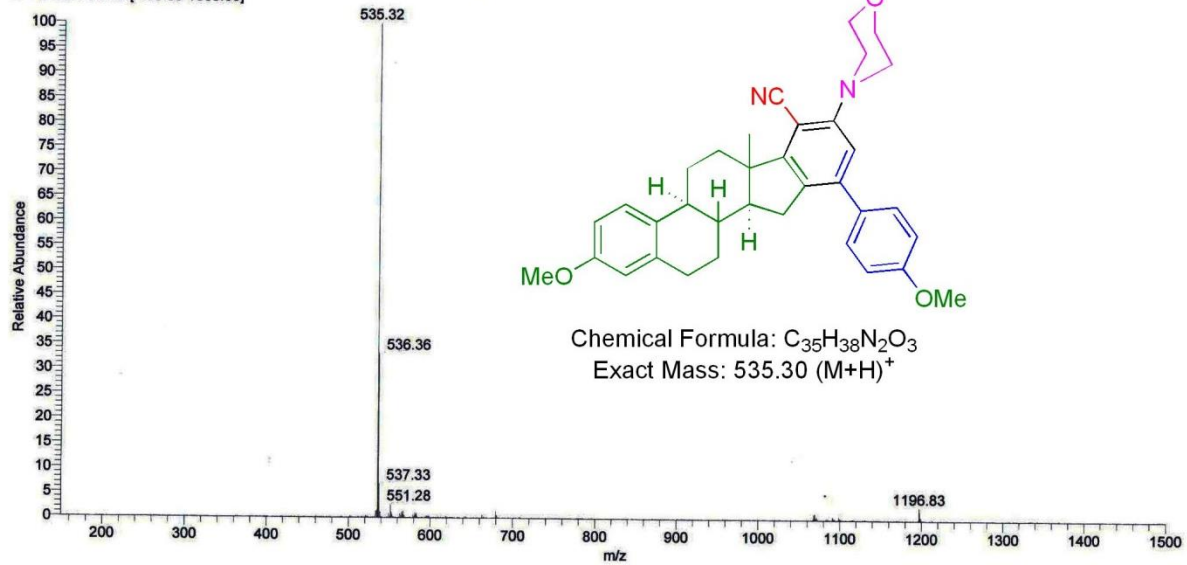
CHANNEL f1
NUC1 13C
P0 12.00 usec
p2 24.00 usec
PL1 -6.00 dB
SFO1 75.4752950 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 25.00 dB
SFO2 300.1312000 MHz

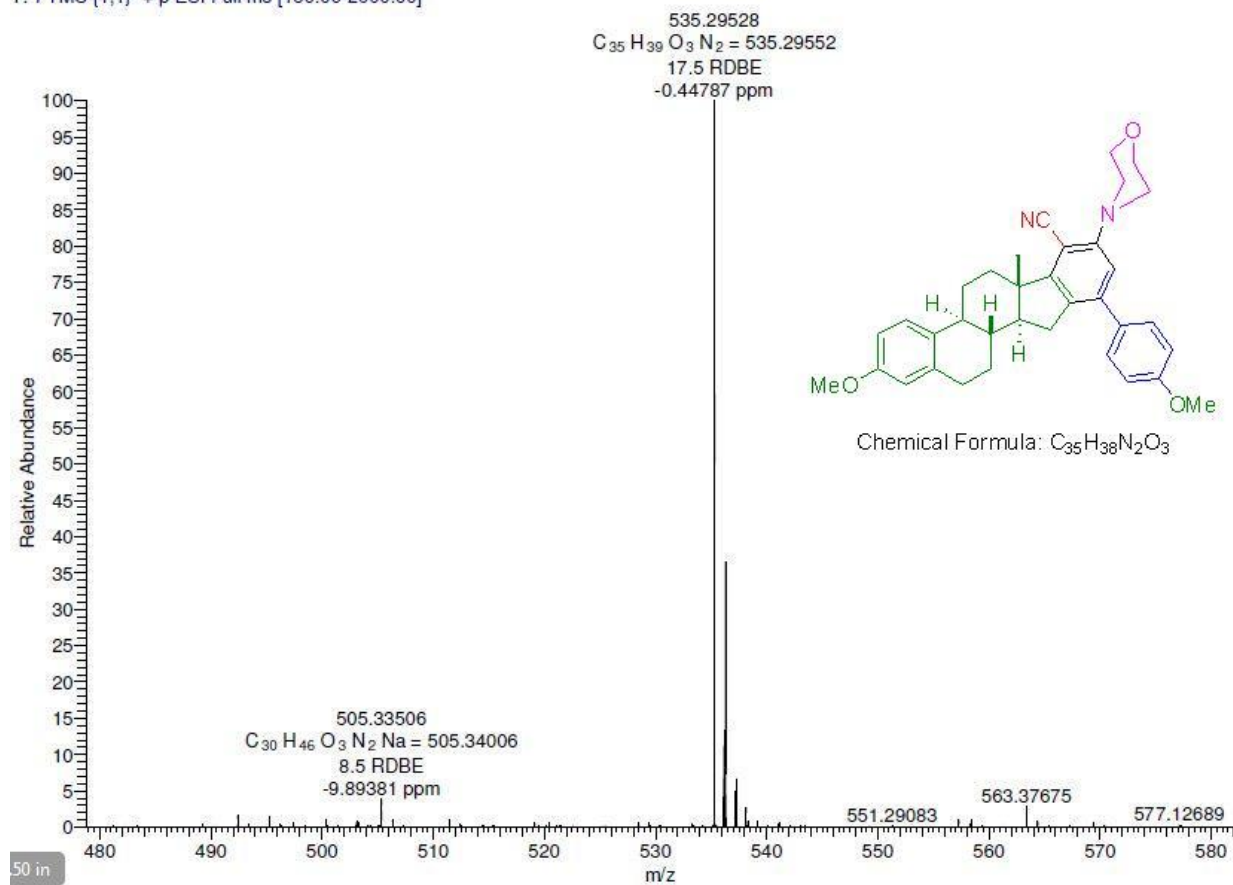
F2 - Processing parameters
SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Sample ID: NR-ATG-260A
Acquisition Date: 02/05/15 14:44:02

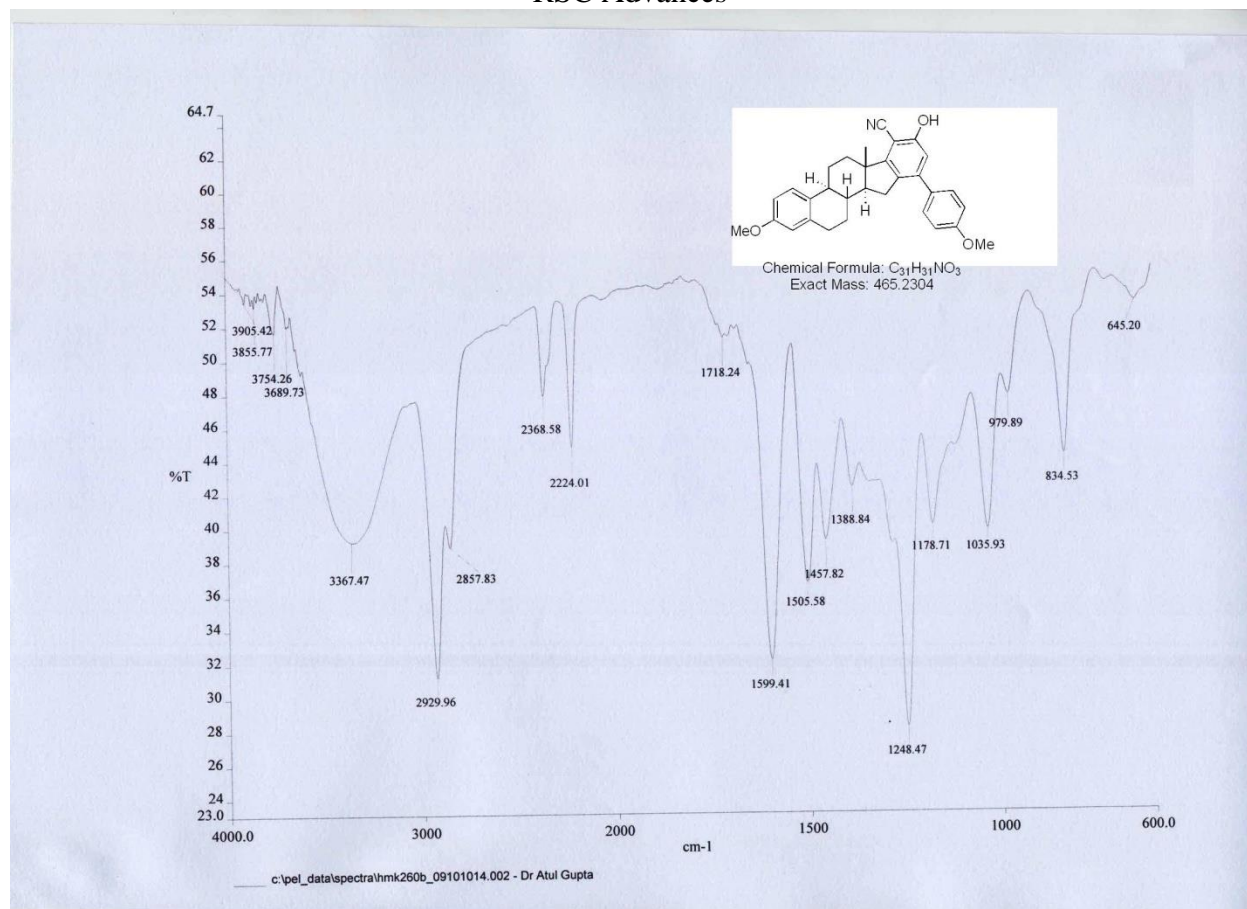
15I05FEB61 #15-36 RT: 0.30-0.70 AV: 22 SB: 2 0.00, 0.00 NL: 5.25E7
T: + c ESI Full ms [150.00-1500.00]



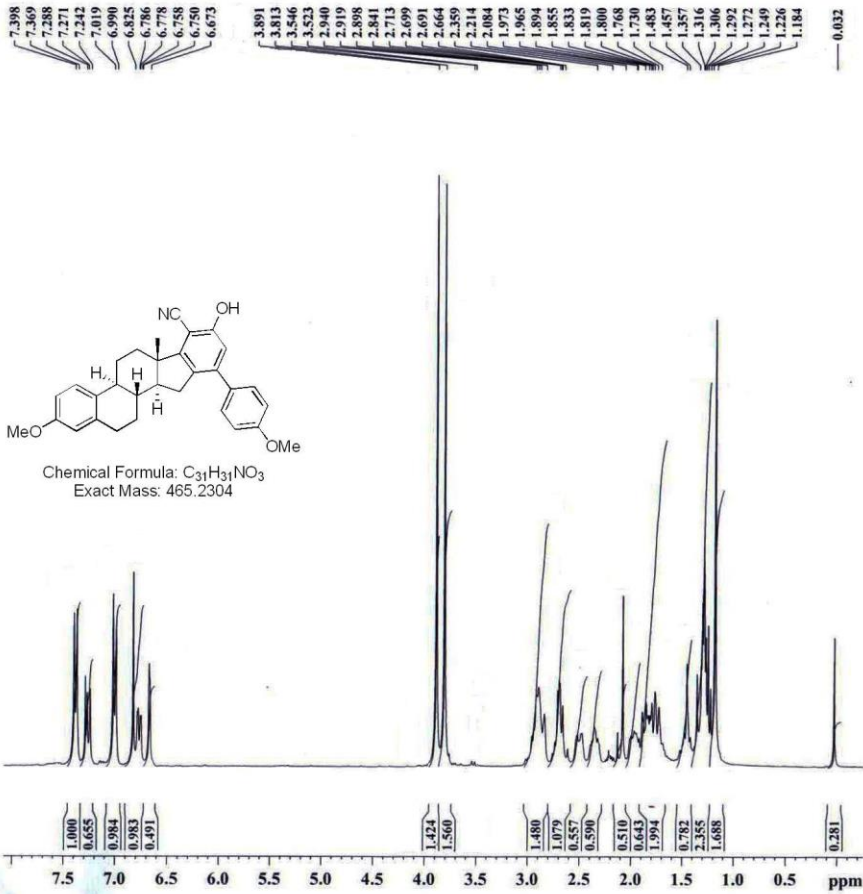
ION TRAP LCQ ADVANTAGE MAX
THERMO ELECTRON CORPORATION

MCS-7D #4-19 RT: 0.02-0.13 AV: 16 NL: 9.22E6
T: FTMS {1,1} +p ESI Full ms [150.00-2000.00]

(6bS,8aS,13aS,13bS)-10-hydroxy-4-methoxy-12-(4-methoxyphenyl)-8a-methyl-2,6b,7,8,8a,9,10,13,13a,13b-decahydro-1H-indeno[2,1-a]phenanthrene-9-carbonitrile (**8d**)



RSC Advances



CIMAP PROTON
PROJECT NO.: mlp-02

Current Data Parameters
NAME atghmk260b.p
EXPNO 1
PROCNO 1

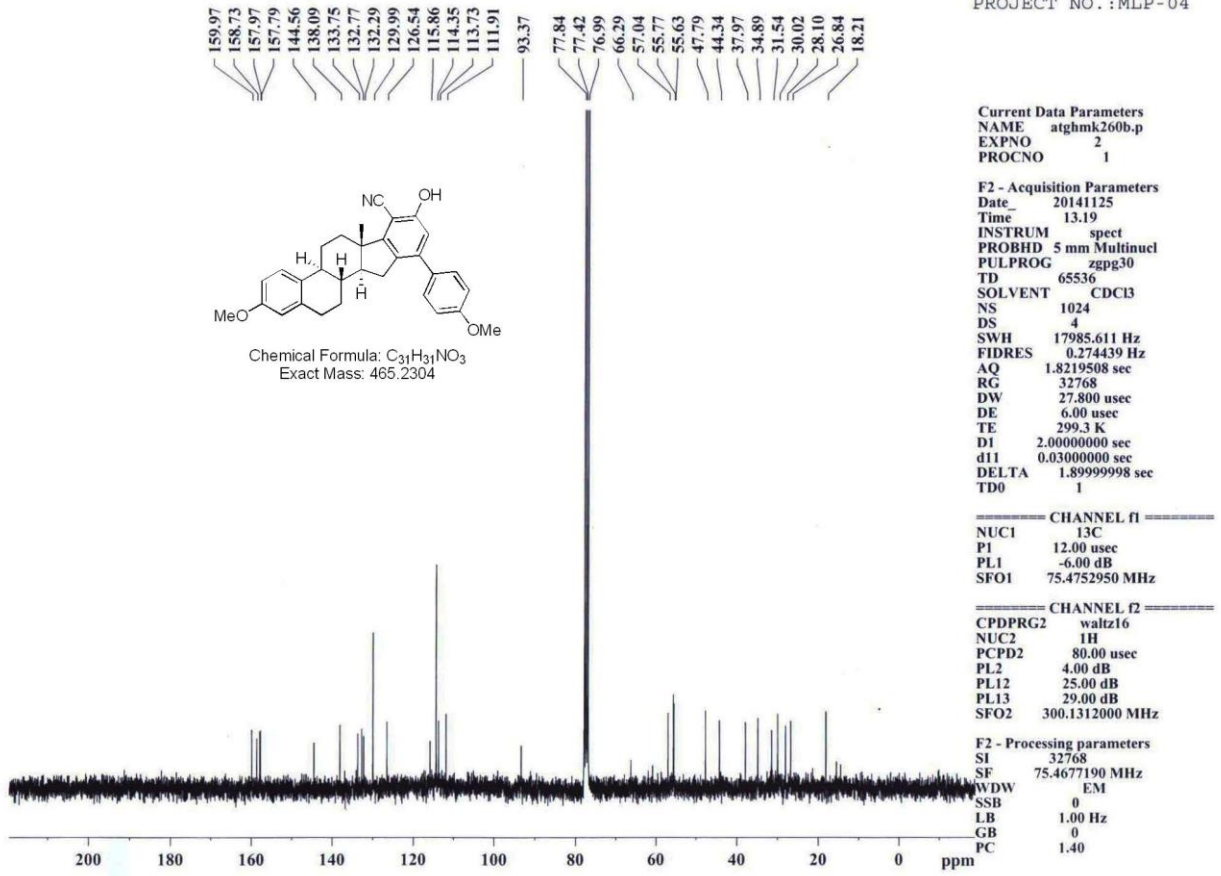
F2 - Acquisition Parameters
Date 20141125
Time 12.52
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 228.1
DW 81.000 usec
DE 6.00 usec
TE 298.5 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
NUC1 1H
PI 7.15 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299974 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

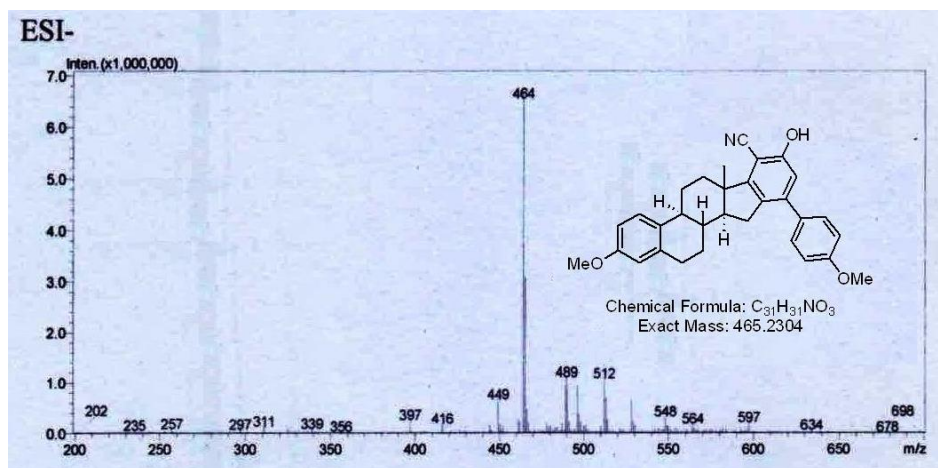
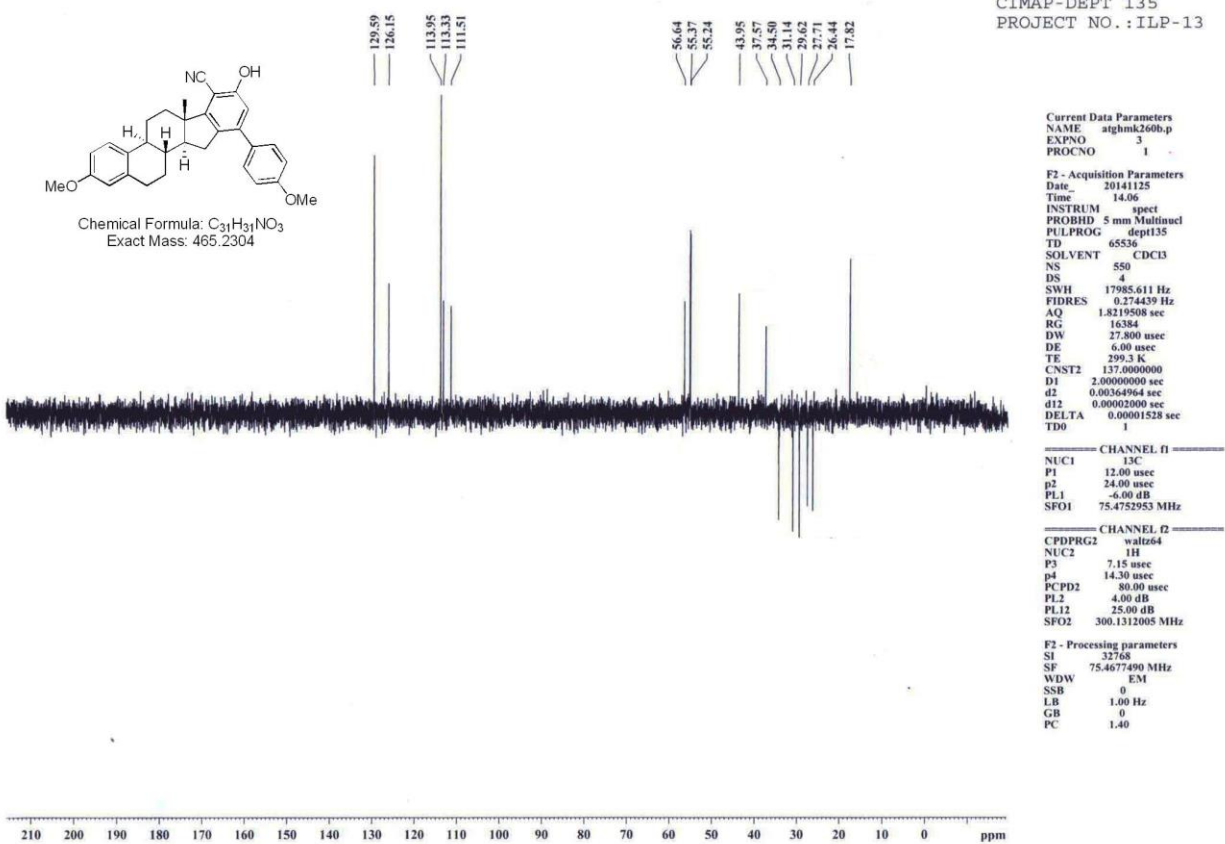
RSC Advances

CIMAP-CARBON
PROJECT NO.:MLP-04

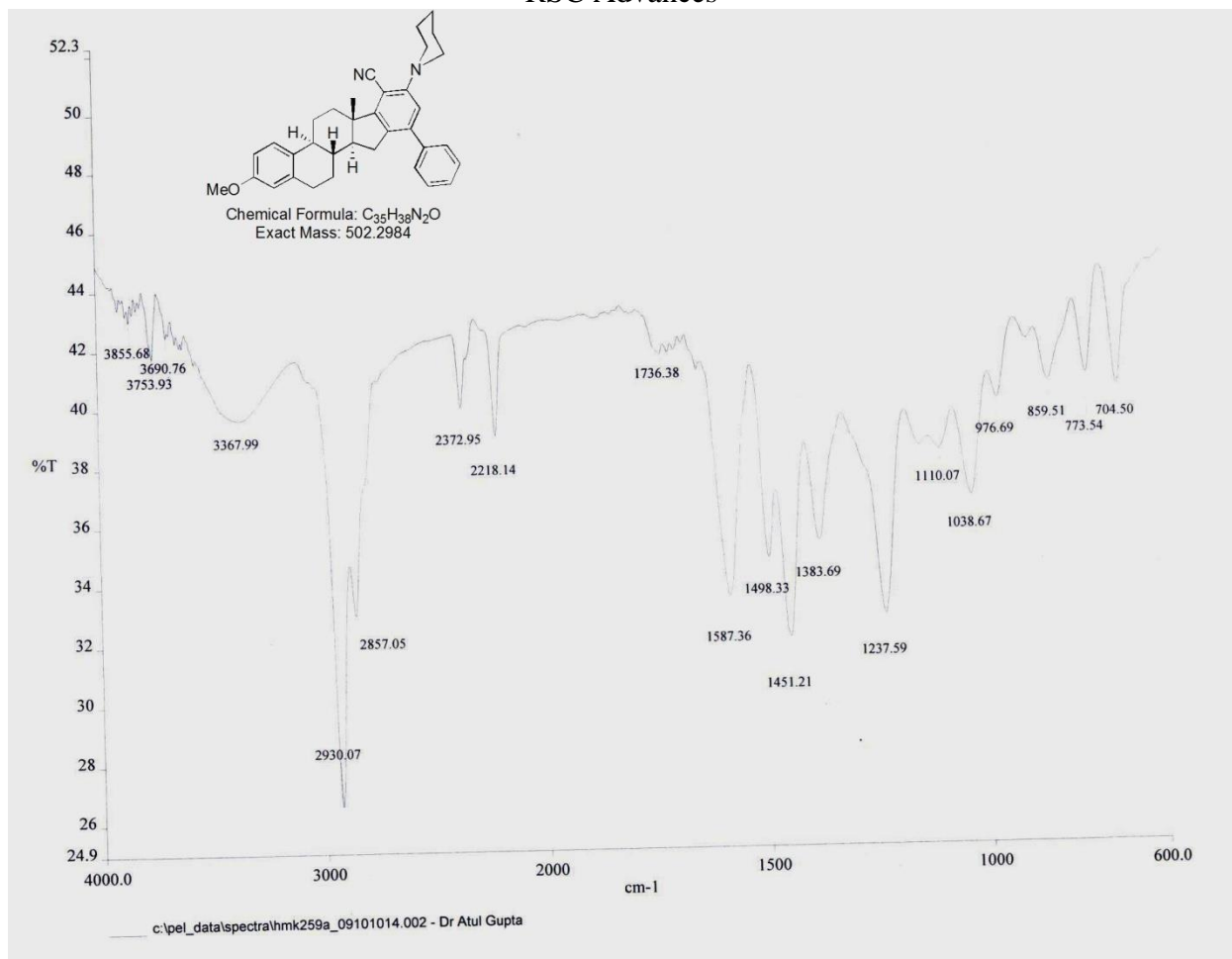


RSC Advances

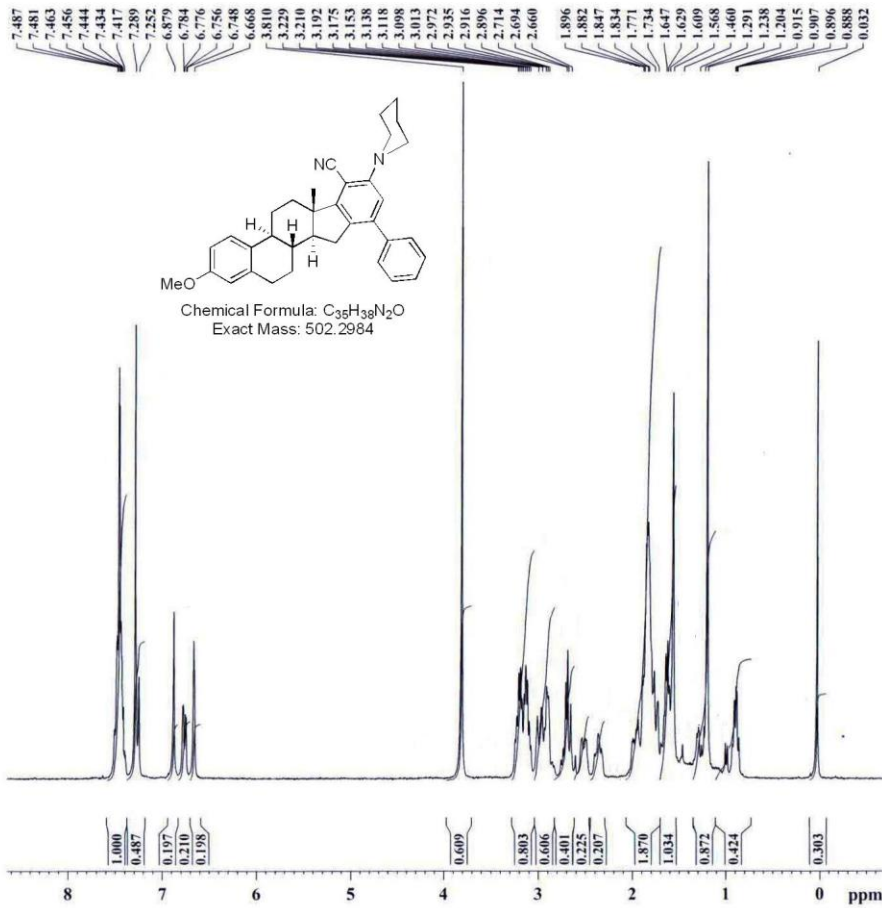
CIMAP-DEPT 135
PROJECT NO.: ILP-13



(+)(6*b*S,8*a*S,13*a*S,13*b*S)-4-methoxy-8*a*-methyl-12-phenyl-10-(piperidin-1-yl)-2,6*b*,7,8,8*a*,13,13*a*,13*b*-octahydro-1*H*-indeno[2,1-*a*]phenanthrene-9-carbonitrile (**7e**)



RSC Advances



CIMAP PROTON
PROJECT NO.: mlp-02

Current Data Parameters
NAME atghmk259ar.p
EXPNO 1
PROCNO 1

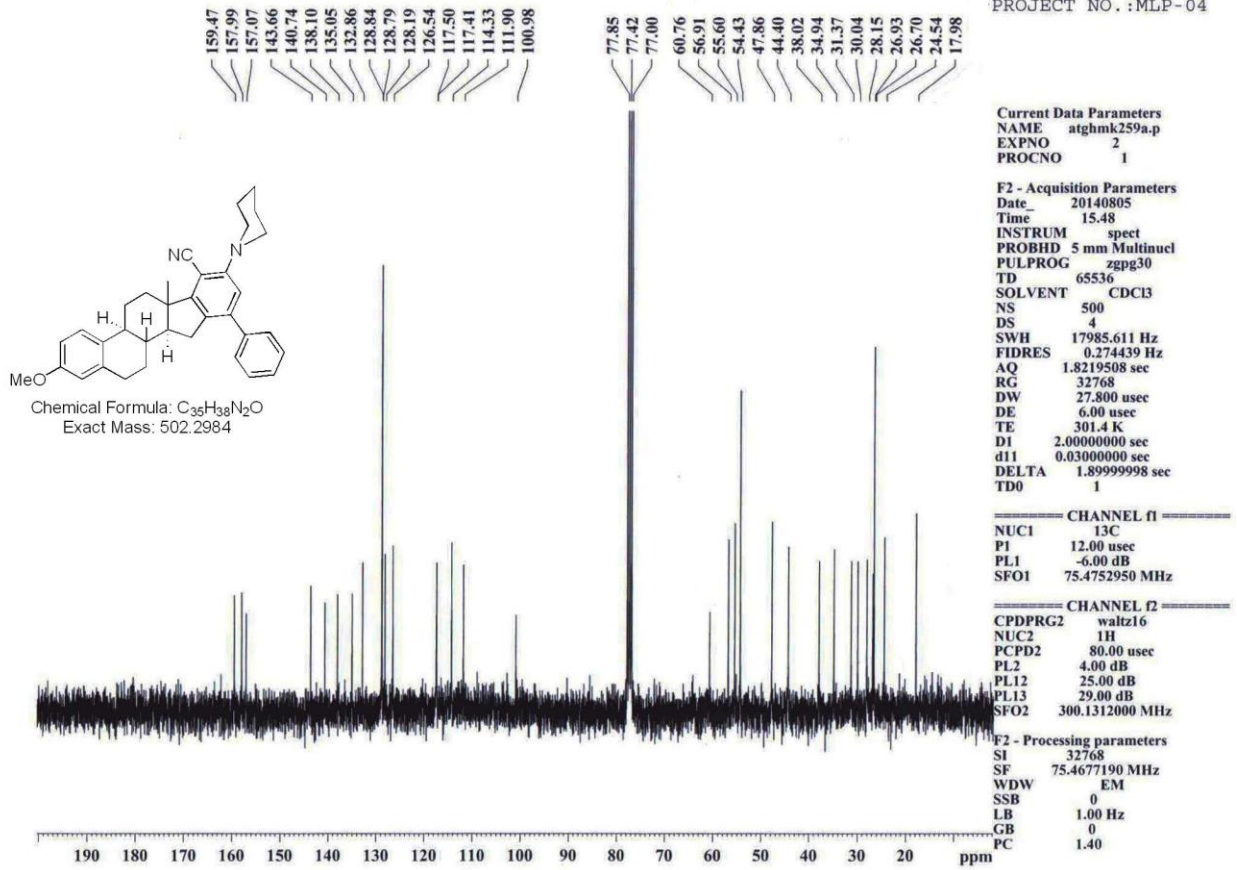
F2 - Acquisition Parameters
Date_ 20140825
Time 16.23
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 812.7
DW 55.600 usec
DE 6.00 usec
TE 302.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 7.15 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299972 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

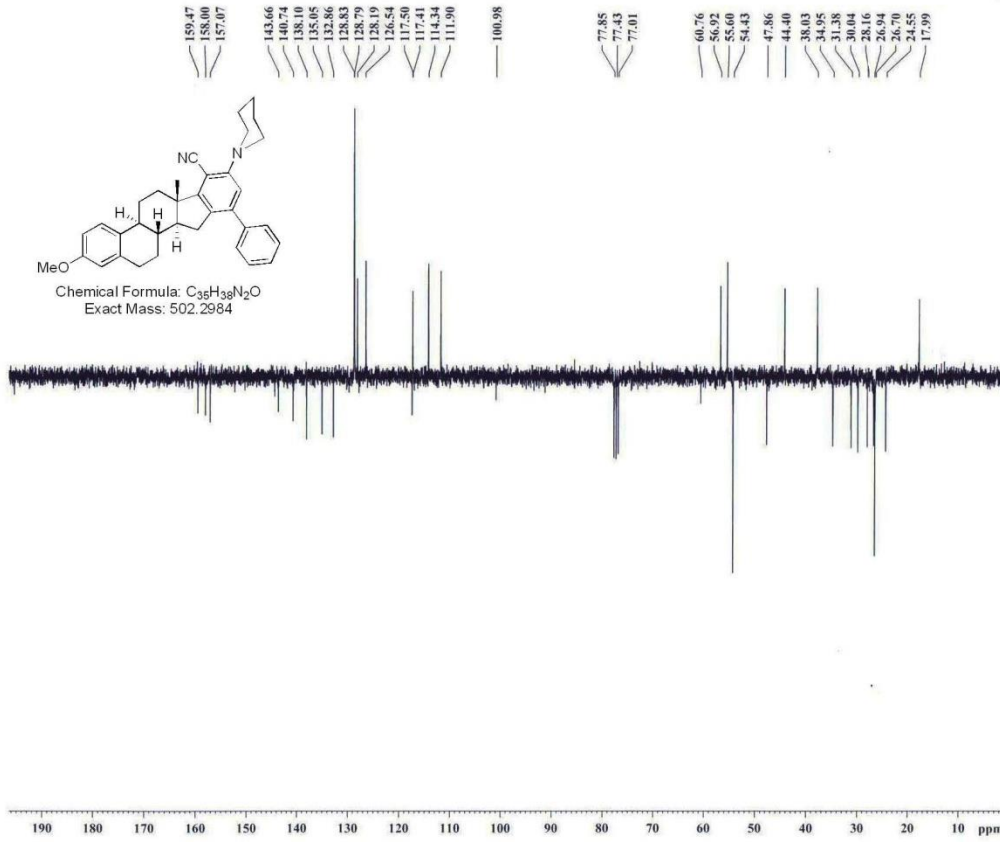
RSC Advances

CIMAP-CARBON
PROJECT NO. :MLP-04



RSC Advances

APT: X, XH2 positiv



Current Data Parameters
NAME atgmk259a.p
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140805
Time 16.30
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG apt
TD 65536
SOLVENT CDCl3
NS 271
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 302.0 K
CNST2 145.000000
CNST1 1.000000
DI 2.0000000 sec
d11 0.0300000 sec
d20 0.00689655 sec
D21 0.0000000 sec
P1 12.00 usec
TD0 1

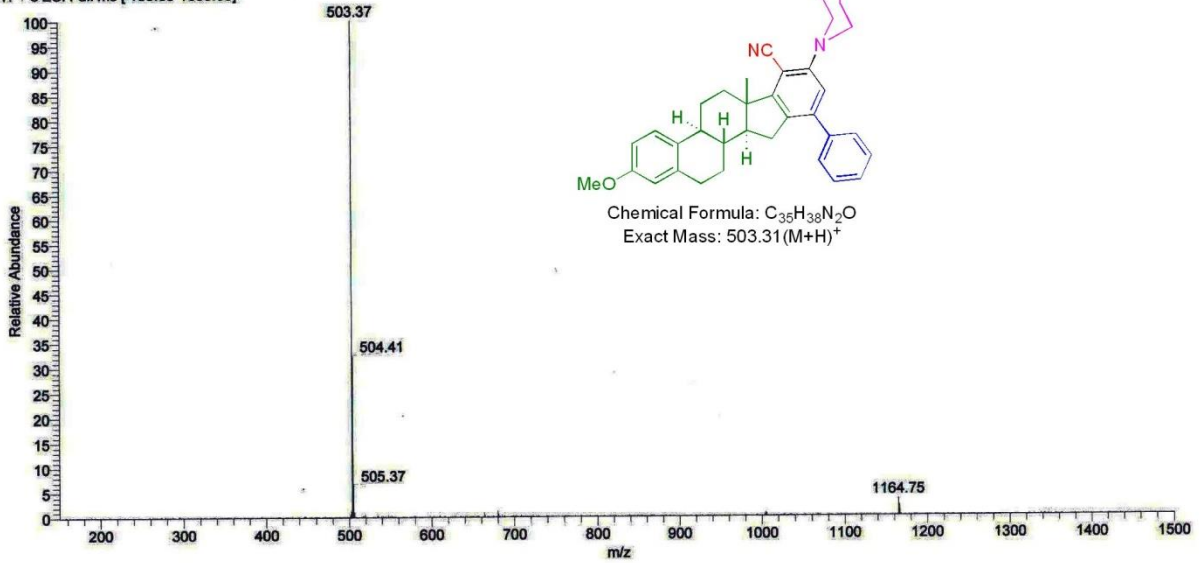
CHANNEL f1
NUC1 13C
P0 12.00 usec
p2 24.00 usec
PL1 -6.00 dB
SFO1 75.4752950 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 25.00 dB
SFO2 300.1312000 MHz

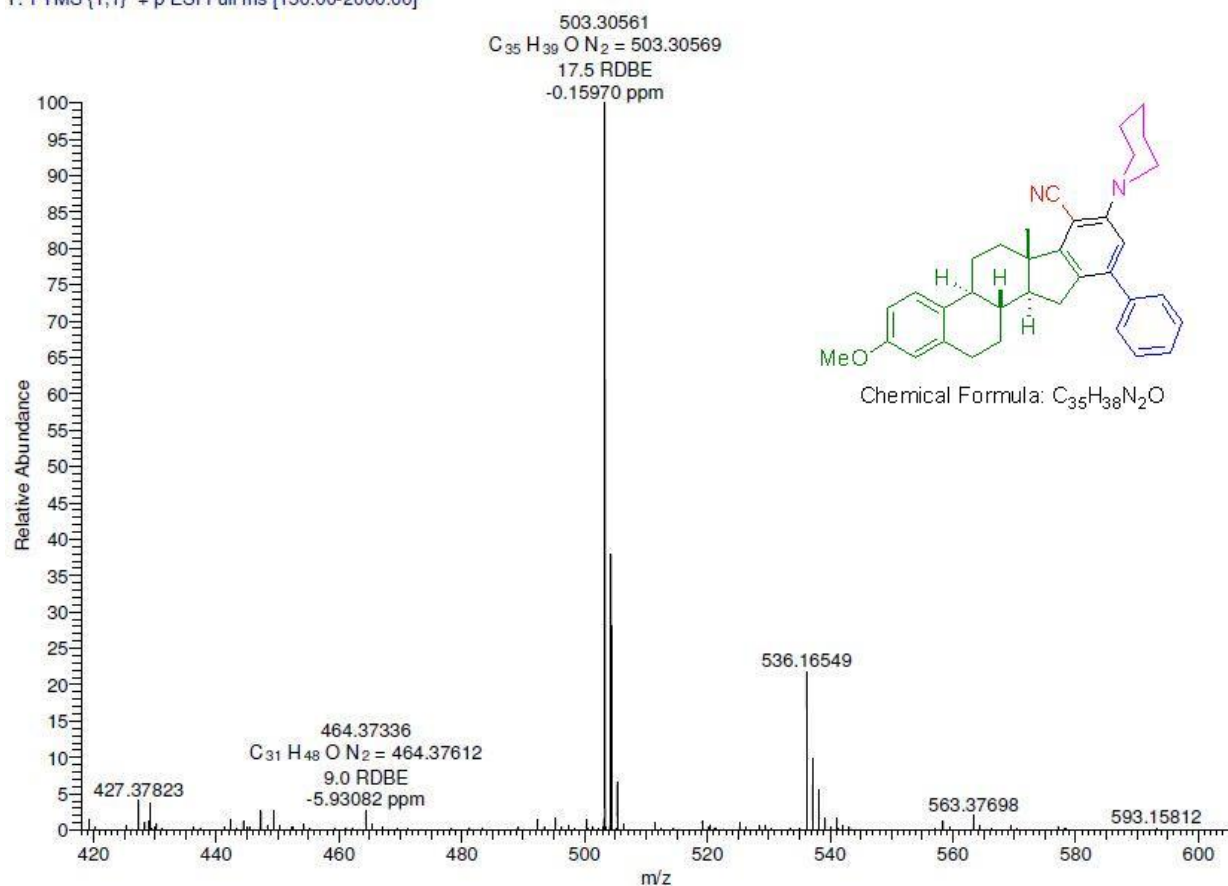
F2 - Processing parameters
SI 32768
SF 75.467190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Sample ID: NR-ATG-259A
Acquisition Date: 02/04/15 14:03:33

15I04FEB54 #15-35 RT: 0.30-0.69 AV: 21 SB: 2 0.01, 0.01 NL: 2.90E7
T: +c ESI Full ms [150.00-1500.00]

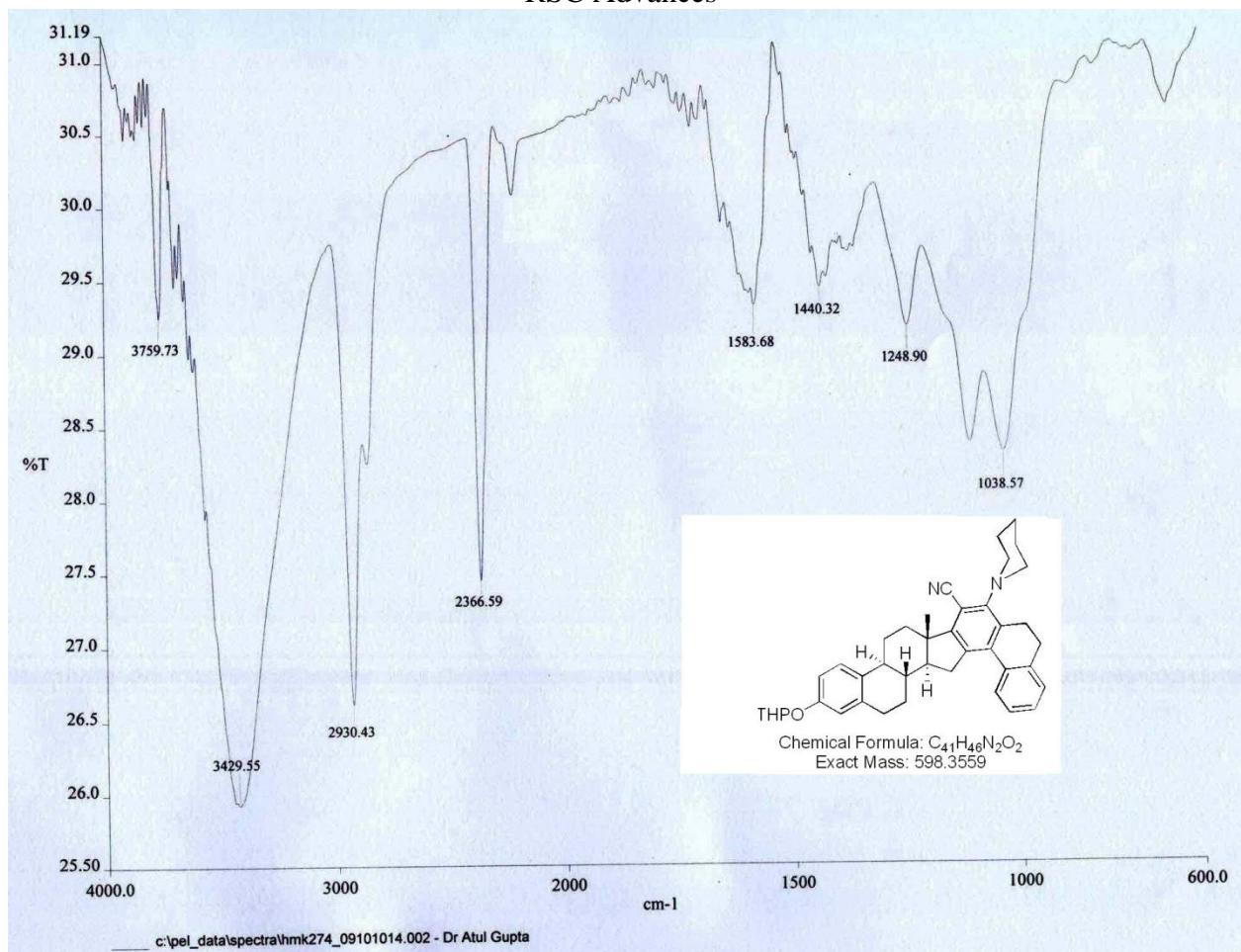


ION TRAP LCQ ADVANTAGE MAX
THERMO ELECTRON CORPORATION

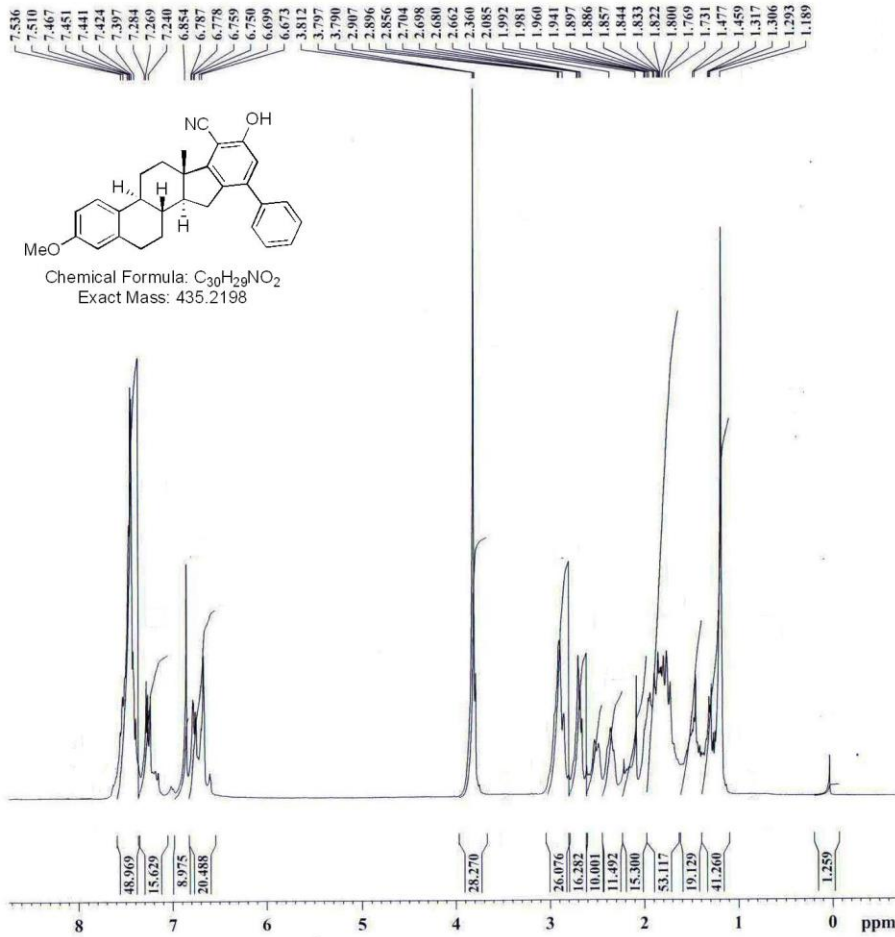
MCS-7E #4-19 RT: 0.02-0.13 AV: 16 NL: 9.83E6
T: FTMS {1,1} + p ESI Full ms [150.00-2000.00]

(6bS,8aS,13aS,13bS)-10-hydroxy-4-methoxy-8a-methyl-12-phenyl-2,6b,7,8,8a,13,13a,13b-octahydro-1H-indeno[2,1-a]phenanthrene-9-carbonitrile (**8e**)

RSC Advances



RSC Advances



CIMAP PROTON
PROJECT NO.: mlp-02

Current Data Parameters
NAME atghmk259b.p
EXPNO 1
PROCNO 1

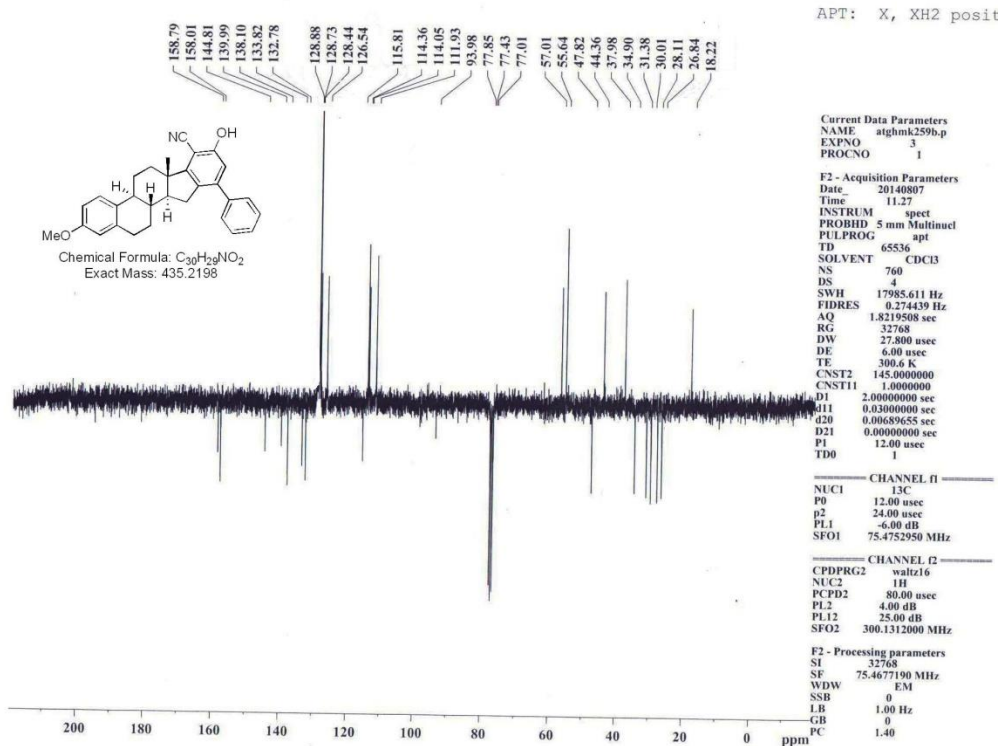
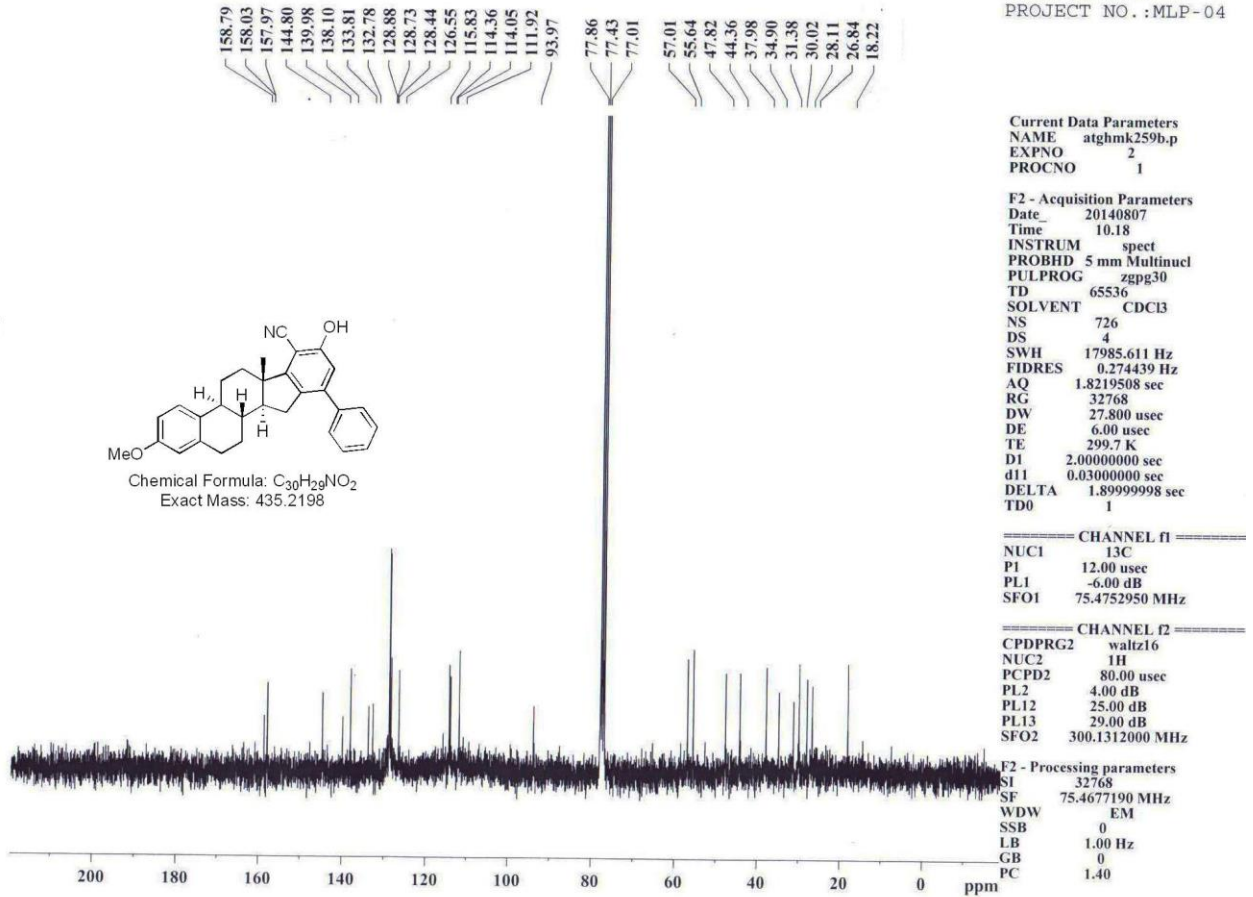
F2 - Acquisition Parameters
Date_ 20140807
Time 10.04
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 17
DS 2
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 128
DW 55.600 usec
DE 6.00 usec
TE 299.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 ====
NUC1 1H
P1 7.15 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

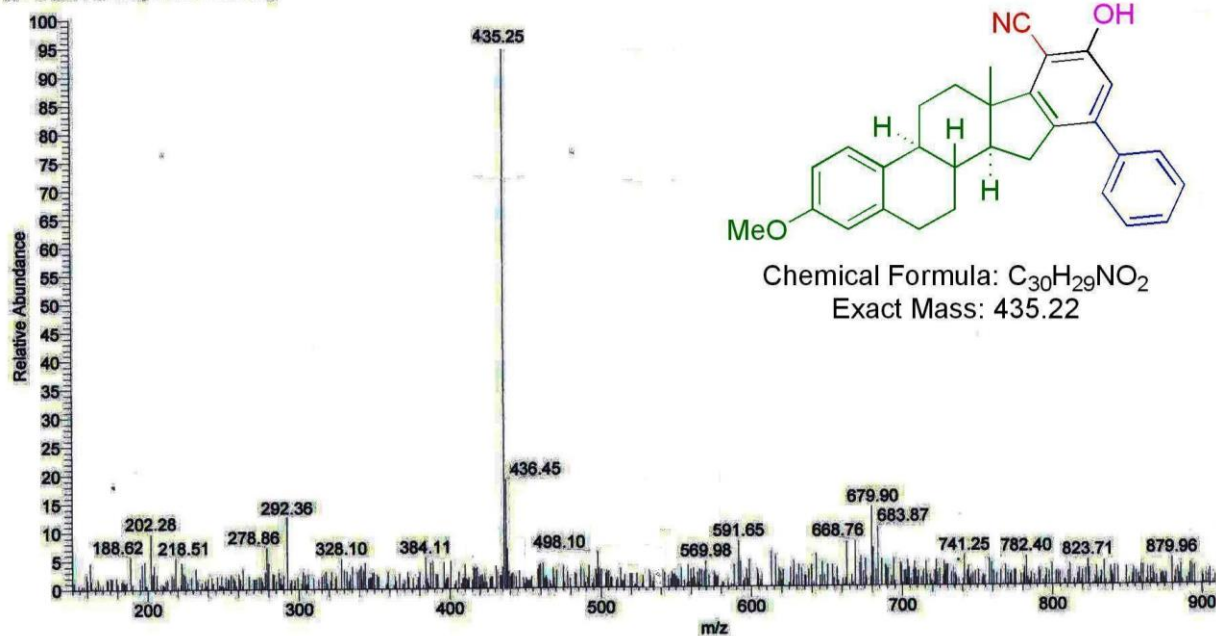
F2 - Processing parameters
SI 32768
SF 300.1299972 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

RSC Advances

CIMAP-CARBON
PROJECT NO.:MLP-04



15I23FEB49 #19-44 RT: 0.30-0.71 AV: 26 SB: 2 0.00, 0.00 NL: 8.01E5
T: + c ESI Full ms [150.00-1000.00]



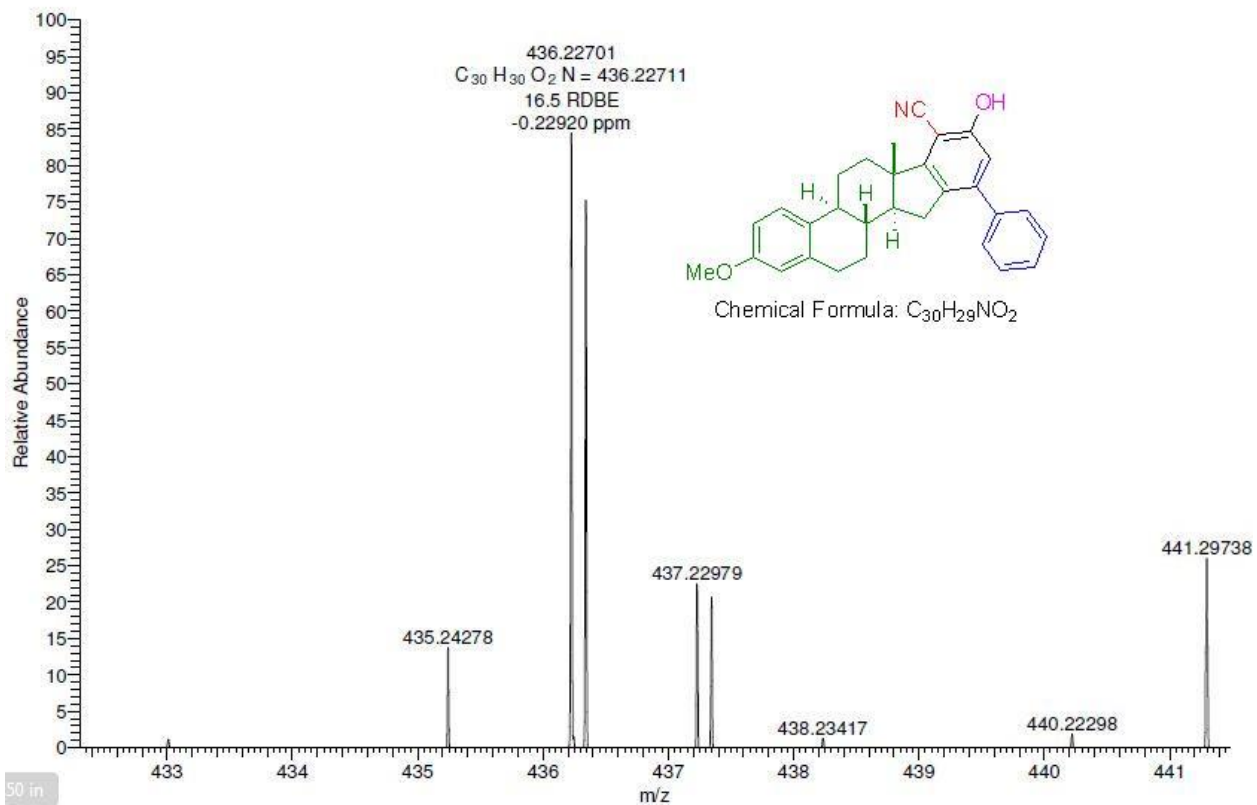
ION TRAP LCQ ADVANTAGE MAX
THERMO ELECTRON CORPORATION

CAIICT HRMS-03.09.2014...MCS-8E
PAVAN

CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
NATIONAL CENTRE FOR MASS SPECTROMETRY

11-05-15 13:11:07

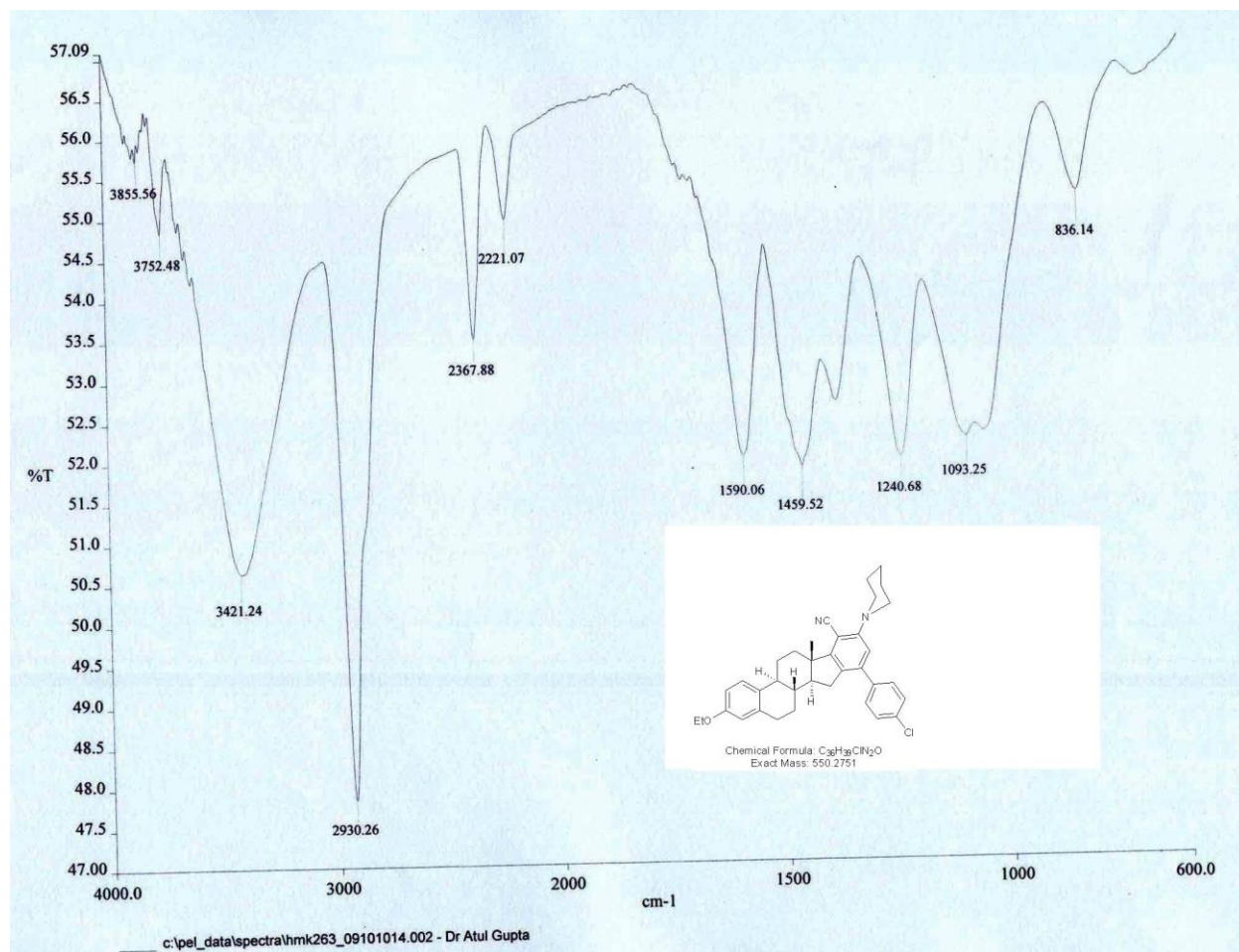
MCS-8E #4-19 RT: 0.02-0.13 AV: 16 NL: 6.28E4
T: FTMS {1,1} + p ESI Full ms [150.00-2000.00]



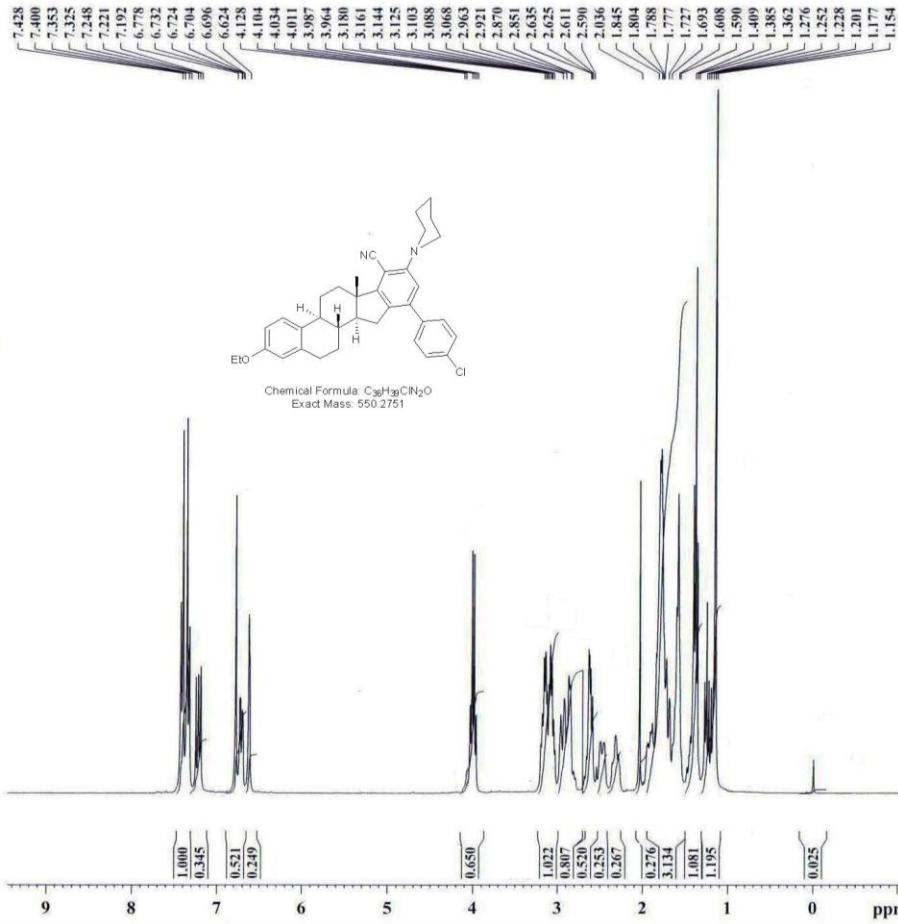
50 in

RSC Advances

(+)(6bS,8aS,13aS,13bS)-12-(4-chlorophenyl)-4-ethoxy-8a-methyl-10-(piperidin-1-yl)-2,6b,7,8,8a,13,13a,13b-octahydro-1*H*-indeno[2,1-*a*]phenanthrene-9-carbonitrile (**7f**)



RSC Advances



CIMAP PROTON
PROJECT NO.: mlp-02

Current Data Parameters
NAME atghmk263.p
EXPNO 1
PROCNO 1

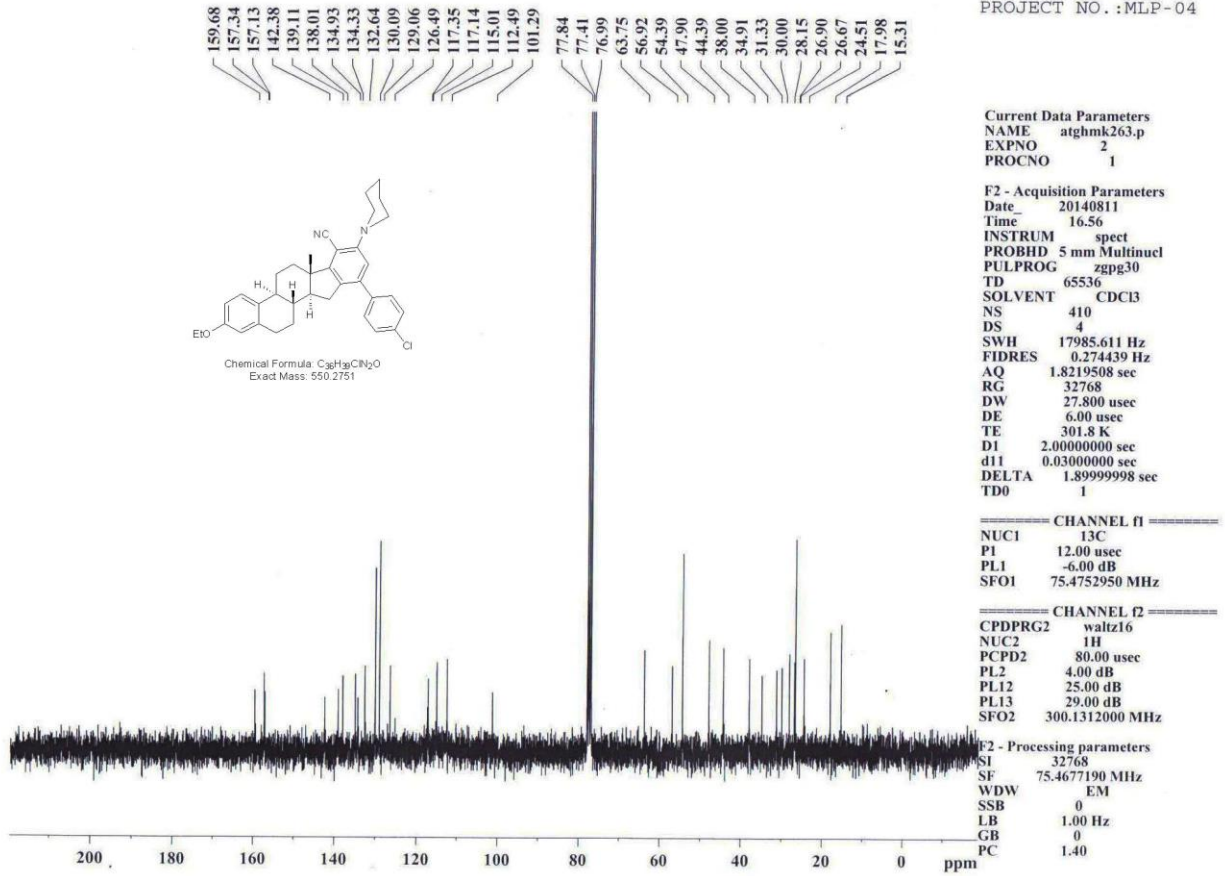
F2 - Acquisition Parameters
Date_ 20140811
Time 16.46
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 23
DS 2
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 161.3
DW 55.600 usec
DE 6.00 usec
TE 301.3 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 7.15 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

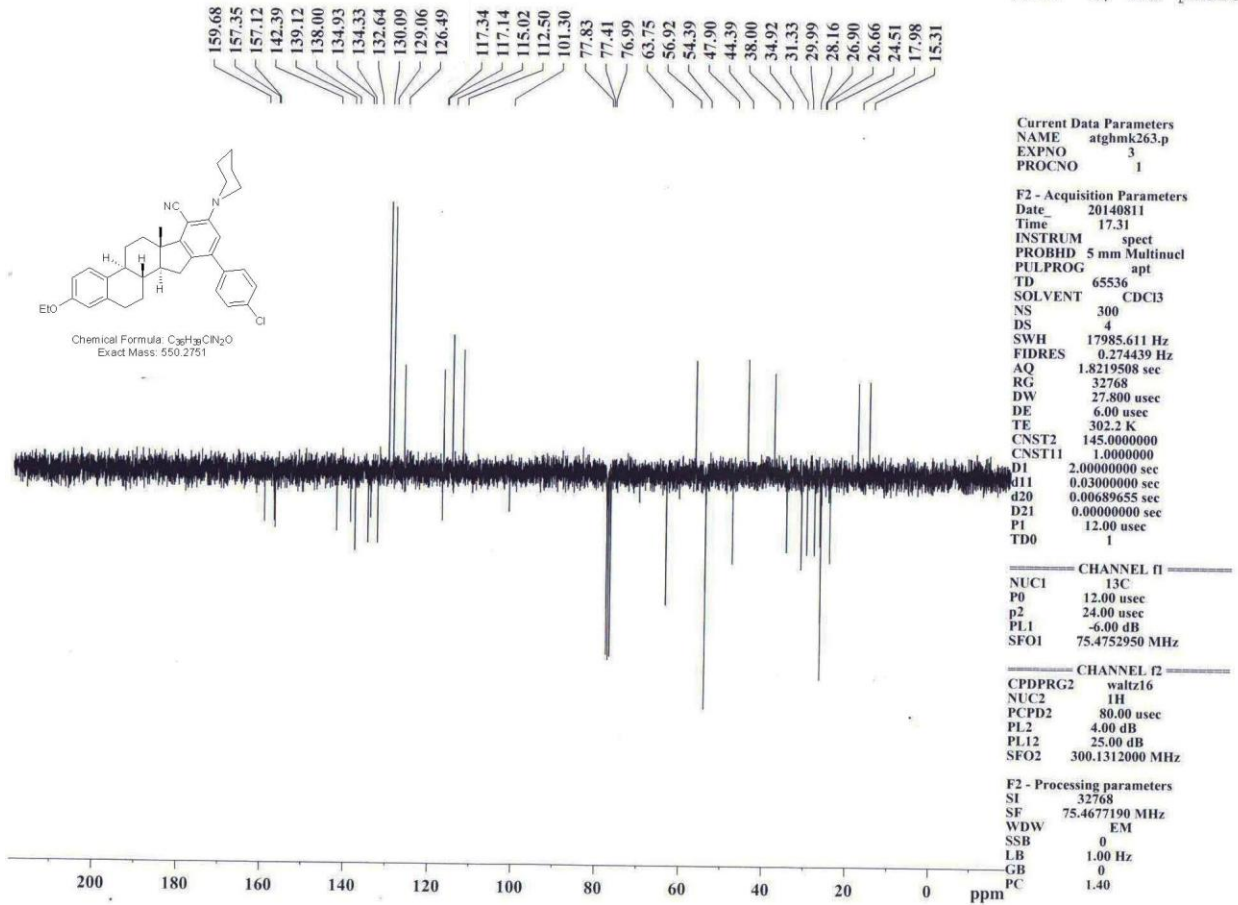
RSC Advances

CIMAP-CARBON
PROJECT NO.: MLP-04



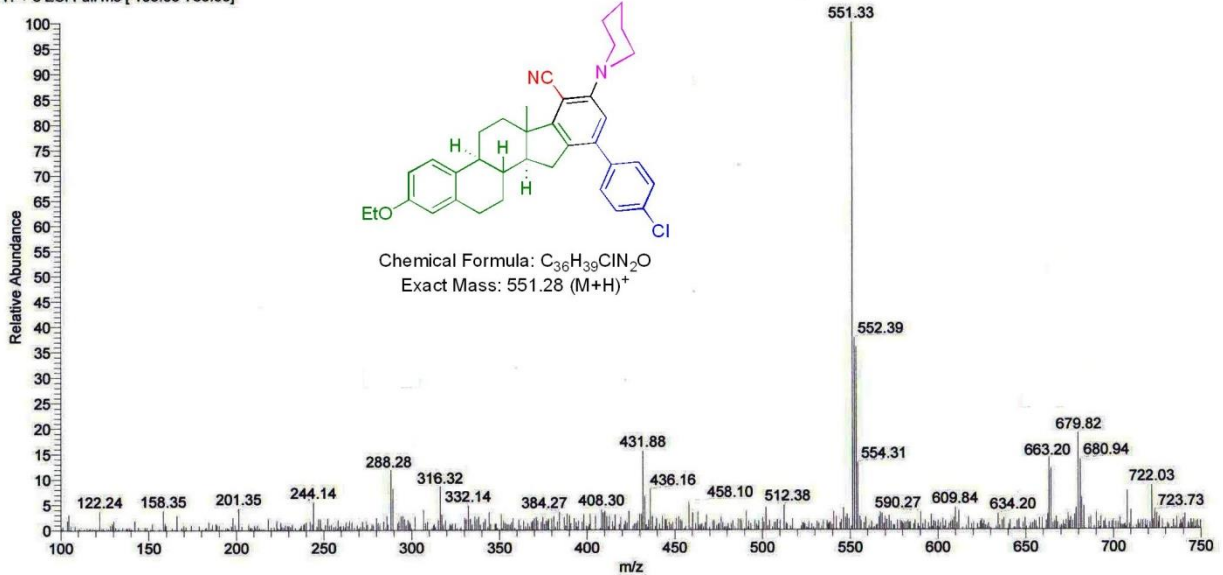
RSC Advances

APT: X, XH2 positi

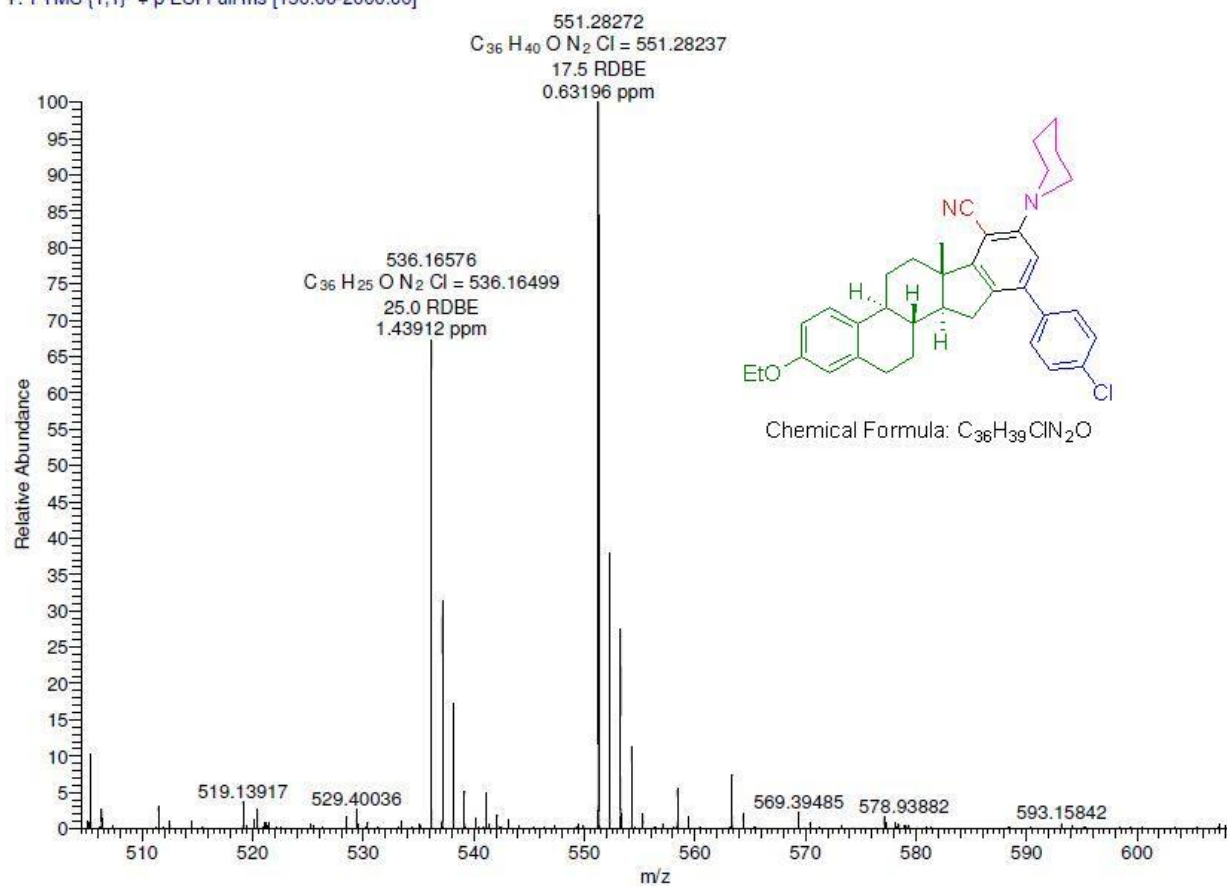


Sample ID: NR-ATG-263
Acquisition Date: 02/03/15 12:21:13

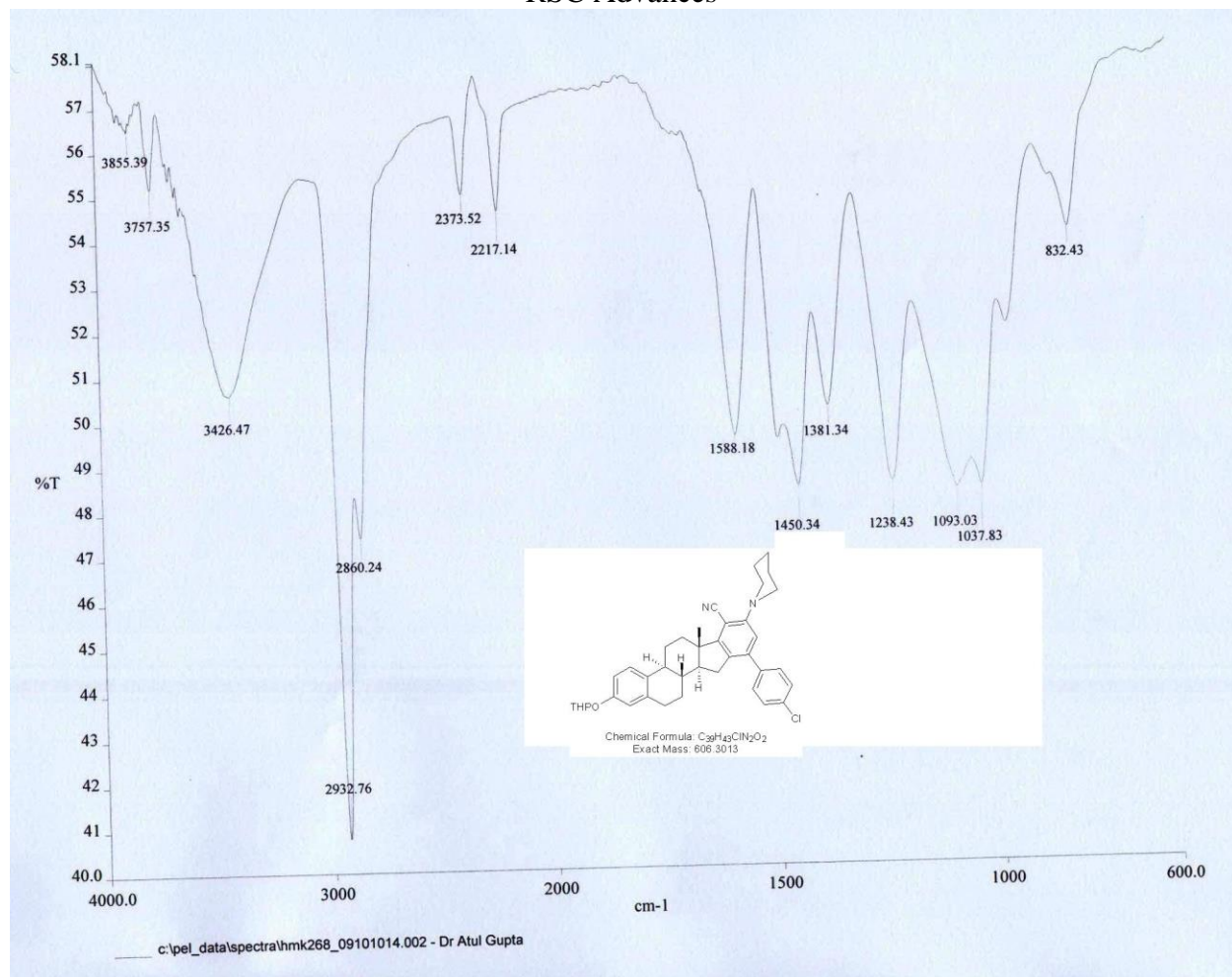
15103FEB02 #23-55 RT: 0.30-0.70 AV: 33 SB: 2 0.01, 0.01 NL: 4.05E6
T: +c ESI Full ms [100.00-750.00]



ION TRAP LCQ ADVANTAGE MAX
THERMO ELECTRON CORPORATION

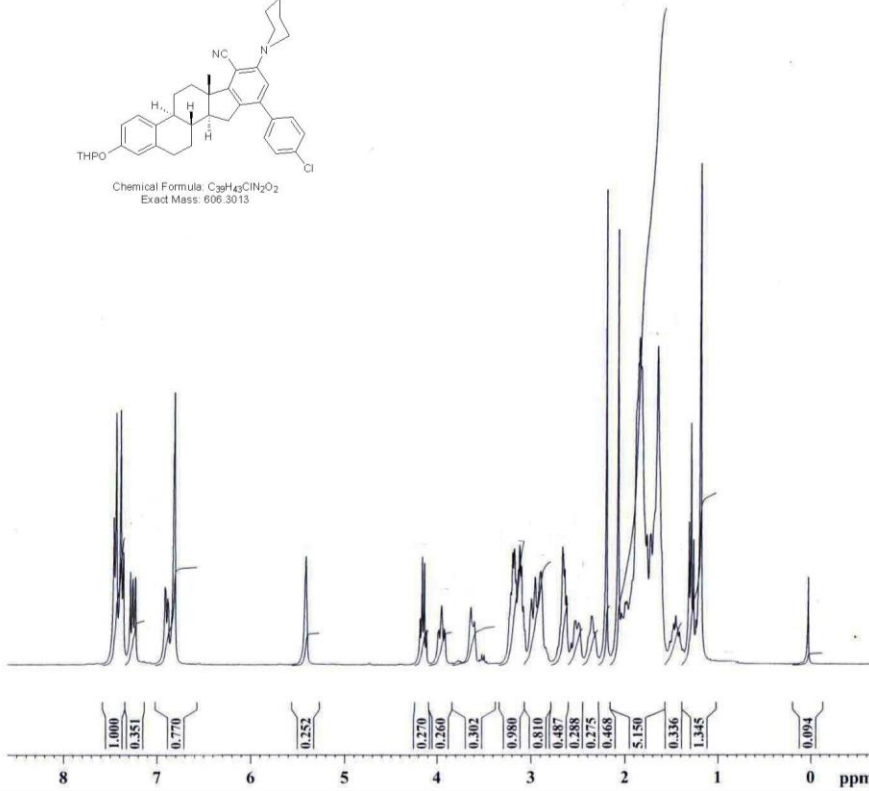
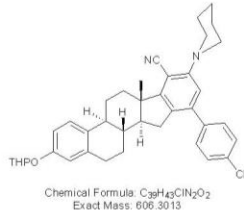
MCS-7F #4-19 RT: 0.02-0.13 AV: 16 NL: 3.22E6
T: FTMS (1,1) + p ESI Full ms [150.00-2000.00]

(+)(6*S*,8*aS*,13*aS*,13*bS*)-12-(4-chlorophenyl)-8*a*-methyl-10-(piperidin-1-yl)-4-(tetrahydrofuran-2-yloxy)-2,6*b*,7,8,8*a*,13, 13*a*,13*b*-octahydro-1*H*-indeno[2,1-*a*]phenanthrene-9-carbonitrile (7g)



RSC Advances

7.464
7.436
7.389
7.361
7.288
7.262
7.233
6.916
6.909
6.888
6.881
6.812
5.416
4.104
4.141
3.955
3.640
3.215
3.196
3.180
3.161
3.138
3.124
3.104
3.084
2.998
2.958
2.901
2.670
2.662
2.647
2.627
2.358
2.199
2.073
2.040
2.000
1.981
1.925
1.855
1.843
1.825
1.766
1.725
1.683
1.647
1.455
1.313
1.289
1.266
1.187
0.032



CIMAP PROTON
PROJECT NO.: mlp-02

Current Data Parameters
NAME atghmk268.p
EXPNO 1
PROCNO 1

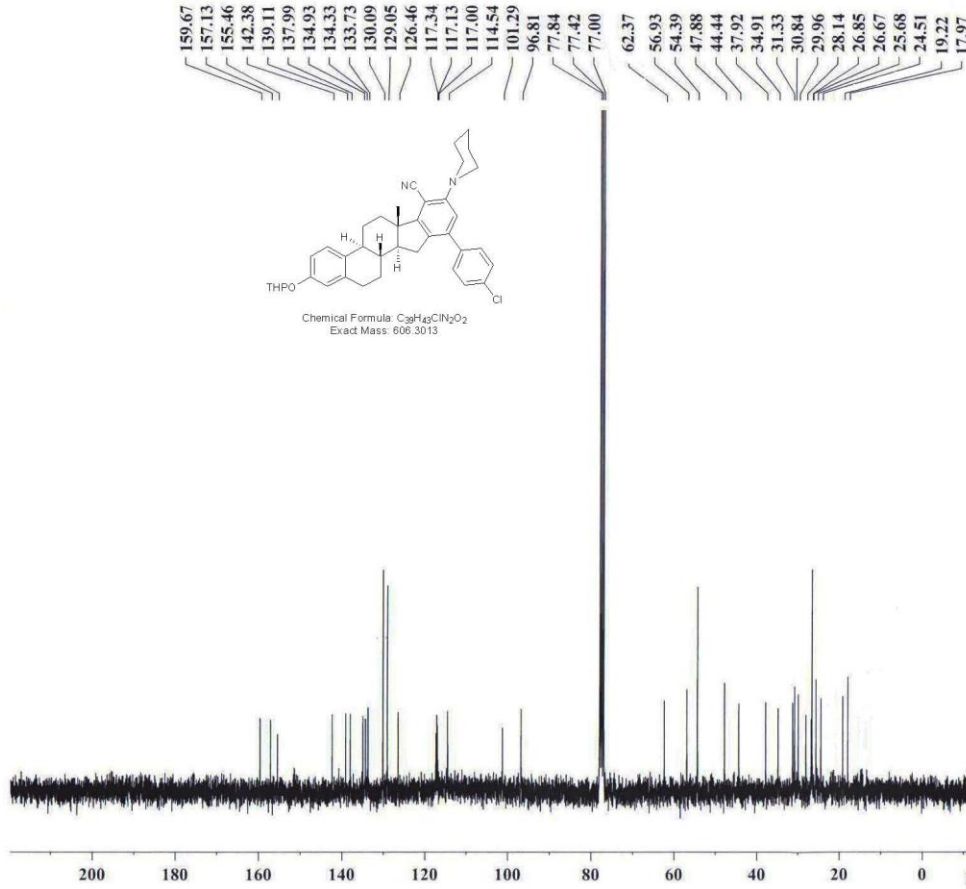
F2 - Acquisition Parameters
Date 20140821
Time 13.55
INSTRUM spect
PROBHD 5 mm Multinuel
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 18
DS 2
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 114
DW 55.600 usec
DE 6.00 usec
TE 301.2 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 7.15 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299972 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

RSC Advances

CIMAP-CARBON
PROJECT NO.: MLP-04



Current Data Parameters
NAME atghmk268.p
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date 20140821
Time 14.16
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1006
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 301.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

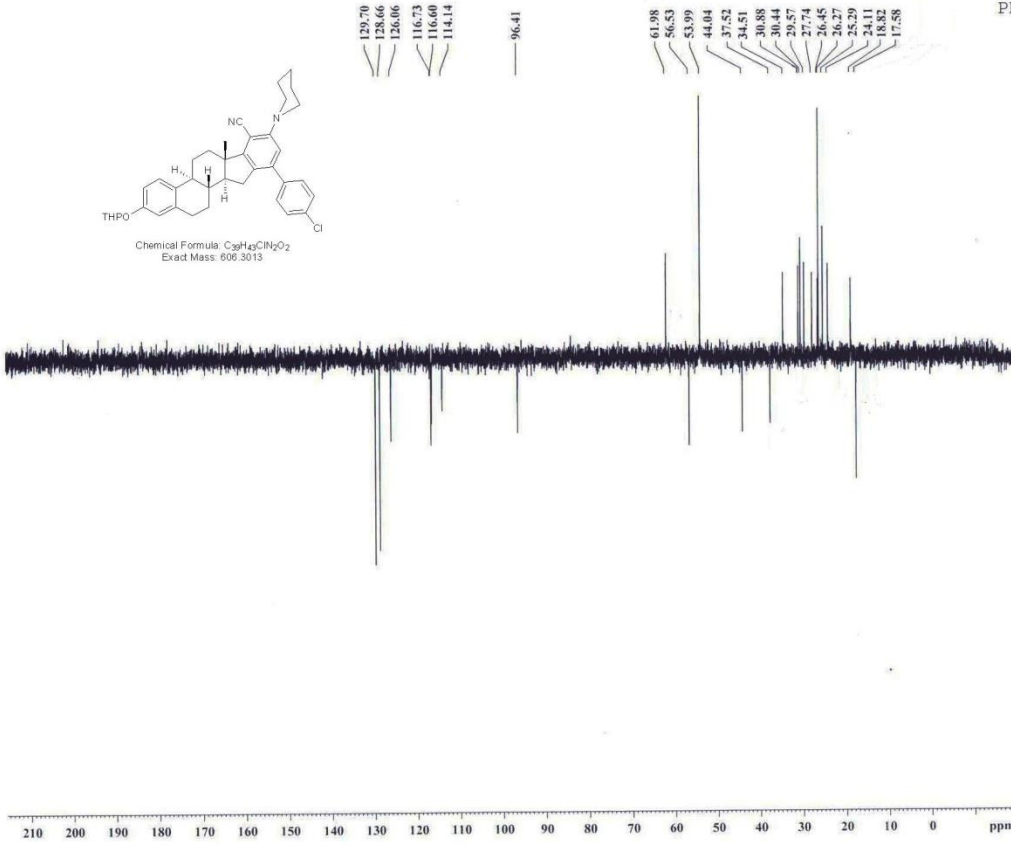
==== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 -6.00 dB
SFO1 75.4752950 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 25.00 dB
PL13 29.00 dB
SFO2 300.1312000 MHz

F2 - Processing parameters
SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

RSC Advances

CIMAP-DEPT 135
PROJECT NO.: ILP-13



Current Data Parameters
NAME aghm1268.p
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140821
Time 15.22
INSTRUM spect
PROBHD 5 mm Multinuc
PULPROG dept135
TD 65536
SOLVENT CDC13
NS 400
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 6.00 usec
TE 302.2 K
CNST2 137.0000000
D1 2.00000000 sec
d2 0.00364964 sec
d12 0.00002000 sec
DELTA 0.00001528 sec
TD0 1

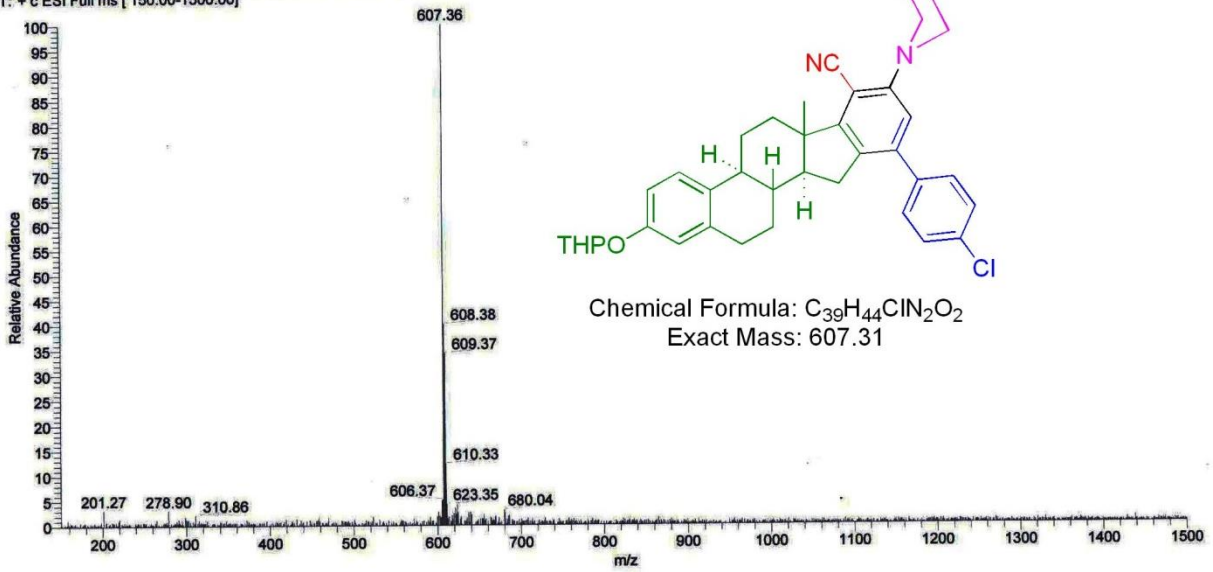
CHANNEL f1
NUC1 13C
P1 12.00 usec
p2 24.00 usec
PL1 -6.00 dB
SFO1 75.4752953 MHz

CHANNEL f2
CPDPRG2 waltz64
NUC2 1H
P3 7.15 usec
p4 14.30 usec
PCPD2 80.00 usec
PL2 4.00 dB
PL12 25.00 dB
SFO2 300.1312065 MHz

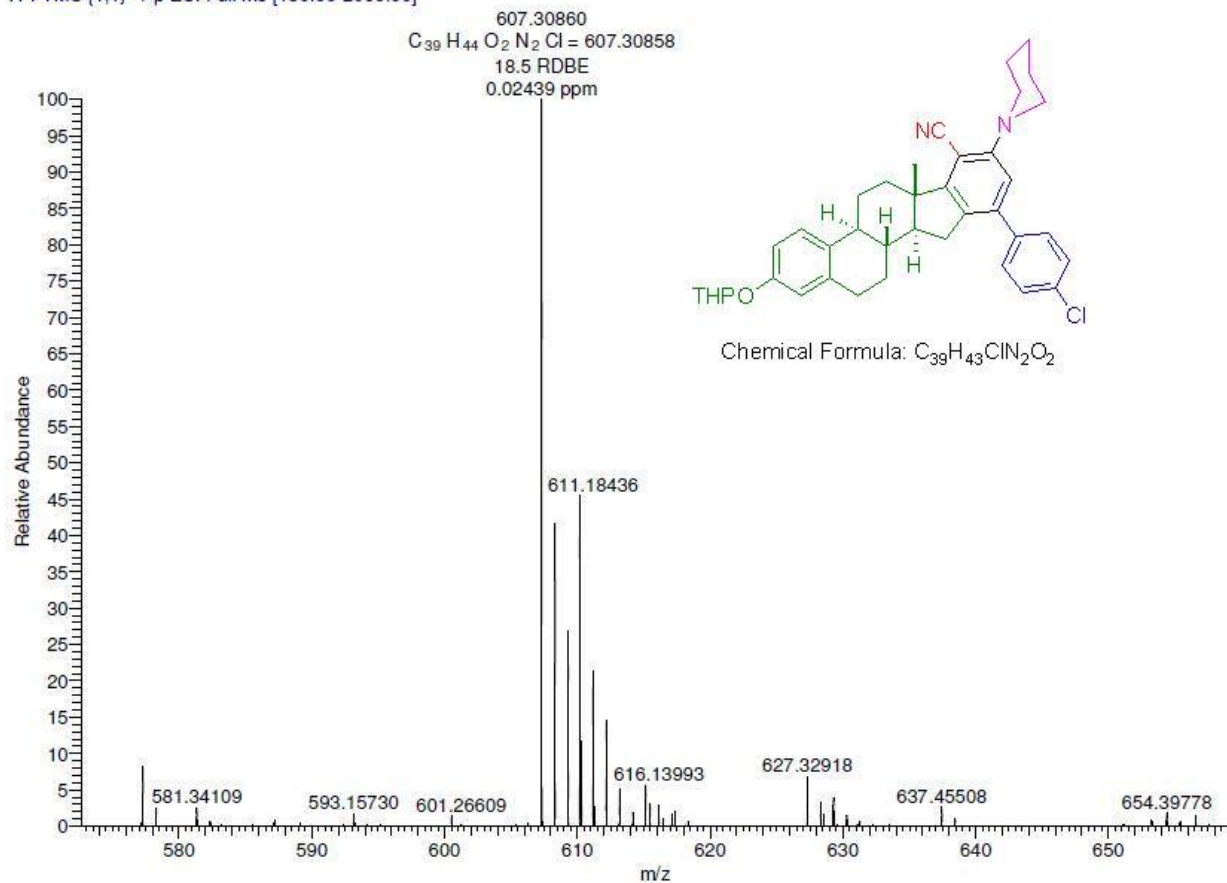
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Data File: 15123FEB50
Original Data Path: 15123FEB50.RAW
Current Data Path: C:\Xcalibur\data\FEB2015\23FEB2015\
Sample ID: NR-ATG-268
Acquisition Date: 02/23/15 13:50:23

15123FEB50 #15-34 RT: 0.30-0.70 AV: 20 SB: 2 0.00, 0.00 NL: 3.97E6
T: + c ESI Full ms [150.00-1500.00]

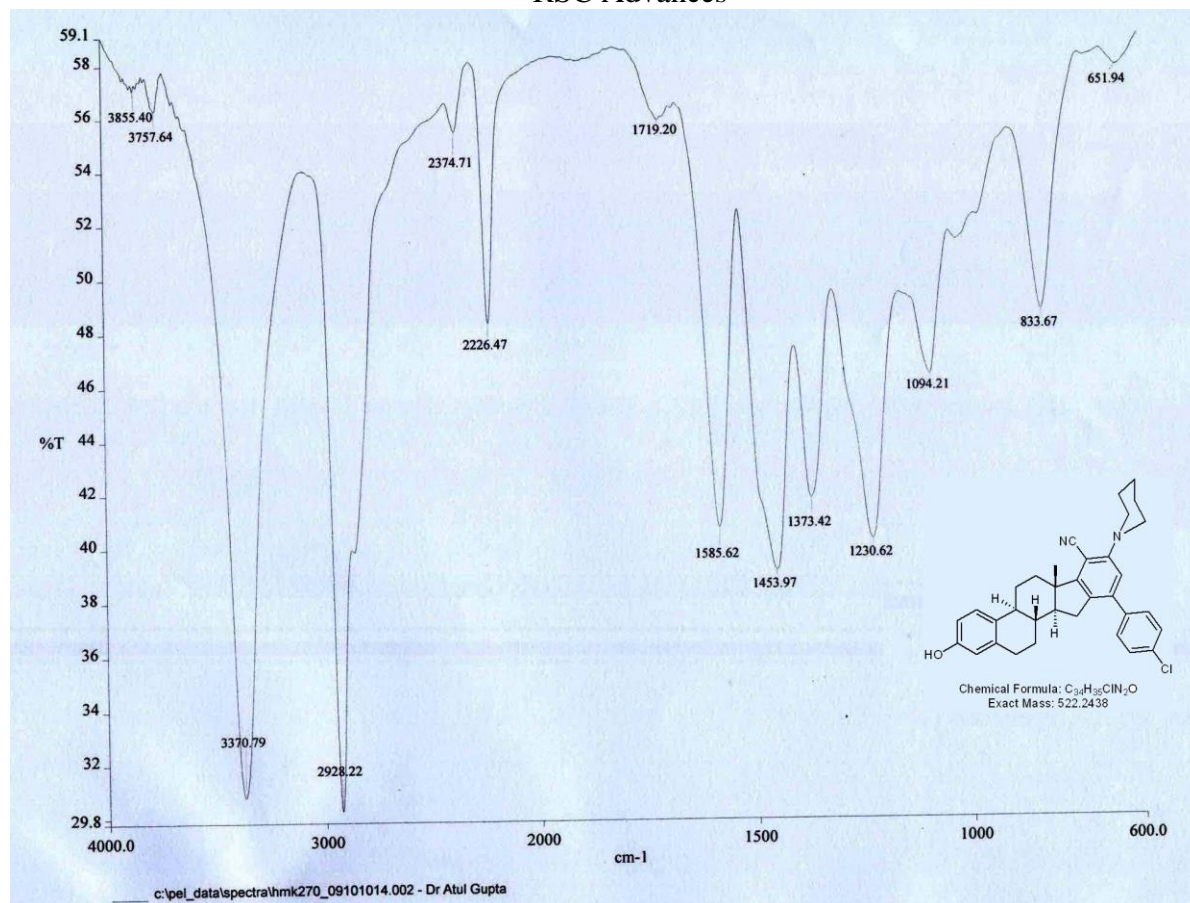


ION TRAP LCQ ADVANTAGE MAX
THERMO ELECTRON CORPORATION

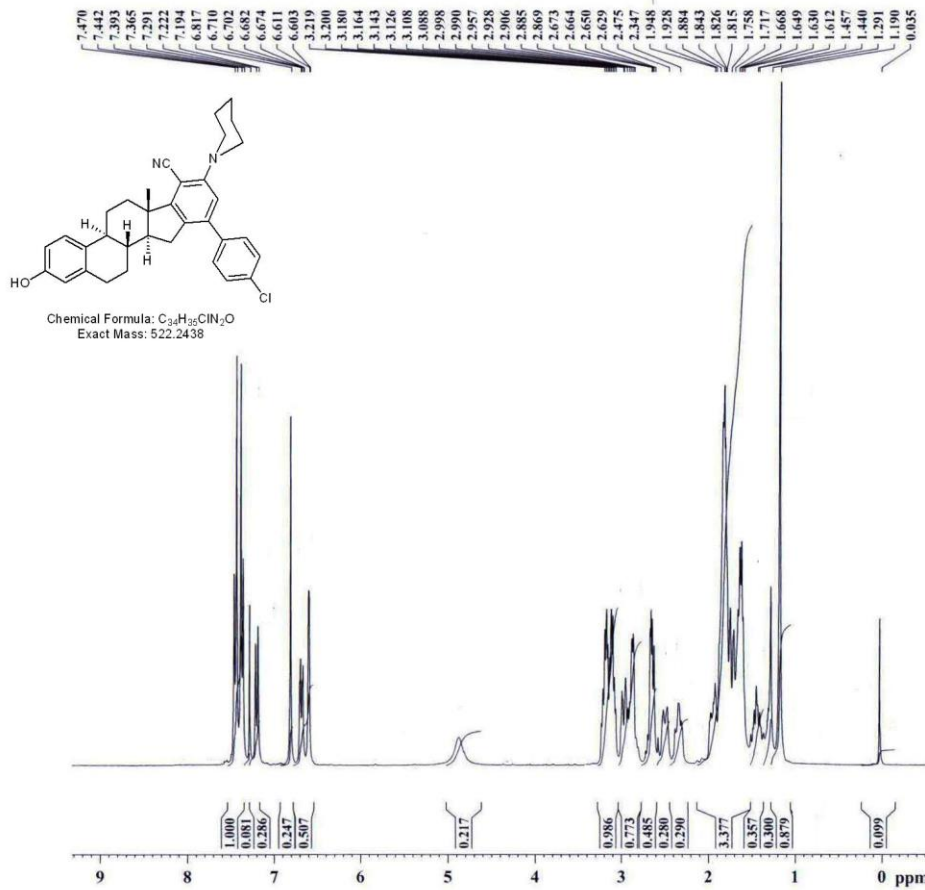


(+)(6bS,8aS,13aS,13bS)-12-(4-chlorophenyl)-4-hydroxy-8a-methyl-10-(piperidin-1-yl)-2,6b,7,8,8a,13,13a,13b-octahydro-1H-indeno[2,1-a]phenanthrene-9-carbonitrile (**7h**)

RSC Advances



RSC Advances



CIMAP PROTON
PROJECT NO.: mlp-02

Current Data Parameters
NAME atghmk270.p
EXPNO 1
PROCNO 1

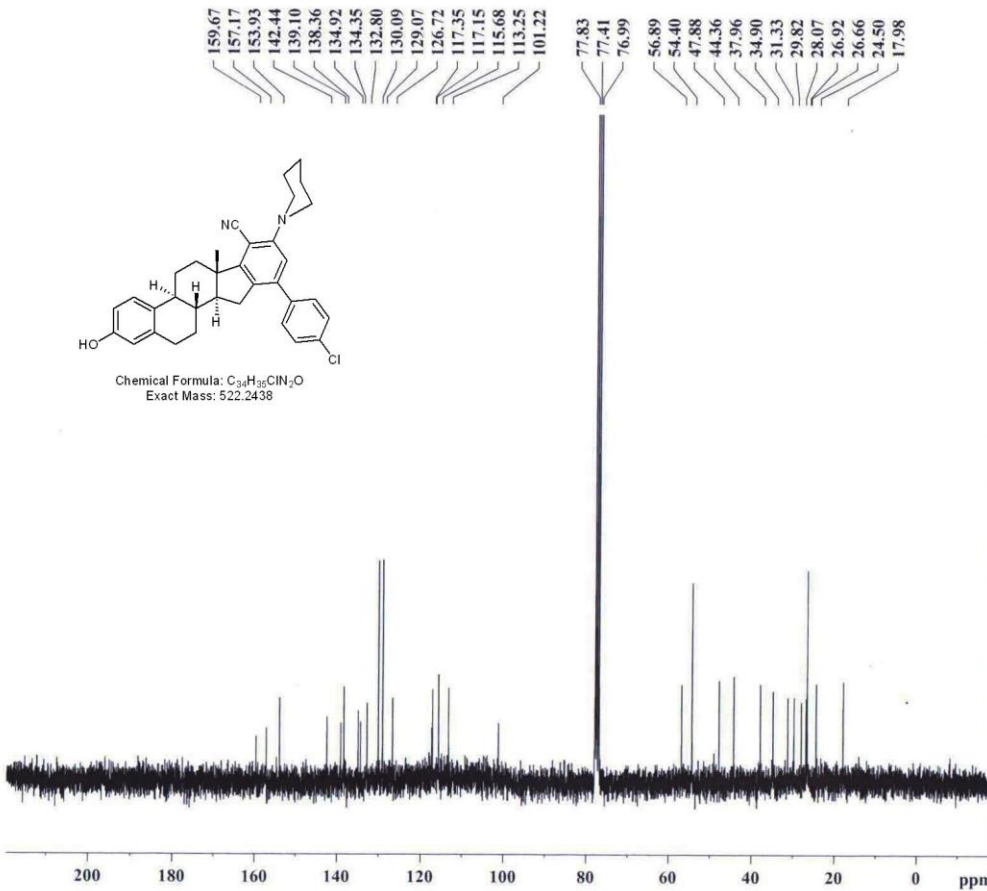
F2 - Acquisition Parameters
Date_ 20140826
Time 13.09
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 62
DS 2
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 181
DW 55.600 usec
DE 6.00 usec
TE 300.7 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 7.15 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299972 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

RSC Advances

CIMAP-CARBON
PROJECT NO.: MLP-04



Current Data Parameters
NAME atghmk270.p
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date 20140903
Time 11.31
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 800
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 301.6 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TD0 1

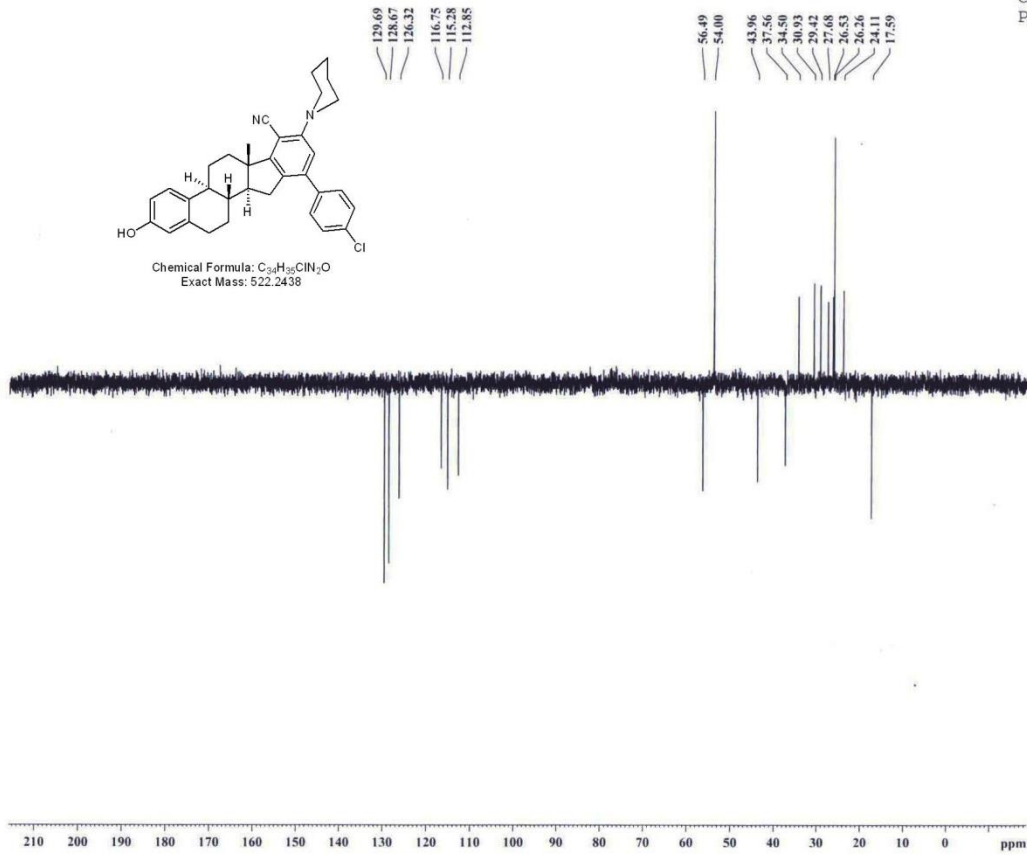
===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 -6.00 dB
SFO1 75.4752950 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 25.00 dB
PL13 29.00 dB
SFO2 300.1312000 MHz

F2 - Processing parameters
SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

RSC Advances

CIMAP-DEPT 135
PROJECT NO.: ILP-13



Current Data Parameters
NAME atgmk270.p
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140903
Time 11:50
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG dept135
TD 65536
SOLVENT CDC13
NS 712
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 6.00 usec
TE 301.6 K
CNST2 137.000000
D1 2.00000000 sec
d2 0.00364964 sec
d12 0.00002000 sec
DELTA 0.00001528 sec
TDO 1

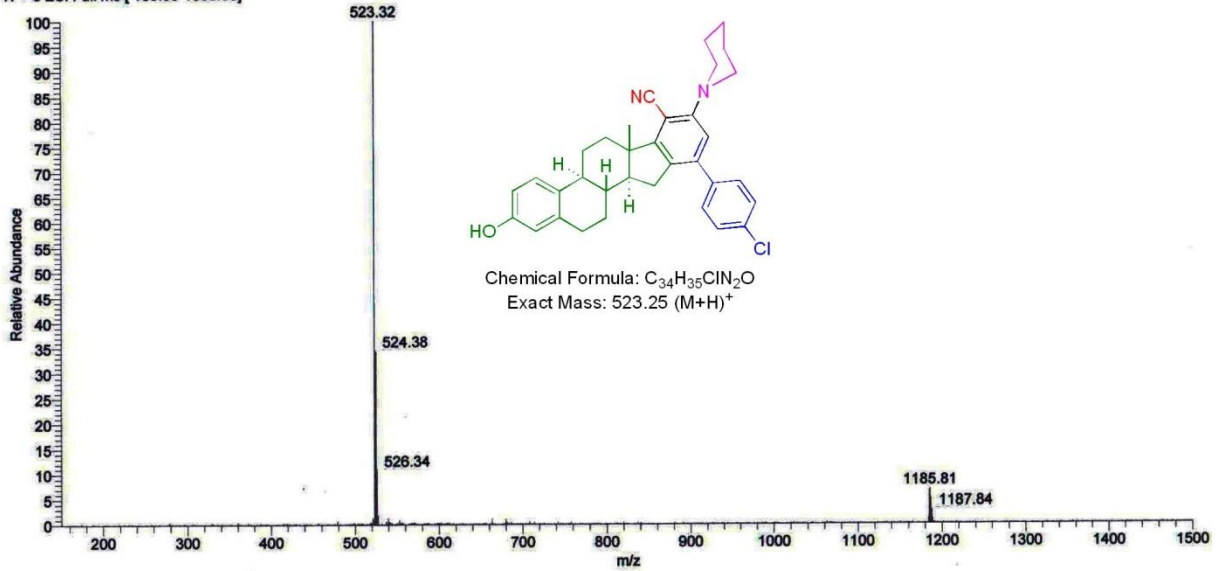
CHANNEL f1
NUC1 13C
P1 12.00 usec
p2 24.00 usec
PL1 -6.90 dB
SFO1 75.4752953 MHz

CHANNEL f2
CPDPRG2 waltz64
NUC2 1H
P3 7.15 usec
p4 14.30 usec
PCPD2 80.00 usec
PL2 4.00 dB
PL12 25.00 dB
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

Sample ID: NR-ATG-270
Acquisition Date: 02/04/15 14:01:35

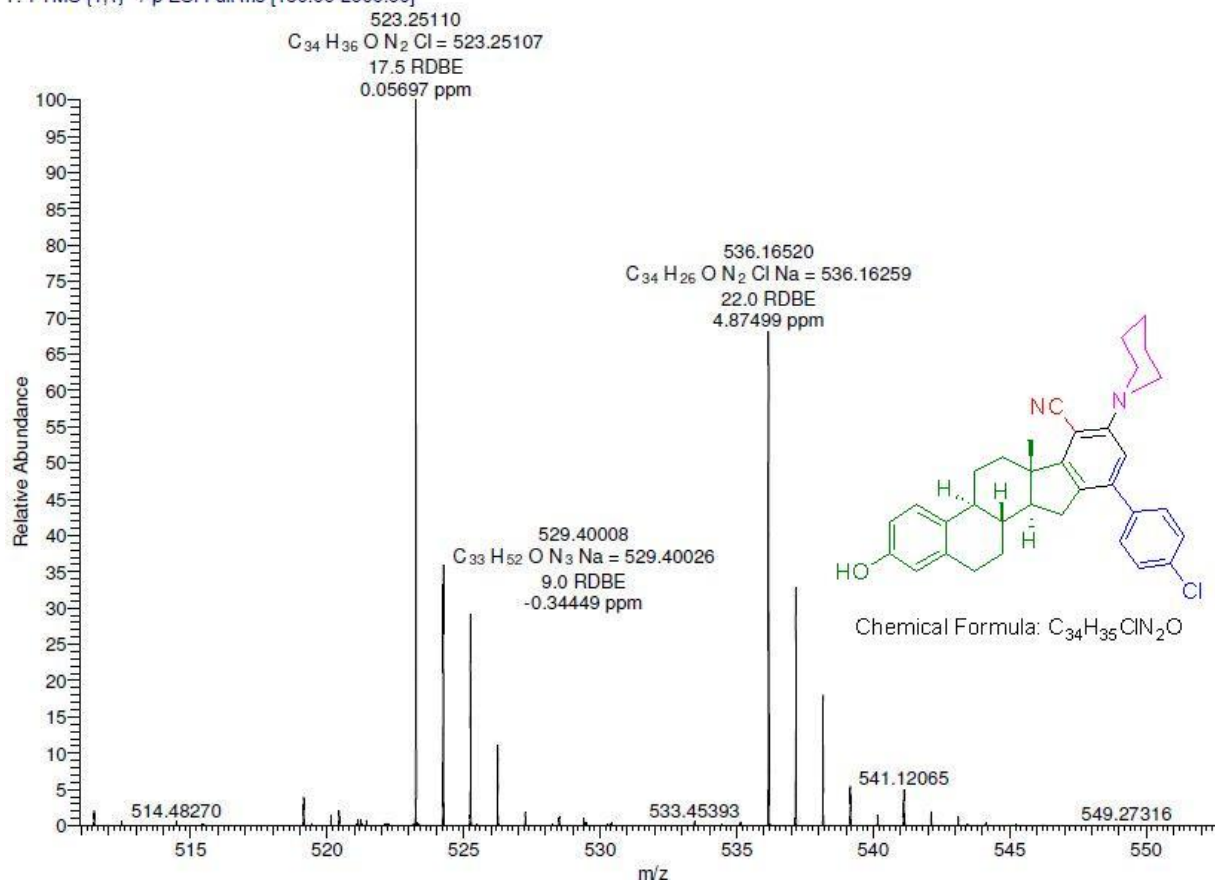
151O4FEB53 #15-35 RT: 0.30-0.70 AV: 21 SB: 2 0.01, 0.01 NL: 2.28E7
T: + c ESI Full ms [150.00-1500.00]



ION TRAP LCQ ADVANTAGE MAX
THERMO ELECTRON CORPORATION

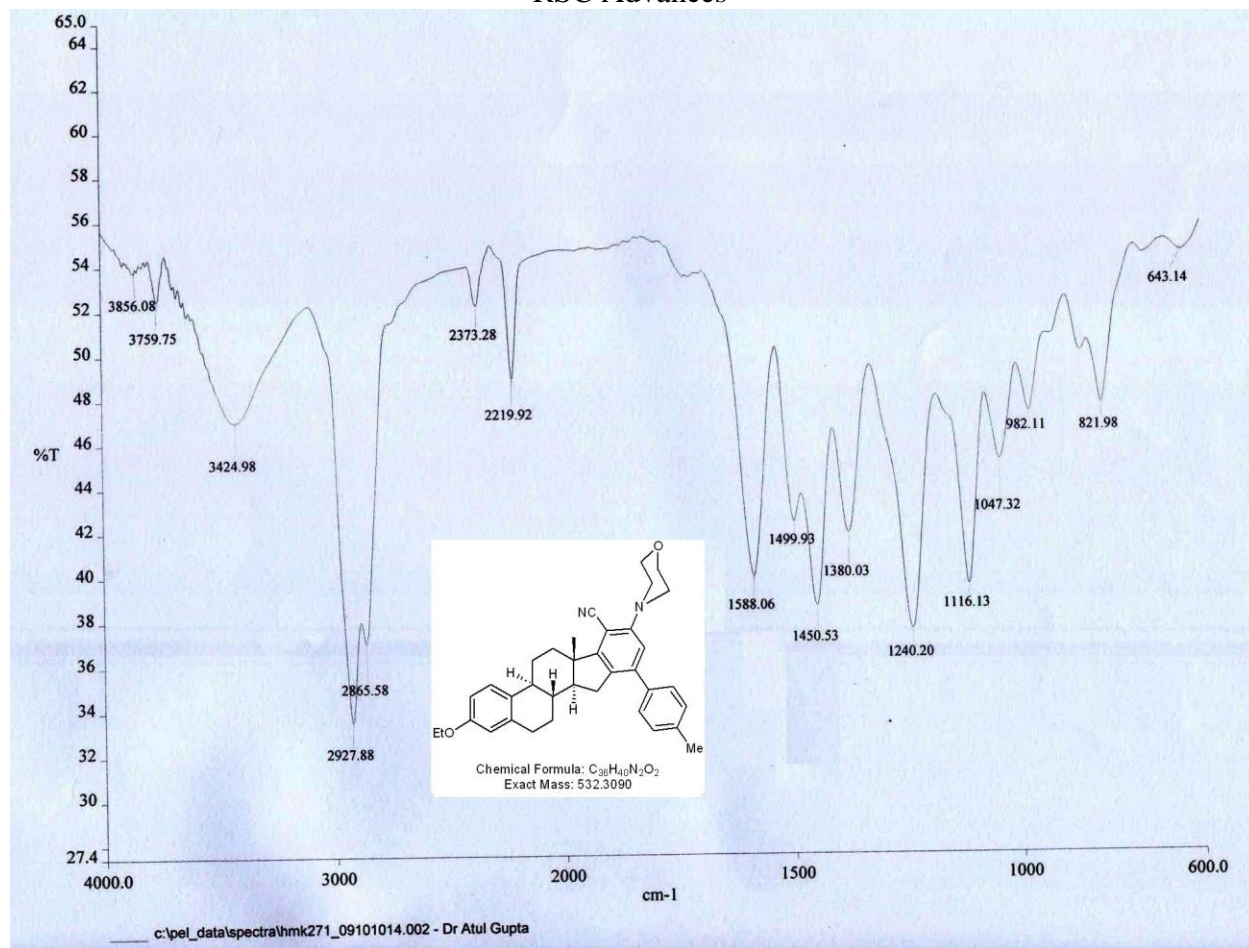
MCS-7H #4-19 RT: 0.02-0.13 AV: 16 NL: 4.36E6

T: FTMS (1,1) + p ESI Full ms [150.00-2000.00]

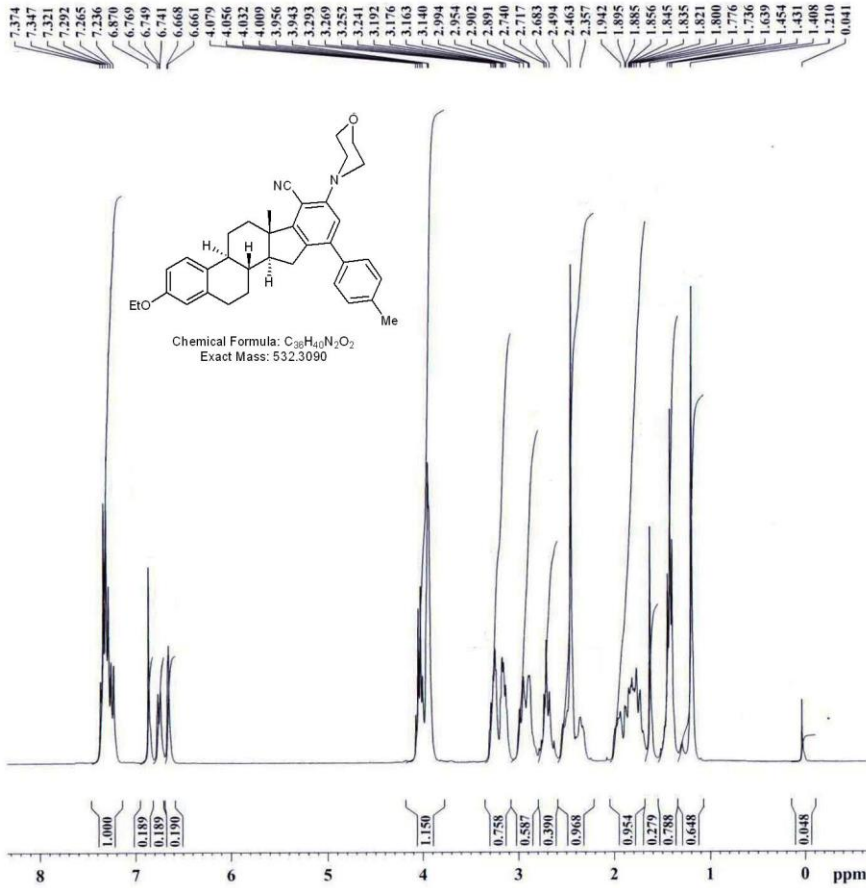


(+)(6bS,8aS,13aS,13bS)-4-ethoxy-8a-methyl-10-morpholino-12-p-tolyl-2,6b,7,8,8a,13,13a,13b-octahydro-1H-indeno[2,1-a]phenanthrene-9-carbonitrile (7i)

RSC Advances



RSC Advances



CIMAP PROTON
PROJECT NO.: mlp-02

Current Data Parameters
NAME atghmk271.p
EXPNO 1
PROCNO 1

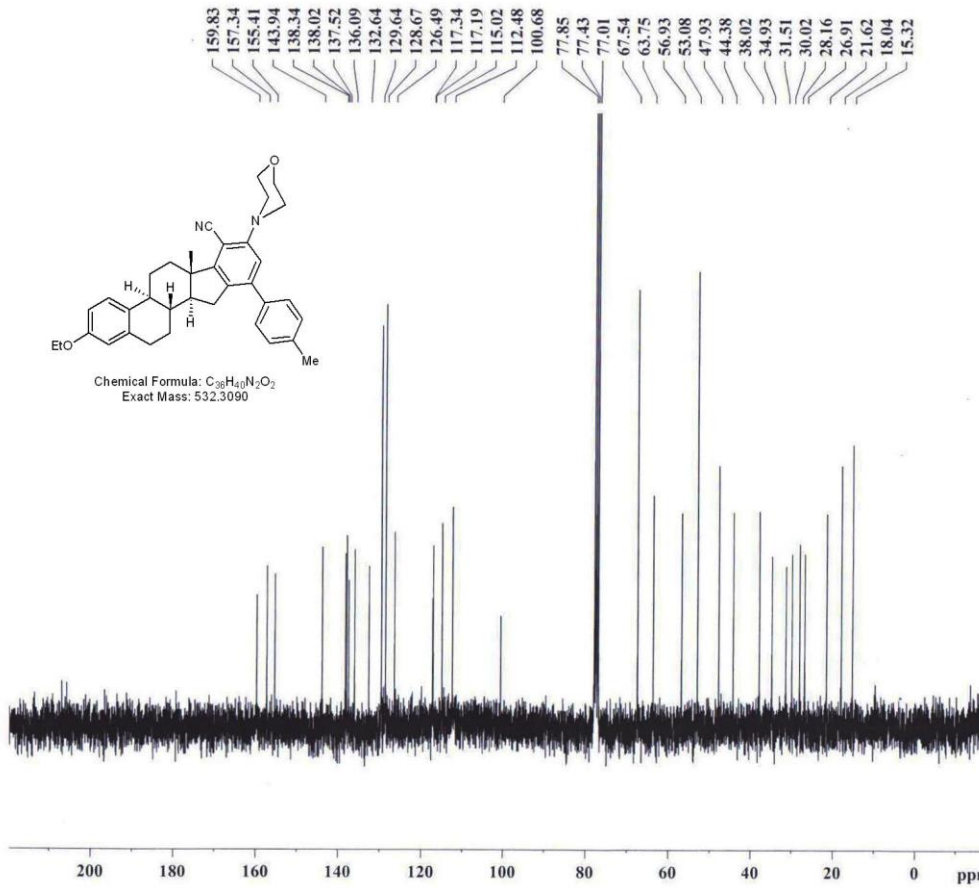
F2 - Acquisition Parameters
Date 20140826
Time 13.01
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 26
DS 2
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 181
DW 55.600 usec
DE 6.00 usec
TE 300.9 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 7.15 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299972 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

RSC Advances

CIMAP-CARBON
PROJECT NO.:MLP-04



Current Data Parameters
NAME atghmk271.p
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140903
Time 10.24
INSTRUM spect
PROBHD 5 mm Multinuel
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 301.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

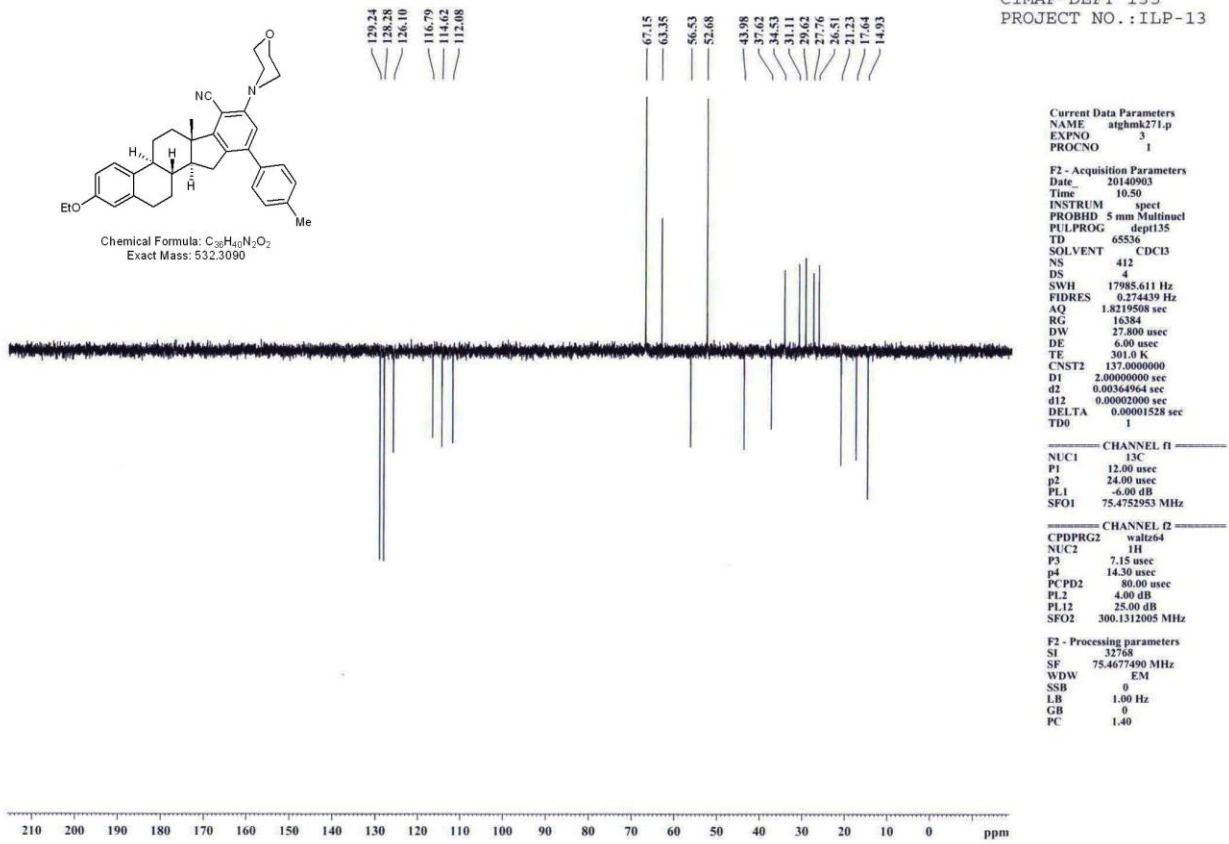
==== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 -6.00 dB
SFO1 75.4752950 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 25.00 dB
PL13 29.00 dB
SFO2 300.1312000 MHz

F2 - Processing parameters
SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

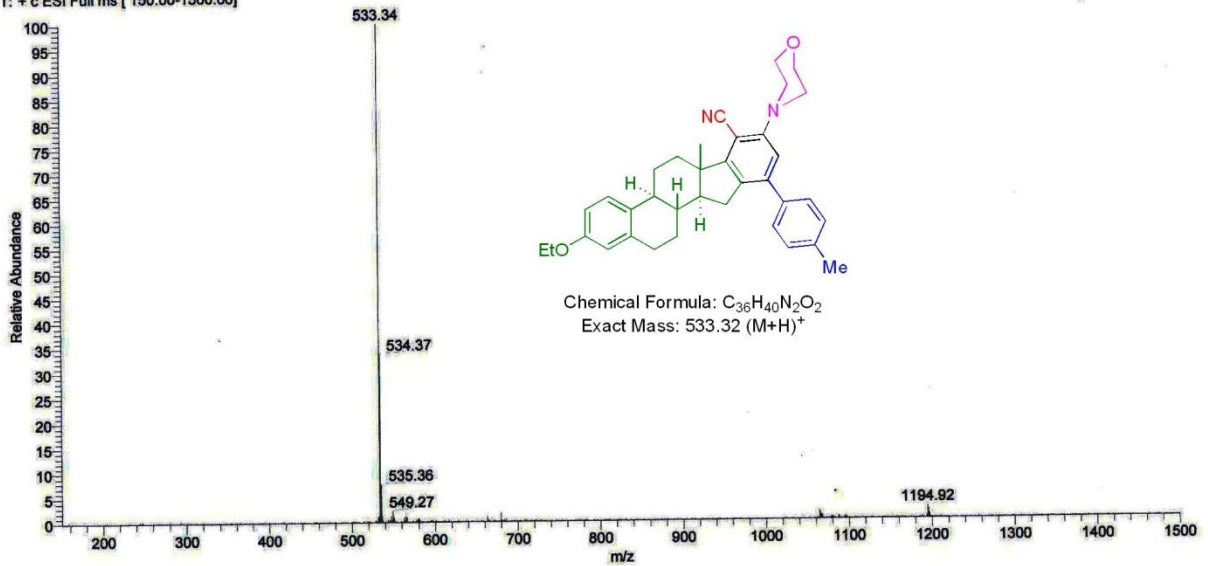
RSC Advances

CIMAP-DEPT 135
PROJECT NO. : ILP-13

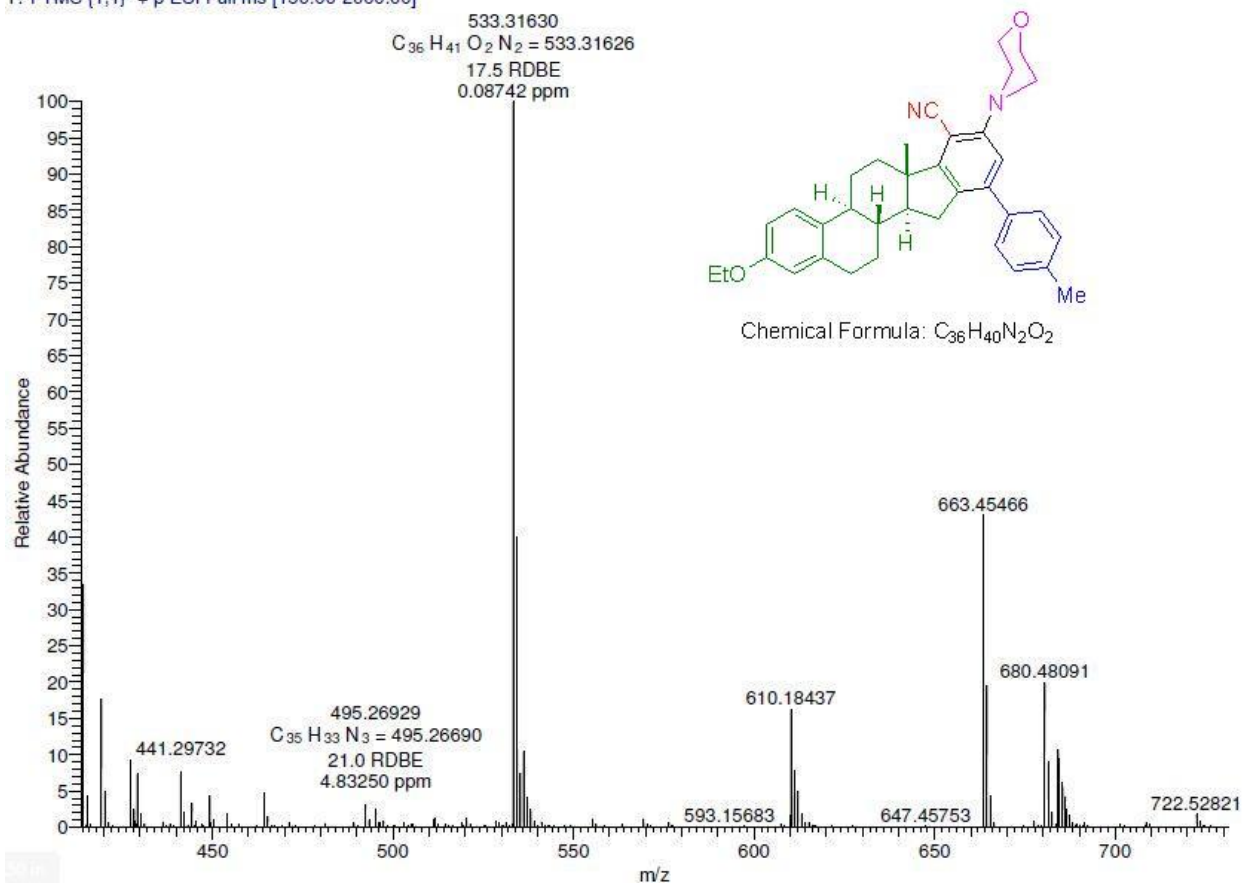


Sample ID: NR-ATG-271
Acquisition Date: 02/04/15 13:59:33

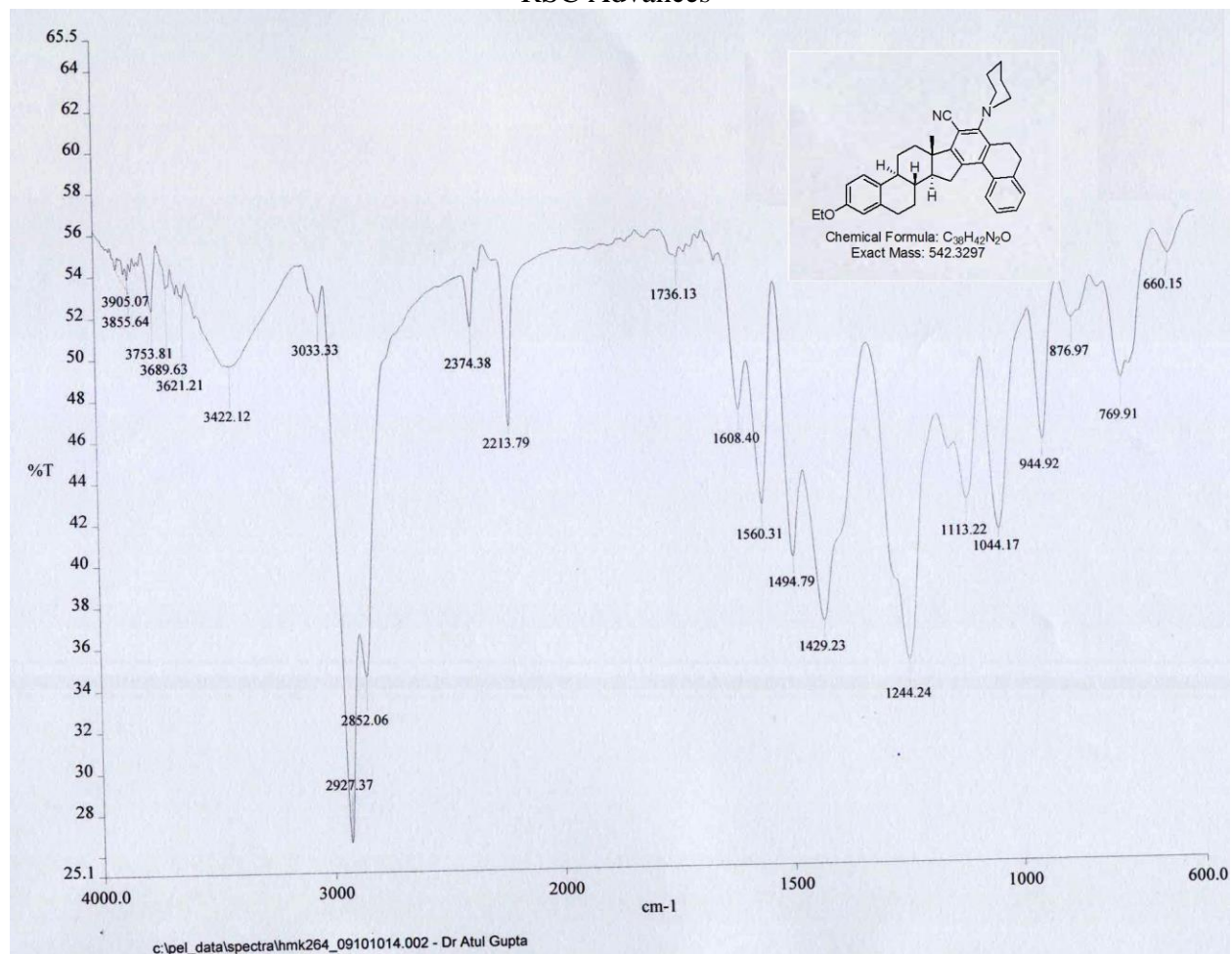
15I04FEB52 #15-35 RT: 0.30-0.70 AV: 21 SB: 2 0.01, 0.01 NL: 2.84E7
T: + c ESI Full ms [150.00-1500.00]



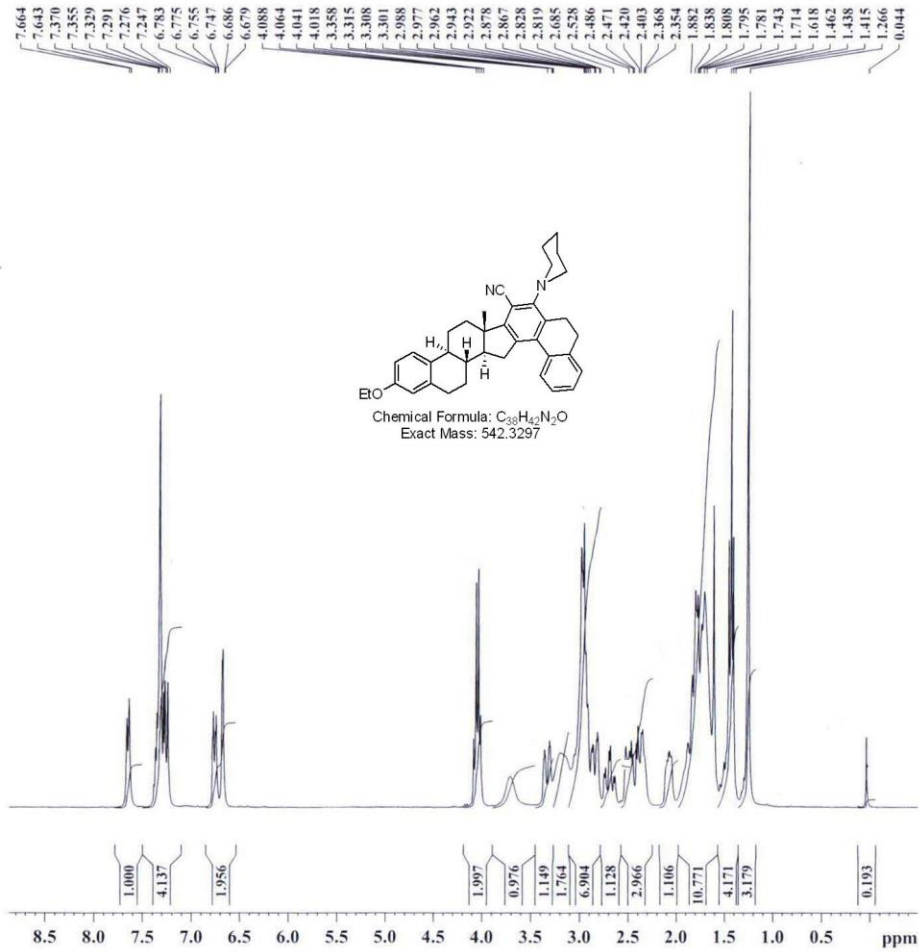
ION TRAP LCQ ADVANTAGE MAX
THERMO ELECTRON CORPORATION

MCS-71 #4-20 RT: 0.02-0.14 AV: 17 NL: 7.75E6
T: FTMS {1,1} + p ESI Full ms [150.00-2000.00]

(+)(6bS,8aS,17aS,17bS)-4-ethoxy-8a-methyl-10-(piperidin-1-yl)-1,2,6b,7,8,8b,11,12,17a,17-decahydro-17H-cyclopenta[*a*:c]bisphenanthrene-9-carbonitrile (**12a**)



RSC Advances



CIMAP PROTON
PROJECT NO.: mlp-02

Current Data Parameters
NAME atghmk264.p
EXPNO 1
PROCNO 1

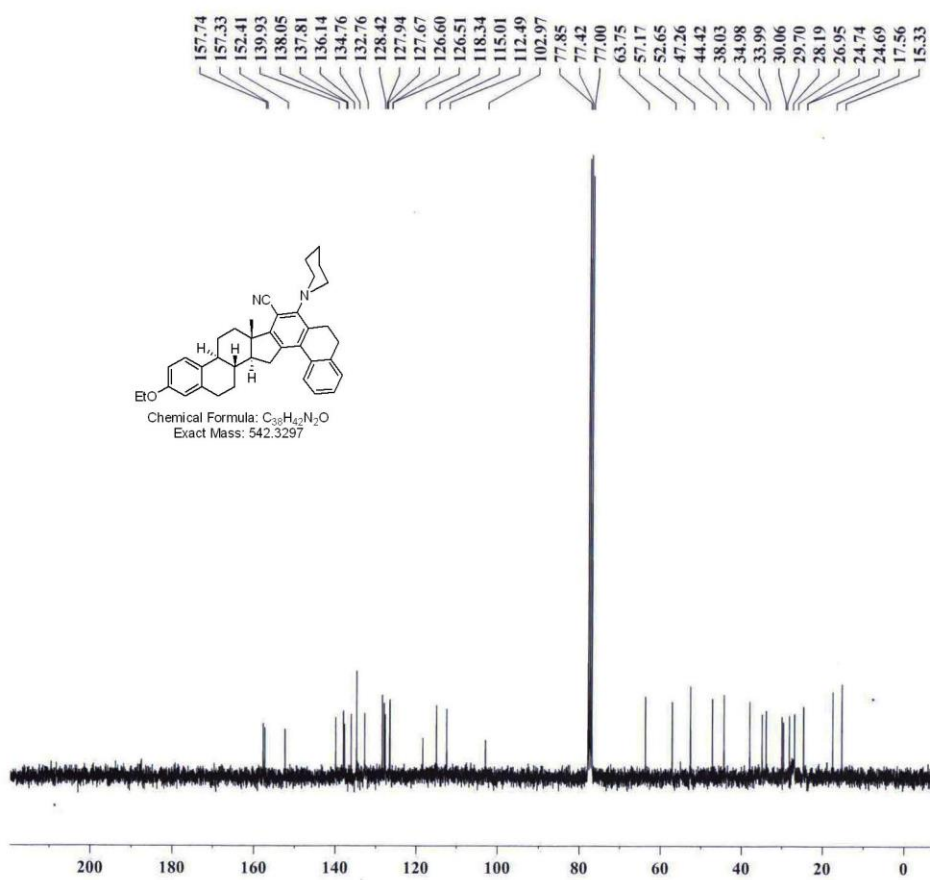
F2 - Acquisition Parameters
Date_ 20140826
Time 13.14
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 181
DW 55.600 usec
DE 6.00 usec
TE 300.5 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 7.15 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299972 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

RSC Advances

CIMAP-CARBON
PROJECT NO.: MLP-04



Current Data Parameters
 NAME atghmk264.p
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date 20140915
 Time 16.05
 INSTRUM spect
 PROBHD 5 mm Multinuc
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 655
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 32768
 DW 27.800 usec
 DE 6.00 usec
 TE 300.9 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.89999998 sec
 TD0 1

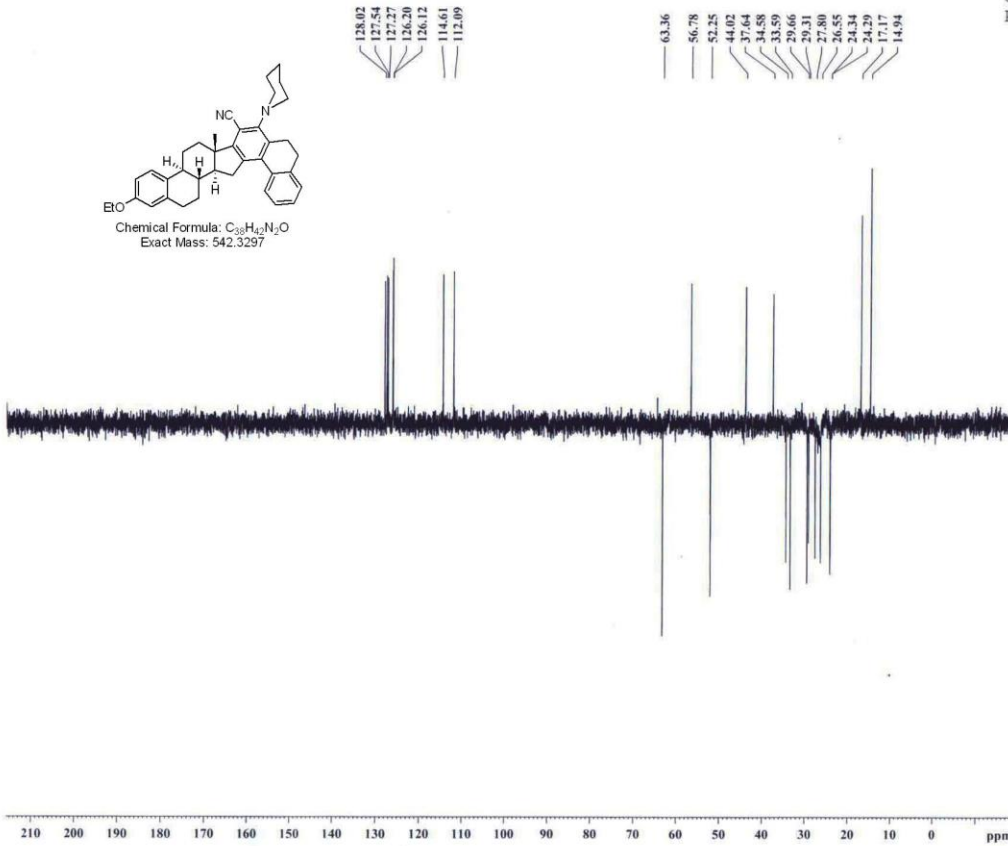
===== CHANNEL f1 =====
 NUC1 13C
 P1 12.00 usec
 PL1 -6.00 dB
 SFO1 75.4752950 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 4.00 dB
 PL12 25.00 dB
 PL13 29.00 dB
 SFO2 300.1312000 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677190 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

RSC Advances

CIMAP-DEPT 135
PROJECT NO. : ILP-13



Current Data Parameters
NAME atghmk264.p
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140915
Time 16.16
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 540
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 6.00 usec
TE 300.9 K
CNST2 137.0000000
D1 2.0000000 sec
d2 0.00364964 sec
d12 0.00002000 sec
DELTA 0.00001528 sec
TD0

CHANNEL f1
NUC1 13C
P1 12.00 usec
p2 24.00 usec
PL1 -4.00 dB
SFO1 75.4752953 MHz

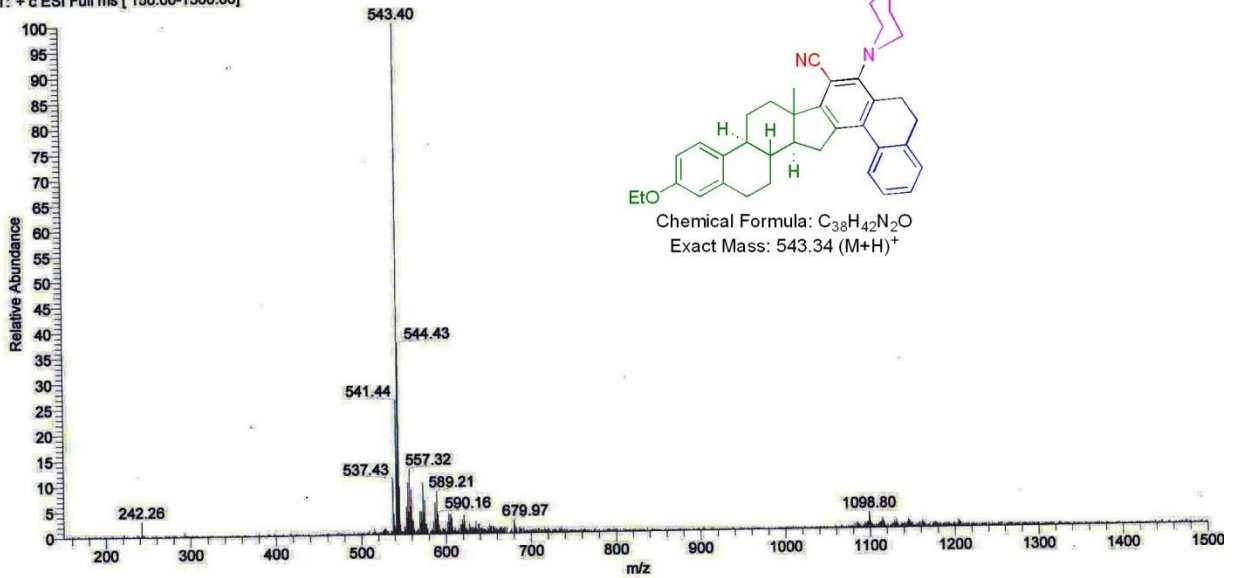
CHANNEL f2
CPDPRG2 waltz164
NUC2 1H
P3 7.15 usec
p4 14.30 usec
PCPD2 80.00 usec
PL2 4.00 dB
PL12 25.00 dB
SFO2 300.1312005 MHz

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

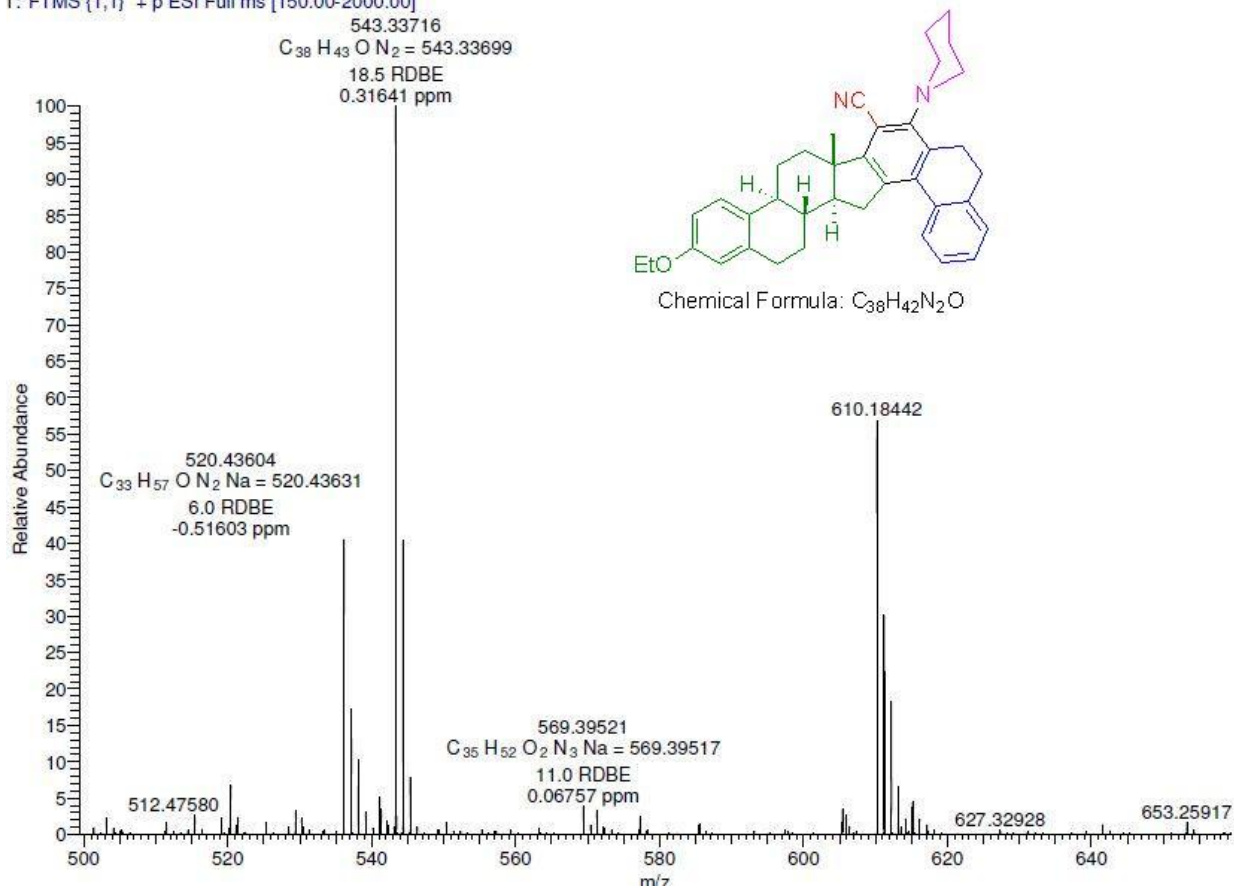
SAIF, CSIR-CDRI, Lucknow

Data File: 15124FEB58
Original Data Path: 15124FEB58.RAW
Current Data Path: C:\Xcalibur\data\FEB2015\24FEB2015\
Sample ID: NR-ATK-264
Acquisition Date: 02/24/15 13:59:59

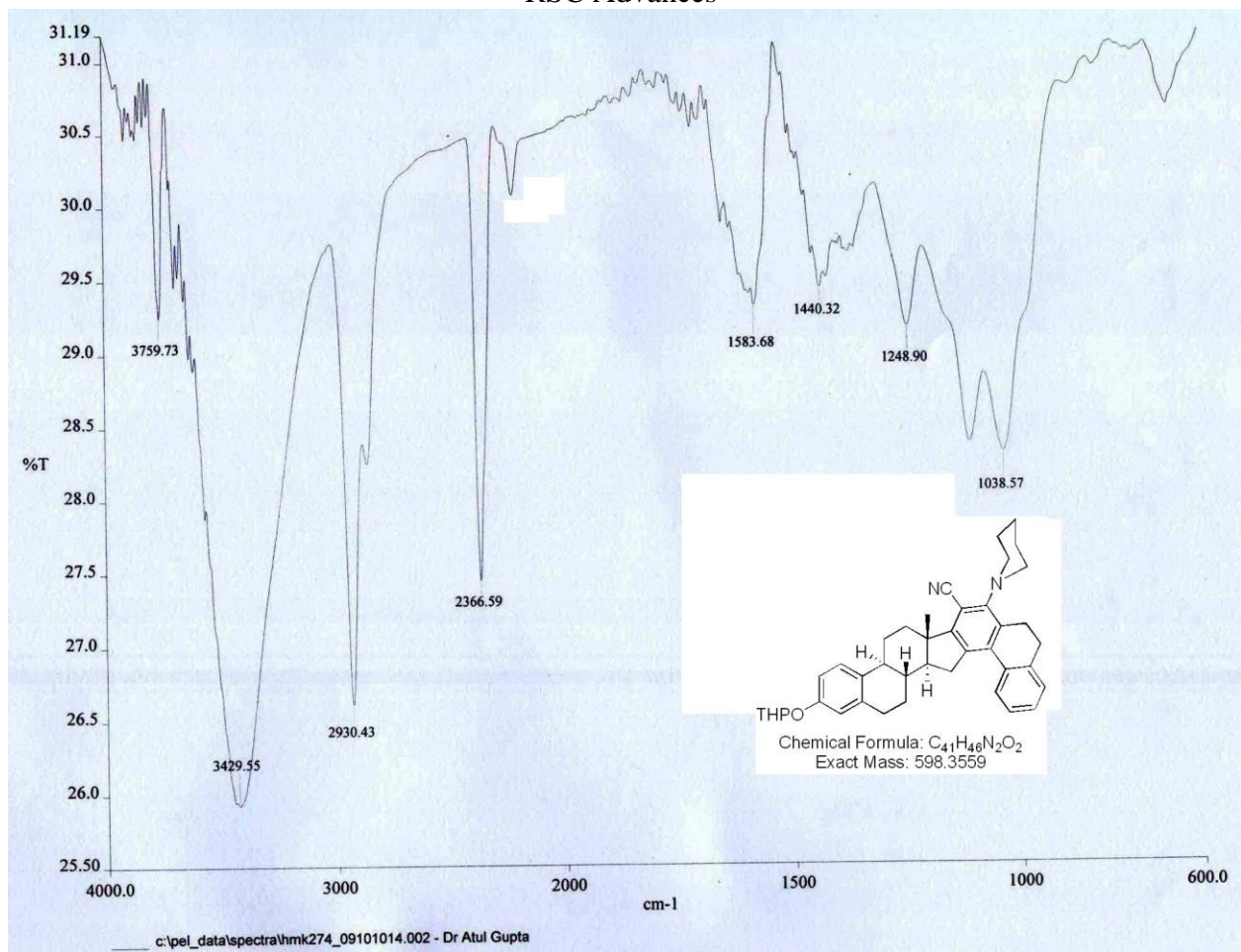
15124FEB58 #15-35 RT: 0.30-0.71 AV: 21 SB: 2 0.00, 0.00 NL: 5.81E6
T: + c ESI Full ms [150.00-1500.00]



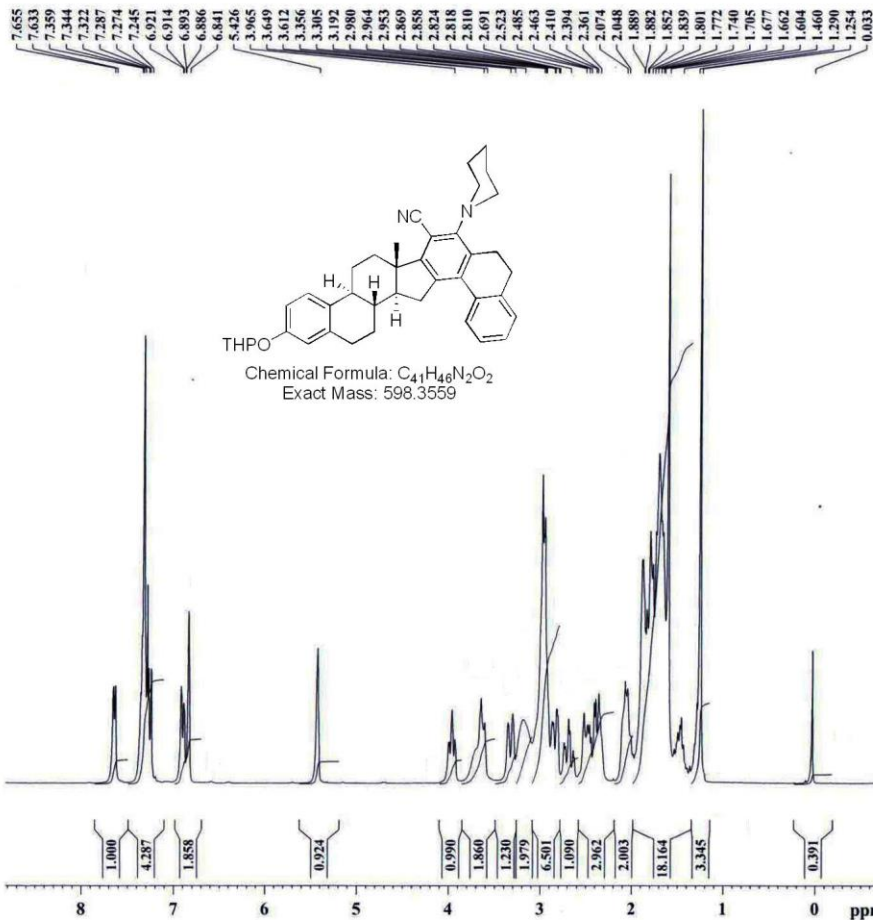
ION TRAP LCQ ADVANTAGE MAX
THERMO ELECTRON CORPORATION

MCS-12A #4-19 RT: 0.02-0.14 AV: 16 NL: 1.71E6
T: FTMS (1,1) + p ESI Full ms [150.00-2000.00]

(+)(6bS,8aS,17aS,17bS)-4-(tetrahydro-2H-pyranoxo)-8a-methyl-10-(piperidin-1-yl)-1,2,6b,7,8,8b,11,12,17a,17-decahydro-17H-cyclopenta[a:c]bisphenanthrene-9-carbonitrile (**12b**)



RSC Advances



CIMAP PROTON
PROJECT NO.: mlp-02

Current Data Parameters
NAME atghmk274.p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date 20140903
Time 12.46
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 256
DW 55.600 usec
DE 6.00 usec
TE 301.7 K
D1 1.00000000 sec
TD0 1

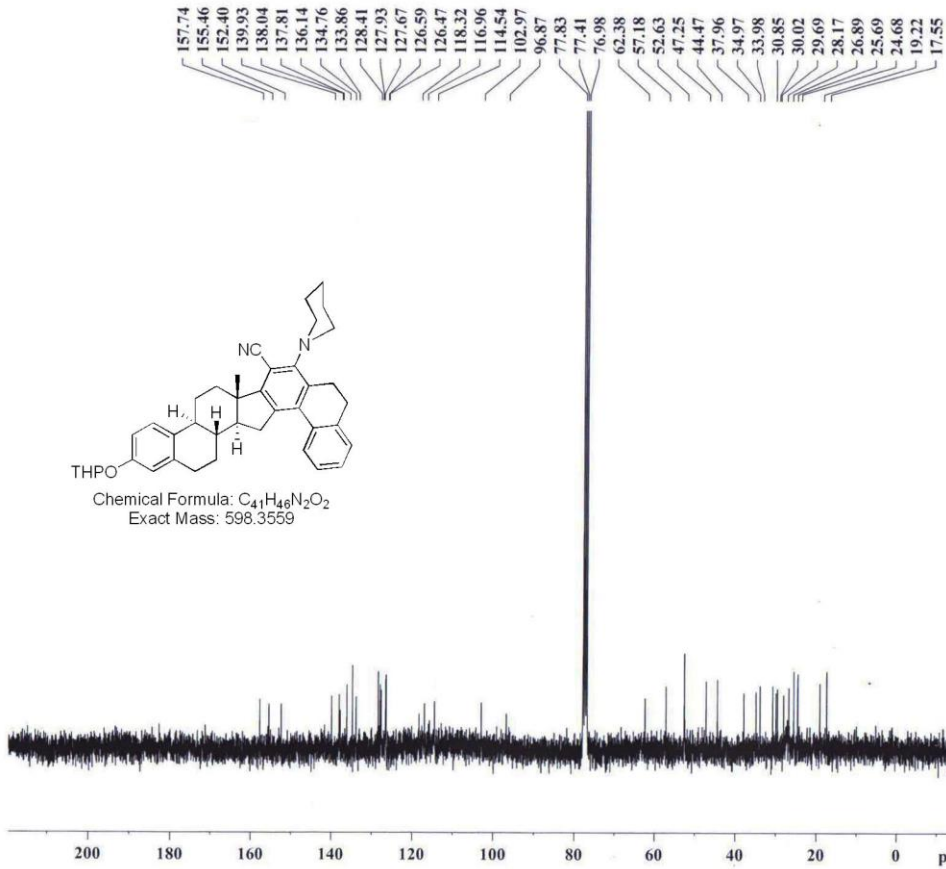
CHANNEL f1
NUC1 1H
P1 7.15 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299972 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

RSC Advances

CIMAP-CARBON
PROJECT NO.: MLP-04

on line



Current Data Parameters
NAME atghmk274.p
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140903
Time 13.02
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 904
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 302.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

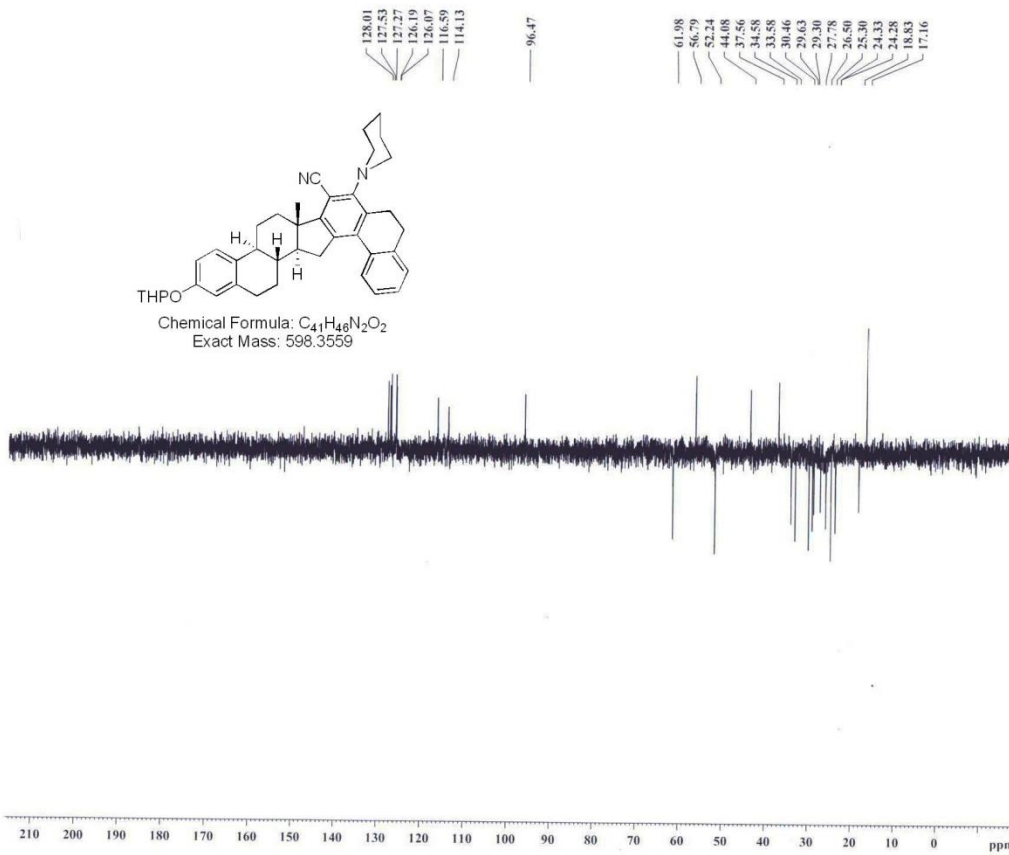
===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 -6.00 dB
SFO1 75.4752950 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 25.00 dB
PL13 29.00 dB
SFO2 300.1312000 MHz

F2 - Processing parameters
SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

RSC Advances

CIMAP-DEPT 135
PROJECT NO. : ILP-13



Current Data Parameters
NAME atgmk274.p
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date 20140903
Time 14.00
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG dep135
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 6.00 usec
TE 302.6 K
CNST2 137.0000000
D1 2.00000000 sec
d2 0.00364964 sec
d12 0.00002000 sec
DELTA 0.00001528 sec
TD0 1

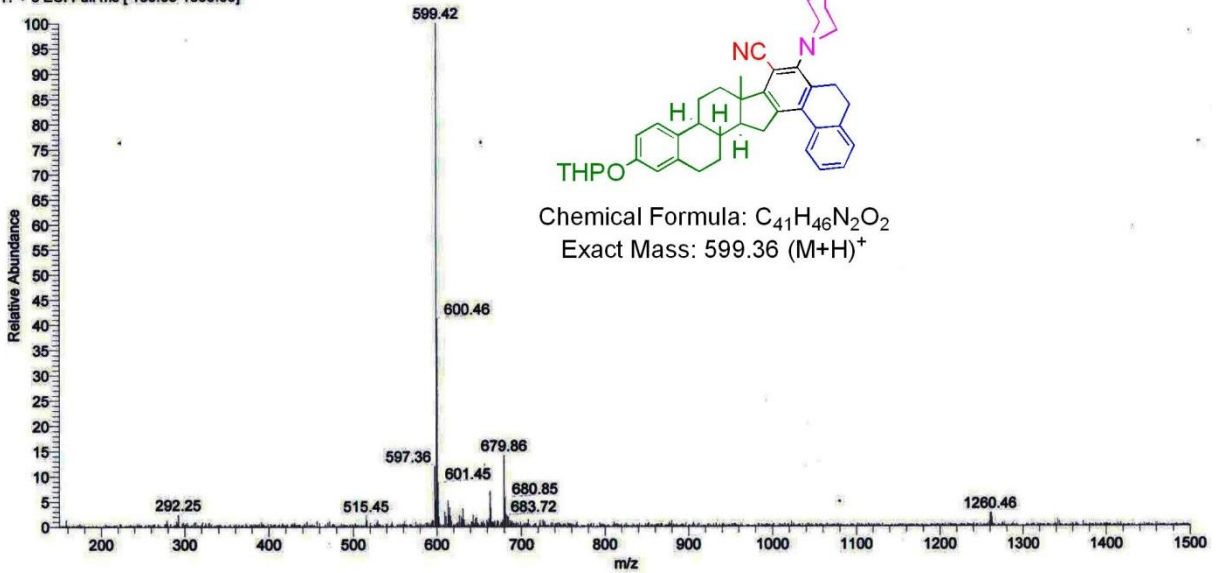
CHANNEL f1
NUC1 13C
P1 12.00 usec
p2 24.00 usec
PL1 -6.00 dB
SFO1 75.4752953 MHz

CHANNEL f2
CPDPRG2 waltz64
NUC2 1H
P3 7.15 usec
p4 14.30 usec
PCPD2 80.00 usec
PL2 4.00 dB
PL12 25.00 dB
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

Sample ID: NR-ATG-274
Acquisition Date: 02/23/15 13:46:20

15123FEB48 #15-35 RT: 0.30-0.71 AV: 21 SB: 2 0.00, 0.00 NL: 6.99E8
T: + c ESI Full ms [150.00-1500.00]



ION TRAP LCQ ADVANTAGE MAX
THERMO ELECTRON CORPORATION

NCS-12B #4-19 RT: 0.02-0.14 AV: 16 NL: 7.42E5

T: FTMS (1,1) + p ESI Full ms [150.00-2000.00]

