

2-(3', 4'-dimethoxybenzylidene) tetralone induces anti-breast cancer activity through microtubule stabilization and activation of reactive oxygen species

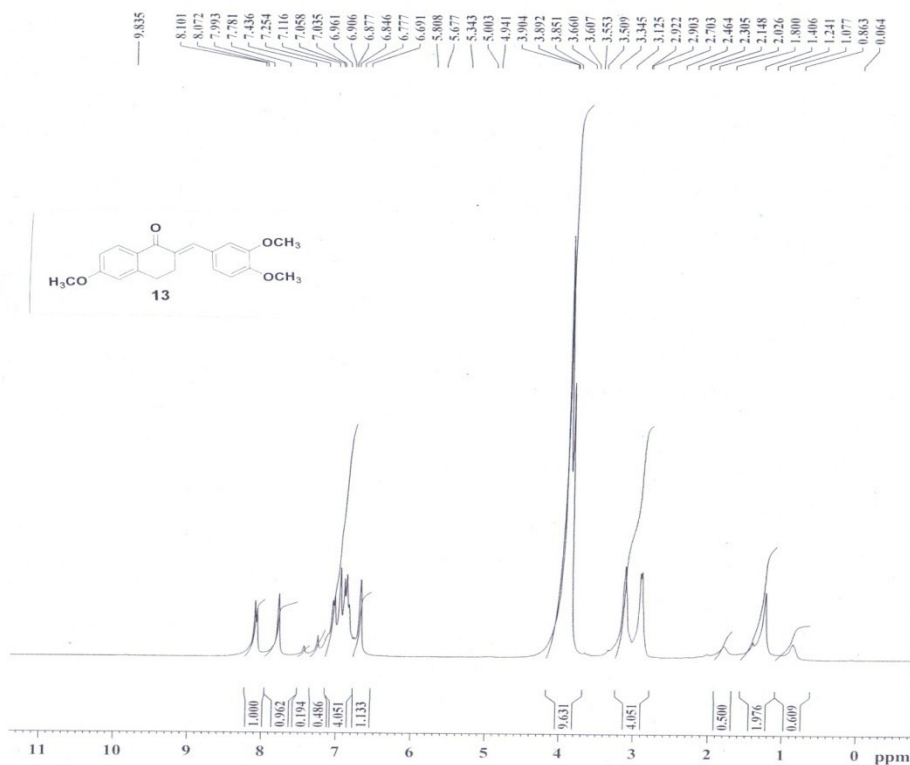
Yashveer Gautam,^{a†} Sonam Dwivedi,^{b†} Ankita Srivastava,^a Hamidullah,^b Arjun Singh,^a D. Chanda,^a Jyotsna Singh,^b Smita Rai,^b Rituraj Konwar,^{b*} and Arvind S. Negi^{a*}

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^b*CSIR-Central Drug Research Institute (CSIR-CDRI), B.S. 10/1, Sector 10, Jankipuram Extension, Sitapur Road, Lucknow-226031, India.*

Spectral data of compounds **13**, **15**, and **19**

Compound **13**: ^1H NMR



CIMAP PROTON
PROJECT NO.: mlp-02

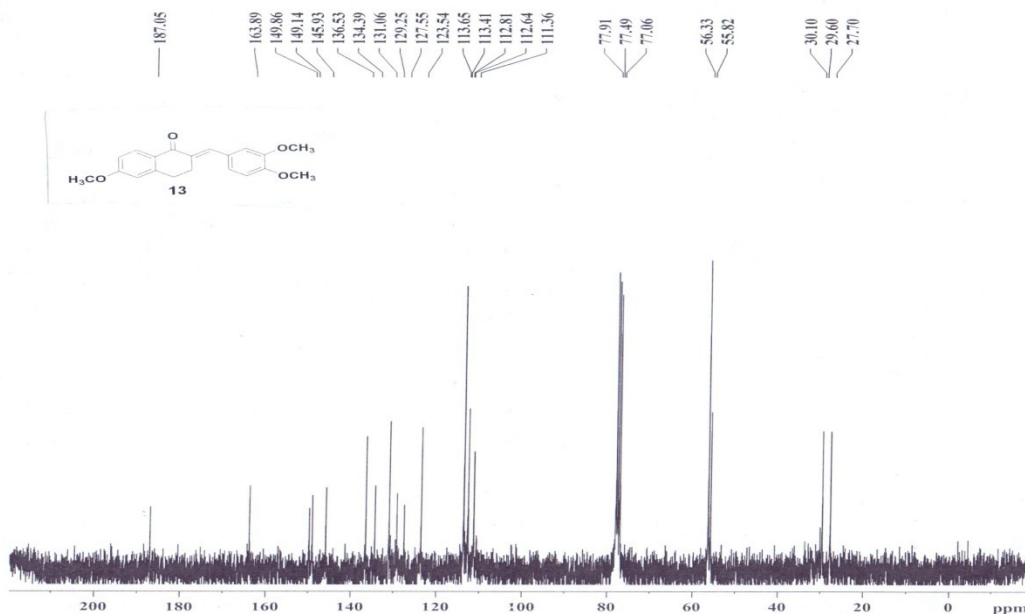
Current Data Parameters
NAME asnjaga.p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121231
Time 13.05
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 22
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 295.6 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 ^1H
P1 6.85 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300071 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

Compound **13**: ^{13}C NMR



CIMAP - CARBON
PROJECT NO.: MLP-04

Current Data Parameters
NAME asnjaga.p
EXPNO 2
PROCNO 1

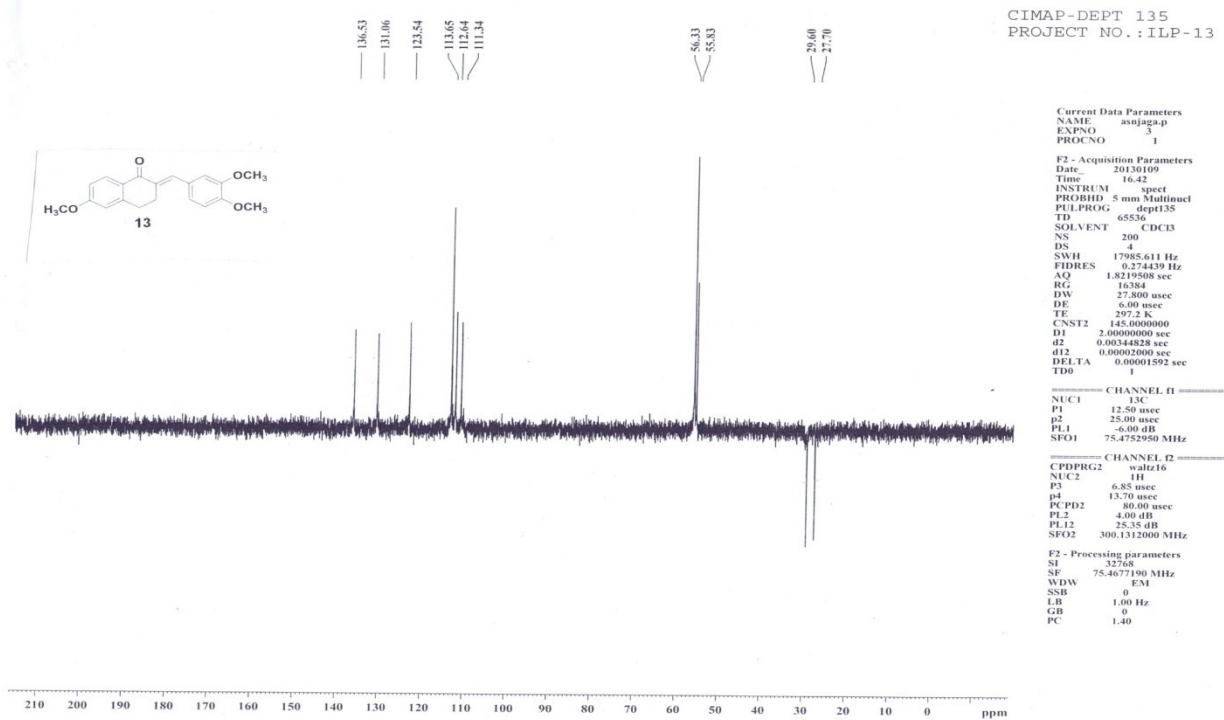
F2 - Acquisition Parameters
Date_ 20130109
Time 16.28
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 350
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 297.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999999 sec
TD0 1

===== CHANNEL f1 =====
NUC1 ^{13}C
P1 12.50 usec
PL1 -6.00 dB
SFO1 75.4752950 MHz

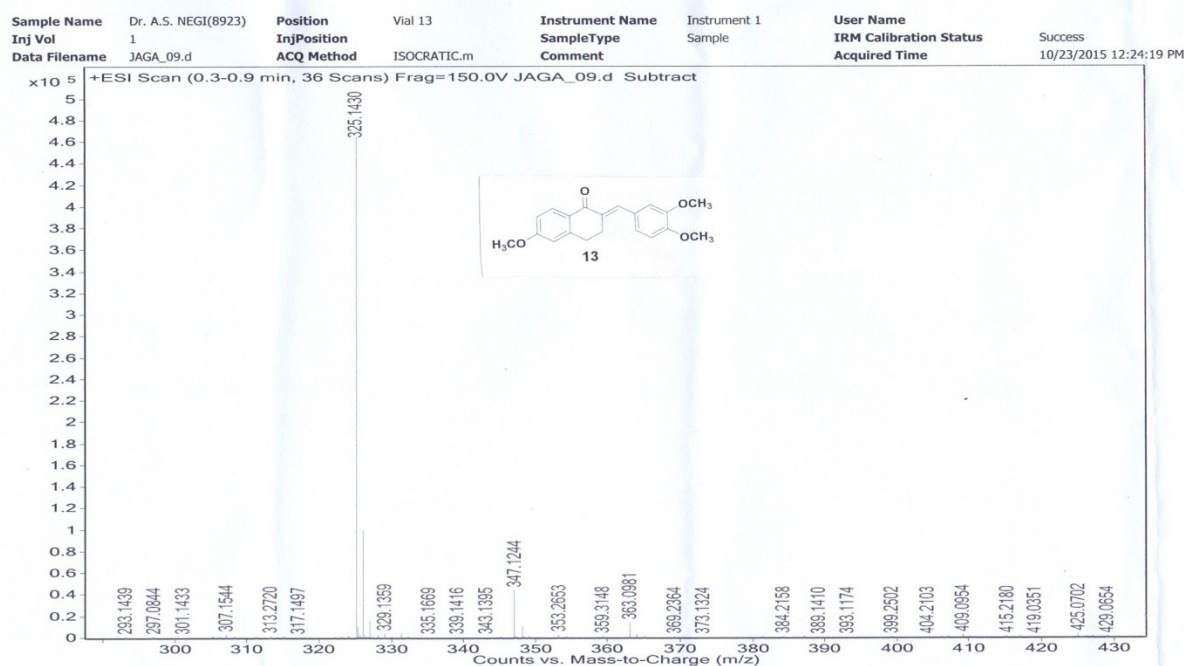
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 ^1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 25.35 dB
PL13 29.61 dB
SFO2 300.1312000 MHz

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

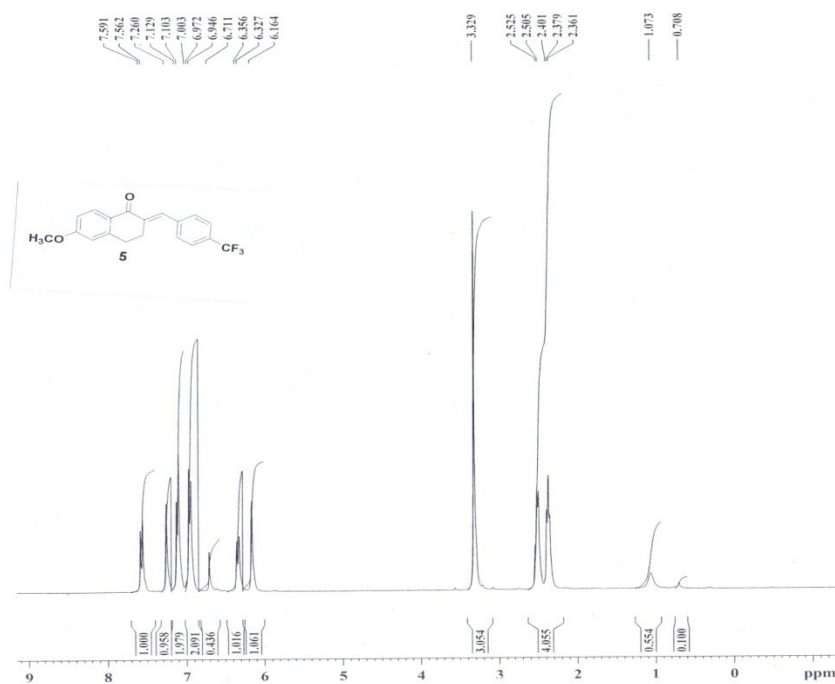
Compound 13: DEPT-135



Compound 13: HRMS



Compound 15: ¹H NMR



CIMAP-PROTON
PROJECT NO.: mlp-02

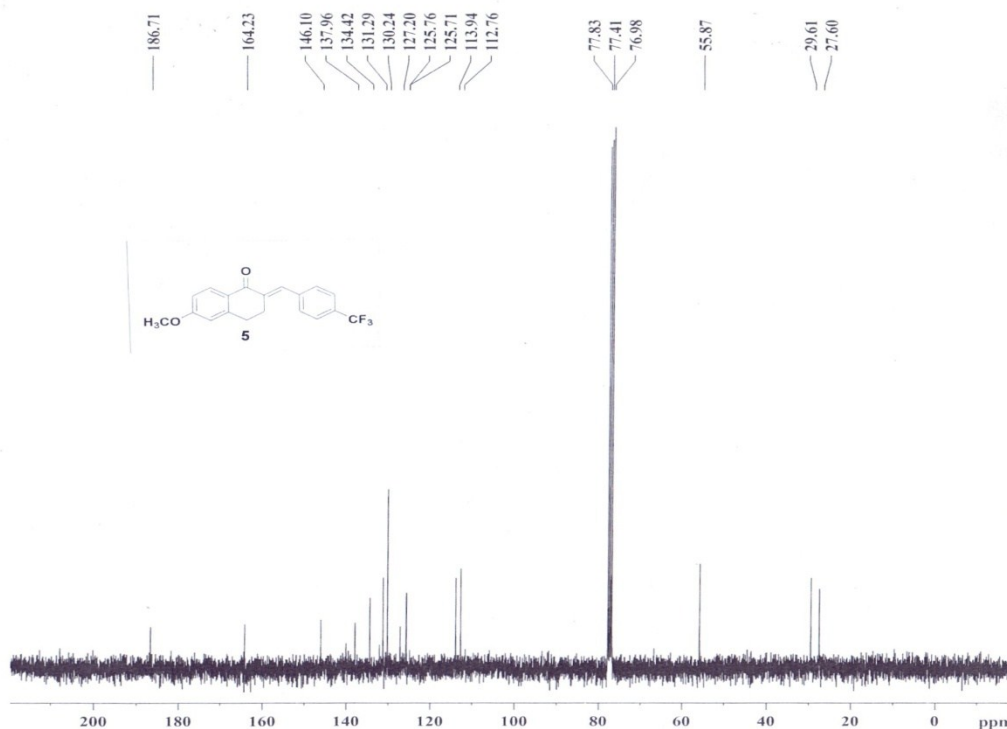
Current Data Parameters
NAME asnaaa1b.p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date 20130418
Time 15.49
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 287.4
DW 55.600 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 6.78 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1301713 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

Compound 15: ¹³C NMR



CIMAP-CARBON
PROJECT NO.: MLP-04

Current Data Parameters
NAME asnaaa1b.p
EXPNO 1
PROCNO 1

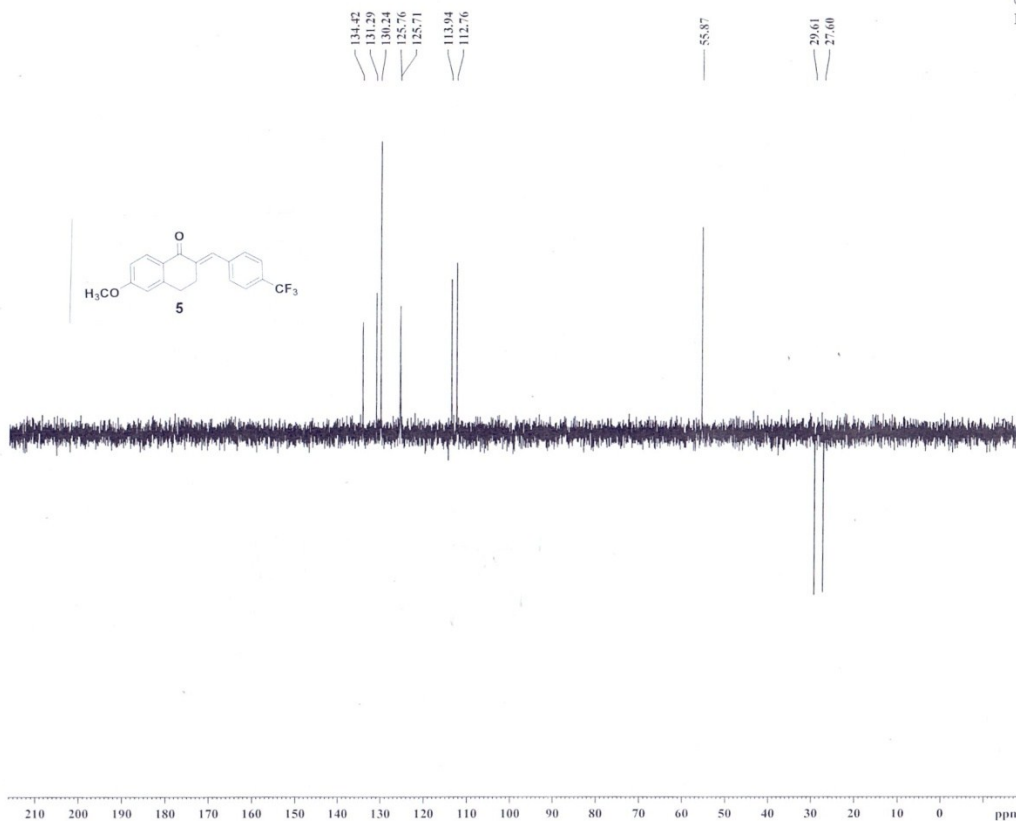
F2 - Acquisition Parameters
Date 20130418
Time 16.07
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 387
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 300.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.60 usec
PL1 -6.00 dB
SFO1 75.4752950 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 25.44 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

Compound 15: DEPT-135



CIMAP-DEPT 135
PROJECT NO.: ILP-13

Current Data Parameters
NAME asnaaab.p
EXPNO 3
PROCNO 1

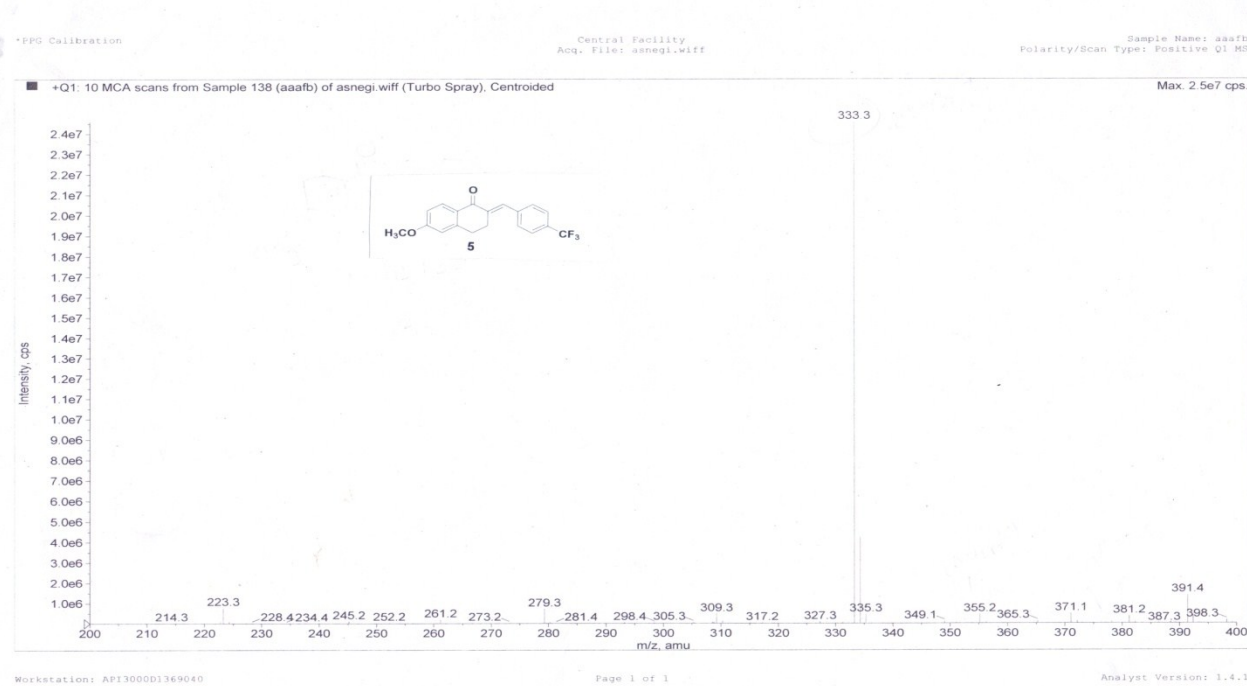
F2 - Acquisition Parameters
Date_ 20130418
Time_ 16.14
INSTRUM spect
PROBHD 5 mm Maltmuact
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 321
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 6.00 usec
TE 300.5 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.0001604 sec
TD0 1

CHANNEL f1
NUC1 13C
P1 12.60 usec
p2 25.20 usec
PL1 -6.00 dB
SFO1 75.4752950 MHz

CHANNEL g2
CPDPRG2 waltz16
NUC2 1H
P3 6.78 usec
pd 13.56 usec
PCPD2 80.00 usec
PL2 4.00 dB
PL12 25.44 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

Compound 15: ESI-Mass

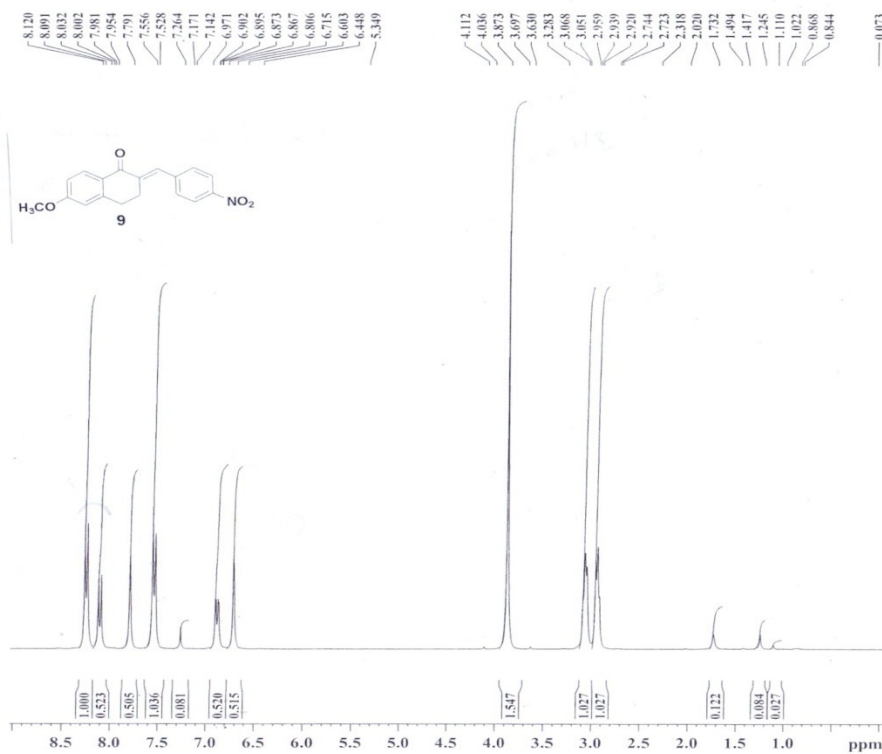


Workstation: API3000D1369040

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Analyst Version: 1.4.1

Compound 19: ¹H NMR



CIMAP-PROTON
PROJECT NO.: mlp-02

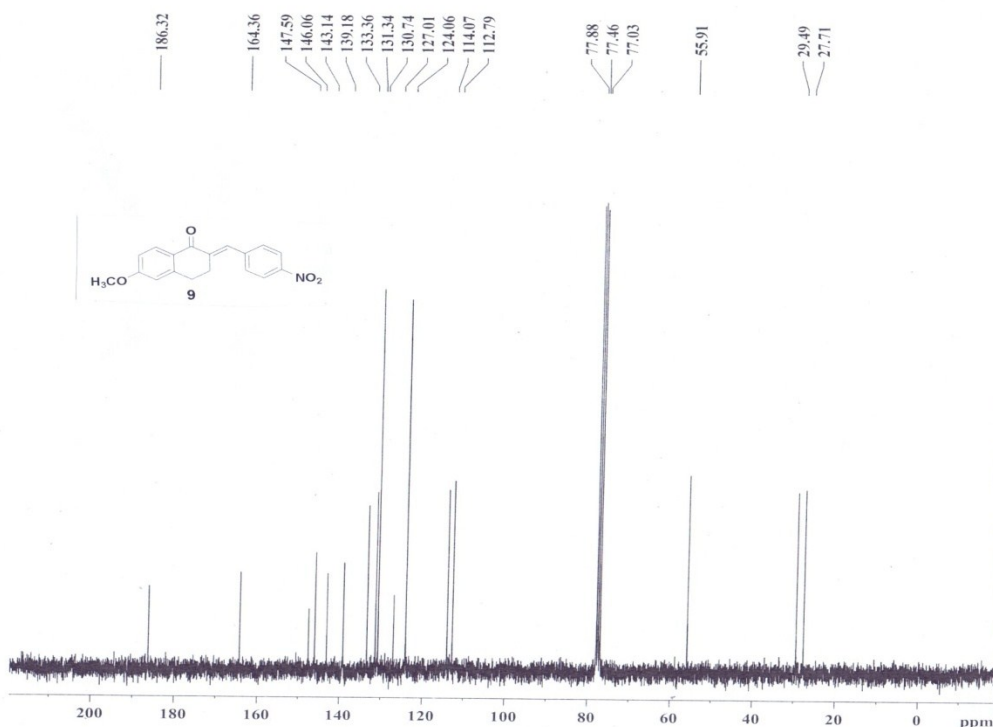
Current Data Parameters
NAME asbbbbit.p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130315
Time 16.04
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 5.308460 sec
RG 128
DW 81.000 usec
DE 6.00 usec
TE 300.3 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 6.78 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

Compound 19: ¹³C NMR



CIMAP-CARBON
PROJECT NO.: MLP-04

Current Data Parameters
NAME asbbbbit.p
EXPNO 2
PROCNO 1

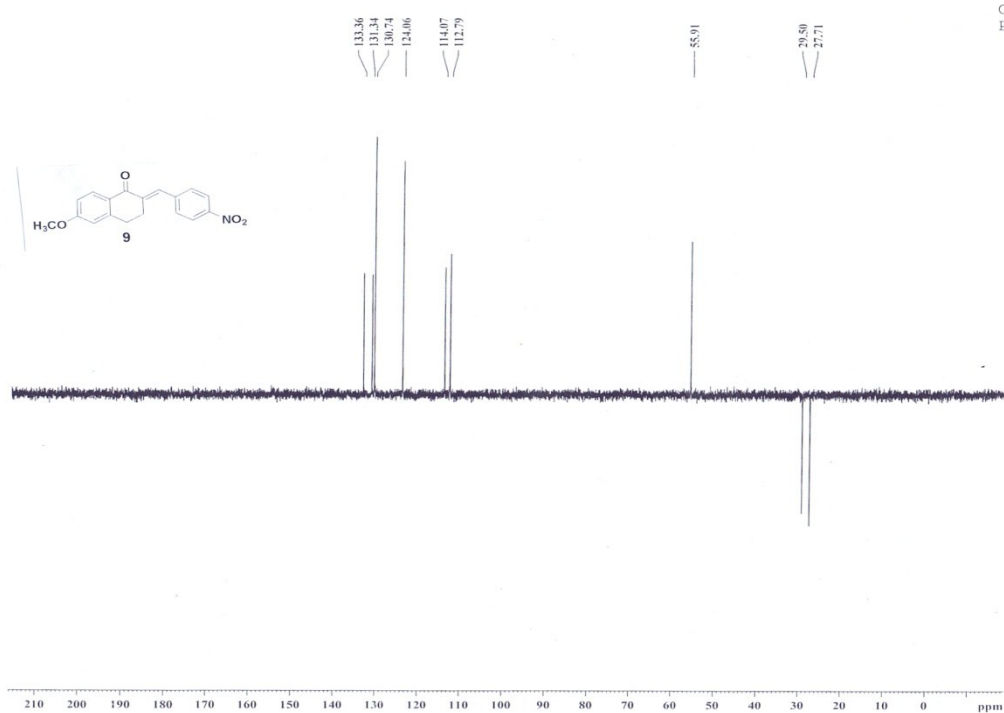
F2 - Acquisition Parameters
Date_ 20130315
Time 16.05
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 300.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.60 usec
PL1 6.00 dB
SFO1 75.4752950 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 25.44 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

Compound 19: DEPT-135



CIMAP-DEPT 135
PROJECT NO.: ILP-13

Current Data Parameters
NAME asbbbnit.p
EXPNO 3
PROCNO 1

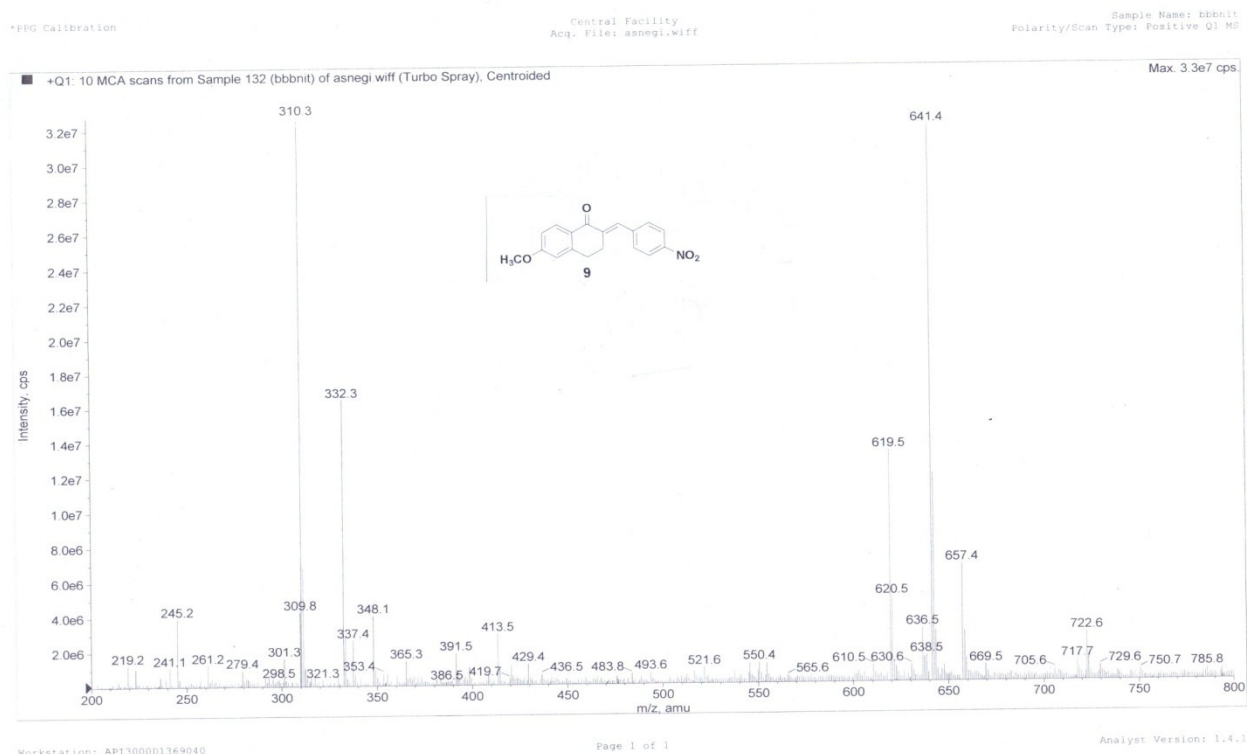
F2 - Acquisition Parameters
Date_ 20130315
Time 16.22
INSTRUM spect
PROBHD 5 mm Multinuc
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 166
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 6.00 usec
TE 300.7 K
CNST2 145.000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001604 sec
TD0 1

CHANNEL f1
NUC1 13C
p1 12.60 usec
p2 25.20 usec
PL1 -6.00 dB
SFO1 75.4752950 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
P3 6.78 usec
p4 13.56 usec
PCPD2 80.00 usec
PI2 4.00 dB
PL12 25.44 dB
SFO2 300.1312000 MHz

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

Compound 19: ESI-Mass



Workstation: API3000D1369040

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