

## SUPPORTING INFORMATION

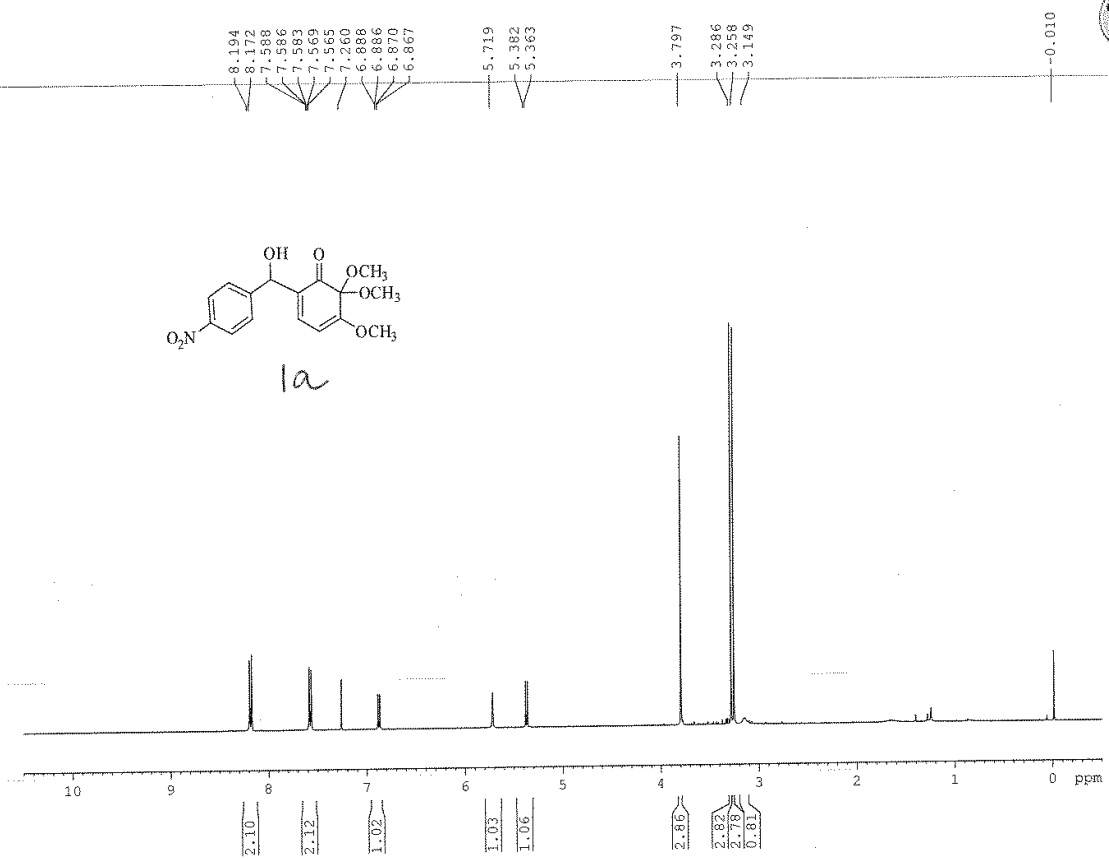
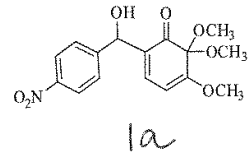
### **Expedient Baylis-Hillman Reaction Protocol to Functionalize Cyclohexa-2,4-dienones**

Santhosh Kumar Chittimalla,\* Manikandan Koodalingam, Chennakesavulu Bandi, Sireesha Putturu and Rajesh Kuppusamy

Medicinal Chemistry Department, AMRI Singapore Research Centre, 61 Science Park Road, #05-01 The Galen, Science Park II, Singapore 117525

Fax: +65 - 63985511

E-mail: [santhosh.chittimalla@amriglobal.com](mailto:santhosh.chittimalla@amriglobal.com); [chemcsk@gmail.com](mailto:chemcsk@gmail.com)



Current Data Parameters  
 NAME SG-MKK-L-P-NO2  
 EXPNO 10  
 PROCNO 1

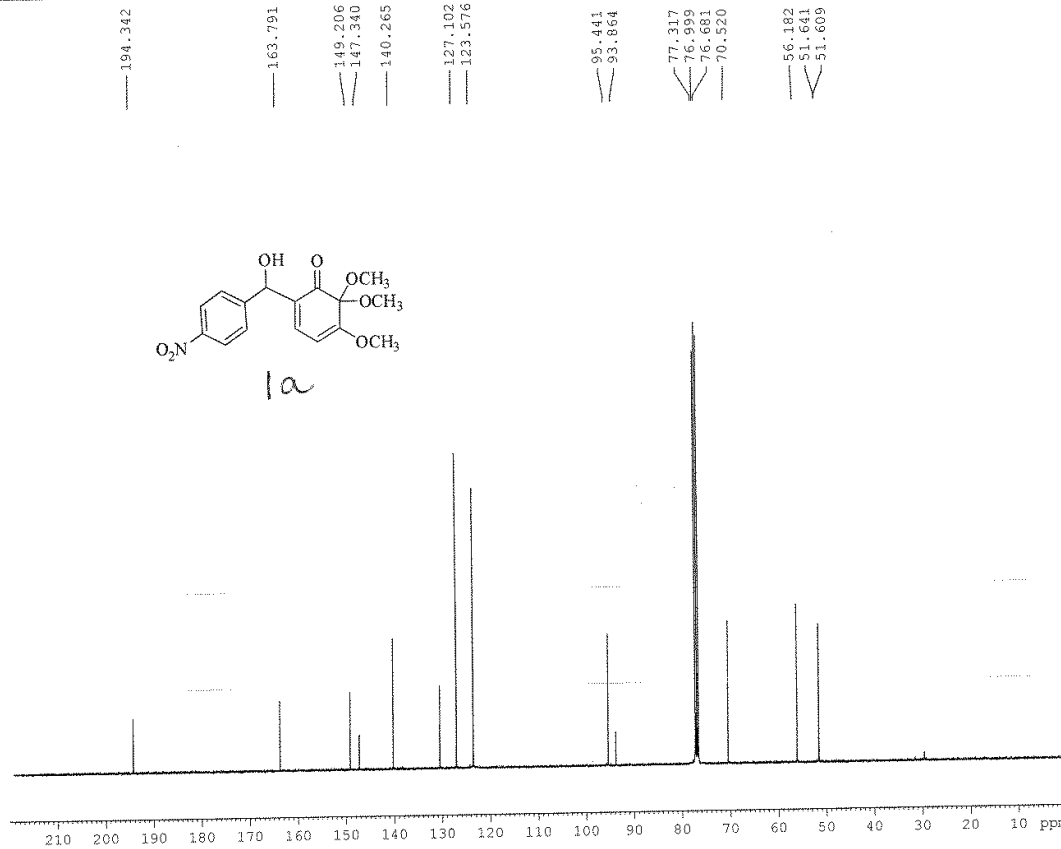
F2 - Acquisition Parameters  
 Date\_ 20130418  
 Time 7.18  
 INSTRUM spect  
 PROBEID 5 mm F4BBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894966 sec  
 RG 71.8  
 DR 62.400 usec  
 DE 6.50 usec  
 FE 300.0 K  
 DI 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.40 usec  
 PL1 -3.00 dB  
 PL1W 19.34582710 W  
 SFO1 400.1318542 MHz

F2 - Processing parameters  
 SI 32768  
 SF 400.1300093 MHz  
 MDW SM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

Name \_\_\_\_\_  
 Date \_\_\_\_\_  
 NB # \_\_\_\_\_

AMRI SRC  
location; 17



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

Current Data Parameters  
NAME 5G-MK-L-E-NO2  
EXNO 20  
PROCNO 1

F2 - Acquisition Parameters  
Date 20150619  
Time 2.01  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 6000  
DS 4  
SMH 23980.814 Hz  
FIDRES 0.265918 Hz  
AQ 1.3664736 sec  
RG 18390.4  
DN 20.850 usec  
DE 6.50 usec  
TE 301.3 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
FDO 1

===== CHANNEL f1 =====  
NUC1 13C  
PI 2.40 usec  
PL1 -4.00 dB  
PL1W 82.02445221 W  
SFO1 100.6228298 MHz

===== CHANNEL f2 =====  
CPDPRG2 waitz16  
NUC2 1H  
PCPD2 80.00 usec  
PI2 -3.00 dB  
PLI2 14.72 dB  
PLI3 15.06 dB  
PLI2W 19.34582110 W  
PLI2W 0.32702974 W  
PLI3W 0.30240381 W  
SFO2 400.1316055 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127711 MHz  
WDW EM  
SSS 0  
LB 1.00 Hz  
GB 0  
FC 1.40

La

ve mode

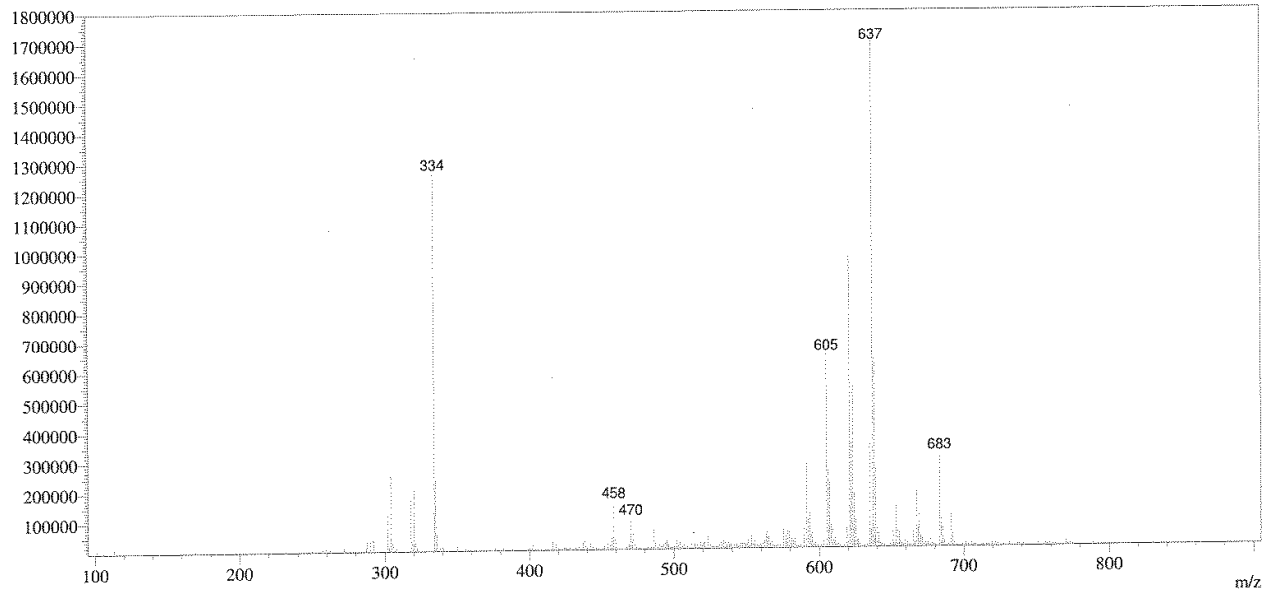
Acquired by : System Administrator  
Sample Name : SG-MKK-L-P-NO2  
Data File : SG-MKK-L-P-NO2.lcd  
Method File : ESI-LCMS Method3.lcm  
Month-Day Acquired : 10/6/2015

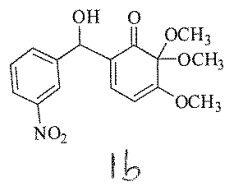
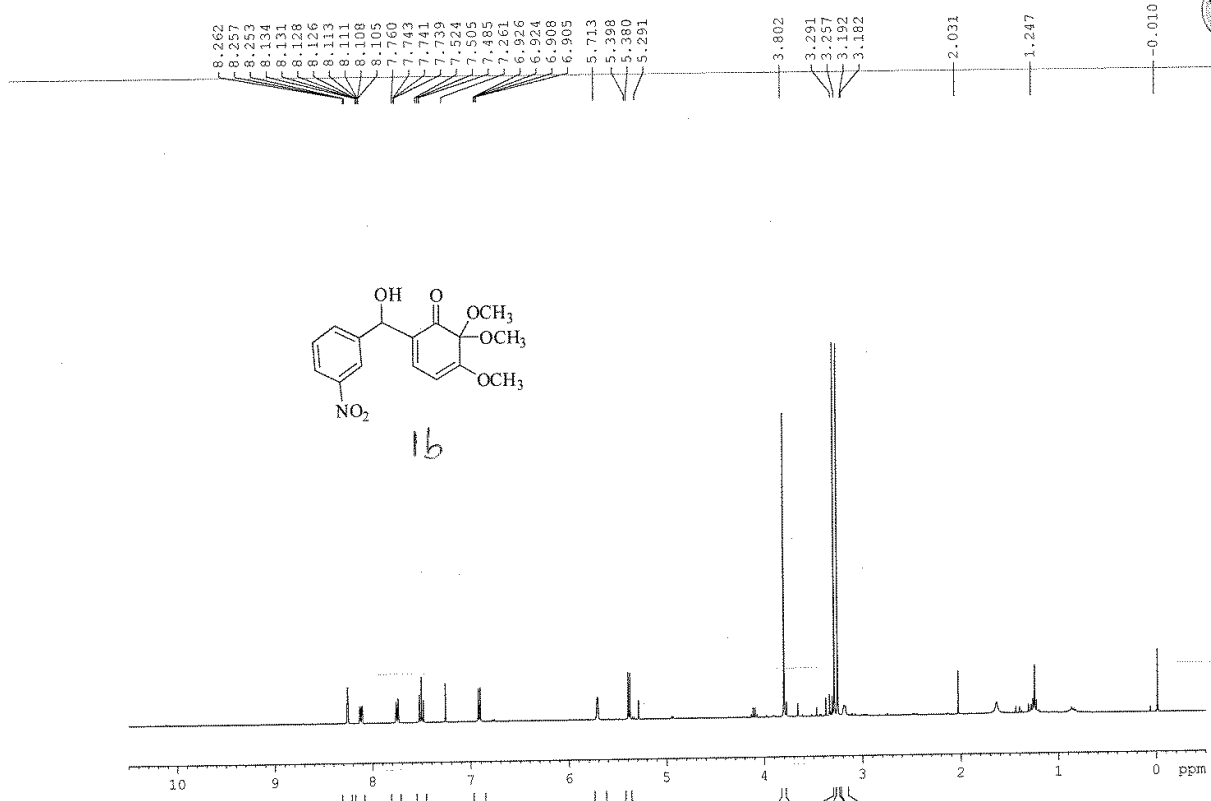
Name	:	_____
Notebook #	:	_____
Date	:	_____



ESI-MS Spectrum

Peak # : 1, Retention Time : 3.116 min  
Base Peak m/z : 637, Base Peak Intensity : 17288351728835  
Polarity : Negative, Event : 1 - 2





Current Data Parameters  
 NAME SG-MRK-L-3-M02  
 EXPNO 23  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150625  
 Time 7.24  
 INSTRUM spect  
 PROBHD 5 mm PABCO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 100  
 DS 2  
 SSB 8012.820 Hz  
 FIDRES 0.132266 Hz  
 AQC 4.0834966 sec  
 RG 71.8  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 300.6 K  
 F1 1.00000000 sec  
 TDG 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.40 usec  
 PL1 -3.00 dB  
 PL1W 19.34582710 W  
 SE01 400.1318542 MHz

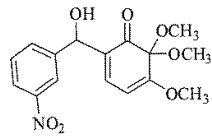
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 SF 400.1300091 MHz  
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 SSB 0  
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 GB 0  
 PC 1.00

Name \_\_\_\_\_  
 Date \_\_\_\_\_  
 NB # \_\_\_\_\_

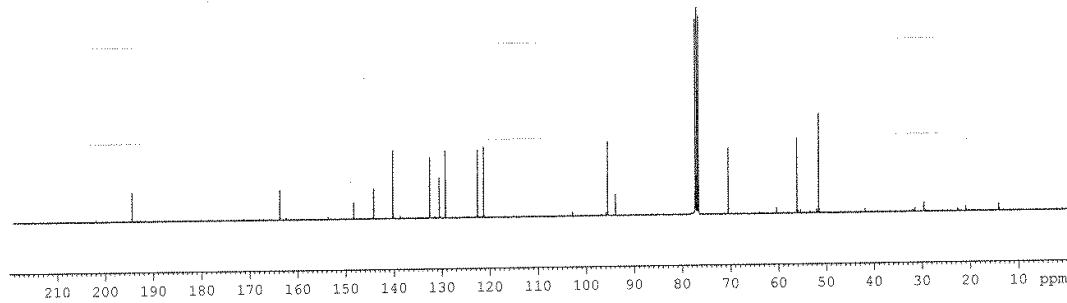
AMRI SRC  
location; 17



194.430  
163.733  
148.360  
144.200  
140.226  
132.555  
130.545  
129.285  
122.574  
121.293  
95.521  
93.899  
77.320  
77.002  
76.884  
70.494  
56.177  
51.625



1b



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

Current Data Parameters  
NAME SC-MKR-L-3-NO2  
EXPNO 20  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150625  
Time 2.51  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 7000  
DS 4  
SWH 23980.814 Hz  
FIDRES 0.365918 Hz  
AQ 1.3664756 sec  
RG 20642.5  
DW 20.850 usec  
DE 6.50 usec  
TE 302.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 13C  
PL 7.40 usec  
PL1 -4.00 dB  
PL1W 82.02445221 W  
SFO1 100.6228298 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -3.00 dB  
PL12 14.72 dB  
PL13 15.06 dB  
PL1W 19.34582710 W  
PL12W 0.32702876 W  
PL13W 0.30240381 W  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127162 MHz  
WDW EM  
SS 0  
LB 1.00 Hz  
GB 0  
PC 1.40

1b

-ve mode

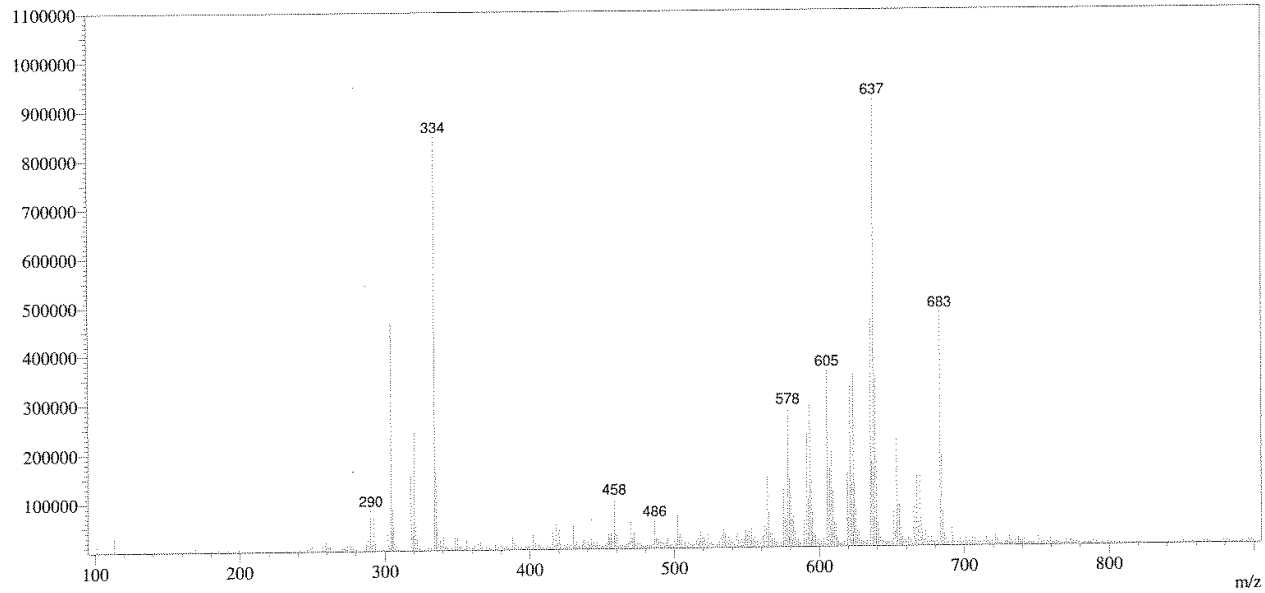
Acquired by : System Administrator  
Sample Name : SG-MKK-L-3-NO2  
Data File : SG-MKK-L-3-NO2.lcd  
Method File : ESI-LCMS Method3.lcm  
Month-Day Acquired : 10/6/2015

Name	:	_____
Notebook #	:	_____
Date	:	_____

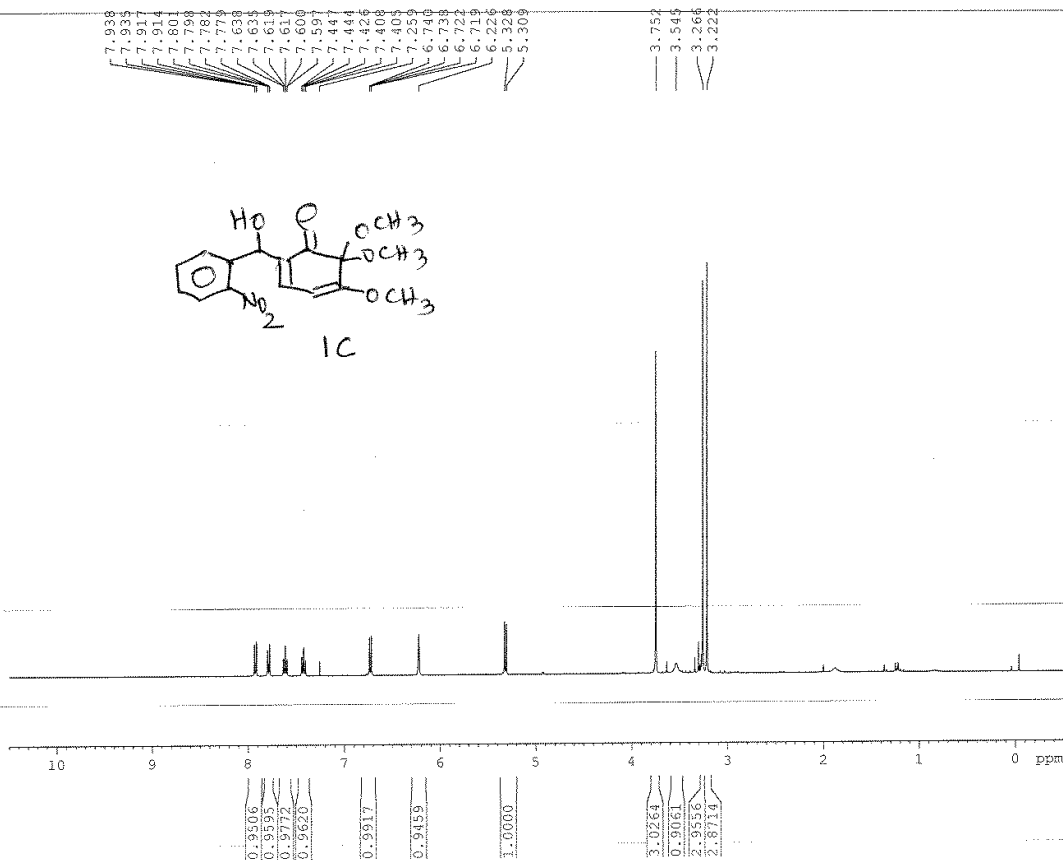


ESI-MS Spectrum

Peak # : 1, Retention Time : 3.116 min  
Base Peak m/z : 637, Base Peak Intensity : 917877917877  
Polarity : Negative, Event : 1 - 2



AMRI; SRC AV400  
location; 18



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB# \_\_\_\_\_

Current Data Parameters  
NAME SG-MKK-L-2-NO2  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150622  
Time 7.26  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 50.8  
DW 62.400 usec  
DE 6.00 usec  
TE 300.0 K  
D1 1.00000000 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 10.70 usec  
PL1 -2.00 dB  
PL1W 14.33185768 W  
SFO1 400.2330895 MHz

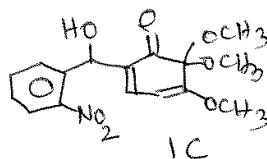
F2 - Processing parameters  
SI 32768  
SF 400.2300119 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



# AMRI SRC location; 17



193.903  
 163.298  
 147.955  
 139.517  
 136.738  
 133.332  
 130.351  
 128.861  
 128.440  
 124.602  
 95.624  
 93.982  
 77.319  
 77.001  
 76.883  
 66.060  
 56.042  
 51.657  
 51.359



Name \_\_\_\_\_  
 Date \_\_\_\_\_  
 NB# \_\_\_\_\_

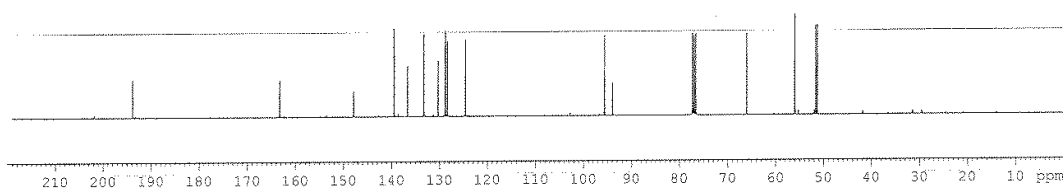
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 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20180623  
 Time\_ 8.12  
 INSTRUM spect  
 PROBRD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 289920  
 FID 65536  
 SOLVENT CDCl3  
 NS 5000  
 DS 4  
 SWH 23980.814 Hz  
 FIDRES 0.365918 Hz  
 AQ 1.3664756 sec  
 RG 14596.5  
 DW 20.850 usec  
 DE 6.50 usec  
 TE 302.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 2.40 usec  
 PL1 -4.00 dB  
 PL1W 82.02445221 W  
 SFO1 100.62282298 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NPK2 1H  
 PCPD2 80.00 usec  
 PL2 -3.00 dB  
 PL12 14.72 dB  
 PL13 15.06 dB  
 PL2W 19.24582710 W  
 PL12W 0.32722976 W  
 PL13W 0.30240381 W  
 SFO2 400.1316095 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6127765 MHz  
 WDN EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



LC

-ve mode

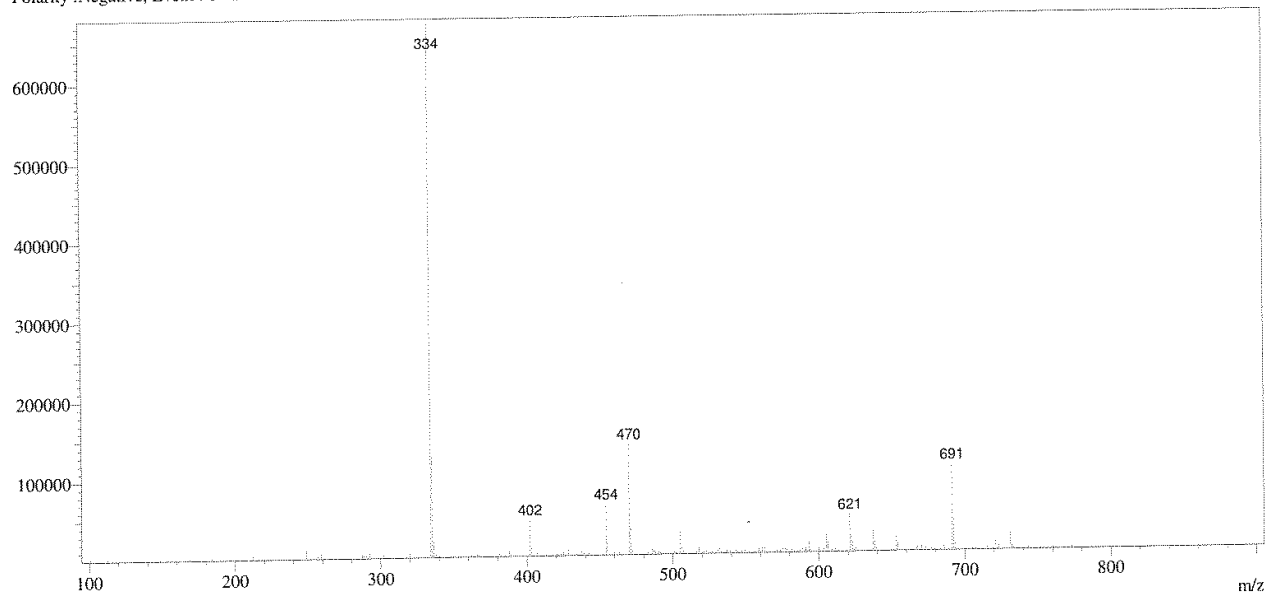
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Data File : SG-MKK-L-2-NO2.lcd  
Method File : ESI-LCMS Method3.lcm  
Month-Day Acquired : 10/8/2015

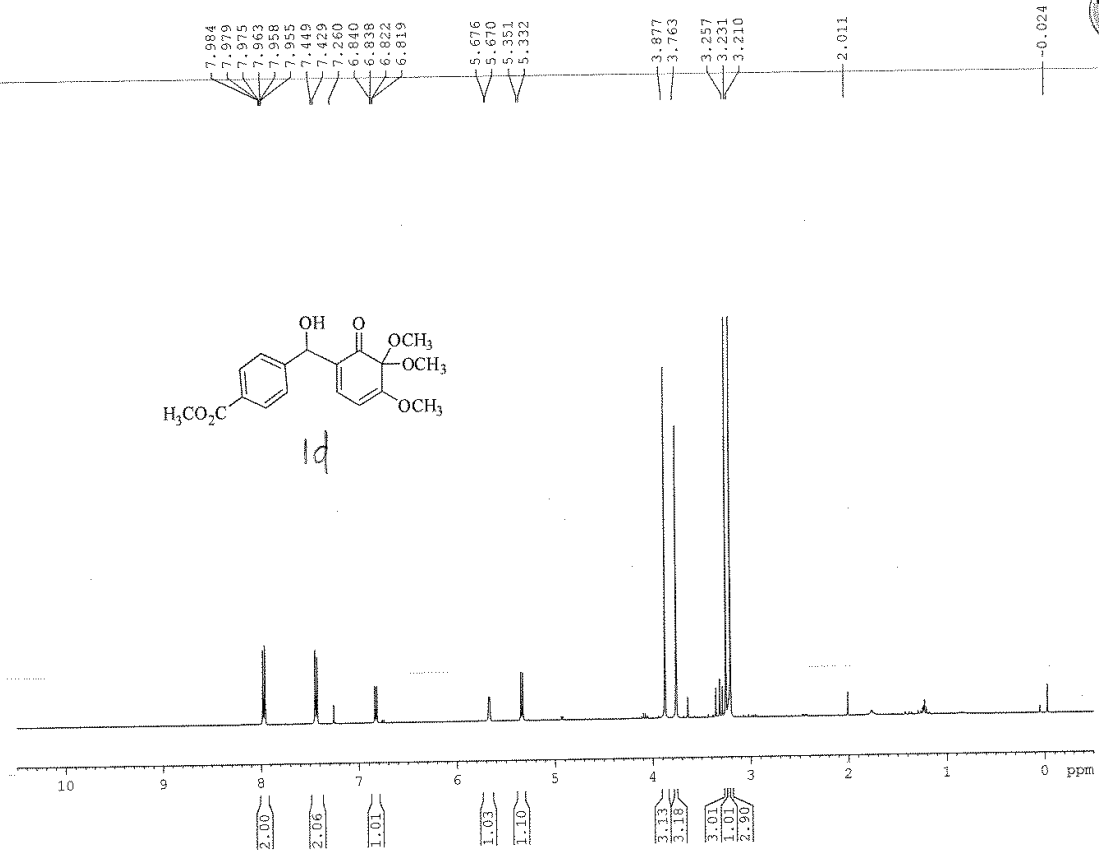
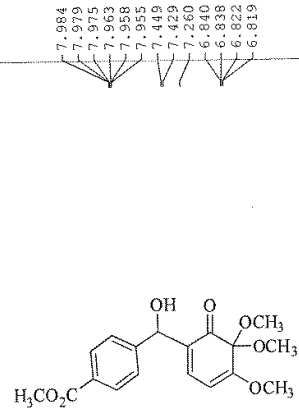
Name	:	_____
Notebook #	:	_____
Date	:	_____



ESI-MS Spectrum

Peak # : 1, Retention Time : 3.016 min  
Base Peak m/z : 334, Base Peak Intensity : 679703679703  
Polarity : Negative, Event : 1 - 2





Current Data Parameters  
 NAME SG-MKK-L-4-CO2Me  
 EXPNO 13  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 20150623  
 Time 3.18  
 INSTRUM spect  
 PROBHD 5 mm FAPBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 160  
 DS 2  
 SWH 8012.920 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894866 sec  
 RG 49.3  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 300.7 K  
 D1 1.0000000 sec  
 TDO 1

===== CHANNEL F1 =====  
 NUCL 1H  
 P1 10.40 usec  
 PL1 -3.00 dB  
 PL1W 19.34982710 W  
 SFO1 400.1318542 MHz

F2 - Processing parameters  
 SI 32768  
 SF 400.1300091 MHz  
 MSB EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

Name \_\_\_\_\_

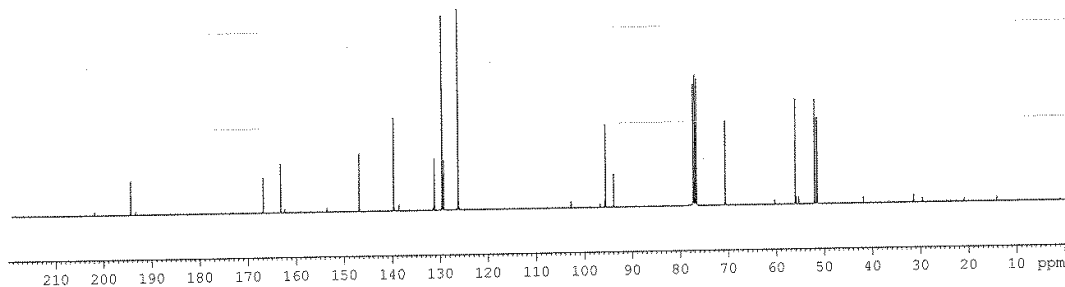
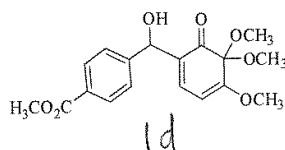
Date \_\_\_\_\_

NB # \_\_\_\_\_

AMRI SRC  
location; 17



194.353  
166.847  
163.211  
146.925  
139.731  
131.234  
129.620  
129.323  
126.275  
86.612  
83.900  
77.320  
77.002  
76.883  
70.671  
56.054  
52.016  
51.554  
51.506



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

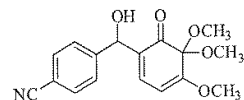
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EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date 20150623  
Time 0.54  
INSTRUM spect  
PROBHD 5 mm PARBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 5000  
DS 4  
SWH 23980.814 Hz  
FIDRES 0.365918 Hz  
AQ 1.3664756 sec  
RG 16384  
DM 20.850 usec  
DE 6.50 usec  
TE 302.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

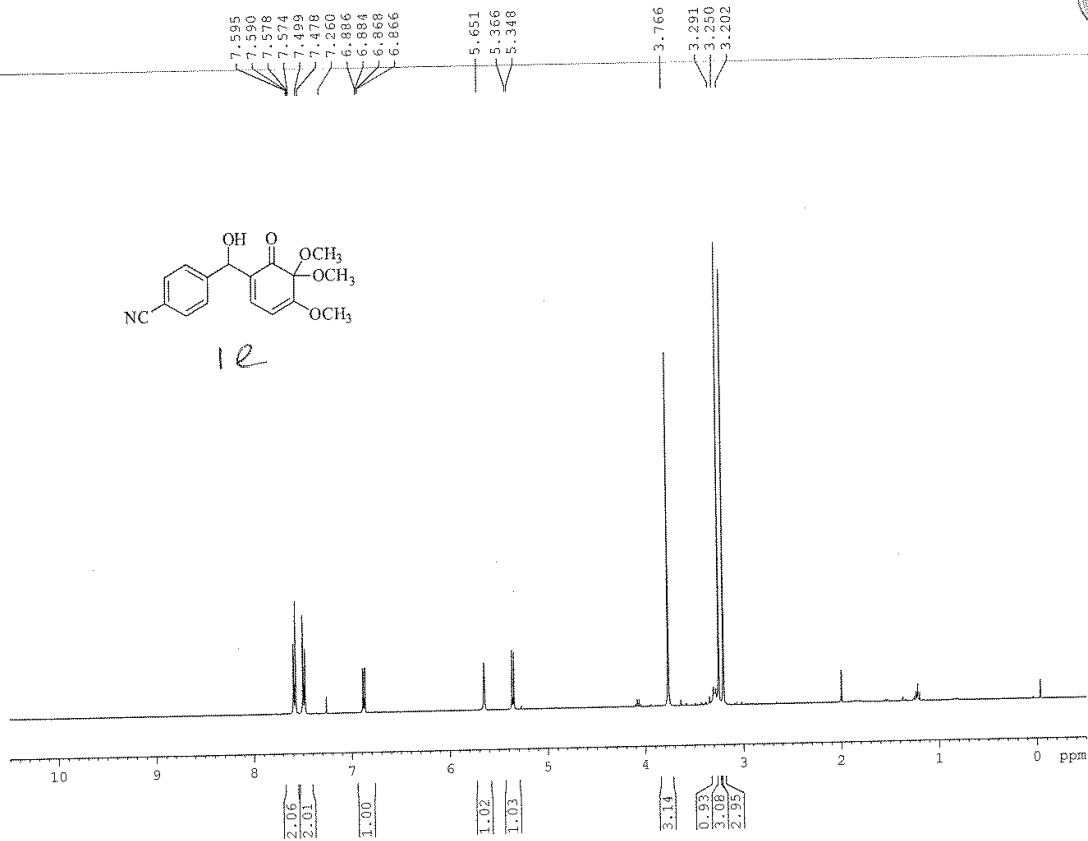
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NUC1 13C  
P1 7.40 usec  
PL1 -4.00 dB  
PL1W 82.02445221 W  
SFO1 100.6228298 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PI2 -3.00 dB  
PL12 14.72 dB  
PL13 15.06 dB  
PL2W 19.34582710 W  
PL12W 0.32702876 W  
PL13W 0.30240381 W  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127738 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



12



Current Data Parameters  
 NAME SG-MKK-L-4-CN  
 EXPRO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150625  
 Time 7.49  
 INSTRUM spect  
 PROBHD 5 mm PABEO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0884966 sec  
 RG 50.8  
 DW 62.400 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 1.0000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUCL 1H  
 FI 10.70 usec  
 PL1 -2.00 dB  
 PL1W 14.33185765 W  
 SFO1 400.2330685 MHz

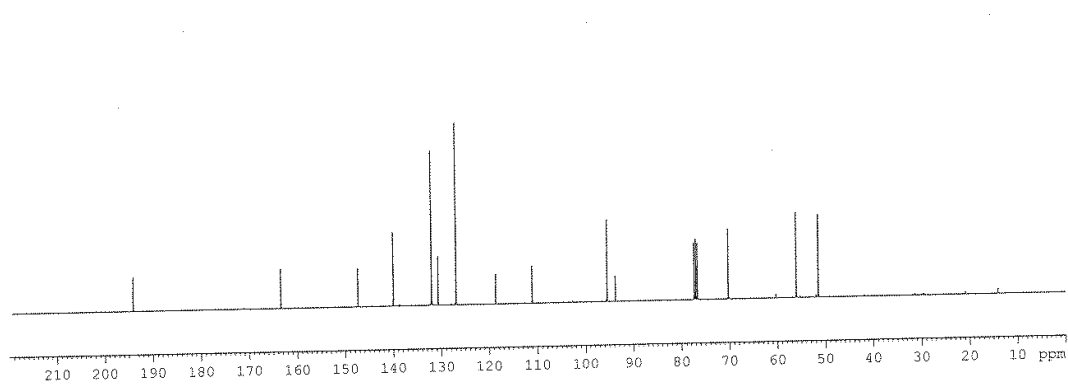
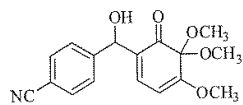
F2 - Processing parameters  
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 SF 400.2330115 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

Name \_\_\_\_\_  
 Date \_\_\_\_\_  
 NB # \_\_\_\_\_

AMRI; SRC AV400  
location; 18



194.150  
163.461  
147.383  
139.999  
132.068  
130.681  
126.949  
118.669  
111.123  
95.494  
93.774  
77.320  
77.001  
76.683  
70.232  
56.082  
51.327  
51.497



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

Current Data Parameters  
NAME SG-MKK-1-4-CN  
EXPNO 20  
PROCNO 1

F2 - Acquisition Parameters  
Date 20150626  
Time 1.55  
INSTRUM spect  
PROBHD 5 mm PABBO BH-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 9000  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 301  
DM 20.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 0.5000000 sec  
D11 0.0300000 sec  
TD0 1

==== CHANNEL F1 =====  
NUC1 13C  
PI 8.60 usec  
PL1 -1.00 dB  
PL1W 44.5811569 W  
SFO1 100.6279769 MHz

==== CHANNEL F2 =====  
CDEPRG2 waitz16  
NUC2 1H  
FOF2 80.00 usec  
PL2 -2.00 dB  
PL12 15.47 dB  
PL13 15.72 dB  
PL2W 14.33185768 W  
PL12W 0.25662708 W  
PL13W 0.24227159 W  
SFO2 400.2316009 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6379238 MHz  
WFF EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

1e

-ve mode

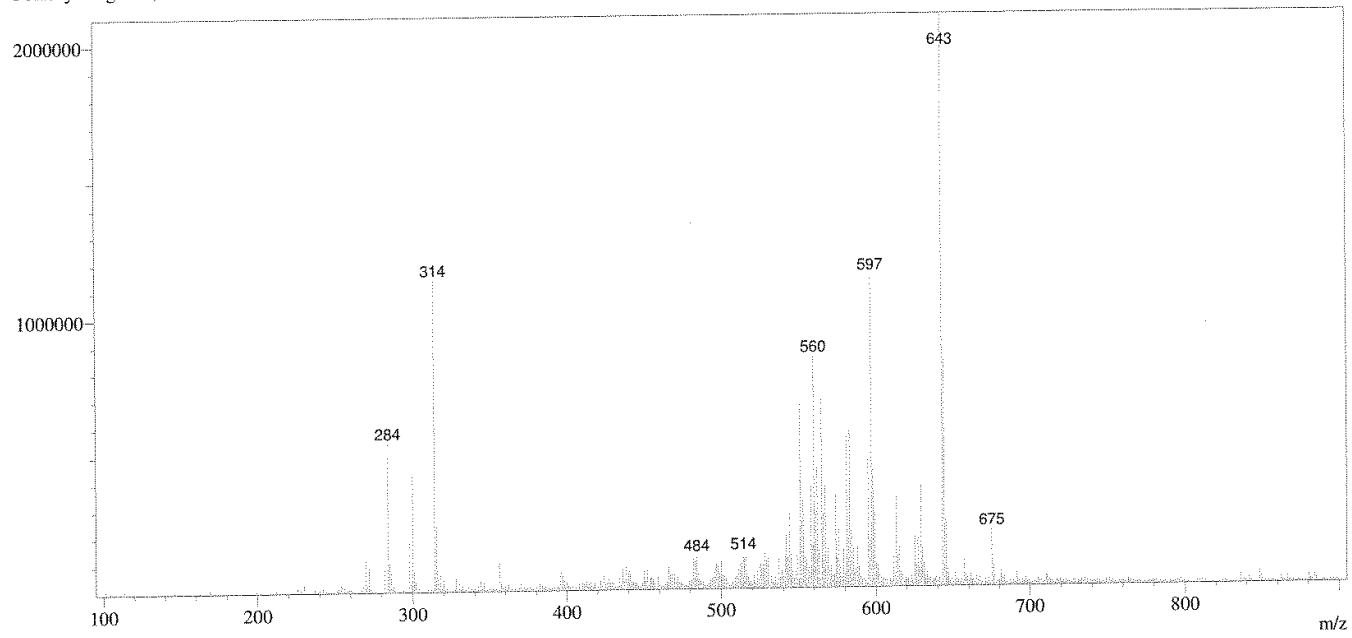
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Method File : ESI-LCMS Method3.lcm  
Month-Day Acquired : 10/6/2015

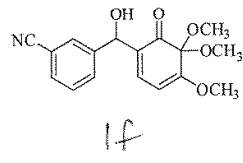
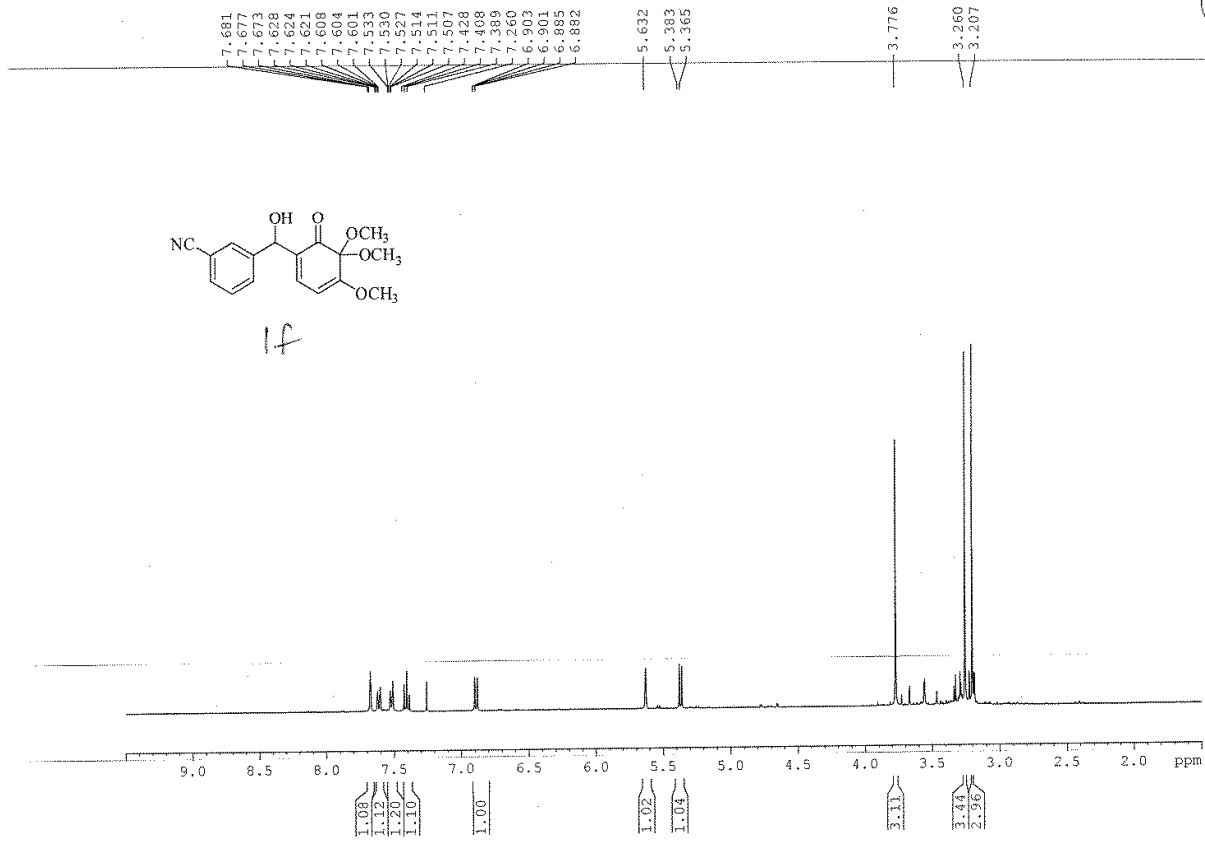
Name	:	_____
Notebook #	:	_____
Date	:	_____



ESI-MS Spectrum

Peak # : 1, Retention Time : 3.016 min  
Base Peak m/z : 643, Base Peak Intensity : 20982912098291  
Polarity : Negative, Event : 1 - 2





Current Data Parameters  
 NAME SG-MRK-1-3-CN  
 EXPHO 20  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 20150725  
 Time 7.33  
 INSTRUM spect  
 PROBRD 5 mm FASBO BS-  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 100  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894966 sec  
 RG 35.9  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 300.0 K  
 DI 1.0000000 sec  
 TDC 1

===== CHANNEL f1 =====  
 NUC1 1H  
 FI 10.40 usec  
 PL1 -3.00 dB  
 PL1W 19.34582710 W  
 SFO1 400.1318542 MHz

F2 - Processing parameters  
 SI 32768  
 SF 400.1300094 MHz  
 WDW EM  
 SSS 0  
 LB 0.30 Hz  
 GB 0  
 FC 1.00

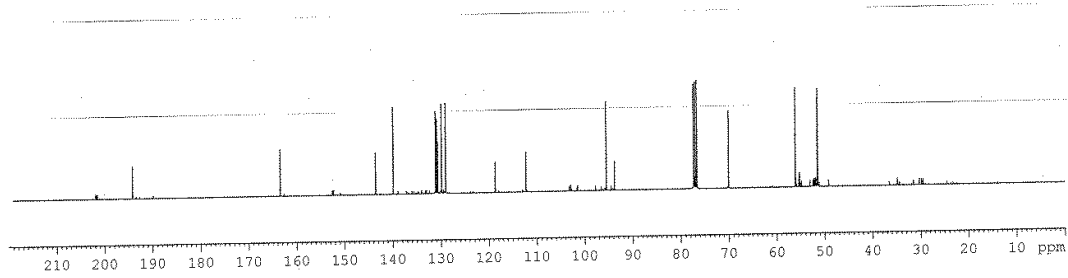
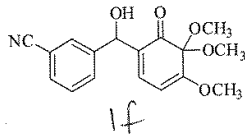
Name \_\_\_\_\_  
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 NB # \_\_\_\_\_



AMRI SRC  
location; 17



194.190  
163.439  
143.578  
139.885  
131.098  
130.849  
130.834  
129.892  
129.041  
118.662  
112.262  
95.509  
93.793  
77.312  
76.894  
76.676  
70.040  
56.092  
51.332  
51.495



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

Current Data Parameters  
NAME SG-MRX-L-3-CN  
EXNO 21  
PROCNO 1

F2 - Acquisition Parameters  
Date 20150725  
Time 14.16  
INSTRUM spect  
PROBRD 5 mm PABBO SB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 7080  
DS 4  
SWH 23980.814 Hz  
FIDRES 0.365918 Hz  
AQ 1.3664756 sec  
RG 7298.2  
DM 20.850 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 7.40 usec  
PL1 -4.00 dB  
PLW 82.02445221 W  
SFO1 100.6228298 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -3.00 dB  
PL12 14.72 dB  
PL13 15.06 dB  
PL2R 19.34582710 W  
PLL2W 0.32702976 W  
PL13W 0.30440381 W  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127780 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

1f -ve mode

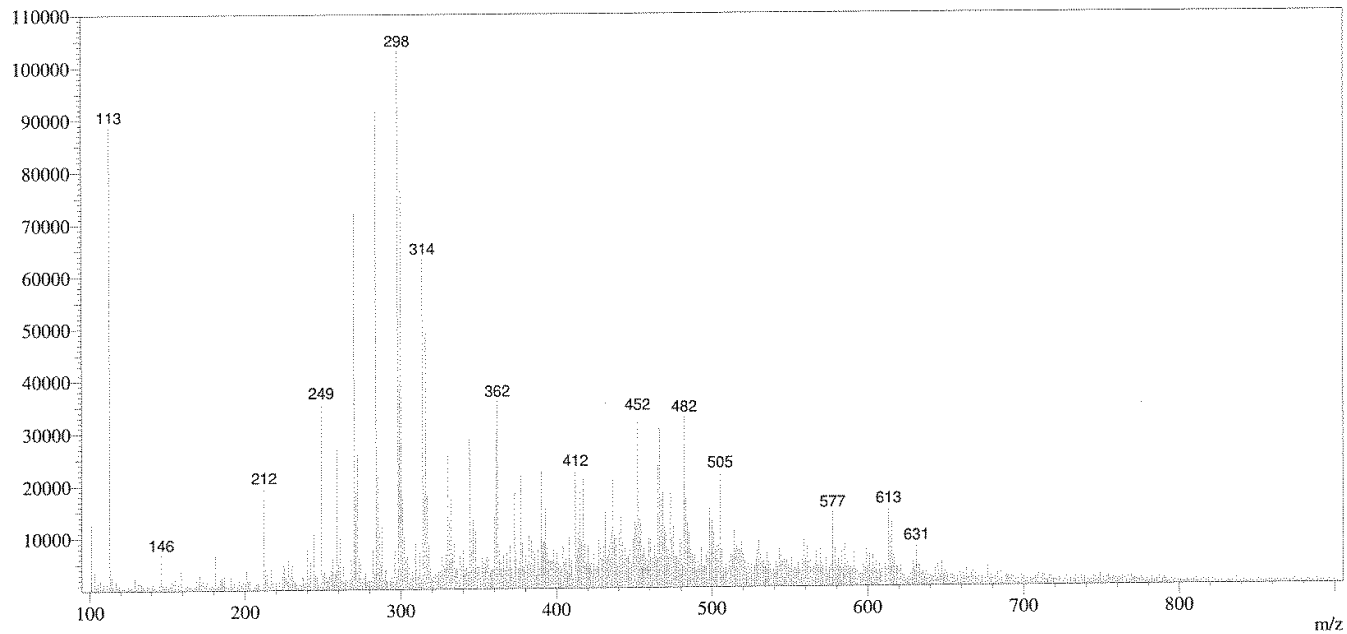
Acquired by : System Administrator  
Sample Name : SG-MKK-L-3-CN  
Data File : SG-MKK-L-3-CN.lcd  
Method File : ESI-LCMS Method3.lcm  
Month-Day Acquired : 10/8/2015

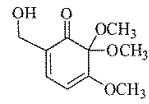
Name	:	_____
Notebook #	:	_____
Date	:	_____



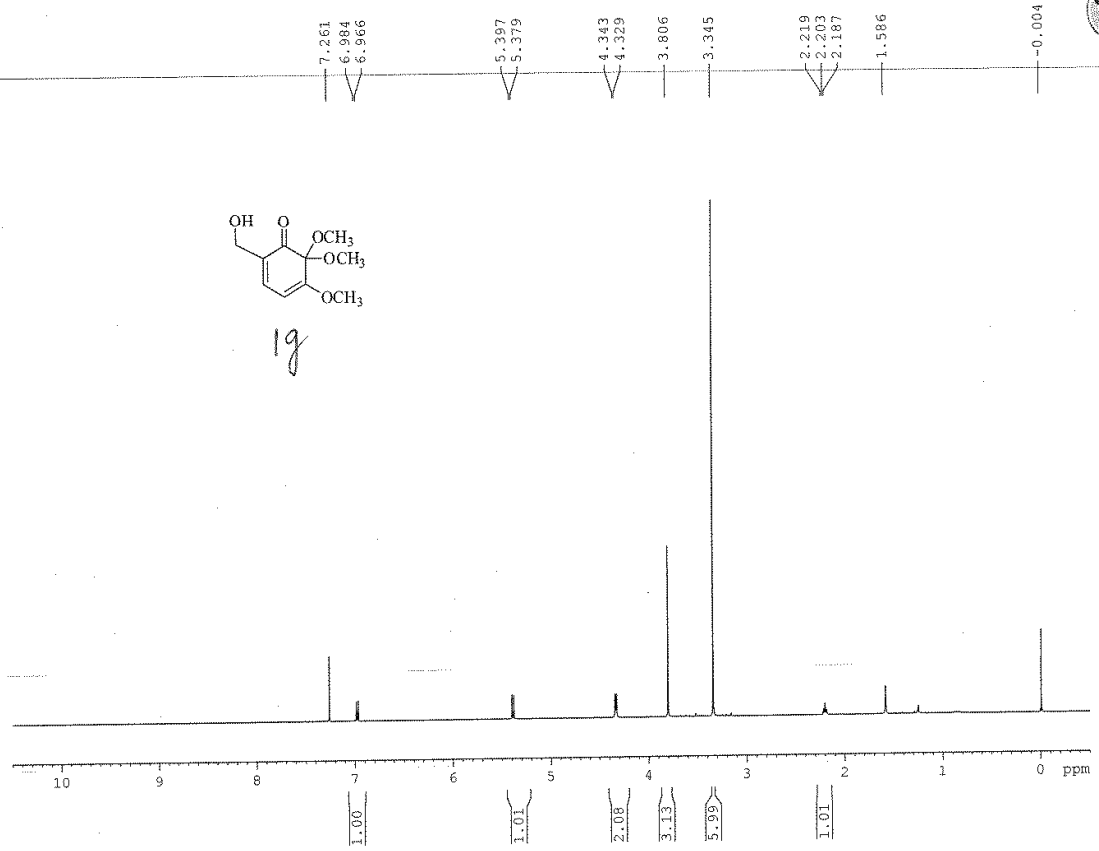
ESI-MS Spectrum

Peak # : 1, Retention Time : 2.649 min  
Base Peak m/z : 298, Base Peak Intensity : 106400106400  
Polarity : Negative, Event : 1 - 2





19



Current Data Parameters  
NAME SG-MKK-L-HCHO  
EXPNO 29  
PROCNO 1

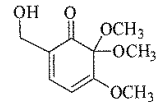
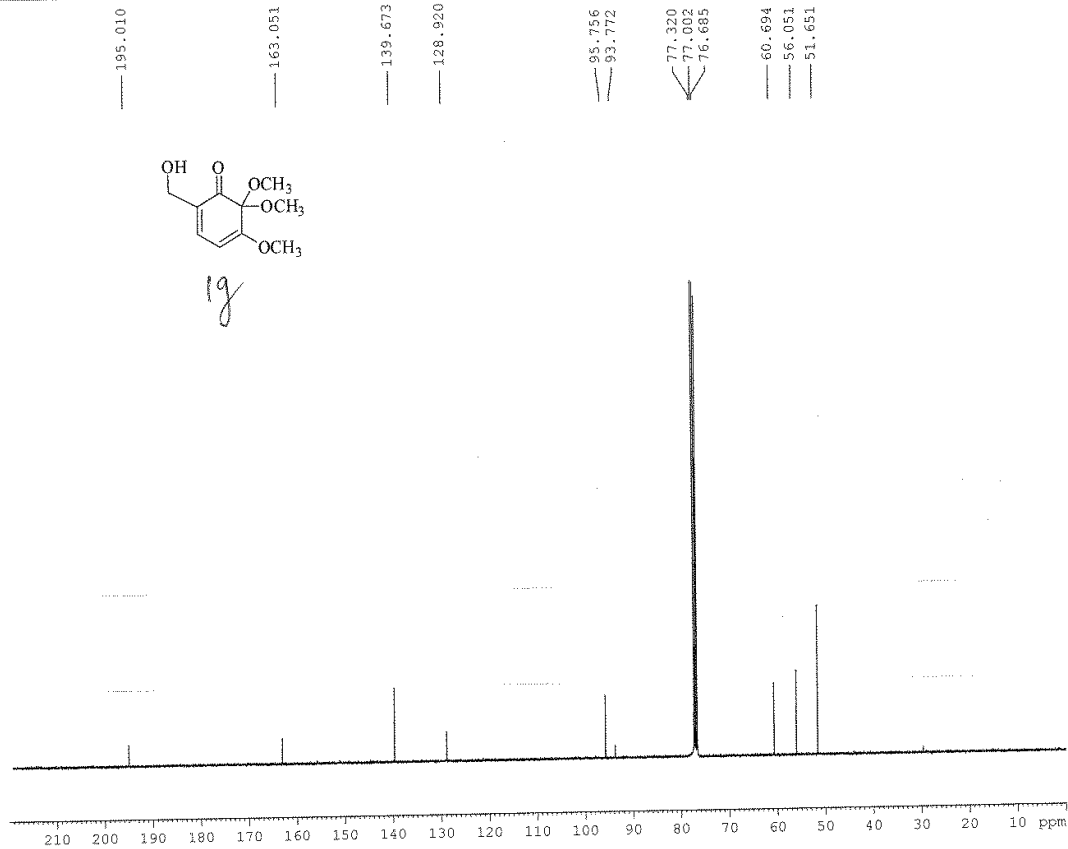
F2 - Acquisition Parameters  
Date\_ 20150626  
Time 7.50  
INSTRUM spect  
PROBHD 5 mm FABRO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 181  
DW 62.400 usec  
DE 6.50 usec  
TE 300.3 K  
SI 1.00000000 sec  
TDS 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 10.40 usec  
PL1 -3.00 dB  
PL1W 19.34582710 W  
SFO1 400.1318542 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1300092 MHz  
WDW EM  
SSB 0  
LB 0 0.30 Hz  
GB 0  
PC 1.00

Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

AMRI SRC  
location; 17



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

Current Data Parameters  
NAME SG-MKK-L-HCHO  
EXPNO 30  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150627  
Time\_ 2.48  
INSTRUM spect  
PROBHD 5 mm PABBO B5-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 7000  
DS 4  
SWH 23980.814 Hz  
FIDRES 0.365918 Hz  
AQ 1.3664756 sec  
RG 16384  
DW 20.850 usec  
DE 6.50 usec  
TE 301.6 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 7.40 usec  
PL1 -4.00 dB  
PL1W 82.02445221 W  
SFO1 100.6228298 MHz

===== CHANNEL f2 =====  
CDEPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -3.00 dB  
PL12 14.72 dB  
PL13 15.06 dB  
PL2W 19.34582710 W  
PL12W 0.32702876 W  
PL13W 0.30240381 W  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127689 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

1g

## AMRI LCMS(ESI) Analysis Report

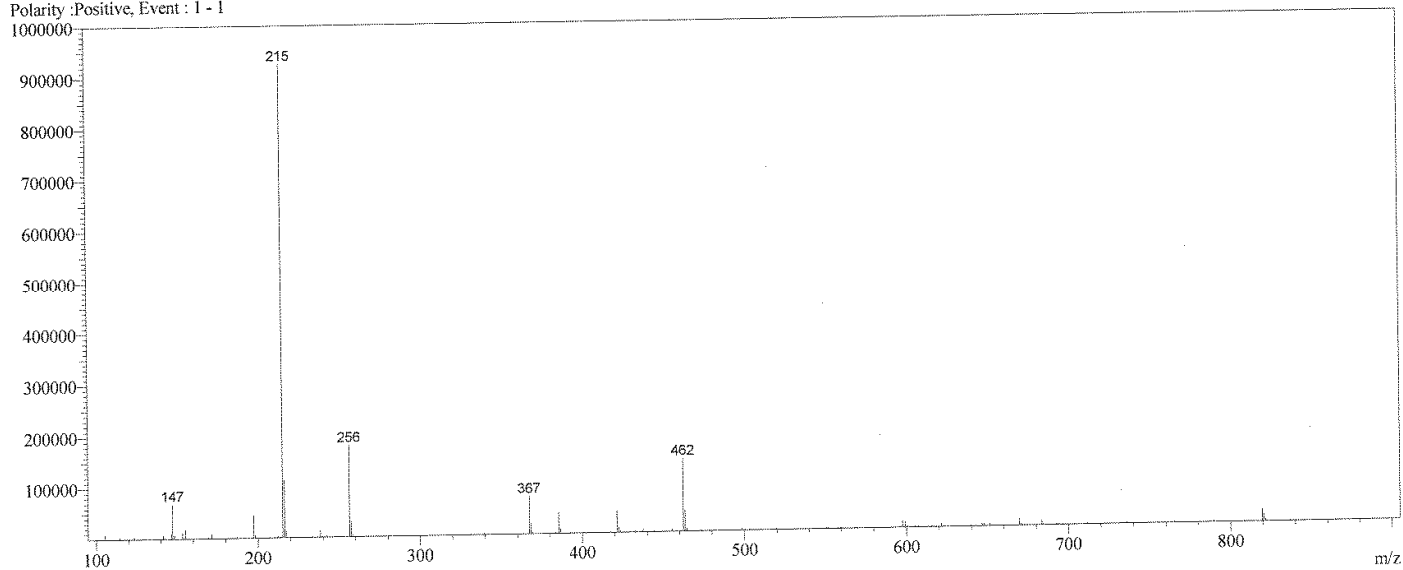
Acquired by : System Administrator  
Sample Name : SG-MKK-L-HCHO  
Data File : SG- MKK-L-HCHO.lcd  
Method File : LCMS-ESI 5 min method.lcm  
Month-Day Acquired : 12/10/2015

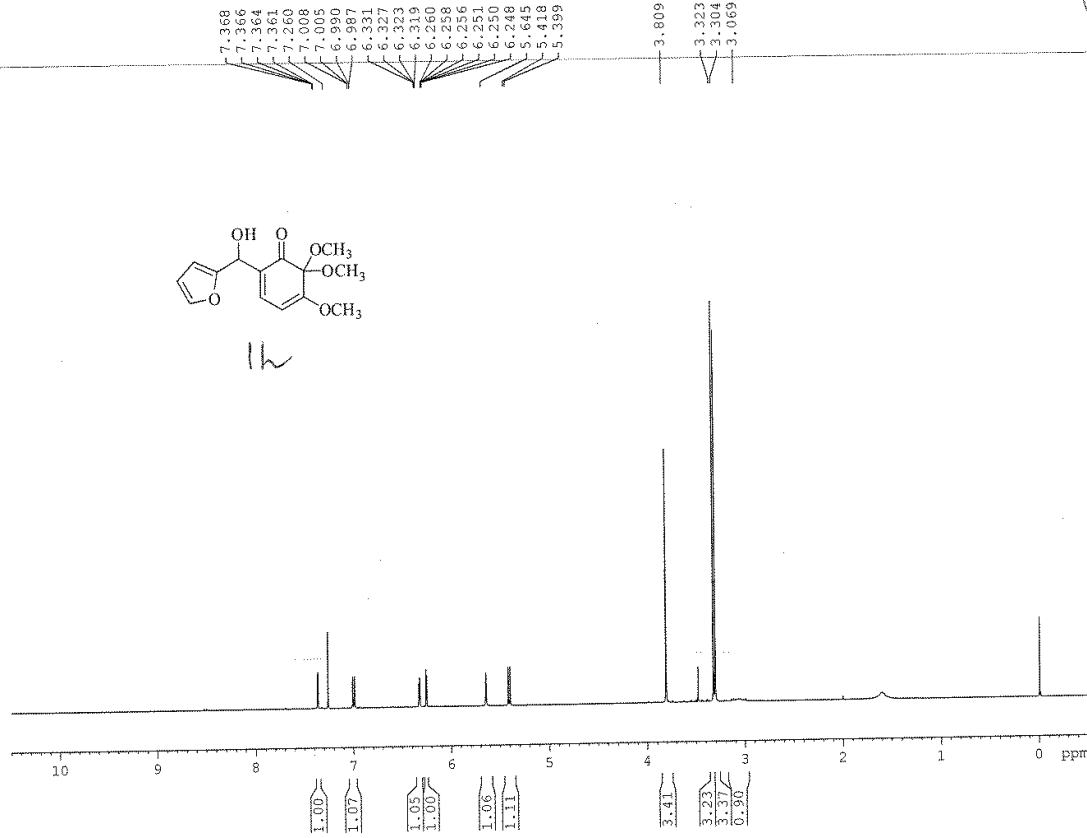
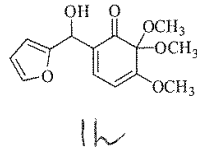
Name	:	_____
Notebook #	:	_____
Date	:	_____



ESI-MS Spectrum

Peak # : 1, Retention Time : 3.753 min  
Base Peak m/z : 215, Base Peak Intensity : 926037926037  
Polarity :Positive, Event : 1 - 1





Current Data Parameters  
NAME SG-MKK-L-Perfural  
EXPNO 40  
PROCNO 1

F2 - Acquisition Parameters  
Date 20150713  
Time 1.04  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 100  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 181  
DW 62.400 usec  
DE 6.50 usec  
TE 302.2 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 10.40 usec  
PL1 -3.00 dB  
PLLN 19.34582710 W  
SF01 400.1318542 MHz

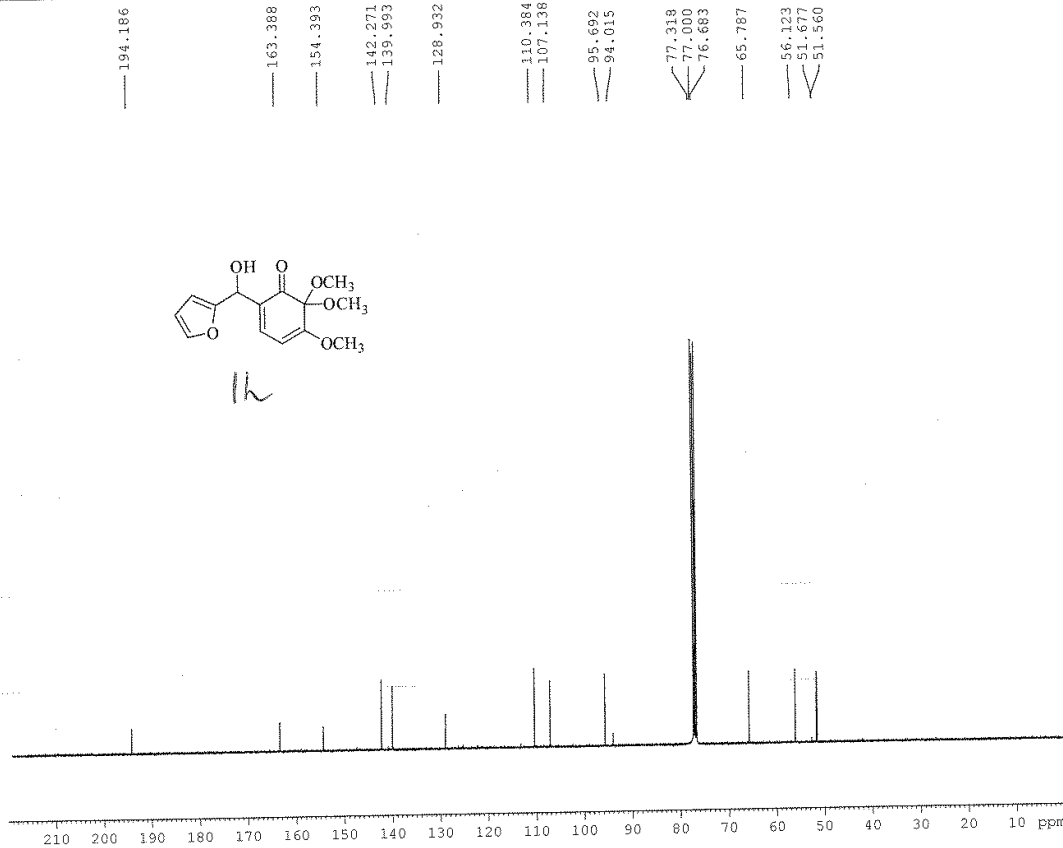
F2 - Processing parameters  
SI 32768  
SF 400.1300093 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Name \_\_\_\_\_

Date \_\_\_\_\_

NB # \_\_\_\_\_

AMRI SRC  
location; 17



194.186  
163.388  
154.393  
142.271  
139.993  
128.932  
110.384  
107.138  
95.692  
94.015  
77.318  
77.000  
76.683  
65.787  
56.123  
51.677  
51.560

Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

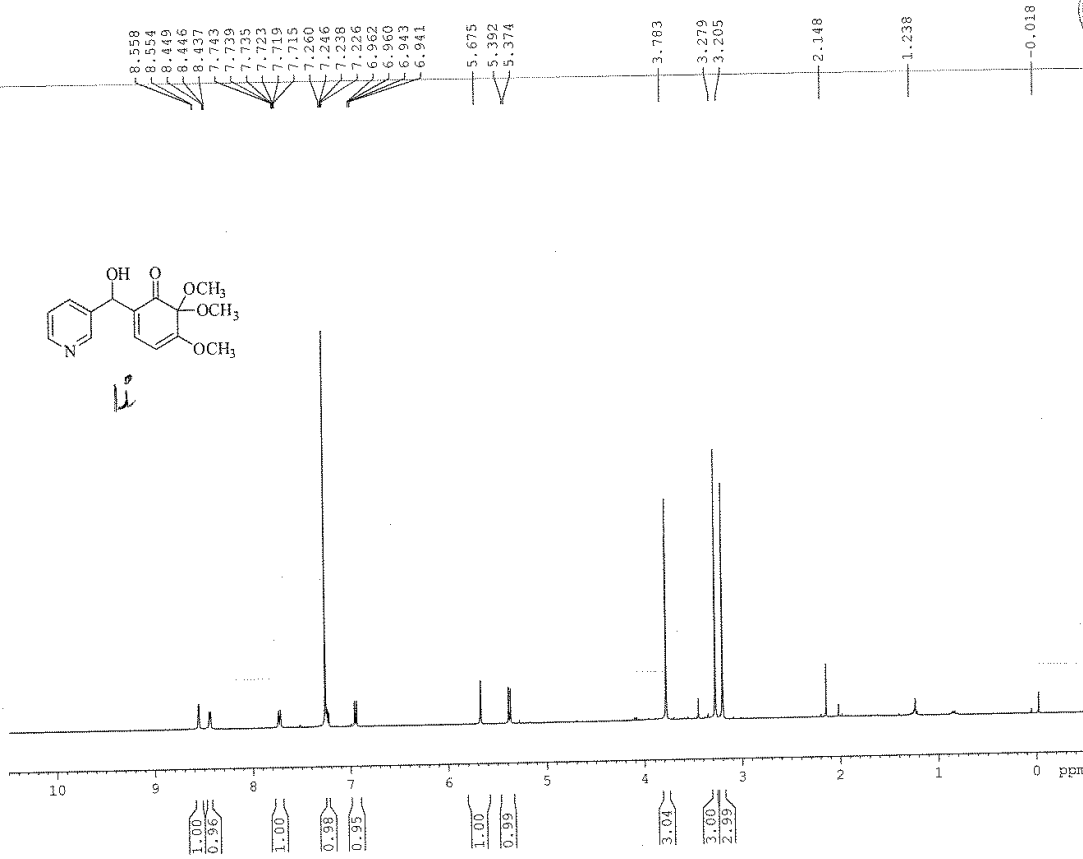
Current Data Parameters  
NAME 3C-MX2-L-Purifural  
EXPNO 41  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150713  
Time 6.51  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 6060  
DS 4  
SWH 23980.814 Hz  
FIDRES 0.365918 Hz  
AQ 1.3864756 sec  
RG 18390.4  
DW 20.850 usec  
DE 6.50 usec  
TE 303.3 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 7.40 usec  
PL1 -4.00 dB  
SFO1 82.02445221 MHz  
SFO2 100.6226298 MHz

===== CHANNEL f2 =====  
CFDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 -3.00 dB  
PL12 14.72 dB  
PL13 15.06 dB  
PL2W 19.34582710 W  
PL12W 0.32702976 W  
PL13W 0.30240381 W  
SFO2 400.1316905 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127692 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



Current Data Parameters  
 NAME SG-MRK-1-3-Py-CHO  
 EXPNO 21  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 20150717  
 Time 15.24  
 INSTRUM spect  
 PROBRD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 OS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894966 sec  
 RG 71.8  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 300.0 K  
 SI 1.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 HNU1 1H  
 F1 10.40 usec  
 PL1 -3.00 dB  
 PL1W 19.34582710 W  
 SFO1 400.1318542 MHz

F2 - Processing parameters  
 SI 32768  
 SF 400.1300092 MHz  
 WDR 3H  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

Name \_\_\_\_\_

Date \_\_\_\_\_

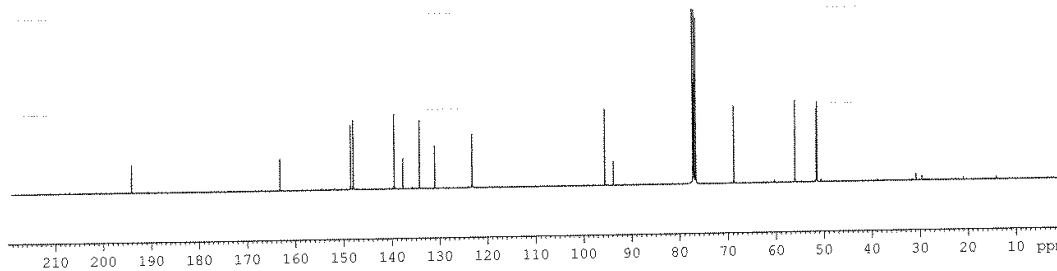
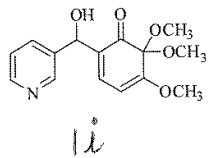
NB # \_\_\_\_\_



AMRI SRC  
location; 17



194.145  
163.256  
148.615  
148.086  
139.555  
137.756  
134.271  
131.093  
123.305  
95.628  
93.868  
77.319  
77.203  
77.000  
76.683  
68.787  
56.102  
51.619  
51.490



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

Current Data Parameters  
NAME SC-MKK-L-3-Py-CHO  
EXPNO 25  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150719  
Time 2.22  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 7000  
DS 4  
SWH 23980.814 Hz  
FIDRES 0.365918 Hz  
AQ 1.3664756 sec  
RG 18390.4  
DM 20.850 usec  
DE 8.50 usec  
TE 300.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
NUC1 13C  
P1 7.40 usec  
PL1 -4.00 dB  
PL1W 82.02445221 W  
SFO1 100.628298 MHz

\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -3.00 dB  
PL12 14.72 dB  
PL13 15.06 dB  
PL2W 19.34582710 W  
PL12W 0.32702976 W  
PL13W 0.30240381 W  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127727 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

11

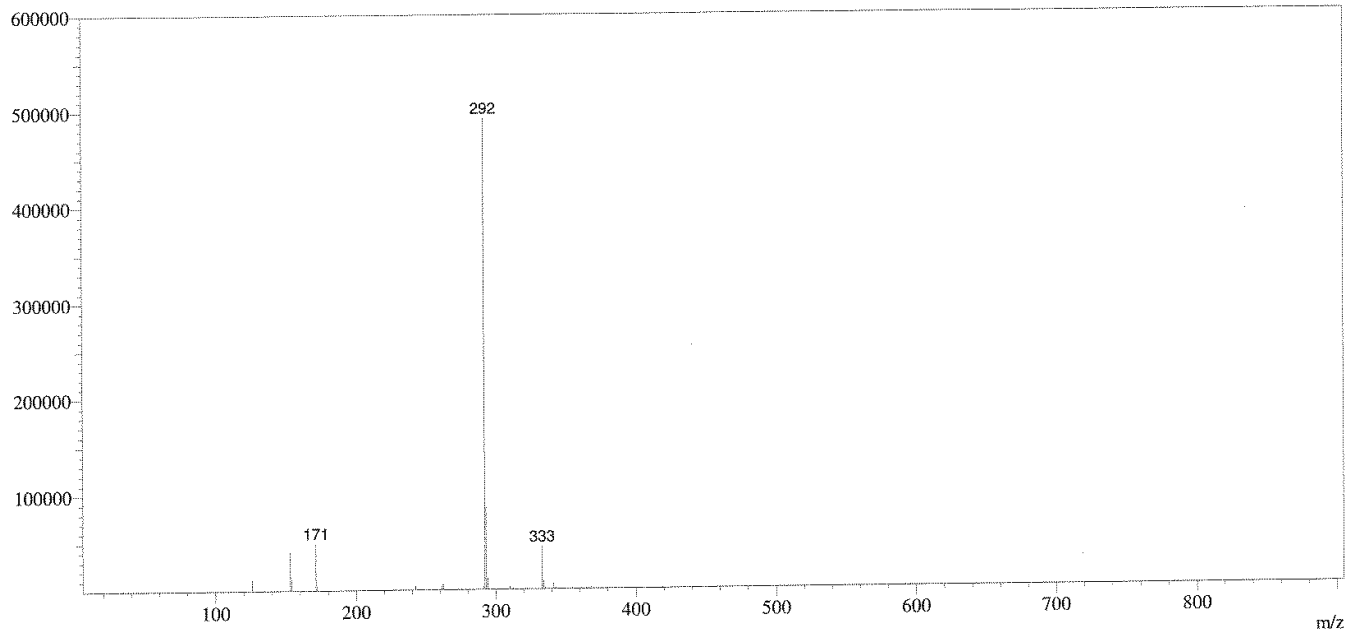
Acquired by : System Administrator  
Sample Name : SG-MKK-L-PY-CHO  
Data File : SG-MKK-L-PY-CHO1.lcd  
Method File : ESI-LCMS Method3.lcm  
Month-Day Acquired : 10/10/2015

Name	:	_____
Notebook #	:	_____
Date	:	_____



ESI-MS Spectrum

Peak # : 1, Retention Time : 0.867 min  
Base Peak m/z : 292, Base Peak Intensity : 492659492659  
Polarity : Positive, Event : 1 - 1



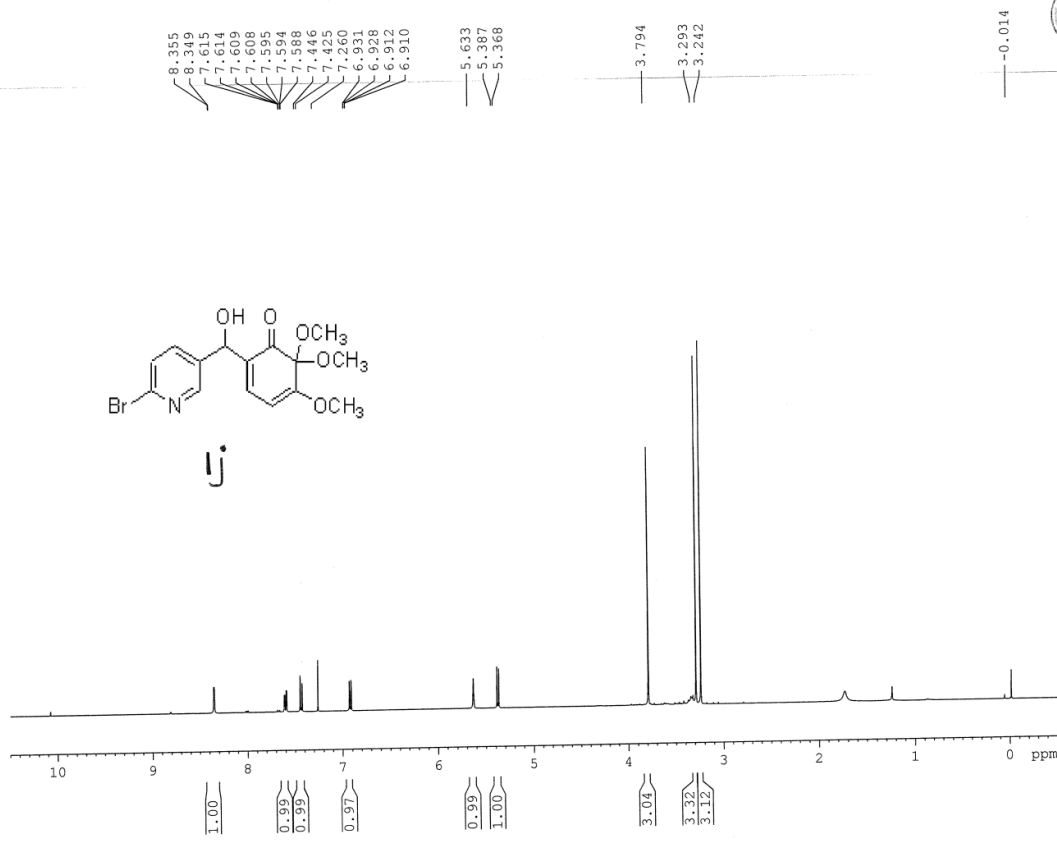
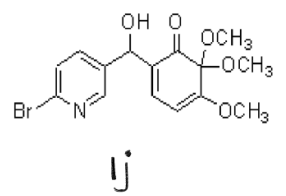


Current Data Parameters  
 NAME SG-BCK-I-26Br-3Py-Q-MAIN  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150729  
 Time 11.53  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 32  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894966 sec  
 RG 90.5  
 LW 62.400 usec  
 DE 6.00 usec  
 TE 300.0 K  
 DI 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.70 usec  
 PL1 -2.00 dB  
 PL1W 14.33185768 W  
 SFO1 400.2330885 MHz

F2 - Processing parameters  
 SI 32768  
 SF 400.2300118 MHz  
 MDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

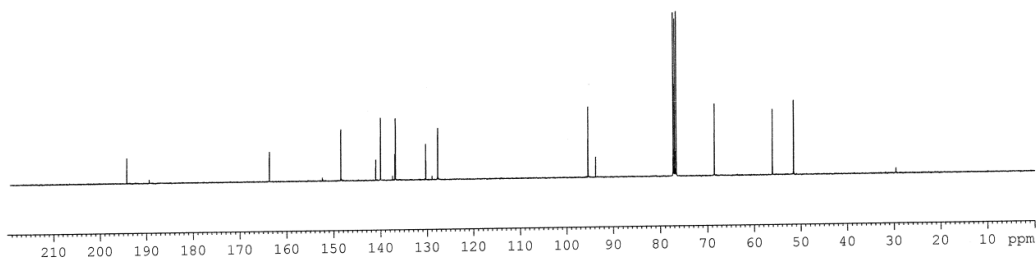
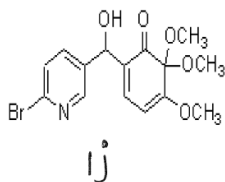


Name \_\_\_\_\_  
 Date \_\_\_\_\_  
 NB # \_\_\_\_\_

AMRI; SRC AV400  
location; 18



194.254  
163.698  
148.531  
141.078  
140.048  
137.003  
136.848  
130.362  
127.754  
95.467  
93.828  
77.317  
76.999  
76.682  
68.577  
56.176  
51.651  
51.614



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

Current Data Parameters  
NAME SG-BCK-I-26Br-3Py-Q-MAIN  
EXFNO 21  
PROCNO 1

F2 - Acquisition Parameters  
Date 20150731  
Time 5.57  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 5000  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 101  
DW 20.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 0.5000000 sec  
D11 0.0300000 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 8.60 usec  
PL1 -1.00 dB  
PL1W 44.58811569 W  
SFO1 100.6479769 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -2.00 dB  
PL12 15.47 dB  
PL13 15.72 dB  
PL2W 14.33185768 W  
PL12W 0.25662708 W  
PL13W 0.24227159 W  
SFO2 400.2316009 MHz

F2 - Processing parameters  
SI 32769  
SF 100.6379176 MHz  
WDW EM  
SBB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

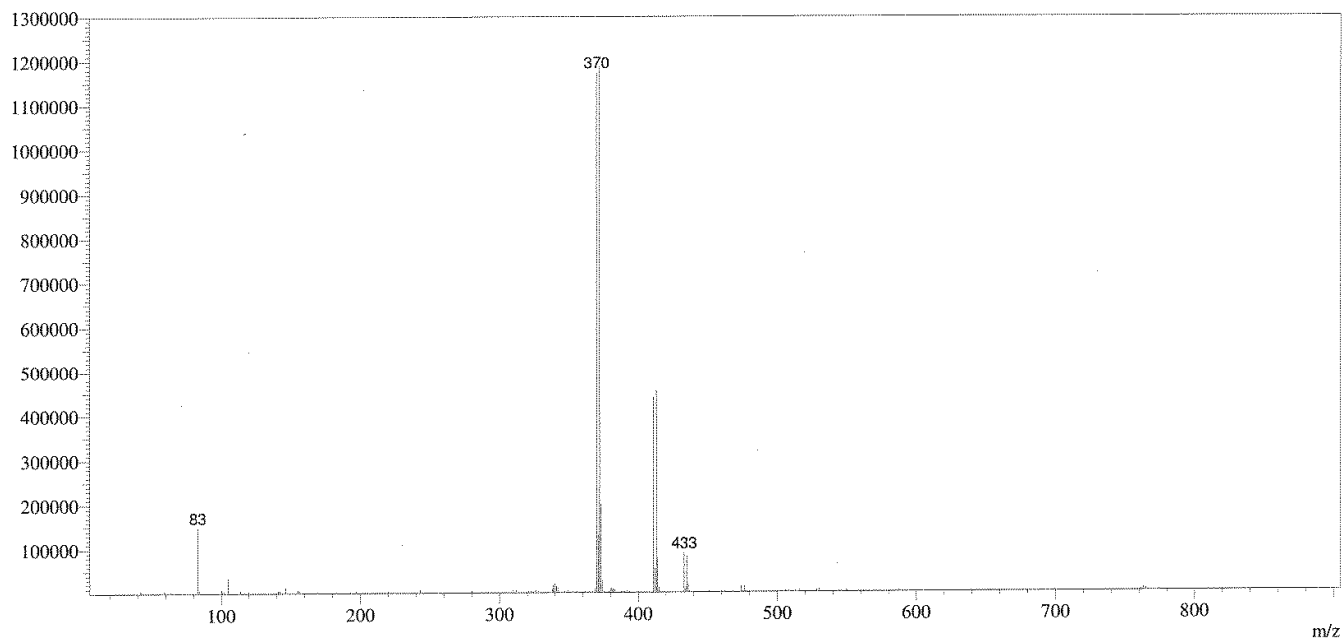
4

Acquired by : System Administrator  
Sample Name : SG-BCK-6-Br-3Py-Qmob-6  
Data File : SG-BCK-6-Br-3Py-Qmob-6.lc  
Method File : ESI-LCMS Method3.lcm  
Month-Day Acquired : 10/7/2015

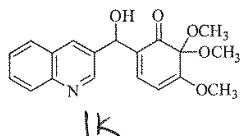
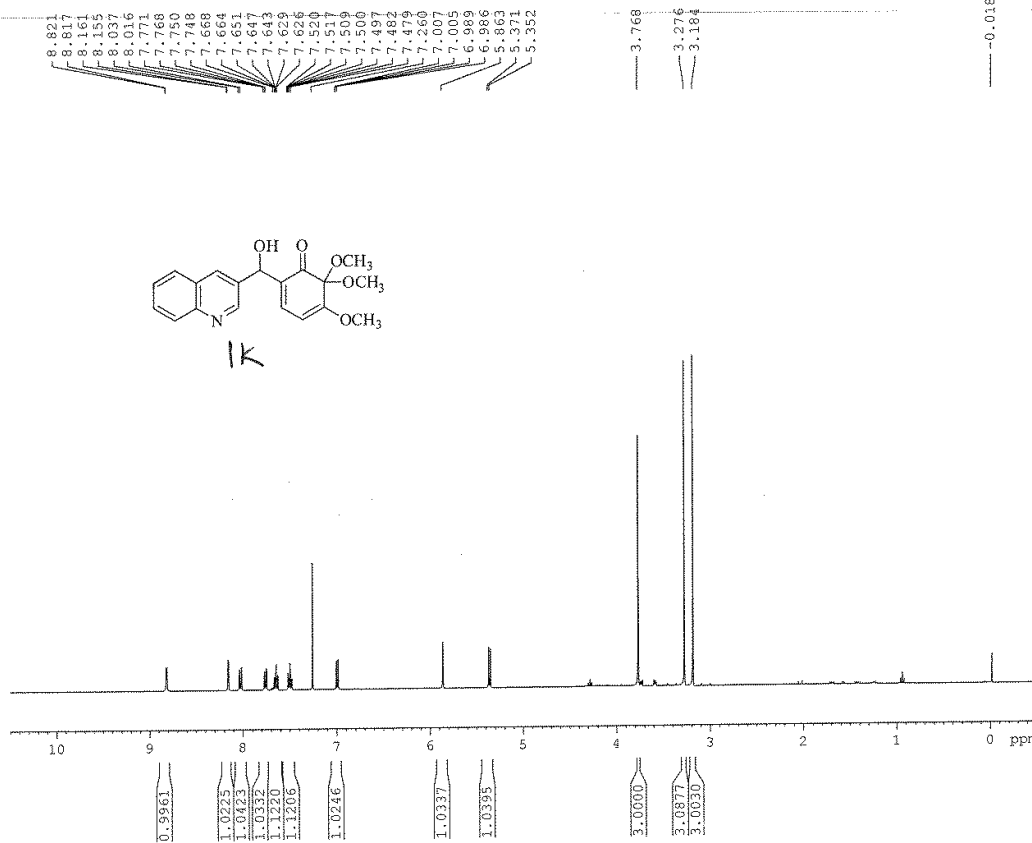


ESI-MS Spectrum

Peak # : 1, Retention Time : 2.567 min  
Base Peak m/z : 372, Base Peak Intensity : 11872591187259  
Polarity : Positive, Event : 1 - 1



AMRI; SRC AV400  
location; 18



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

Current Data Parameters  
NAME SG-SKC-1-23Quin-Q-MAIN  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date 20150731  
Time 19.24  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 64  
DW 62.400 usec  
DE 6.00 usec  
TE 300.0 K  
D1 1.00000000 sec  
TDO 1

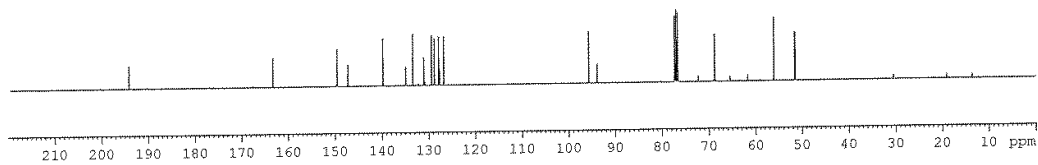
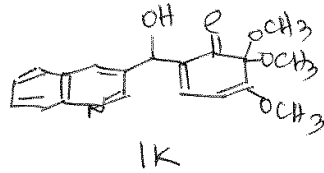
==== CHANNEL f1 =====  
NUC1 1H  
P1 10.70 usec  
PL1 -2.00 dB  
PL1W 14.33185768 W  
SFO1 400.2330885 MHz

F2 - Processing parameters  
SI 32768  
SF 400.2300118 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

AMRI; SRC AV400  
location; 18



194.148  
163.293  
149.579  
147.263  
139.810  
134.931  
133.407  
131.054  
129.412  
129.000  
127.689  
126.799  
95.689  
93.882  
77.317  
76.999  
76.681  
68.790  
56.087  
51.616  
51.506



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

Current Data Parameters  
NAME SG-SKC-I-23Quin-Q-MAIN  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150731  
Time 23.10  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TE 65.536  
SOLVENT CDCl3  
NS 4000  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 801.6  
DW 20.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 0.50000000 sec  
D11 0.03000000 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 8.60 usec  
PL1 -1.00 dB  
PL1W 44.58811569 W  
SFO1 100.6479769 MHz

===== CHANNEL f2 =====  
CPDPRG2 waitz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -2.00 dB  
PL12 15.47 dB  
PL13 15.72 dB  
PL2W 14.33185768 W  
PL12W 0.25662708 W  
PL13W 0.24227159 W  
SFO2 400.2316009 MHz

F2 - Processing parameters  
SI 32768  
SP 100.6379195 MHz  
RDM ZH  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

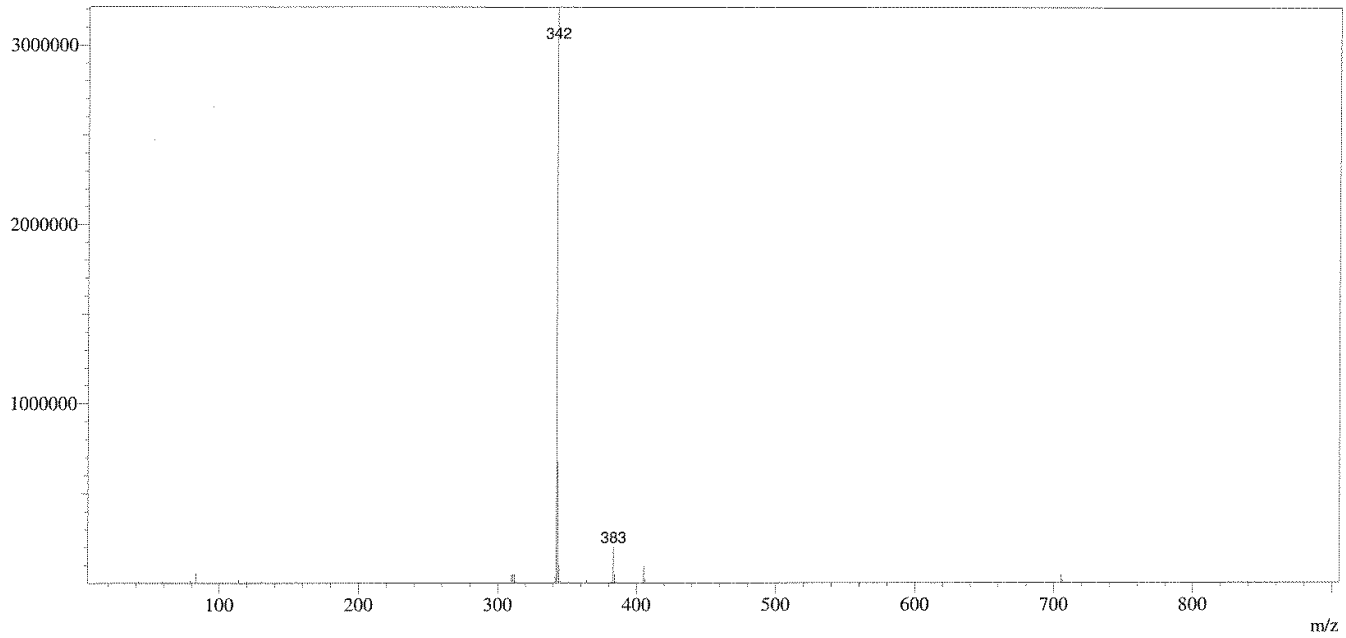
IK

Acquired by : System Administrator  
Sample Name : SG-BCK-NIN-9  
Data File : SG-BCK-4-QuinCHO-Qmob-9  
Method File : ESI-LCMS Method3.lcm  
Month-Day Acquired : 10/8/2015



ESI-MS Spectrum

Peak # : 1, Retention Time : 1.700 min  
Base Peak m/z : 342, Base Peak Intensity : 32125863212586  
Polarity : Positive, Event : 1 - 1





AMRI; SRC AV400  
location; 18

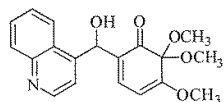


8.917  
8.131  
8.111  
8.109  
7.806  
7.804  
7.785  
7.783  
7.715  
7.710  
7.709  
7.697  
7.693  
7.683  
7.672  
7.664  
7.654  
7.644  
7.619  
7.615  
7.512  
7.504  
7.498  
7.494  
7.491  
7.477  
7.473  
7.260  
6.537  
6.535  
6.518  
6.516  
6.507  
5.222  
5.203

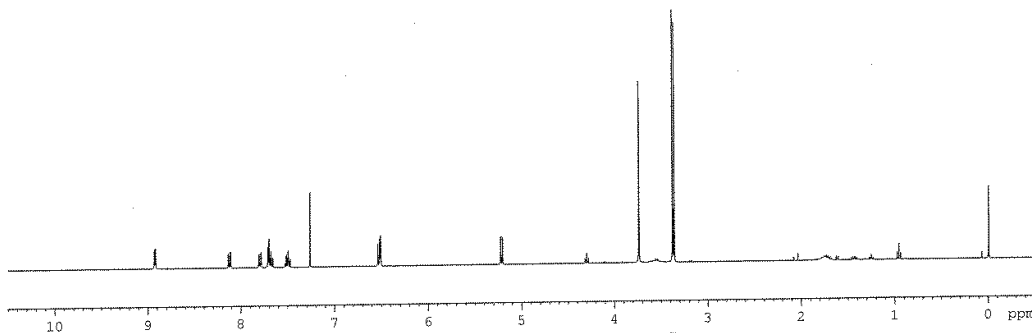
3.735  
3.376  
3.358

0.006

Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_



12



1.0073  
1.0210  
1.0373  
2.1888  
1.1864  
1.0639  
0.9717  
1.0246  
3.1191  
2.7887  
3.1611

Current Data Parameters  
NAME SG-BCK-i-24Quin-Q-MAIN  
EXPNO 20  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150729  
Time\_ 18.32  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 32  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 181  
DW 62.400 usec  
DE 6.00 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

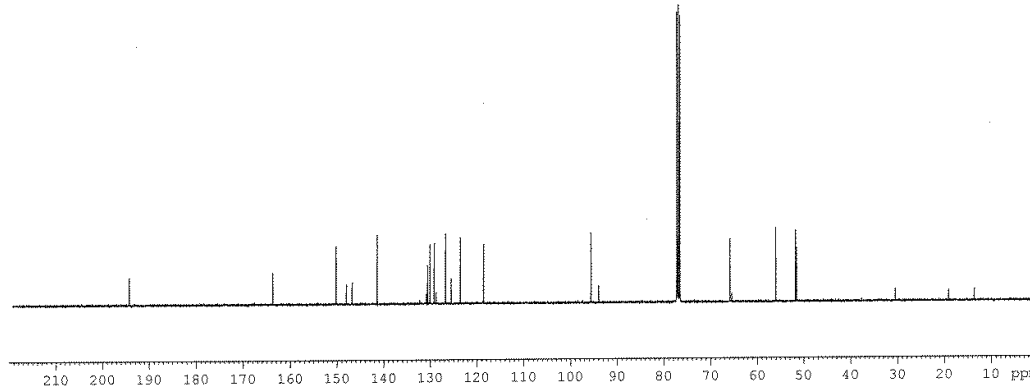
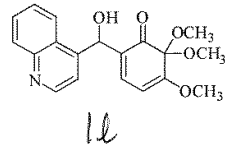
==== CHANNEL f1 =====  
NUC1 1H  
P1 10.70 usec  
PL1 -2.00 dB  
PL1W 14.33185768 W  
SF01 400.2330885 MHz

F2 - Processing parameters  
SI 32768  
SF 400.2300118 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

AMRI; SRC AV400  
location; 18



194.346  
163.772  
150.295  
148.053  
146.844  
141.453  
130.620  
130.133  
129.208  
126.772  
125.568  
123.602  
118.616  
85.660  
83.997  
77.319  
77.001  
76.684  
65.925  
56.123  
51.851  
51.644



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

Current Data Parameters  
NAME SC-BOX-1-2402in-Q-MAIN  
EXPNO 31  
PROCNO 1

F2 - Acquisition Parameters  
Date 20150730  
Time 23.50  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT cbr13  
NS 5000  
DS 4  
SWH 24938.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631888 sec  
RG 71.8  
RW 20.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 0.5000000 sec  
D11 0.03600000 sec  
TD0 1

----- CHANNEL f1 -----  
NUC1 13C  
P1 8.60 usec  
PL1 -1.00 dB  
PLW 44.58811569 K  
SFO1 100.6479769 MHz

----- CHANNEL f2 -----  
CQDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -2.00 dB  
PL12 15.47 dB  
PL13 15.72 dB  
PL2W 14.33185768 W  
PL12W 0.25662708 W  
PL13W 0.24271159 W  
SFO2 400.2516009 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6379159 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

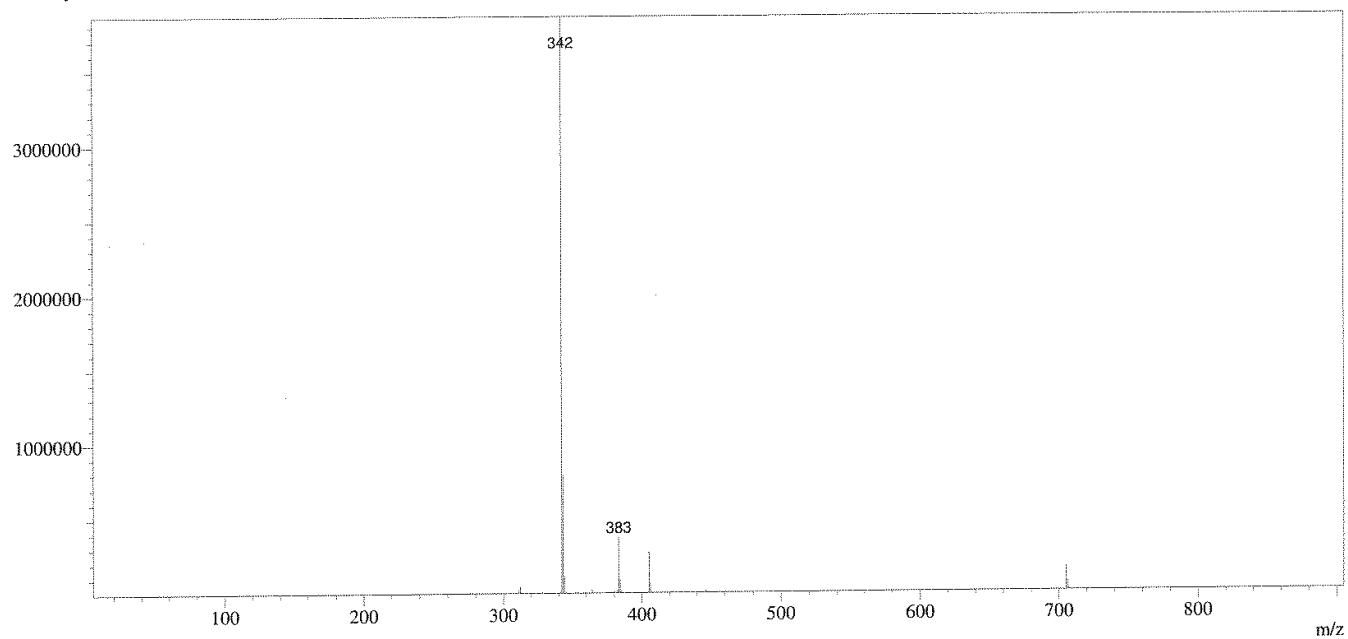
12

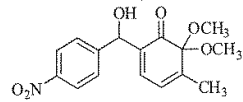
Acquired by : System Administrator  
Sample Name : SG-BCK-3-QuinCHO-Qmob-7  
Data File : SG-BCK-3-QuinCHO-Qmob-7  
Method File : ESI-LCMS Method3.lcm  
Month-Day Acquired : 10/7/2015



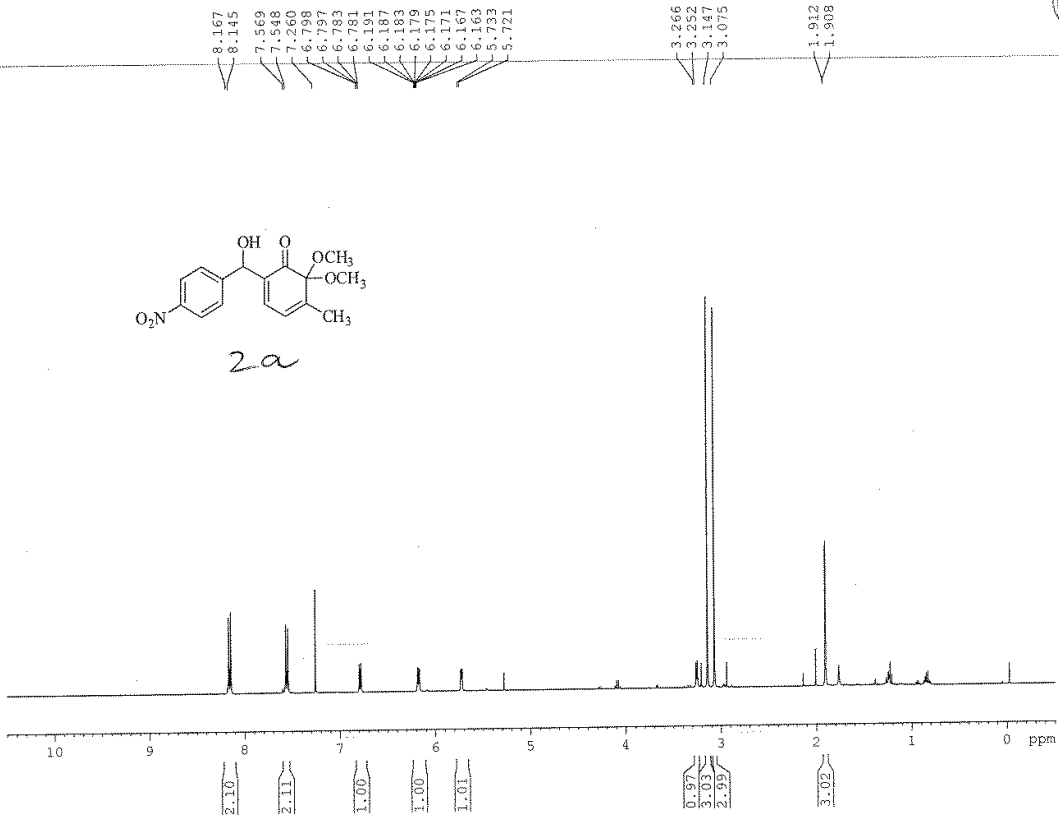
ESI-MS Spectrum

Peak # : 1, Retention Time : 2.167 min  
Base Peak m/z : 342, Base Peak Intensity : 38670113867011  
Polarity : Positive, Event : 1 - 1





2a



Current Data Parameters  
 NAME SG-MKK-L-N-Me-P-R02  
 EXPNO 20  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150712  
 Time 7.23  
 INSTRUM spect  
 PROBRD 5 mm FAPBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 100  
 DS 2  
 SSWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894966 sec  
 RG 35.9  
 DR 62.400 usec  
 DE 6.50 usec  
 TE 301.8 K  
 D1 1.0000000 sec  
 FDD 1

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.40 usec  
 PL1 -3.00 dB  
 PLLW 19.34582710 W  
 SFO1 400.1316542 MHz

F2 - Processing parameters  
 SI 32768  
 SF 400.1300092 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

Name \_\_\_\_\_

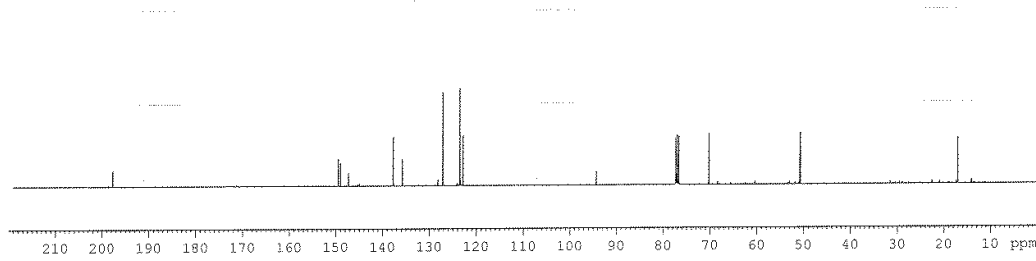
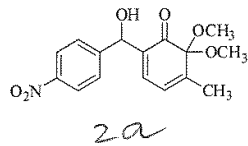
Date \_\_\_\_\_

NB # \_\_\_\_\_

AMRI SRC  
location; 17



197.739  
149.494  
149.020  
147.349  
137.754  
135.791  
127.144  
123.555  
122.851  
94.305  
77.321  
77.003  
76.685  
70.217  
50.778  
50.695  
17.059



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

Current Data Parameters  
NAME SG-MKK-L-M-Me-F-NO2  
EXPNO 21  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150712  
Time 12.12  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 5000  
DS 4  
SWH 23980.814 Hz  
FREQES 0.365918 Hz  
AQ 1.3664756 sec  
RG 18390.4  
DW 20.850 usec  
DE 6.50 usec  
TE 303.2 K  
D1 2.0000000 sec  
D11 0.0500000 sec  
TDD 1

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
NUC1 13C  
P1 7.40 usec  
PL1 -4.00 dB  
PL1W 82.02445221 W  
SFO1 100.6282299 MHz

\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
CPOBPG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -3.00 dB  
PL12 14.72 dB  
PL13 15.06 dB  
PL2W 19.34592710 W  
PL12W 8.32702976 W  
PL13W 6.30240381 W  
SFO2 400.1316095 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127729 MHz  
WDW EM  
SFR 0  
L8 1.00 Hz  
GB 0  
PC 1.40

2a -ve mode

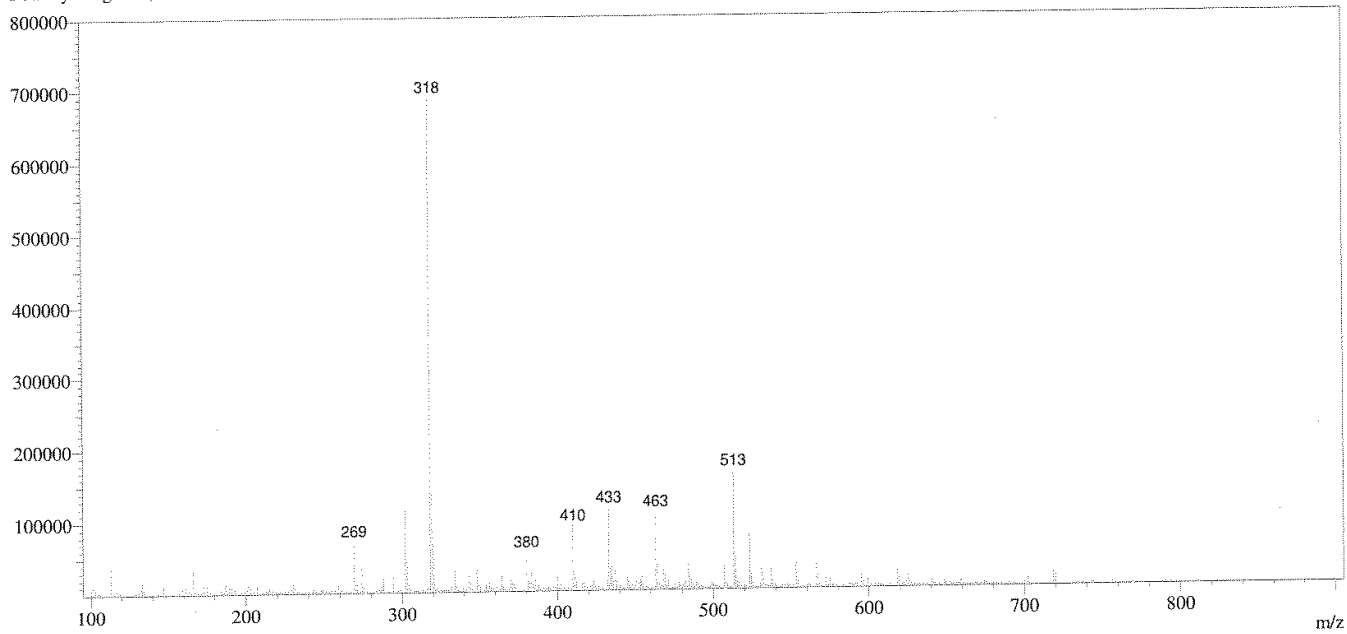
Acquired by : System Administrator  
Sample Name : SG- MKK-L-Me-P-NO2  
Data File : SG- MKK-L-Me-P-NO2.lcd  
Method File : ESI-LCMS Method3.lcm  
Month-Day Acquired : 10/11/2015

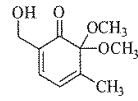
Name	:	_____
Notebook #	:	_____
Date	:	_____



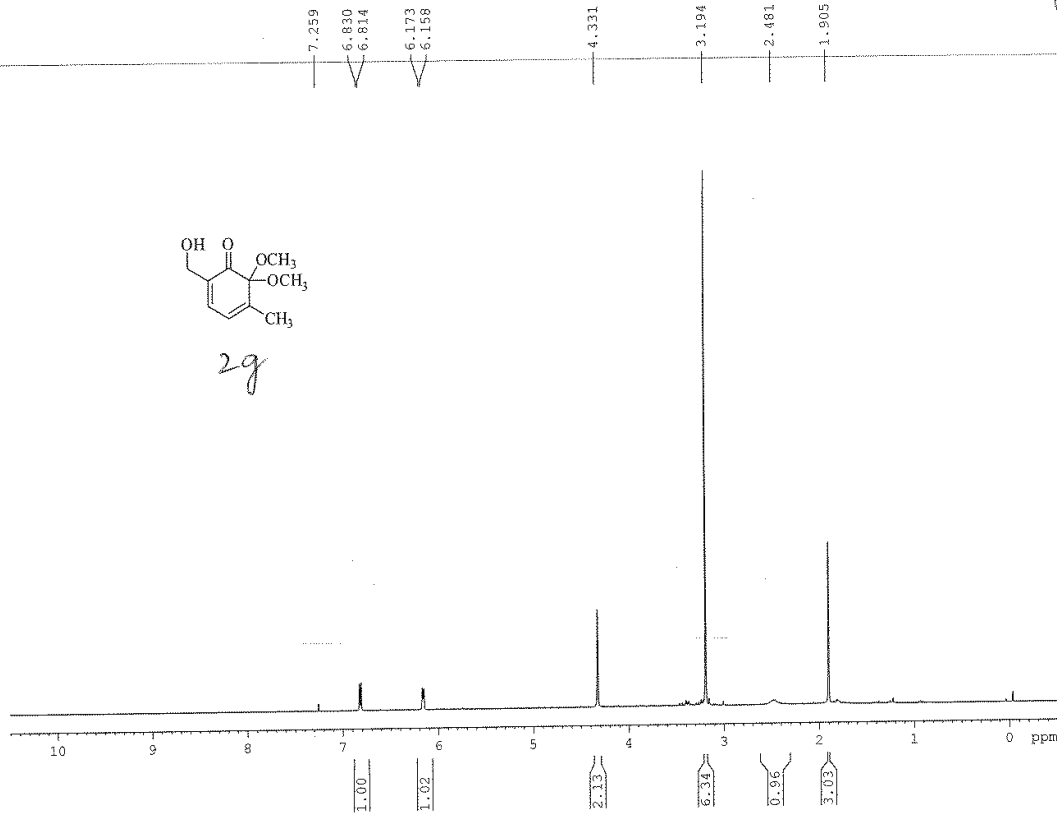
ESI-MS Spectrum

Peak # : 1, Retention Time : 2.849 min  
Base Peak m/z : 318, Base Peak Intensity : 690753690753  
Polarity : Negative, Event : 1 - 2





2g



Current Data Parameters  
NAME SG-MKK-1-M-Me-HCHO  
EXPNO 30  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150712  
Time\_ 16.13  
INSTRUM spect  
PROBHD 5 mm PARBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 100  
DS 2  
SMH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 35.5  
DM 62.400 usec  
DE 6.50 usec  
TE 302.4 K  
D1 1.0000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 10.40 usec  
PL1 -3.00 dB  
PL1W 19.34582710 W  
SFO1 400.1318542 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1300037 MHz  
WDW EM  
SSB 0  
LA 0.30 Hz  
GB 0  
PC 1.00

Name \_\_\_\_\_

Date \_\_\_\_\_

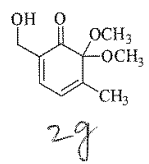
NB # \_\_\_\_\_

# AMRI SRC location; 17



198.370  
148.240  
137.271  
134.094  
123.145  
94.121  
77.315  
76.997  
76.679  
60.080  
50.756  
16.945

Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_



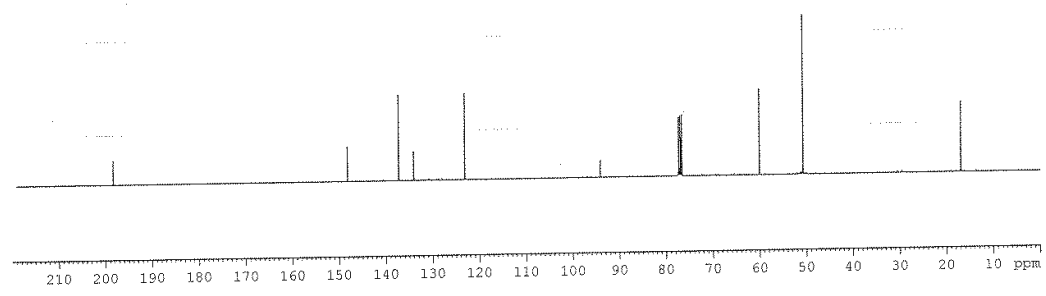
Current Data Parameters  
NAME SG-MKN-L-M-Hc-HCHO  
EXPRO 31  
PROCNO 1

F2 - Acquisition Parameters  
Date 20150712  
Time 21.03  
INSTRUM spect  
PROBHD 5 mm PABO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 6000  
DS 4  
SWH 23960.814 Hz  
FIDRES 0.365918 Hz  
AQ 1.3664756 sec  
RG 16384  
DW 20.850 usec  
DE 6.50 usec  
TE 303.4 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1

==== CHANNEL F1 =====  
NUC1 13C  
P1 7.40 usec  
PL1 -4.00 dB  
PL1X 82.02445221 W  
SFO1 100.6228298 MHz

==== CHANNEL F2 =====  
CQDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -3.00 dB  
PL12 14.72 dB  
PL13 15.06 dB  
PL2W 18.34582710 W  
PL12W 0.32702876 W  
PL13W 0.30240381 W  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127726 MHz  
WDW EM  
SSB 0  
IB 0 1.00 Hz  
GB 0  
PC 1.40

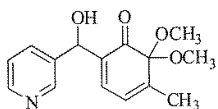




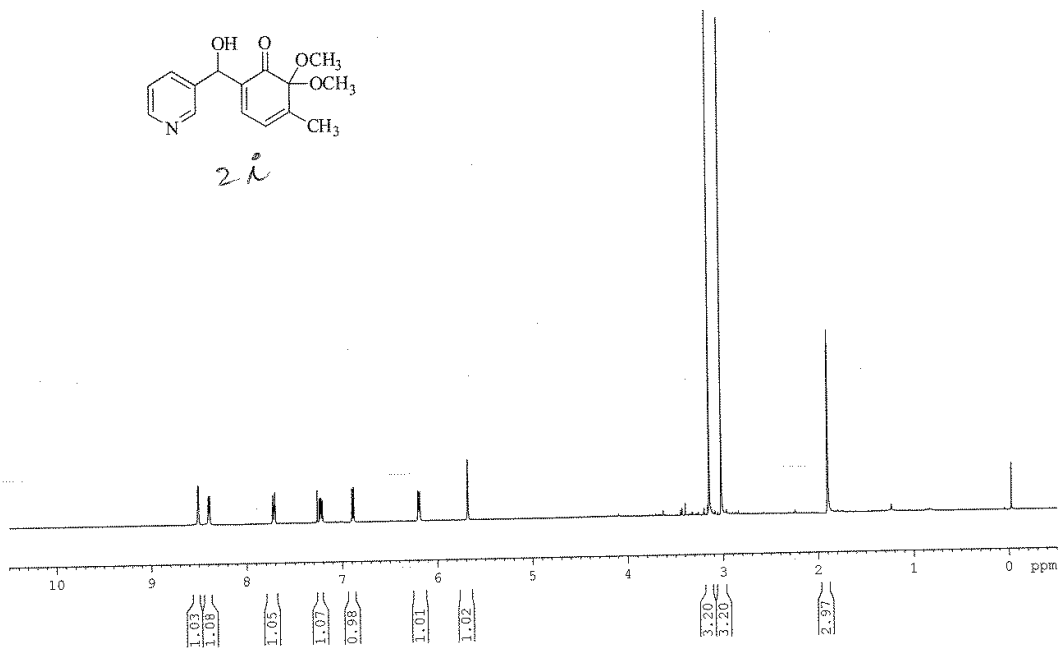
8.509  
8.504  
8.500  
8.396  
8.388  
8.384  
7.727  
7.723  
7.719  
7.709  
7.708  
7.703  
7.699  
7.260  
7.238  
7.237  
7.226  
7.225  
7.219  
7.217  
7.206  
7.205  
6.895  
6.893  
6.879  
6.877  
6.200  
6.187  
6.183  
5.680

3.150  
3.024  
1.906  
1.902

-0.022



2.1



Current Data Parameters  
NAME SG-MKK-L-Me-3-Py-CHO  
EXPNO 20  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20130724  
Time 21:13  
INSTRUM spect  
PROBHD 5 mm F400 BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 100  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 57  
SW 62.400 usec  
DE 6.50 usec  
TE 300.0 K  
DI 1.06000000 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 10.40 usec  
PL1 -3.00 dB  
PL1W 19.34582710 W  
SFO1 400.1318542 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1300093 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
FC 1.00

Name \_\_\_\_\_

Date \_\_\_\_\_

NB # \_\_\_\_\_

AMRI SRC  
location; 17



197.447

148.770  
148.567  
148.073  
137.780  
137.004  
136.385  
134.392

123.349  
123.045

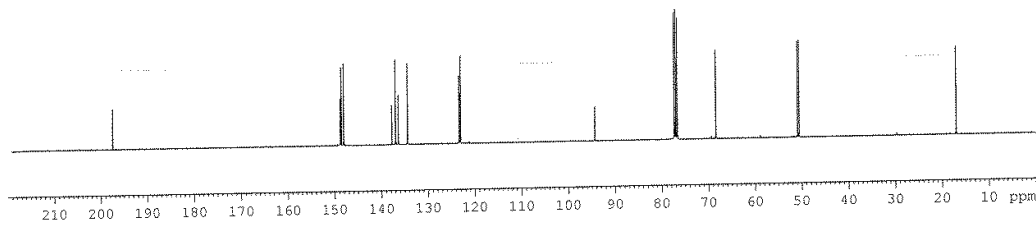
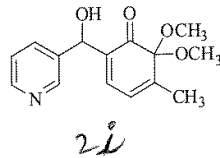
94.314

77.320  
77.001  
76.684

68.410

50.867  
50.569

17.016



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

Current Data Parameters  
NAME SG-MKK-L-Me-3-Py-CHO  
EXPNO 21  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150225  
Time 4.01  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
FID 65536  
SOLVENT CDCl3  
NS 7000  
DS 4  
SWH 23980.814 Hz  
FIDRES 0.365918 Hz  
AQ 1.3664706 sec  
RG 8192  
DW 20.850 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1

CHANNEL f1  
NUC1 13C  
P1 7.40 usec  
PL1 -4.00 dB  
PL1W 82.02445221 W  
SFO1 100.6228236 MHz

CHANNEL f2  
CPDPRG2 waltz16  
NUC2 1H  
P2 80.00 usec  
PL2 -3.00 dB  
PL12 14.72 dB  
PL13 15.06 dB  
PL2W 19.34582710 W  
PL12W 0.32702976 W  
PL13W 0.30240381 W  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127725 MHz  
WDW EM  
SFB 0  
LB 1.00 Hz  
GB 0  
EC 1.46

21

Acquired by : System Administrator  
Sample Name : SG-MKK-L-Me-PY-CHO  
Data File : SG-MKK-L-Me-PY-CHO.lcd  
Method File : ESI-LCMS Method3.lcm  
Month-Day Acquired : 10/8/2015

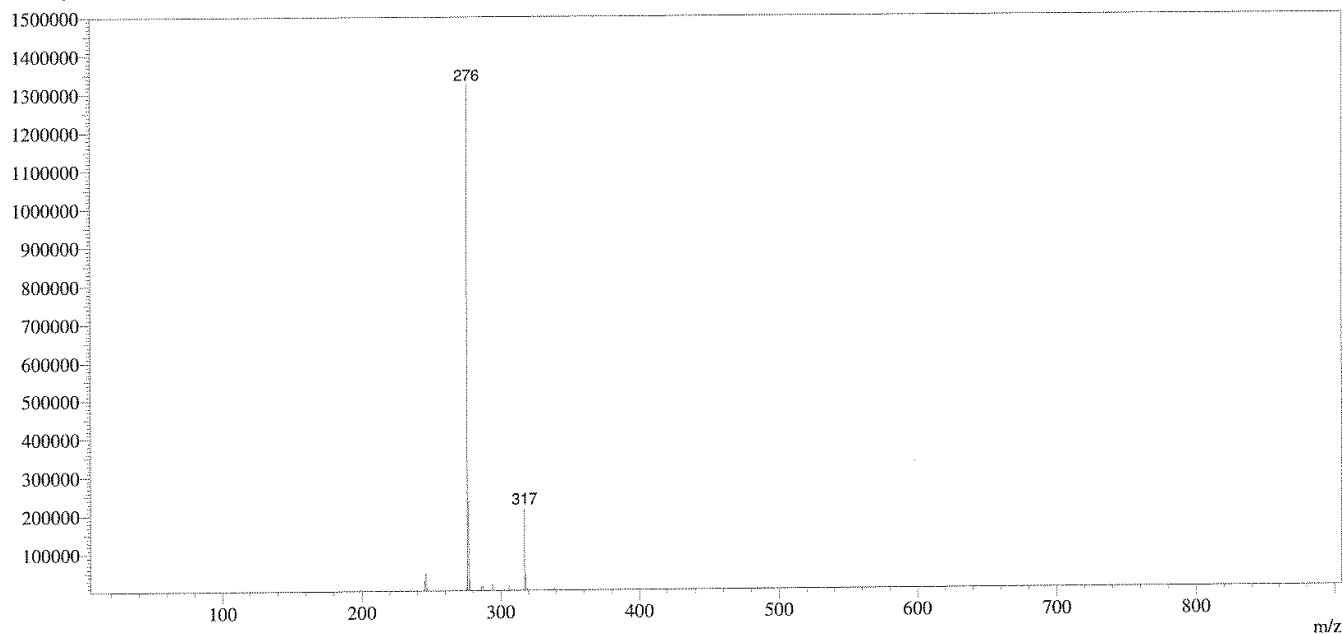
Name	:	_____
Notebook #	:	_____
Date	:	_____



**AMRI**<sup>®</sup>  
Albany Molecular Research Inc.

ESI-MS Spectrum

Peak # : 1, Retention Time : 1.267 min  
Base Peak m/z : 276, Base Peak Intensity : 13229131322913  
Polarity : Positive, Event : 1 - 1



7.302  
7.266  
7.268  
7.011  
7.007  
7.003  
6.995  
6.991  
6.987

4.474  
4.471

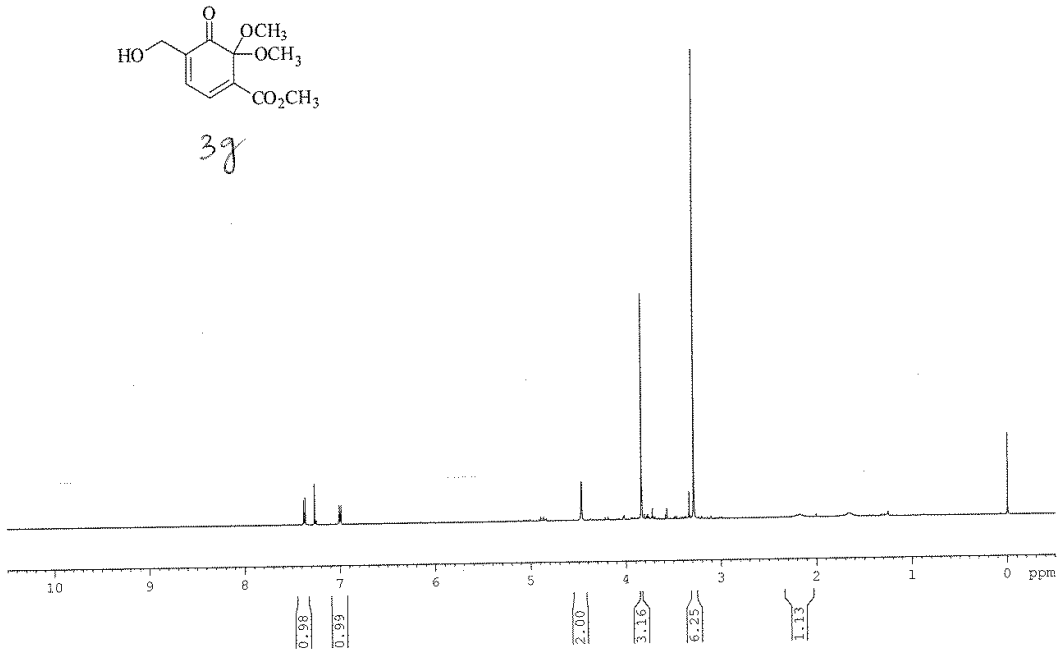
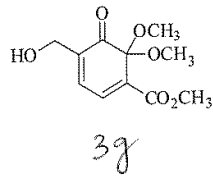
3.843

3.292

2.187  
2.171  
2.142

1.658

— 0.000



Current Data Parameters  
NAME SG-MKK-L-CO2Me-HCHO  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150822  
Time 13.35  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 100  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 114  
DM 62.400 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.0000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 10.40 usec  
PL1 -3.00 dB  
PLLW 19.34592710 W  
SFO1 400.1318542 MHz

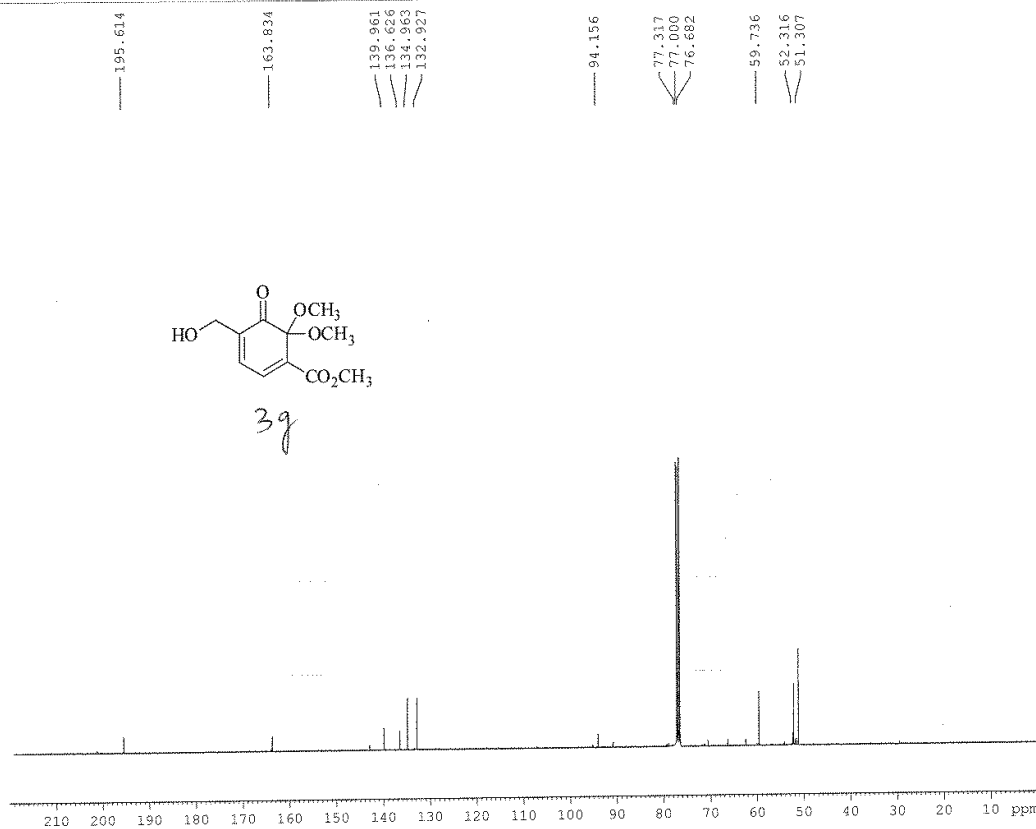
F2 - Processing parameters  
SI 32768  
SF 400.1300060 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Name \_\_\_\_\_

Date \_\_\_\_\_

NB # \_\_\_\_\_

AMRI SRC  
location; 17



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

Current Data Parameters  
NAME SG-MKK-L-CO2Me-HCHO  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150822  
Time 23.09  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 10000  
DS 4  
SWH 23980.814 Hz  
FIDRES 0.365918 Hz  
AQ 1.3664756 sec  
RG 9195.2  
DW 20.850 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 7.40 usec  
PL1 -4.00 dB  
EL1W 82.02445221 W  
SFO1 100.6282298 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -3.00 dB  
PL12 14.72 dB  
PL13 15.08 dB  
PL2W 19.34582710 W  
PL12W 0.32702876 W  
PL13W 0.30240381 W  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127708 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

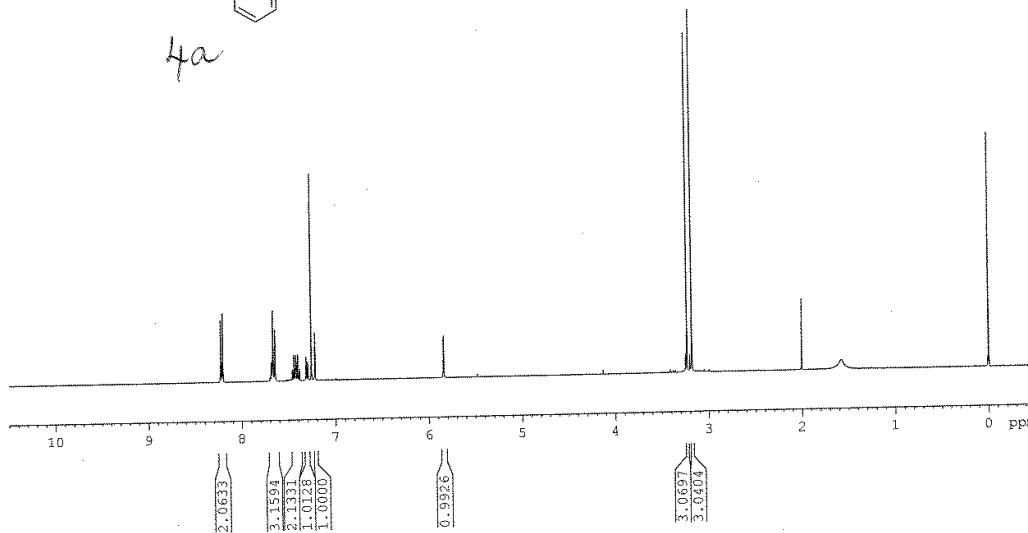
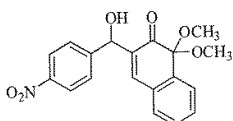
AMRI; SRC AV400  
location; 18



8.226  
8.221  
8.209  
8.204  
8.198  
7.687  
7.683  
7.669  
7.668  
7.650  
7.647  
7.464  
7.460  
7.448  
7.447  
7.443  
7.442  
7.432  
7.420  
7.406  
7.402  
7.387  
7.383  
7.316  
7.312  
7.298  
7.294  
7.260  
7.221  
5.841

3.233  
3.181

Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_



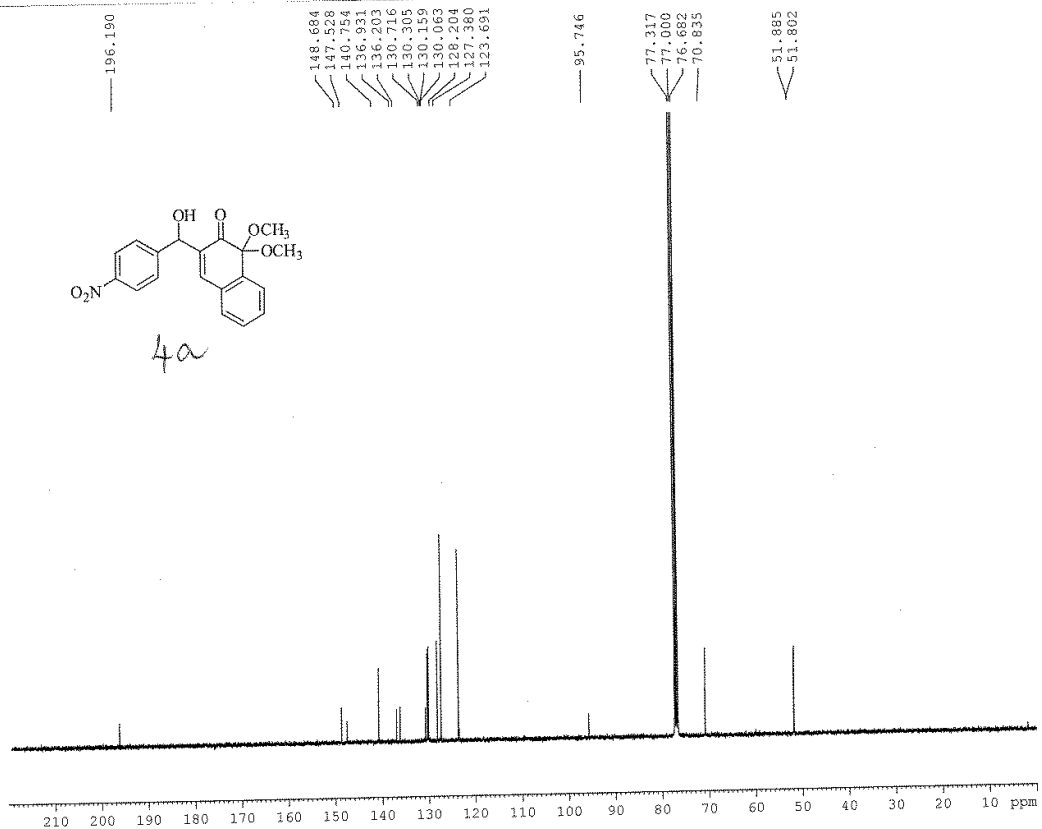
Current Data Parameters  
NAME SG-RKP-L-4-NO2-NAP  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150723  
Time 21.07  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 181  
DW 62.400 usec  
DE 6.00 usec  
TE 300.0 K  
D1 1.00000000 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 10.70 usec  
PL1 -2.00 dB  
PL1W 14.33185768 W  
SFO1 400.2330885 MHz

F2 - Processing parameters  
SI 32768  
SE 400.2300118 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

AMRI; SRC AV400  
location; 18



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

Current Data Parameters  
NAME SG-RK7-L-4-NO2-NAP  
EXPNO 12  
PROCNO 1

F2 - Acquisition Parameters  
Date 20150724  
Time 1.26  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 8000  
DS 4  
SWH 24698.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 80.5  
DM 20.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 0.5000000 sec  
D11 0.0300000 sec  
TDO 1

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
NUC1 13C  
P1 8.60 usec  
PL1 -1.90 dB  
PL1W 44.56811569 W  
SFO1 100.6479769 MHz

\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
CH2PRG2 waltz16  
NUC2 1H  
PCPD2 60.00 usec  
PL2 -2.00 dB  
PL12 15.47 dB  
PL13 15.72 dB  
PL2W 14.33185768 W  
PL12W 0.25662708 W  
PL13W 0.24227159 W  
SFO2 400.2316009 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6379156 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

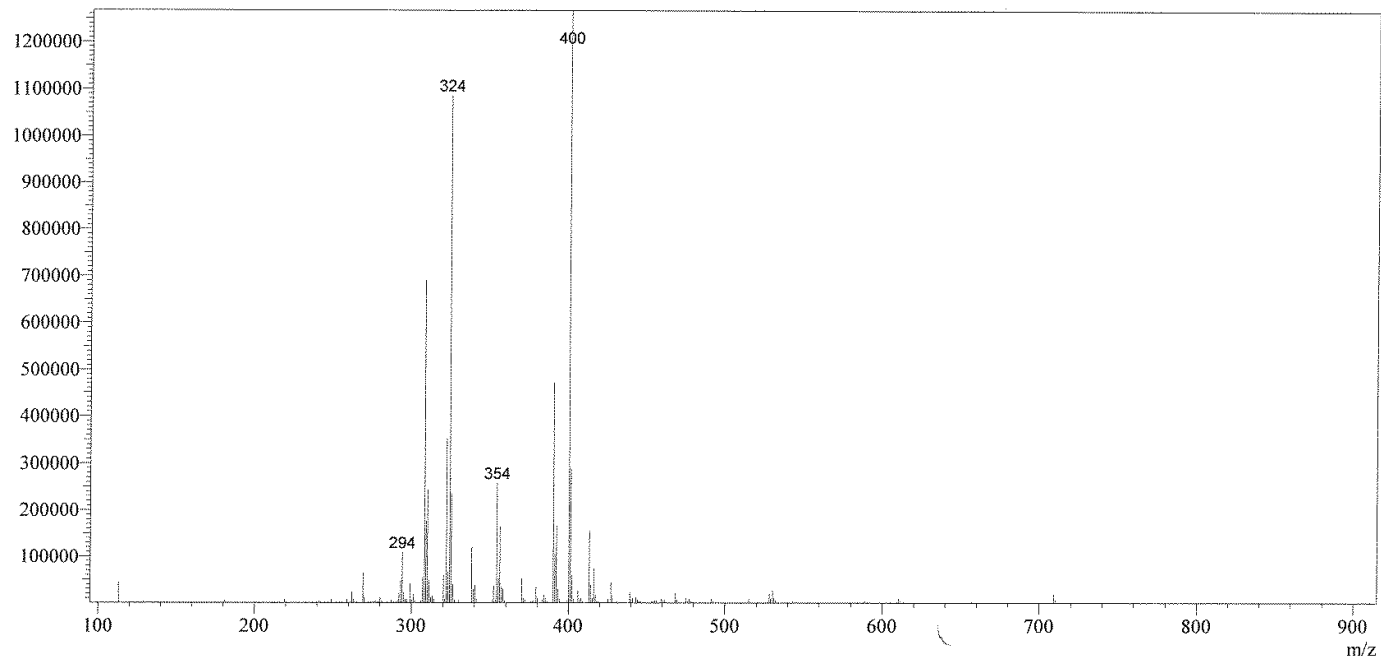
Acquired by : System Administrator  
Sample Name : SG-BCK-2-Naphth-p-NO2-Ph  
Data File : SG-BCK-2-Naphth-p-NO2-Ph  
Method File : ESI-LCMS Method3.lcm  
Month-Day Acquired : 10/7/2015

4a



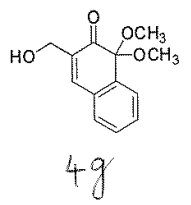
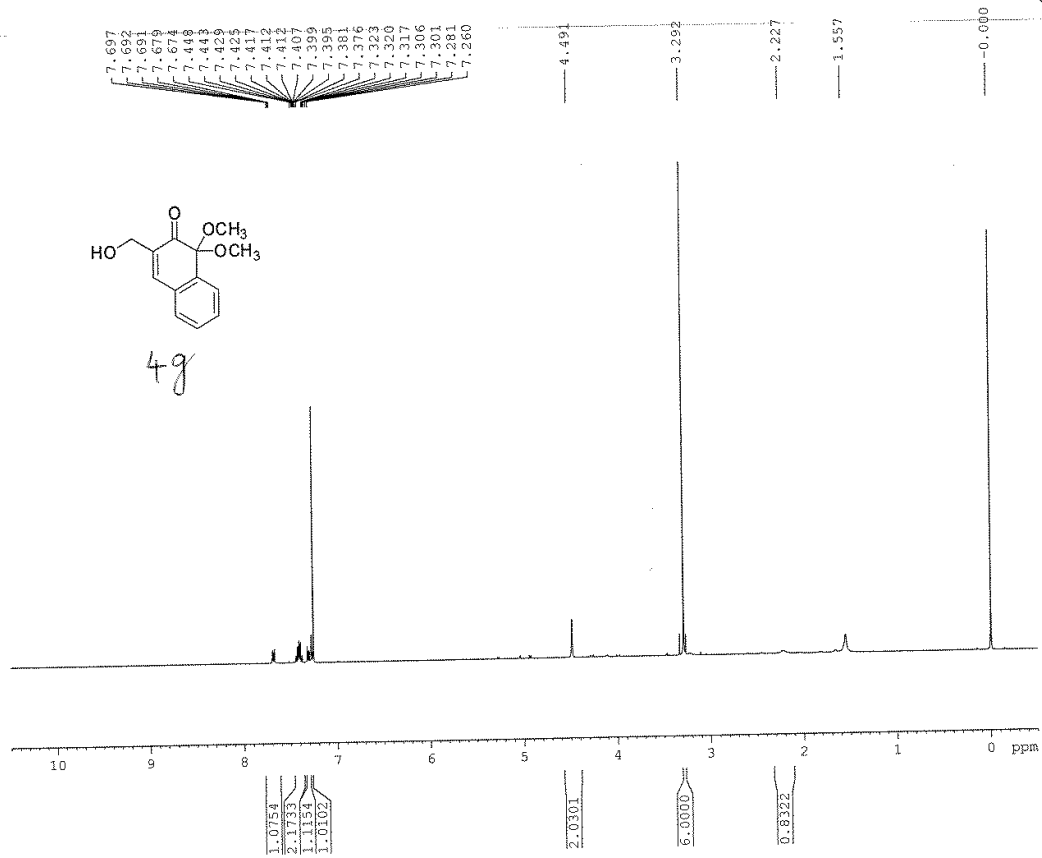
ESI-MS Spectrum

Peak # : 1, Retention Time : 3.149 min  
Base Peak m/z : 400, Base Peak Intensity : 12670381267038  
Polarity : Negative, Event : 1 - 2





AMRI; SRC AV400  
location; 18



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

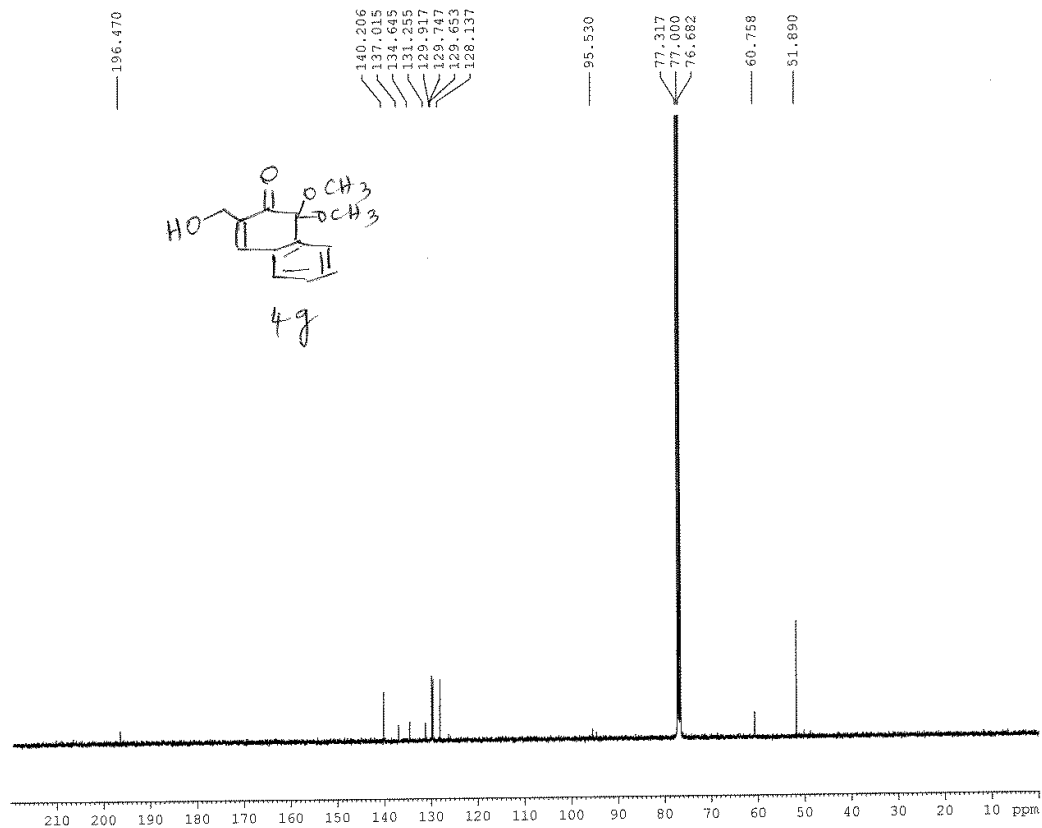
Current Data Parameters  
NAME SG-RKP-L-NAP-FORM  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150724  
Time 8.26  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 287  
DW 62.400 usec  
DE 6.00 usec  
TE 300.0 K  
D1 1.0000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 10.70 usec  
PL1 -2.00 dB  
PL1W 14.33185768 W  
SF01 400.2330885 MHz

F2 - Processing parameters  
SI 32768  
SF 400.2300121 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
FC 1.00

AMRI; SRC AV400  
location; 18



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

Current Data Parameters  
NAME SG-RKP-L-NAP-FORM  
EXPNO 21  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150725  
Time 12.21  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TE 65.36  
SOLVENT CDCl3  
NS 16000  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 101  
DW 20.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 0.50000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 8.60 usec  
PL1 -1.60 dB  
PL1W 44.58811569 W  
SF01 100.6479769 MHz

===== CHANNEL f2 =====  
CEDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -2.00 dB  
PL12 15.47 dB  
PL13 15.72 dB  
PL2W 14.33185768 W  
PL12W 0.25662708 W  
PL13W 0.24227159 W  
SF02 400.2316009 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6379149 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

AMRI; SRC AV400  
location; 18

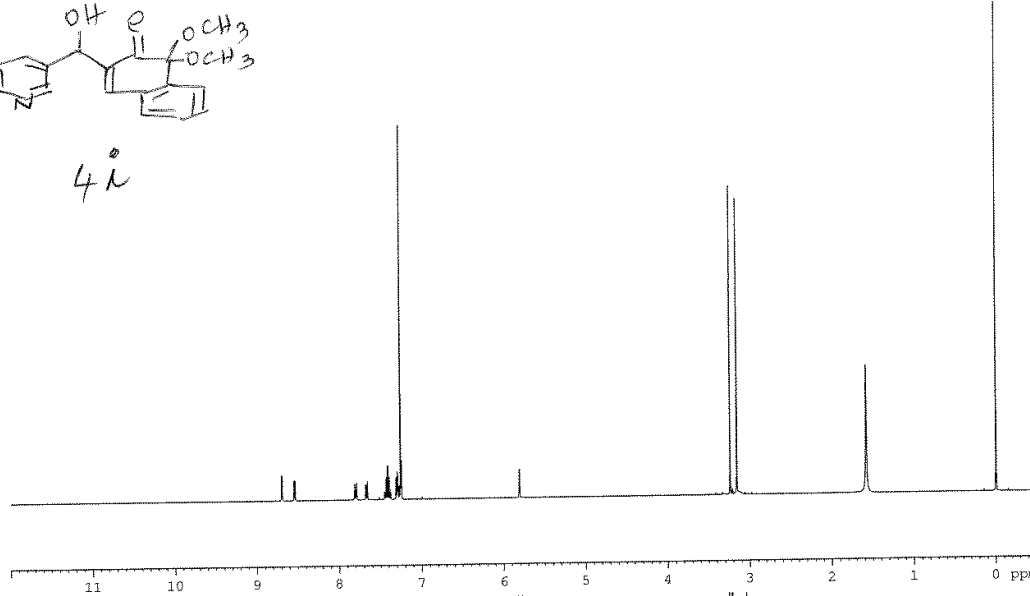
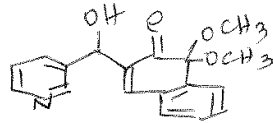


8.703  
8.697  
8.553  
8.549  
8.541  
8.537  
7.818  
7.814  
7.810  
7.809  
7.800  
7.799  
7.794  
7.790  
7.789  
7.788  
7.679  
7.666  
7.661  
7.655  
7.451  
7.436  
7.433  
7.433  
7.419  
7.414  
7.401  
7.397  
7.382  
7.378  
7.316  
7.310  
7.308  
7.298  
7.295  
7.289  
7.288  
7.277  
7.276  
7.261  
7.250  
5.811  
3.242  
3.161  
3.137

1.586

-0.500

Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB# \_\_\_\_\_



1.0060  
0.9960  
1.0173  
1.0172  
2.1278  
2.1372  
1.0608  
0.9984  
3.0048  
3.2197

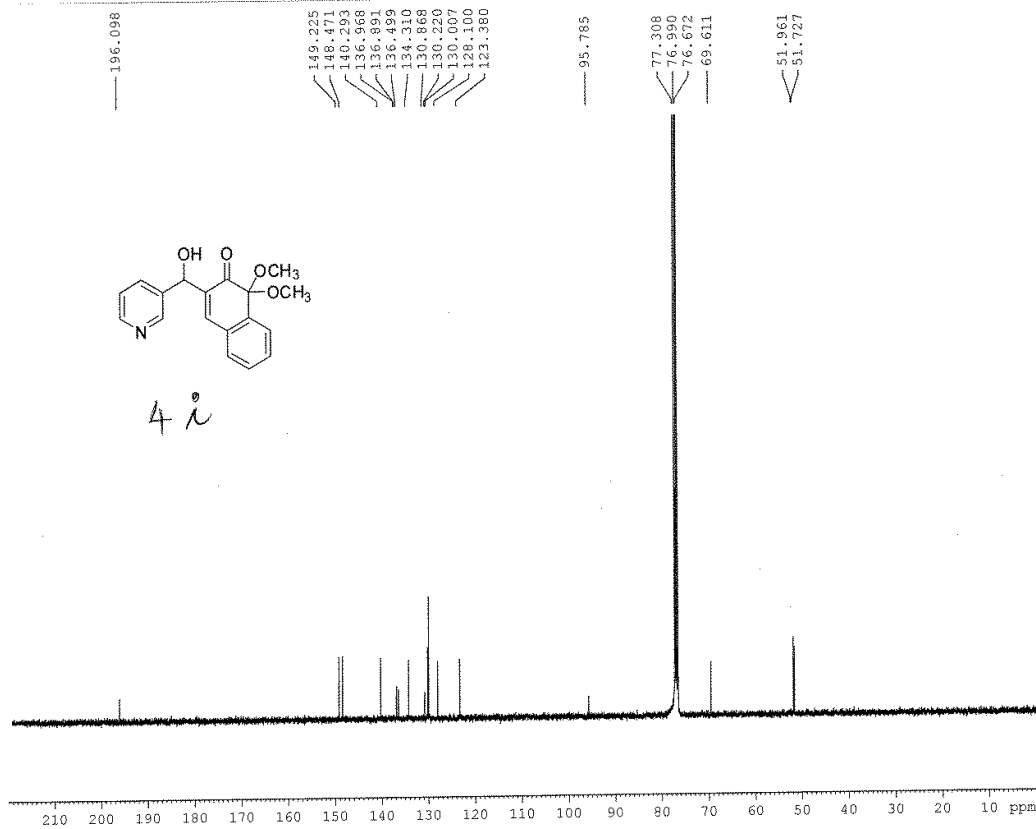
Current Data Parameters  
NAME SG-RKP-L-2-NAP-PYR-1  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150729  
Time 7.38  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 181  
DW 62.400 usec  
DE 6.00 usec  
TE 300.0 K  
D1 1.00000000 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 10.70 usec  
PL1 -2.00 dB  
PLW 14.33185768 W  
SFO1 400.2330885 MHz

F2 - Processing parameters  
SI 32768  
SF 400.2300116 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

AMRI SRC  
location; 17



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

Current Data Parameters  
NAME SG-RKP-L-2-N-PY  
EXNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150801  
Time 6.43  
INSTRUM spect  
PROBHD 5 mm PABBO ER-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 10000  
DS 4  
SMH 23980.814 Hz  
FIDRES 0.365918 Hz  
AQ 1.3684736 sec  
RG 18390.4  
DN 20.850 usec  
DE 6.50 usec  
TE 300.2 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 7.40 usec  
PL1 -4.00 dB  
PL1W 82.02445221 W  
SFO1 100.6228298 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -3.00 dB  
PL12 14.72 dB  
PL13 15.06 dB  
PL2W 19.34582710 W  
PL12W 0.32702976 W  
PL13W 0.30240381 W  
SFO2 400.1316005 MHz

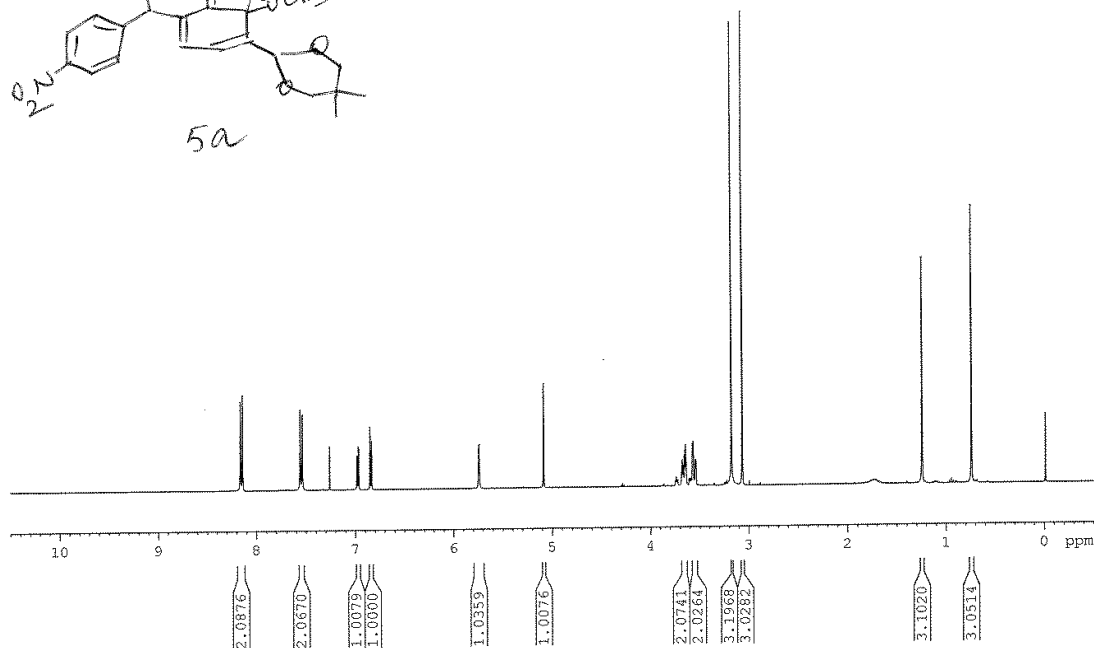
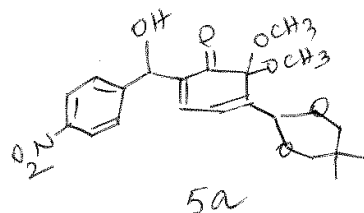
F2 - Processing parameters  
SI 32768  
SF 100.6127766 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
EC 1.40

AMRI; SRC AV400  
location; 18



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

8.169  
8.133  
8.119  
8.116  
8.111  
8.116  
8.158  
7.358  
7.354  
7.337  
7.331  
7.260  
6.984  
6.981  
6.968  
6.965  
6.851  
6.835  
5.742  
5.087  
3.176  
3.066  
1.242  
0.740  
-0.014



Current Data Parameters  
NAME SG-SIR-3Kt1-NO2PhCHO-DMAP  
EXPNO 10  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20150801  
Time 11.37  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 64  
DW 62.400 usec  
DE 6.00 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 10.70 usec  
PL1 -2.00 dB  
PL1W 14.33185768 W  
SFO1 400.2330885 MHz

F2 - Processing parameters  
SI 32768  
SF 400.2300118 MHz  
WDR EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

AMRI; SRC AV400  
location; 18



196.211

148.662

147.422

146.394

137.869

136.117

127.245

125.145

123.592

95.967

93.854

77.767

77.313

76.996

76.678

70.112

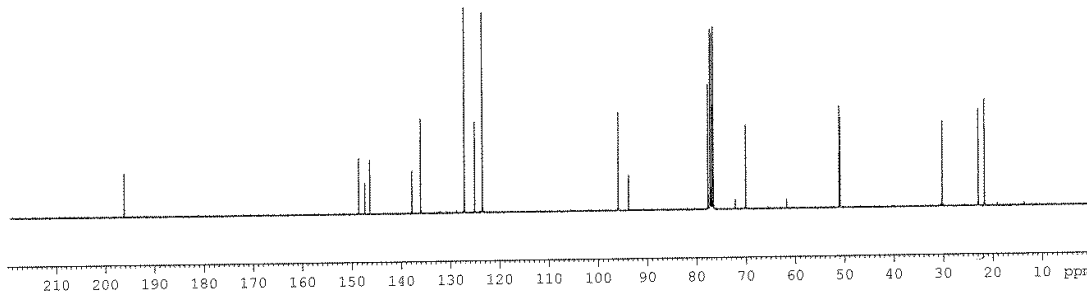
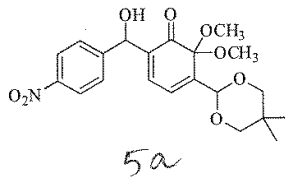
51.151

50.996

30.246

22.950

21.723



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

Current Data Parameters  
NAME SG-SIR-3kt1-NO2PHCHO-DMAP  
EXPNO 11  
PROCNO 1

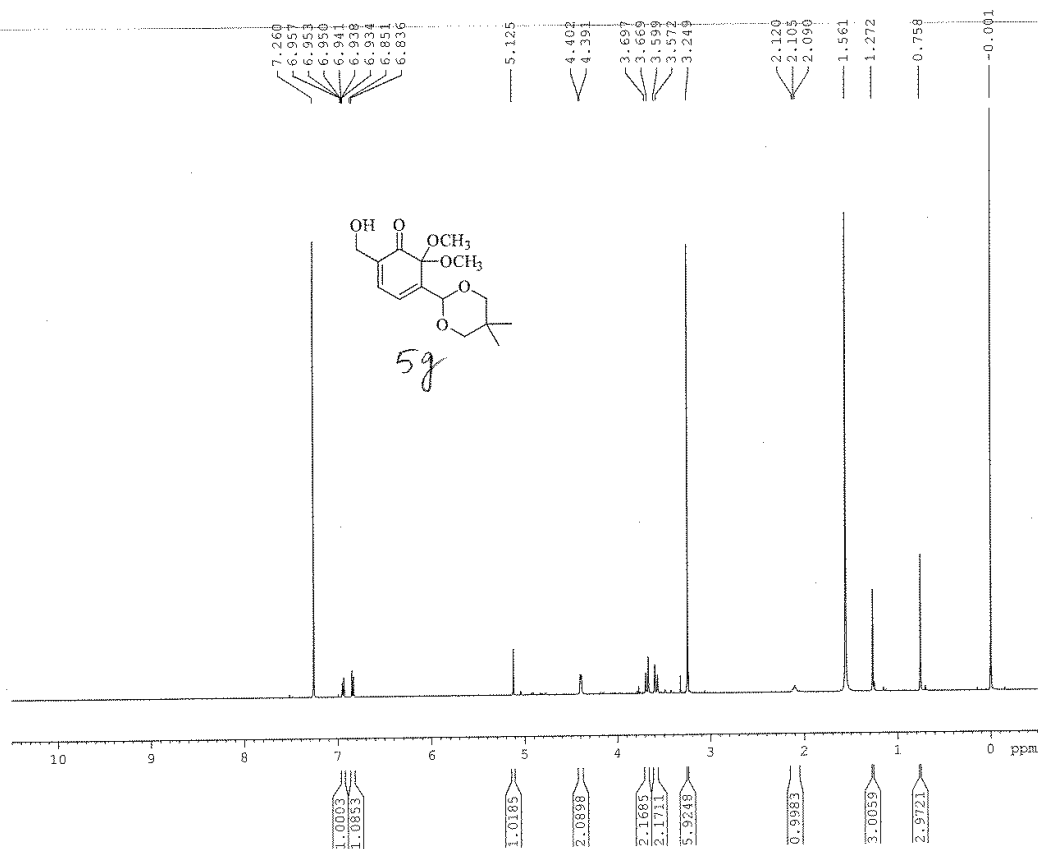
F2 - Acquisition Parameters  
Date\_ 20150801  
Time\_ 13.31  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CECL3  
NS 3493  
DS 4  
SMH 24036.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 101  
DN 20.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 0.5000000 sec  
D11 0.0300000 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 8.60 usec  
PL1 -1.00 dB  
PL1W 44.58811589 W  
SFO1 100.6479769 MHz

===== CHANNEL f2 =====  
CDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -2.00 dB  
PL12 15.47 dB  
PL13 15.72 dB  
PCW 14.33185768 W  
PL12W 0.25662708 W  
PL13W 0.24227158 W  
SFO2 400.2316009 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6379189 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

AMRI; SRC AV400  
location; 18



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

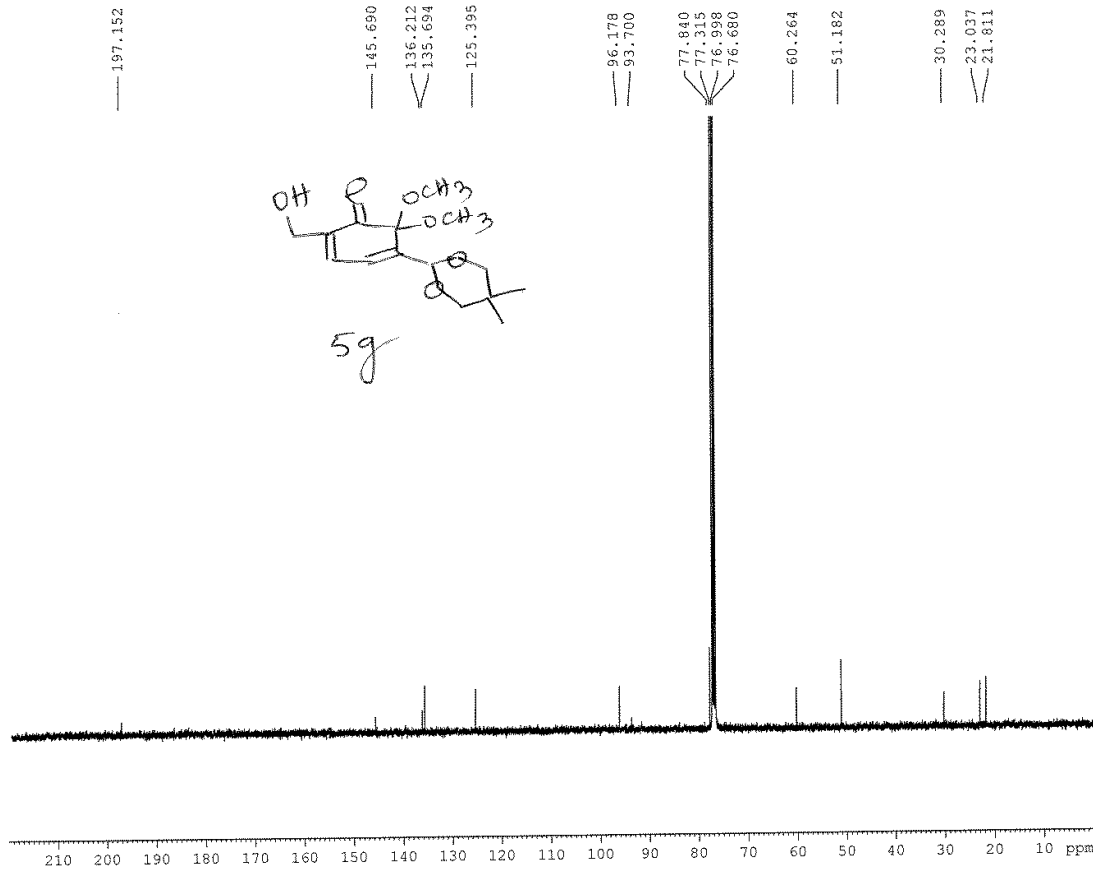
Current Data Parameters  
NAME SG-SIR-3KTL-HCHO-DMAP-PDT  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date 20150807  
Time 0.09  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 322  
DW 62.400 usec  
DE 6.00 usec  
TE 300.0 K  
D1 1.0000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 10.70 usec  
PL1 -2.00 dB  
PL1W 14.33185768 W  
SFO1 400.2330885 MHz

F2 - Processing parameters  
SI 32768  
SF 400.2300118 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

AMRI; SRC AV400  
location; 18



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

Current Data Parameters  
NAME SG-SIR-3KTL-13CNO-DMAP-PDT  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150807  
Time\_ 5.31  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 10000  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366788 Hz  
AQ 1.3631988 sec  
RG 80.6  
DW 20.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 0.5000000 sec  
D11 0.0300000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 8.60 usec  
PL1 -1.00 dB  
PL1W 44.58811569 W  
SFO1 100.6479769 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -2.00 dB  
PL12 15.47 dB  
PL13 15.72 dB  
PL2W 14.33185768 W  
PL12W 0.25662708 W  
PL13W 0.24227159 W  
SFO2 400.2316009 MHz

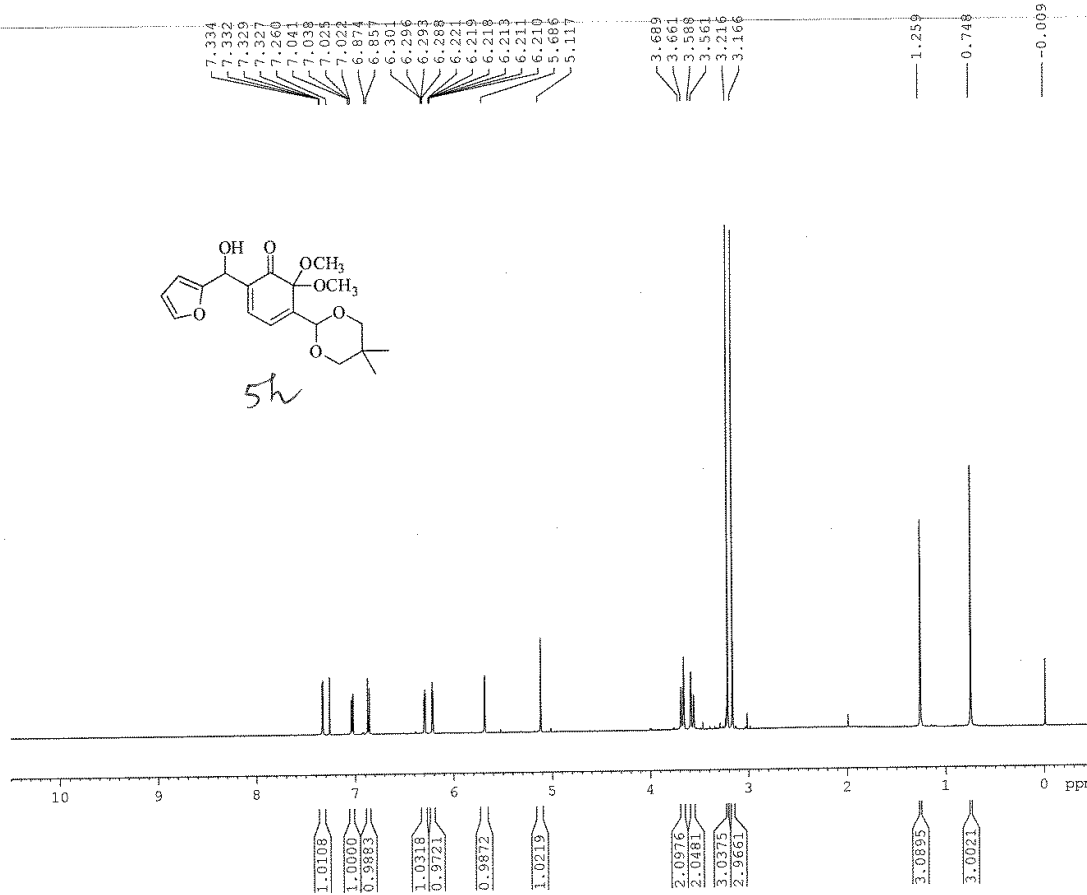
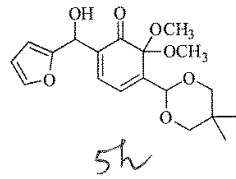
F2 - Processing parameters  
SI 32768  
SF 100.6379151 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
FC 1.40



AMRI SRC  
location; 17



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_



Current Data Parameters  
NAME 5G-SIR-3kl-dsap-furcho-pdt  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150721  
Time 21.09  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT cdcl3  
NS 15  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 71.8  
DW 62.400 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TDO 1

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
NUC1 1H  
P1 10.40 usec  
PL1 -3.00 dB  
PL1F 19.34582710 W  
SFO1 400.1318542 MHz

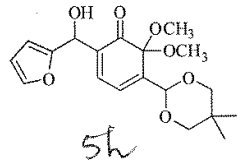
F2 - Processing parameters  
SI 32768  
SF 400.1300094 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

AMRI SRC  
location; 17



196.000  
153.862  
145.984  
142.391  
136.144  
125.348  
110.424  
107.350  
96.095  
93.935  
77.793  
77.318  
77.000  
76.682  
65.115  
51.316  
50.954  
30.266  
22.997  
21.774

Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_



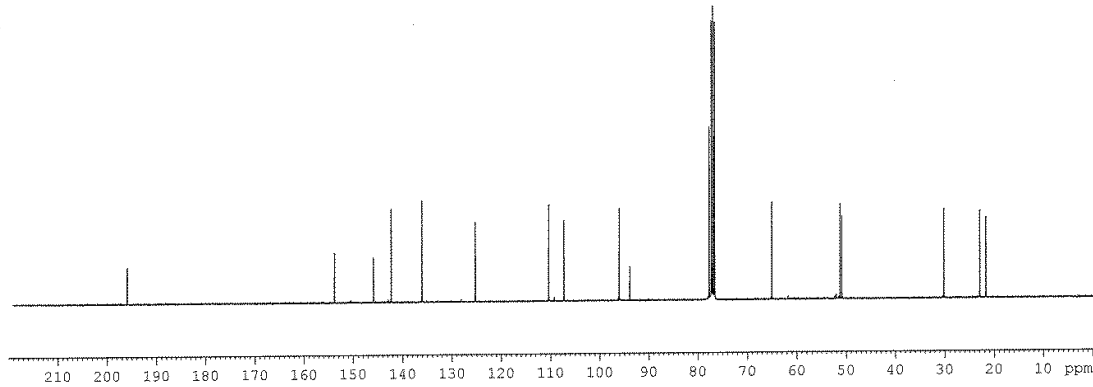
Current Data Parameters  
NAME SG-SIR-3kt1-dmap-furcho-pdt  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date 20150722  
Time 1.58  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 5000  
DS 4  
SWH 23980.814 Hz  
FIDRES 0.365918 Hz  
AQ 1.3664756 sec  
RG 13004  
DW 20.850 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 7.40 usec  
PL1 -4.00 dB  
PL1W 82.02445221 W  
SFO1 100.6228238 MHz

==== CHANNEL f2 =====  
CPDPRG2 waitz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -3.00 dB  
PL12 14.72 dB  
PL13 15.06 dB  
PL12W 19.34582719 W  
PL12W 0.32702976 W  
PL13W 0.30240381 W  
SFO2 400.1316005 MHz

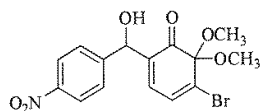
F2 - Processing parameters  
SI 32768  
SF 100.6127718 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



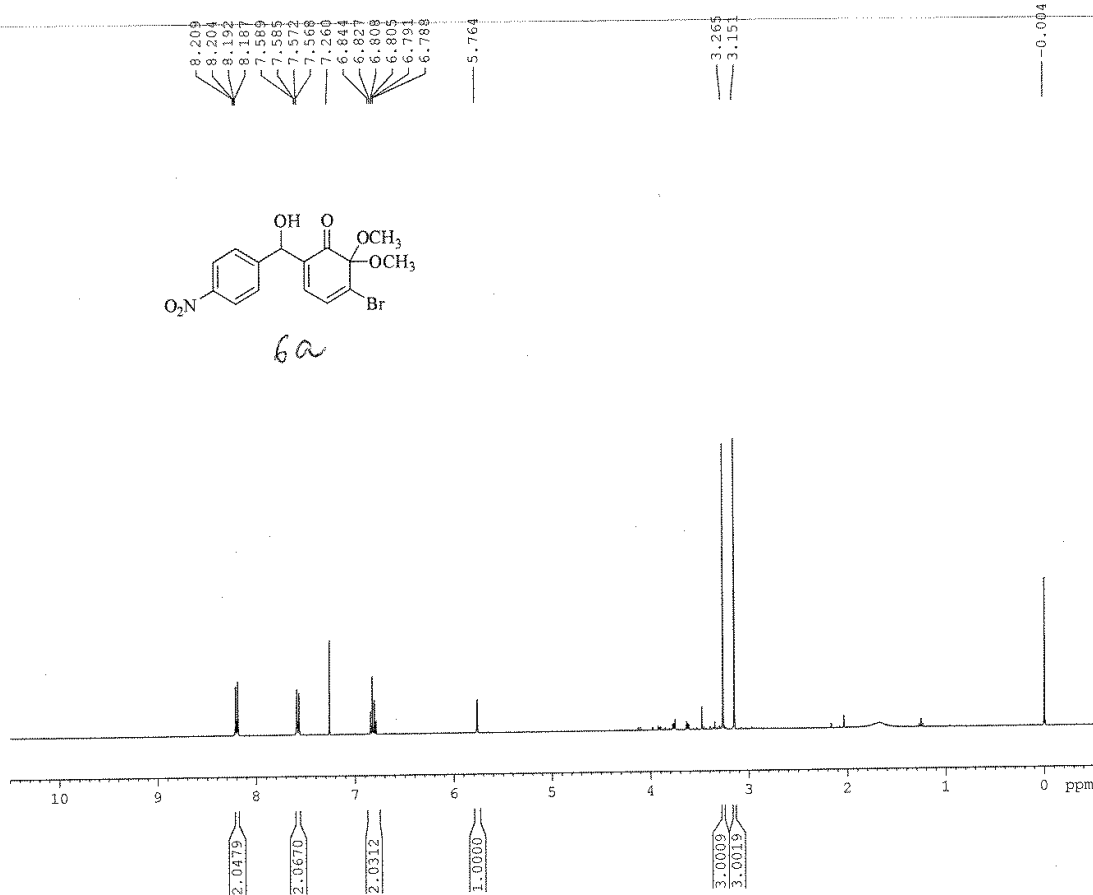
AMRI; SRC AV400  
location; 18



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_



6a



Current Data Parameters  
NAME SG-SIR-NO2PhCHO-3Br-DMAP  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150801  
Time 18.40  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 181  
DW 62.400 usec  
DE 6.00 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

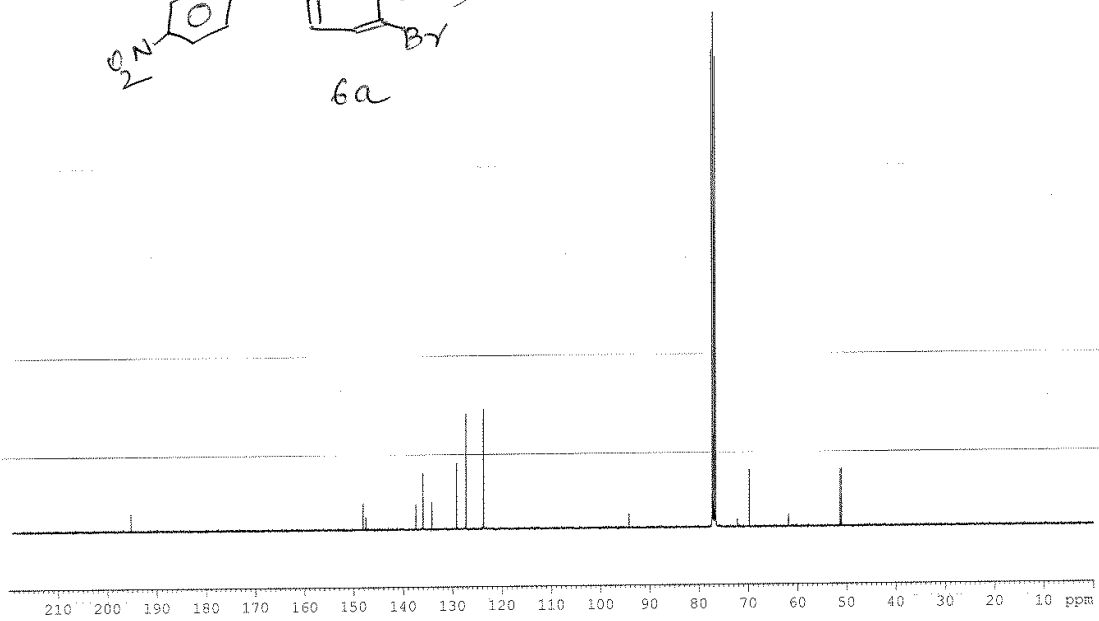
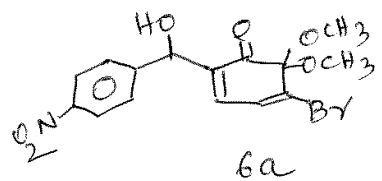
==== CHANNEL f1 =====  
NUC1 1H  
P1 10.70 usec  
PL1 -2.00 dB  
PL1W 14.33185768 W  
SFO1 400.2330885 MHz

F2 - Processing parameters  
SI 32768  
SF 400.2300118 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

AMRI; SRC AV400  
location; 18



195.298  
148.154  
147.611  
137.461  
136.025  
134.230  
129.215  
127.303  
123.764  
94.226  
77.318  
77.000  
76.683  
69.821  
51.376  
51.136



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

Current Data Parameters  
NAME SG-SIR-N02PhCHO-3Br-DMAP  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150802  
Time 0.03  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 10000  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631986 sec  
RG 71.8  
DW 20.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 0.5000000 sec  
D11 0.03000000 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 8.60 usec  
PL1 -1.00 dB  
PL1R 44.5811569 W  
SFO1 100.6479769 MHz

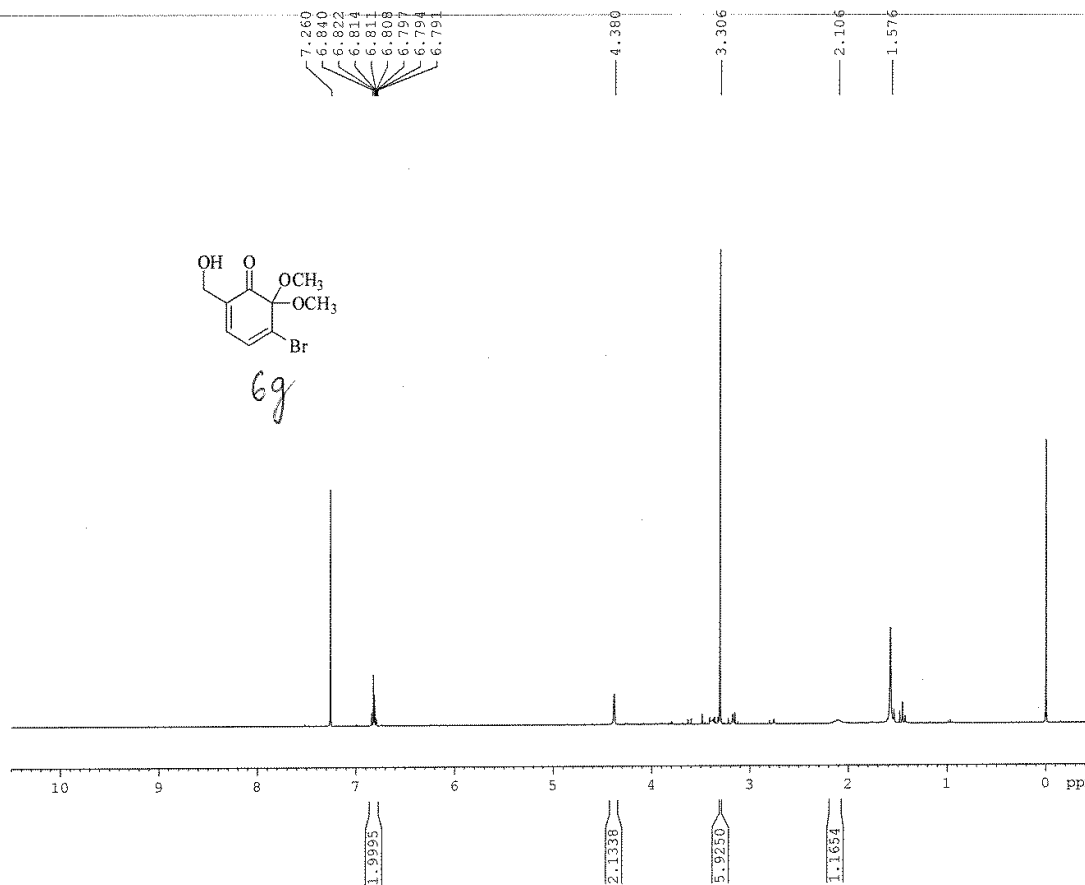
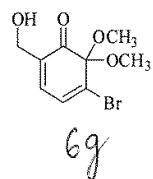
===== CHANNEL f2 =====  
CPEPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -2.00 dB  
PL12 15.47 dB  
PL13 15.72 dB  
PL2W 14.33185768 W  
PL12W 0.25662708 W  
PL13W 0.24227159 W  
SFO2 400.2316009 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6379150 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

AMRI; SRC AV400  
location; 18



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB# \_\_\_\_\_



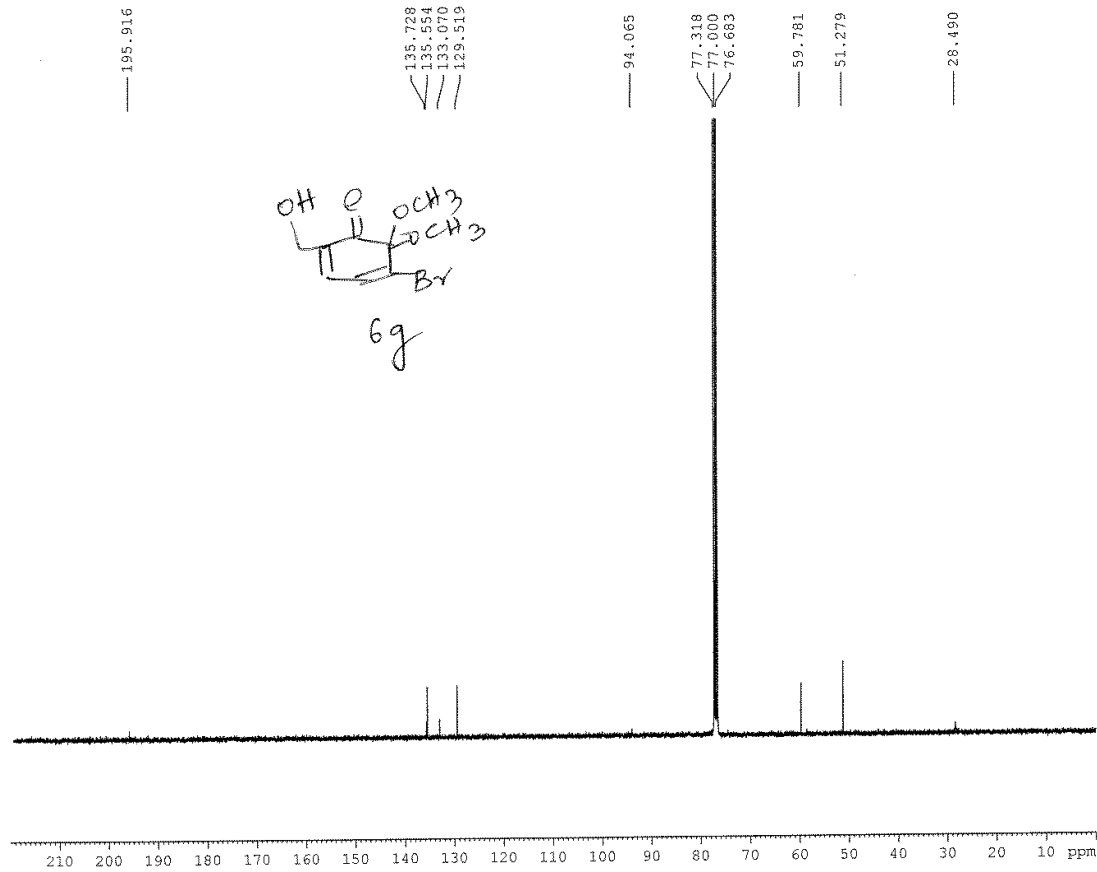
Current Data Parameters  
NAME SG-SIR-3Br-HCHO-PDT-DMAP  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150807  
Time\_ 21.09  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 181  
DW 62.400 usec  
DE 6.00 usec  
TE 300.0 K  
D1 1.00000000 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 10.70 usec  
PL1 -2.00 dB  
PL1W 14.33185768 W  
SFO1 400.2330885 MHz

F2 - Processing parameters  
SI 32768  
SF 400.2300120 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

AMRI; SRC AV400  
location; 18



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

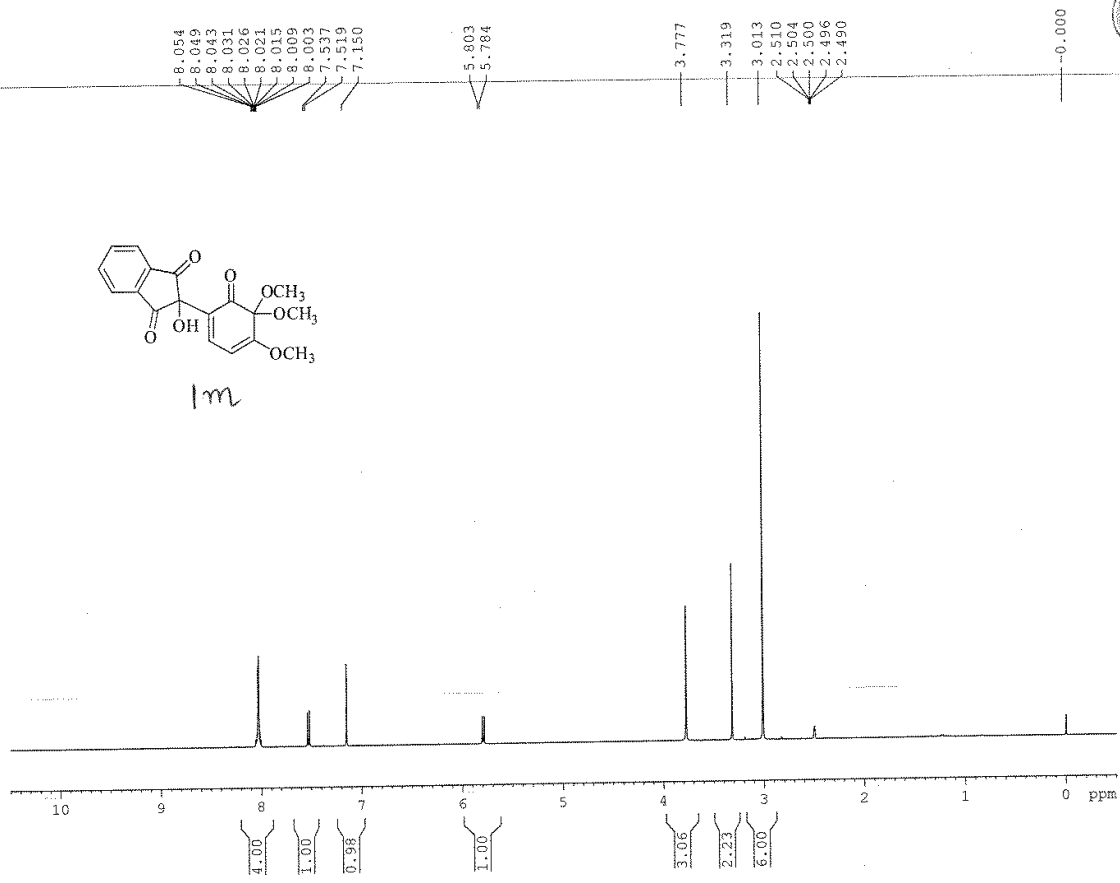
Current Data Parameters  
NAME SG-81R-3Br-CHO-PDT-DMAP  
EXPRO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date 20150808  
Time 2.32  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 10000  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 101  
DW 20.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 0.50000000 sec  
D11 0.03000000 sec  
TD0 1

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
NUC1 13C  
PI 8.60 usec  
PL1 -1.00 dB  
PL1W 44.58811569 W  
SFO1 100.6479769 MHz

\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -2.00 dB  
PL12 15.47 dB  
PL13 15.72 dB  
PL2W 14.33185768 W  
PL12W 0.25662708 W  
PL13W 0.24227159 W  
SFO2 400.2316099 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6379151 MHz  
WDW EM  
SFB 0  
LE 1.00 Hz  
GB 0  
PC 1.40



8.054  
8.049  
8.043  
8.031  
8.026  
8.021  
8.015  
8.009  
8.003  
7.537  
7.519  
7.150  
5.803  
5.784  
3.777  
3.319  
3.013  
2.510  
2.504  
2.500  
2.496  
2.490  
-0.000

Current Data Parameters  
 NAME SG-MKK-L-NINHYDRIN  
 EXPNO 13  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150704  
 Time 23.24  
 INSTRUM spect  
 PROBRD 5 mm PABBO BE-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 FQ 4.0894966 sec  
 RG 71.8  
 DM 62.400 usec  
 DE 6.50 usec  
 TE 300.2 K  
 D1 1.00000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.40 usec  
 PL1 -3.00 dB  
 PL1W 19.34582710 W  
 SFOL 400.1318542 MHz

F2 - Processing parameters  
 SI 32768  
 SF 400.1300029 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

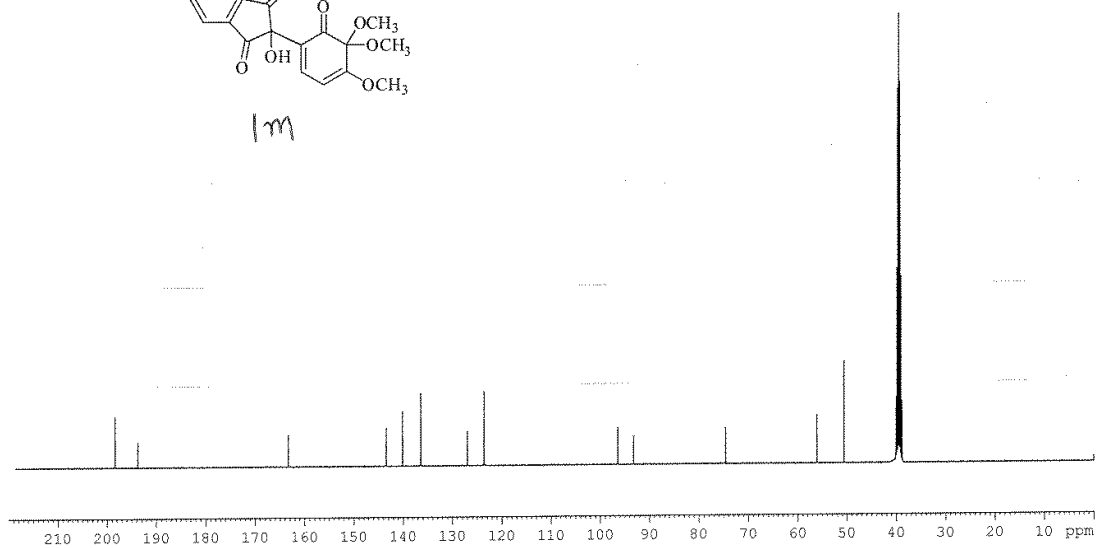
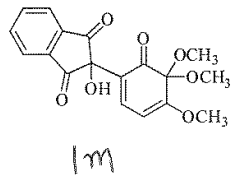
Name \_\_\_\_\_  
 Date \_\_\_\_\_  
 NB # \_\_\_\_\_

# AMRI SRC location; 17



198.462  
 193.822  
  
 163.374  
  
 143.488  
 140.183  
 136.454  
  
 127.033  
 123.634  
  
 96.485  
 93.275  
  
 74.651  
  
 56.171  
 50.689  
 40.125  
 39.916  
 39.708  
 39.499  
 39.290  
 39.082  
 38.873

Name \_\_\_\_\_  
 Date \_\_\_\_\_  
 NB # \_\_\_\_\_



**Current Data Parameters**  
 NAME SG-MKK-L-NINHYDRIN  
 EXPNO 10  
 PROCNO 1  
  
**F2 - Acquisition Parameters**  
 Date\_ 20150704  
 Time 20.02  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 6000  
 DS 4  
 SWH 23980.814 Hz  
 FIDRES 0.365918 Hz  
 AQ 1.3664756 sec  
 RG 11585.2  
 DW 20.850 usec  
 DE 8.50 usec  
 TE 301.3 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1  
  
**===== CHANNEL f1 =====**  
 NUCL1 13C  
 P1 7.40 usec  
 PL1 -4.00 dB  
 PL1W 62.02445221 W  
 SF01 100.6228298 MHz  
  
**===== CHANNEL f2 =====**  
 CPDPRG2 waltz16  
 NUCL2 1H  
 PCPD2 80.00 usec  
 PL2 -3.00 dB  
 PL12 14.72 dB  
 PL13 15.06 dB  
 PL2W 19.34582710 W  
 PL12W 6.32702976 W  
 PL13W 0.30240381 W  
 SF02 400.1316005 MHz  
  
**F2 - Processing parameters**  
 SI 32768  
 SF 100.6128205 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



17

-ve mode

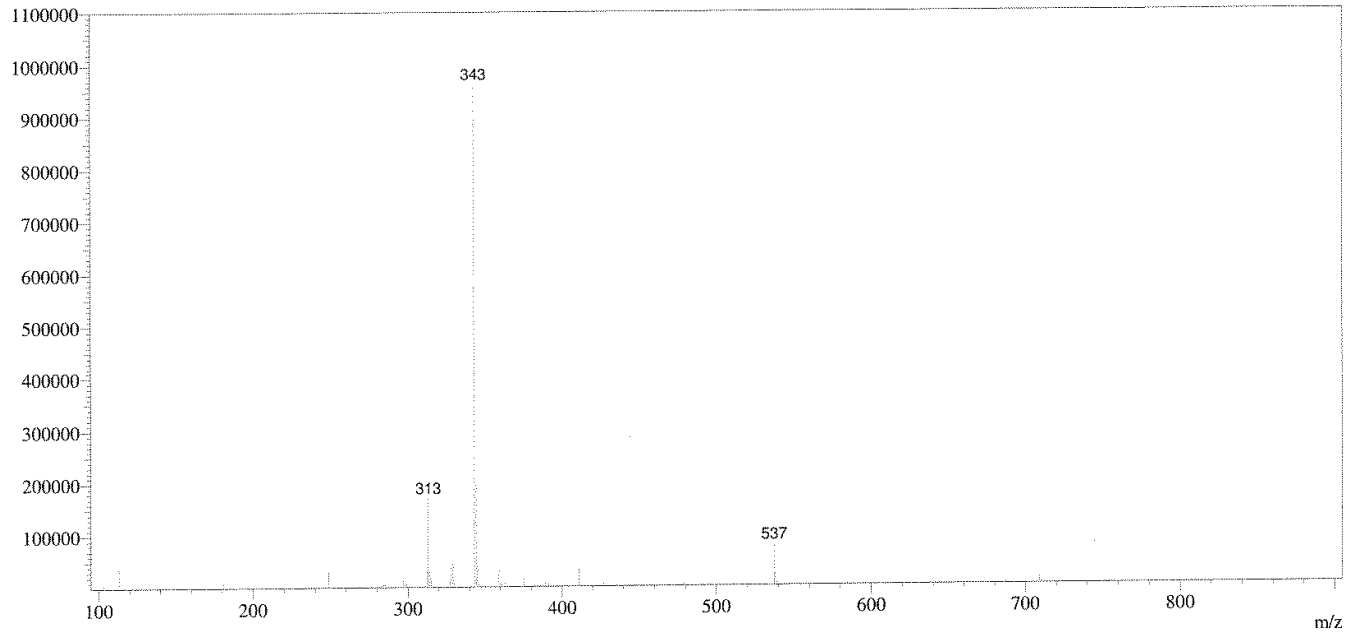
Acquired by : System Administrator  
Sample Name : SG-MKK-L-Nin  
Data File : SG-MKK-L-Nin.lcd  
Method File : ESI-LCMS Method3.lcm  
Month-Day Acquired : 10/6/2015

Name	:	_____
Notebook #	:	_____
Date	:	_____



ESI-MS Spectrum

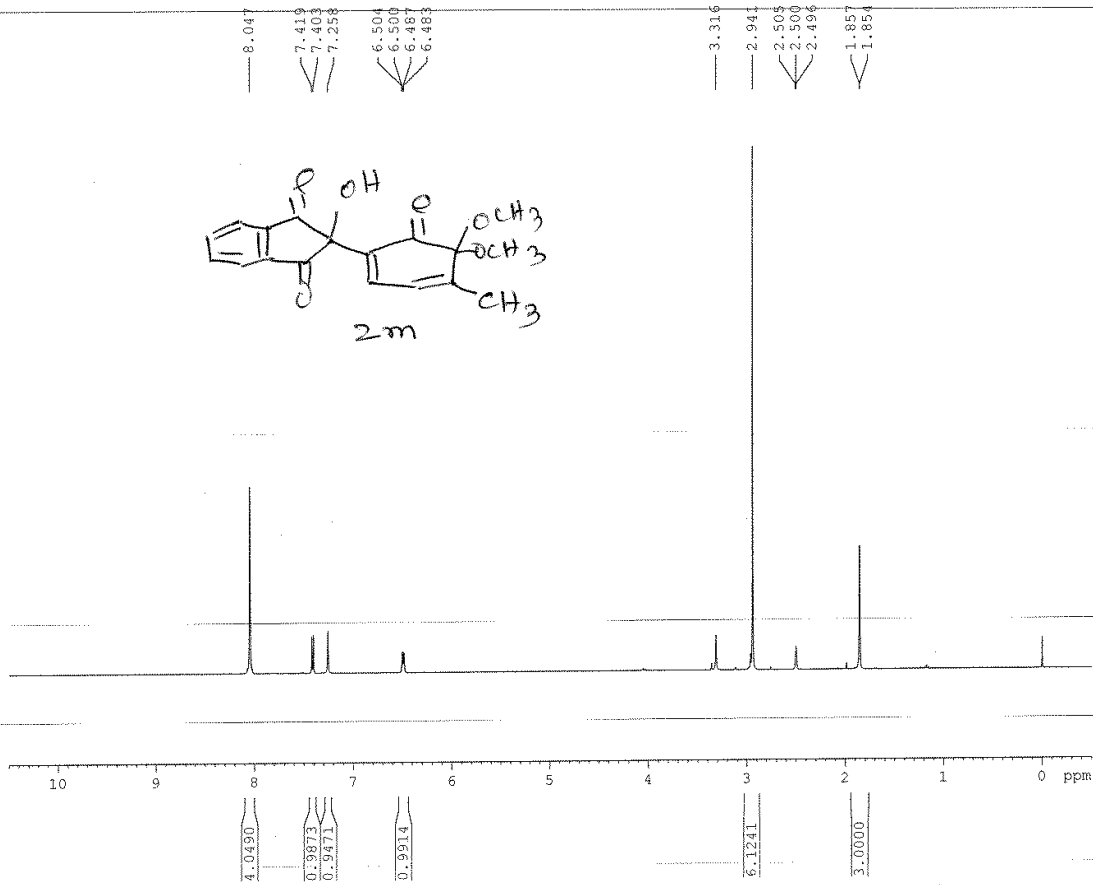
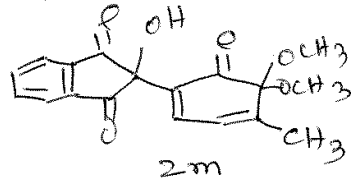
Peak # : 1, Retention Time : 2.516 min  
Base Peak m/z : 343, Base Peak Intensity : 963626963626  
Polarity : Negative, Event : 1 - 2



AMRI; SRC AV400  
location; 18



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_



Current Data Parameters  
NAME SG-BCK-I-23Me-Nin-MAIN  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150804  
Time 21.06  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 90.5  
DW 62.400 usec  
DE 6.00 usec  
TE 300.0 K  
D1 1.00000000 sec  
TDO 1

==== CHANNEL f1 =====  
NUC1 1H  
PI 10.70 usec  
PL1 -2.00 dB  
PL1W 14.33185768 W  
SFO1 400.2330885 MHz

F2 - Processing parameters  
SI 32768  
SF 400.2300049 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

AMRI; SRC AV400  
location; 18



198.039  
197.636

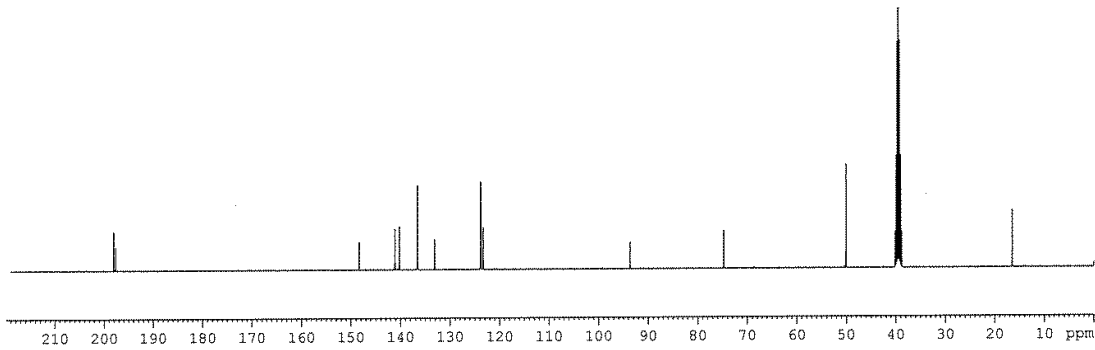
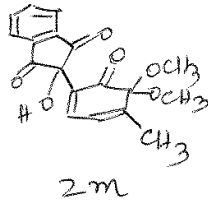
148.348  
141.114  
140.227  
136.571  
133.131  
123.836  
123.325

93.682

74.800

50.103  
40.150  
39.941  
39.733  
39.524  
39.315  
39.106  
38.898

16.543



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

NAME SG-BCK-I-23Me-Nin-MAIN  
EXPNO 11  
PROCNO 1  
Date\_ 20150805  
Time 1.25  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 8000  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 101  
DW 20.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 0.5000000 sec  
D11 0.0300000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 8.60 usec  
PL1 -1.00 dB  
PL1W 44.58811569 W  
SFO1 100.6479769 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -2.00 dB  
PL12 15.47 dB  
PL13 15.72 dB  
PL2W 14.33185768 W  
PL12W 0.25662708 W  
PL13W 0.24227159 W  
SFO2 400.2316009 MHz  
SI 32768  
SF 100.6379633 MHz  
WDM EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

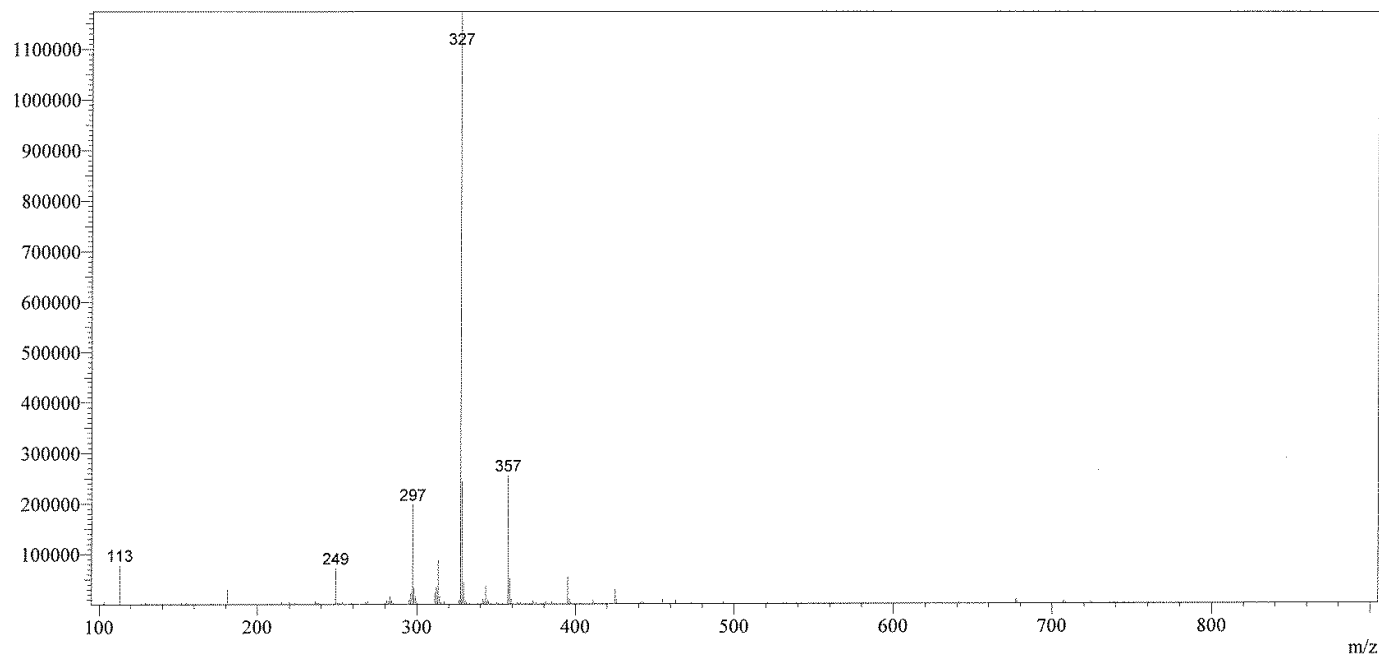
2m -ve mode

Acquired by : System Administrator  
Sample Name : SG-BCK-3-Me-NIN-4  
Data File : SG-BCK-3-Me-NIN-4.lcd  
Method File : ESI-LCMS Method3.lcm  
Month-Day Acquired : 10/7/2015



ESI-MS Spectrum

Peak # : 1, Retention Time : 2.749 min  
Base Peak m/z : 327, Base Peak Intensity : 11738881173888  
Polarity : Negative, Event : 1 - 2

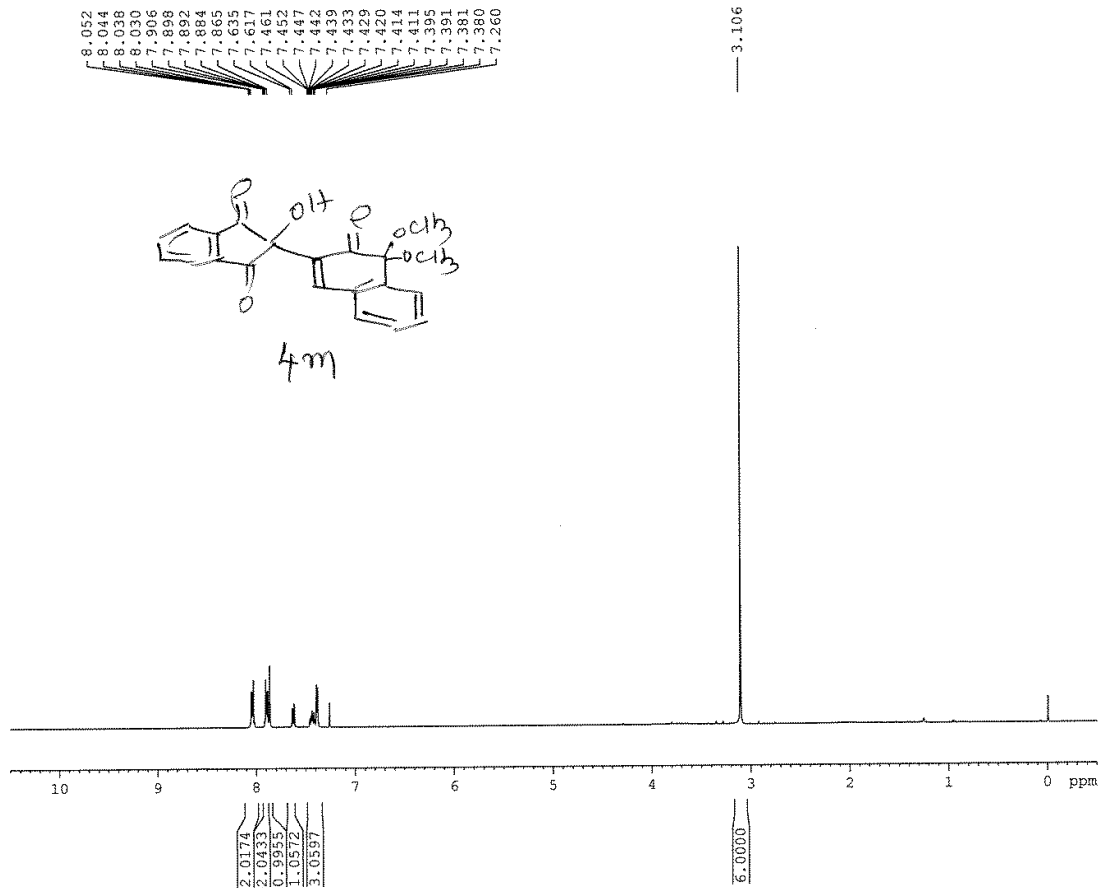
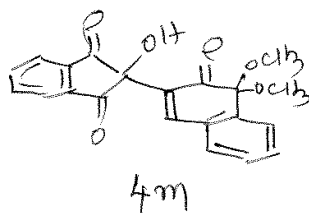


AMRI; SRC AV400  
location; 18



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

8.052  
8.044  
8.038  
8.030  
7.906  
7.898  
7.892  
7.884  
7.865  
7.635  
7.617  
7.461  
7.452  
7.447  
7.442  
7.439  
7.433  
7.429  
7.420  
7.414  
7.411  
7.395  
7.391  
7.381  
7.380  
7.260



NAME SG-BCK-I-2Naph-Nin-MAIN  
EXPNO 10  
PROCNO 1  
Date\_ 20150728  
Time\_ 7.37  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 80.6  
DW 62.400 usec  
DE 6.00 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 10.70 usec  
PL1 -2.00 dB  
PL1W 14.33185768 W  
SF01 400.2330885 MHz  
SI 32768  
SF 400.2300117 MHz  
WDB EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

AMRI; SRC AV400  
location; 18



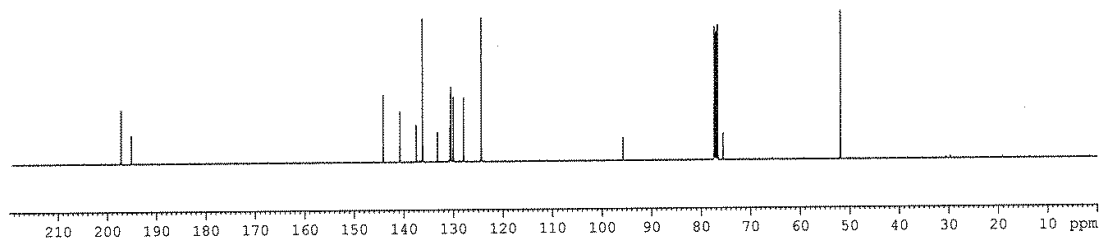
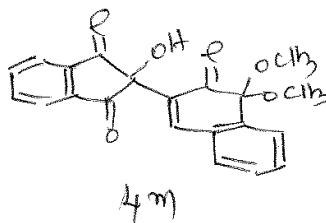
197.230  
195.102

144.154  
140.769  
137.485  
136.240  
133.212  
130.676  
130.555  
130.502  
130.034  
127.956  
124.378

95.736

77.319  
77.001  
76.683  
75.578

51.863



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

NAME SG-BCK-I-2Naph-Nin-MAIN  
EXPNO 11  
PROCNO 1  
Date\_ 20150728  
Time 23.47  
INSTRUM spect  
PROBHD 5 mm FABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 5000  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 80.6  
DW 20.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 0.50000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
F1 6.60 usec  
PL1 -1.00 dB  
PL1W 44.58811569 W  
SFO1 100.6479769 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -2.00 dB  
PL12 15.47 dB  
PL13 15.72 dB  
PL2W 14.33185768 W  
PL12W 0.25662708 W  
PL13W 0.24227159 W  
SFO2 400.2316009 MHz  
SI 32768  
SF 100.6379183 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

4m

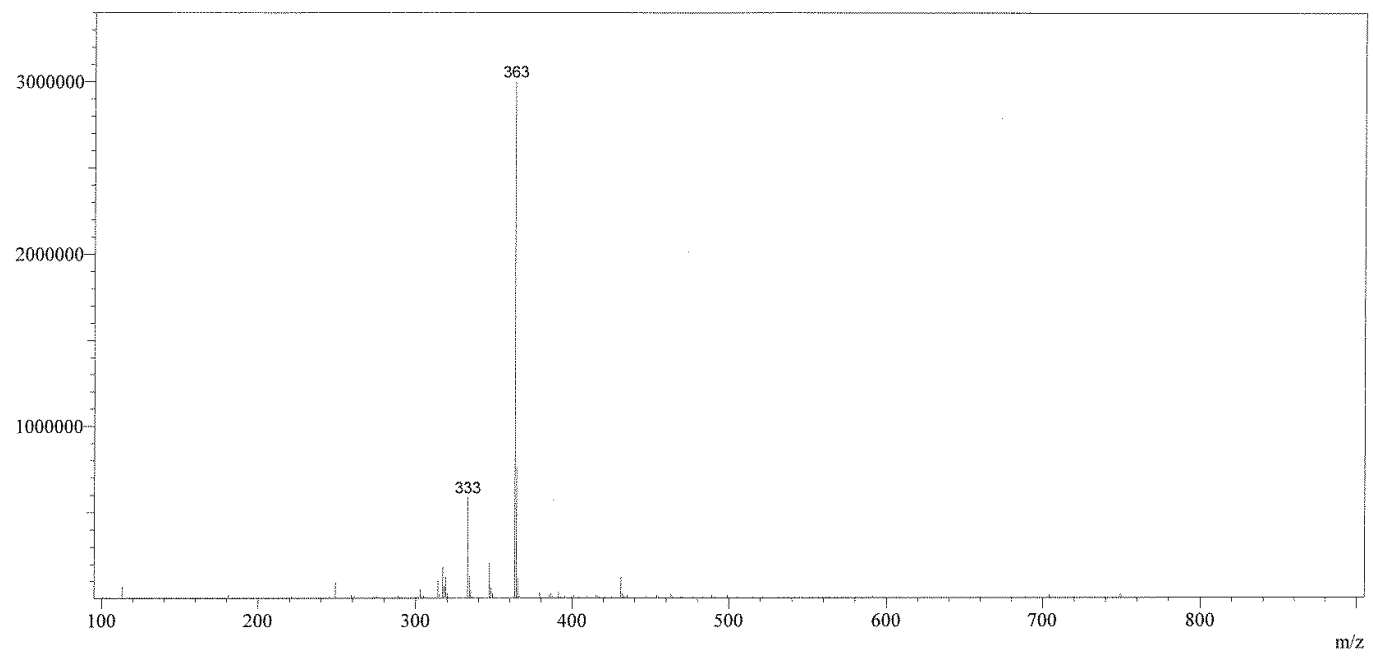
-ve mode

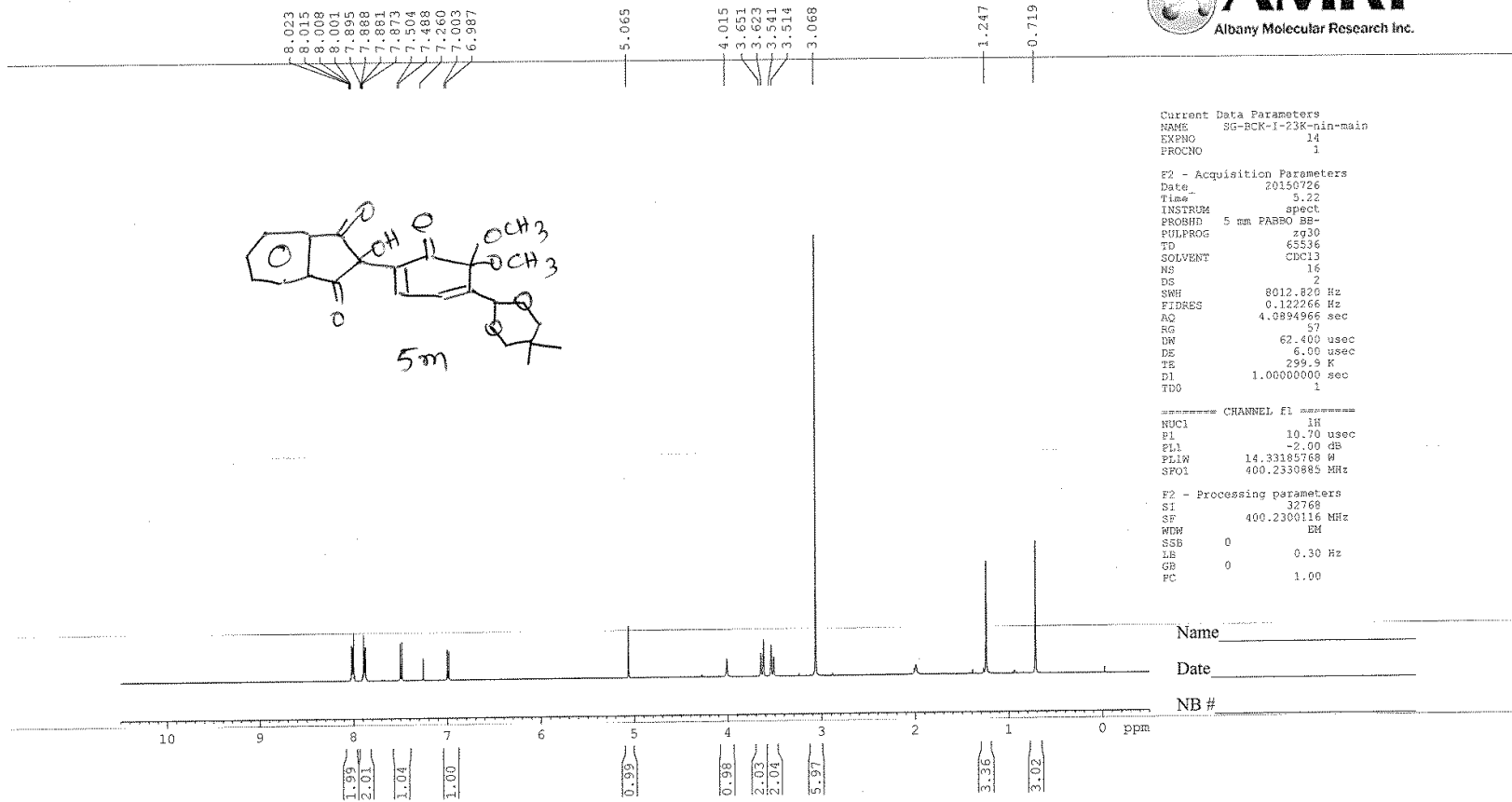
Acquired by : System Administrator  
Sample Name : SG-BCK-2Naphth-NIN-2  
Data File : SG-BCK-2Naphth-NIN-2.lcd  
Method File : ESI-LCMS Method3.lcm  
Month-Day Acquired : 10/7/2015



ESI-MS Spectrum

Peak # : 1, Retention Time : 2.983 min  
Base Peak m/z : 363, Base Peak Intensity : 30036363003636  
Polarity : Negative, Event : 1 - 2







AMRI; SRC AV400  
location; 18



196.904  
196.387

146.499  
140.673  
139.749  
136.176  
135.207  
125.937  
124.361

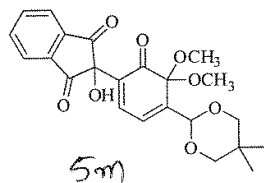
95.974  
93.934

77.728  
77.320  
77.002  
76.685  
75.390

51.167

30.236  
22.958  
21.733

Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_



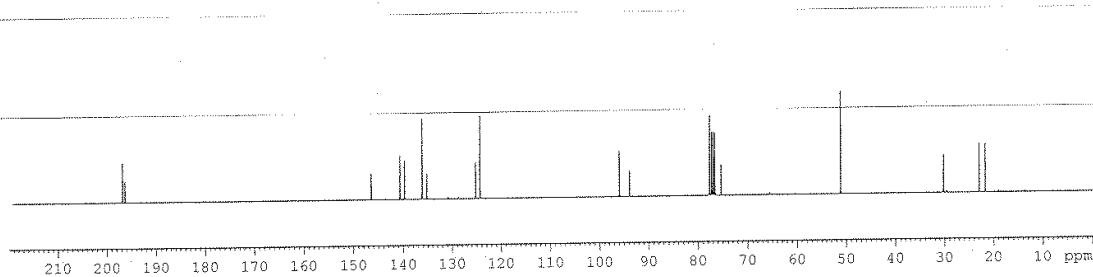
Current Data Parameters  
NAME SG-BCK-I-23K-nin-main  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150726  
Time 5.20  
INSTRUM spect  
PROBHD 5 mm FAPBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CCl3  
NS 8000  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366796 Hz  
AQ 1.3631988 sec  
RG 101  
DW 20.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 0.5000000 sec  
D11 0.0300000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 8.60 usec  
PL1 -1.00 dB  
PLW 44.5881569 W  
SFO1 100.6279769 MHz

===== CHANNEL f2 =====  
CPDPRG2 walzr16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -2.00 dB  
PL12 15.47 dB  
PL13 15.72 dB  
PL2W 14.33185768 W  
PL12W 0.25662708 W  
PL13W 0.24227159 W  
SFO2 400.2316009 MHz

F2 - Processing parameters  
S1 32768  
SF 100.6279155 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



5m

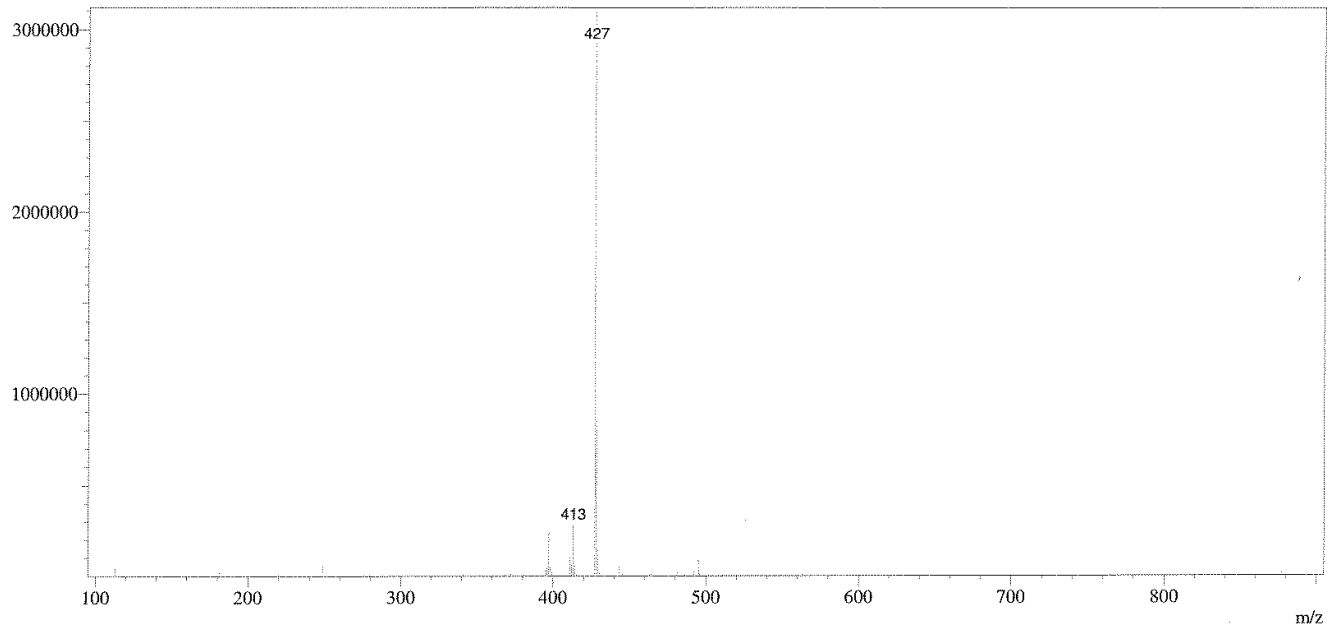
-ve mode

Acquired by : System Administrator  
Sample Name : SG-BCK-3K-NIN-10  
Data File : SG-BCK-3K-NIN-10.lcd  
Method File : ESI-LCMS Method3.lcm  
Month-Day Acquired : 10/8/2015



ESI-MS Spectrum

Peak # : 1, Retention Time : 3.049 min  
Base Peak m/z : 427, Base Peak Intensity : 31220743122074  
Polarity : Negative, Event : 1 - 2



AMRI; SRC AV400  
location; 18

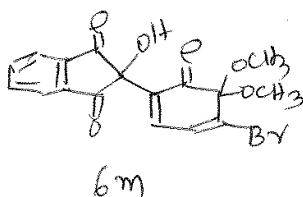


Name \_\_\_\_\_

Date \_\_\_\_\_

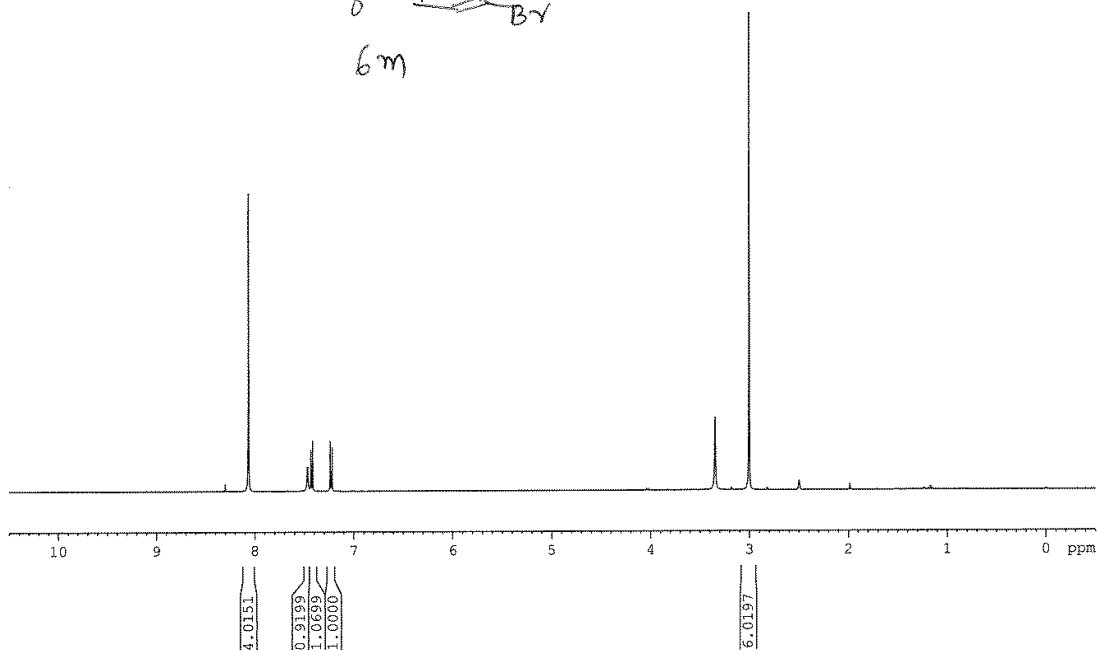
NB # \_\_\_\_\_

8.065  
7.468  
7.434  
7.416  
7.238  
7.220  
3.350  
3.007  
2.508  
2.504  
2.500  
2.495

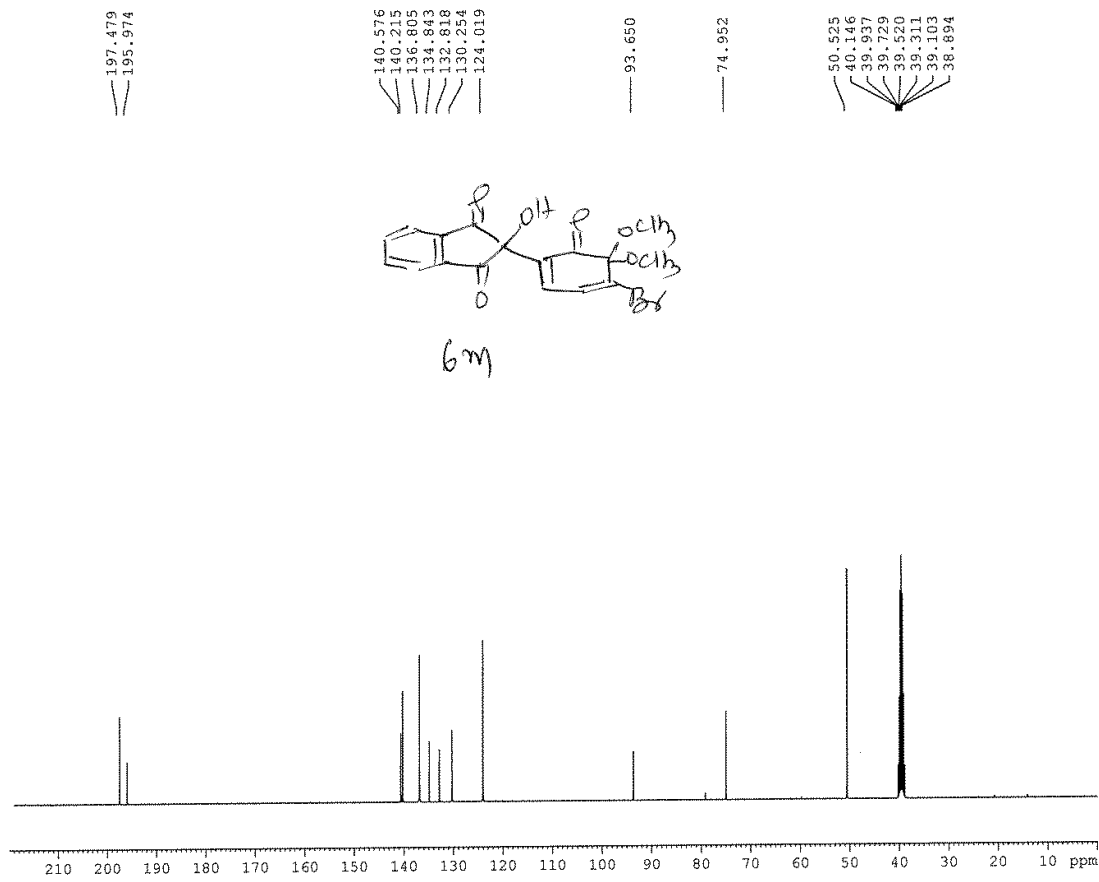


NAME SG-BCK-I-23Br-nin-main  
EXPNO 10  
PROCNO 1  
Date\_ 20150726  
Time\_ 9.41  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 64  
DW 62.400 usec  
DE 6.00 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
PI 10.70 usec  
PL1 -2.00 dB  
PL1W 14.33165768 W  
SFO1 400.2330885 MHz  
SI 32768  
SF 400.2300052 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



AMRI; SRC AV400  
location; 18



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

```

NAME      SG-BCK-I-23Br-nin-main
EXPNO     11
PROCNO    1
Date_     20150726
Time      13.59
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD        65536
SOLVENT   DMSO
NS        8000
DS        4
SWH        24038.461 Hz
FIDRES    0.366798 Hz
AQ        1.3631988 sec
RG        101
DW        20.800 usec
DE        6.50 usec
TE        300.0 K
D1        0.50000000 sec
D11       0.03000000 sec
TDO       1
  
```

```

===== CHANNEL f1 =====
NUC1      13C
P1        8.60 usec
PL1       -1.00 dB
PL1W      44.56811569 W
SFO1      100.6479769 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       -2.00 dB
PL12      15.47 dB
PL13      15.72 dB
PL2W      14.33185768 W
PL12W     0.25662708 W
PL13W     0.24227159 W
SFO2      400.2316009 MHz
SI        32768
SF        100.6379613 MHz
WEN       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```

6m

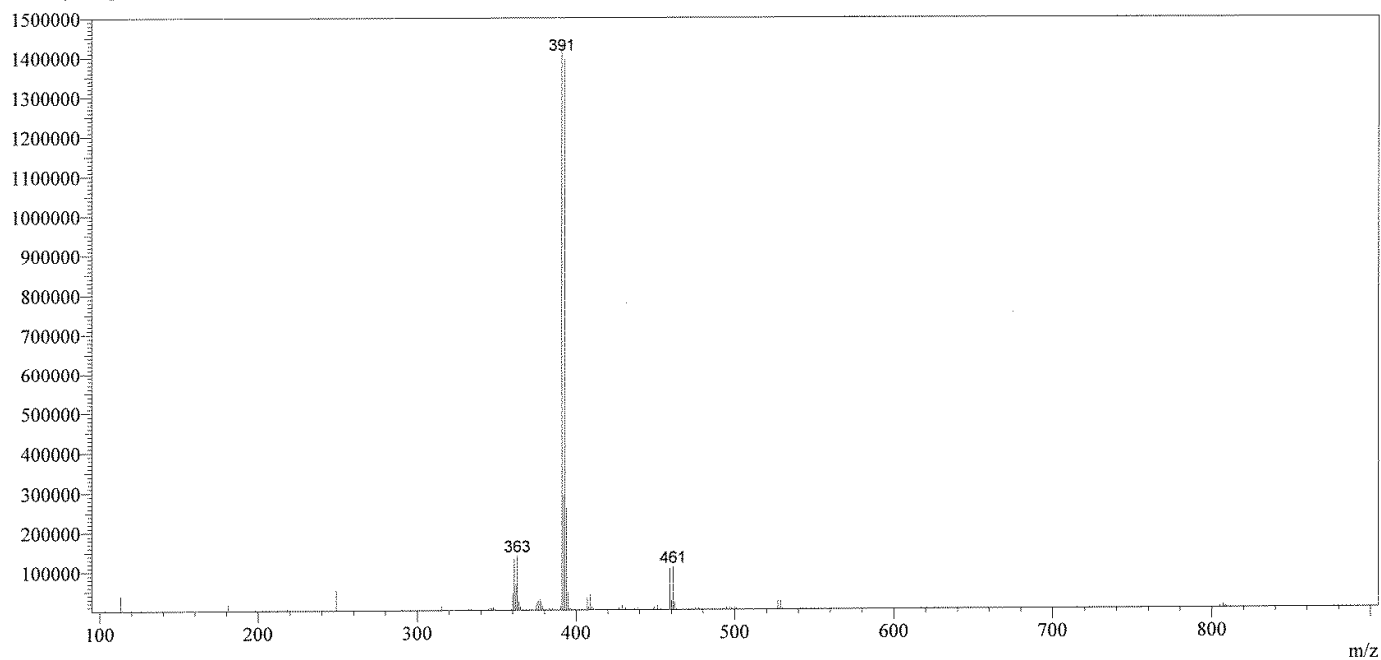
-ve mode

Acquired by : System Administrator  
Sample Name : SG-BCK-3Br-NIN-1  
Data File : SG-BCK-3Br-NIN-1.lcd  
Method File : ESI-LCMS Method3.lcm  
Month-Day Acquired : 10/7/2015



ESI-MS Spectrum

Peak # : 1, Retention Time : 2.849 min  
Base Peak m/z : 391, Base Peak Intensity : 14364051436405  
Polarity : Negative, Event : 1 - 2



AMRI; SRC AV400  
location; 18

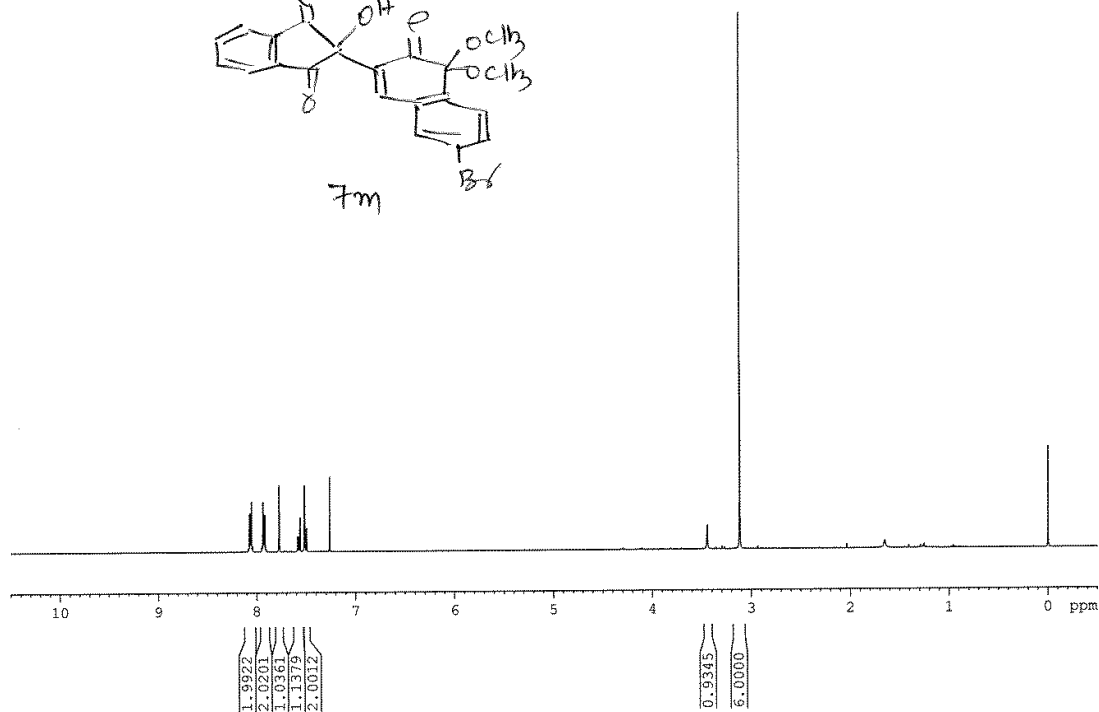
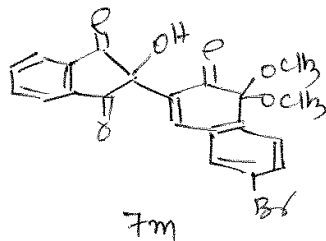


Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

8.074  
8.066  
8.060  
8.052  
7.937  
7.929  
7.923  
7.915  
7.773  
7.585  
7.580  
7.565  
7.560  
7.517  
7.495  
7.261

3.448  
3.120

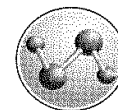
-0.000



NAME SG-BCK-1-26Br-2Naph-Nin-MAIN  
EXPNO 10  
PROCNO 1  
Date\_ 20150728  
Time\_ 7.43  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 181  
DW 62.400 usec  
DE 6.00 usec  
TE 300.0 K  
D1 1.0000000 sec  
TDO 1

----- CHANNEL f1 -----  
NUC1 1H  
P1 10.70 usec  
PL1 -2.00 dB  
PL1W 14.33185768 W  
SFO1 400.2330885 MHz  
SI 32768  
SF 400.2300115 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

AMRI; SRC AV400  
location; 18



**AMRI**

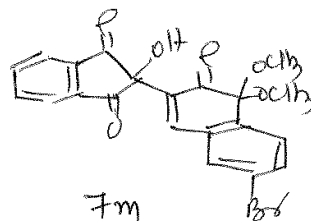
196.810  
194.556

142.440  
140.768  
136.386  
136.284  
134.484  
133.252  
132.879  
132.428  
129.600  
124.498  
124.096

95.528

77.318  
77.000  
76.683  
75.590

51.917



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

```

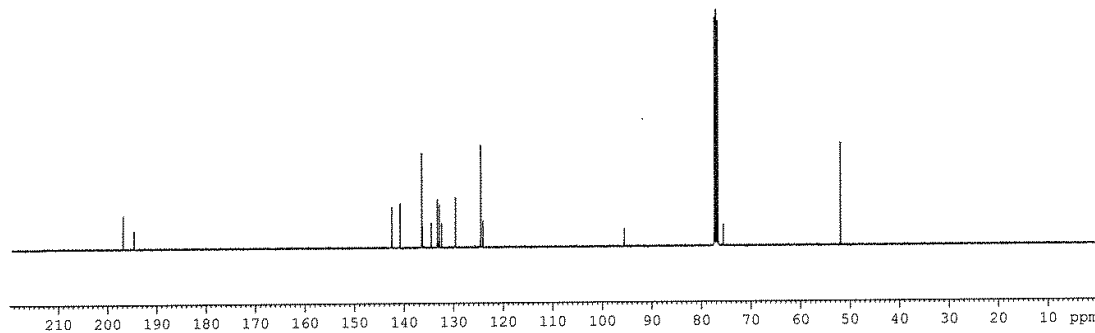
NAME      SG-BCK-I-26Br-2Naph-Min-MAIN
EXPNO     1
PROCNO    1
Date_     20150729
Time      5.02
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS        5000
DS        4
SWH       24038.461 Hz
FIDRES    0.366798 Hz
AQ        1.3631988 sec
RG        101
DW        20.800 usec
DE        6.50 usec
TE        300.0 K
D1        0.5000000 sec
D11       0.0300000 sec
TD0       1
  
```

```

***** CHANNEL f1 *****
NUC1      13C
P1        8.60 usec
PL1       -1.00 dB
PL1W     44.58811569 W
SFO1     100.6479769 MHz
  
```

```

***** CHANNEL f2 *****
CEDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       -2.00 dB
PL12     15.47 dB
PL13     15.72 dB
PL2W     14.33185768 W
PL12W    0.25662708 W
PL13W    0.24227159 W
SFO2     400.2316009 MHz
SI        32768
SF        100.6379159 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```



7m

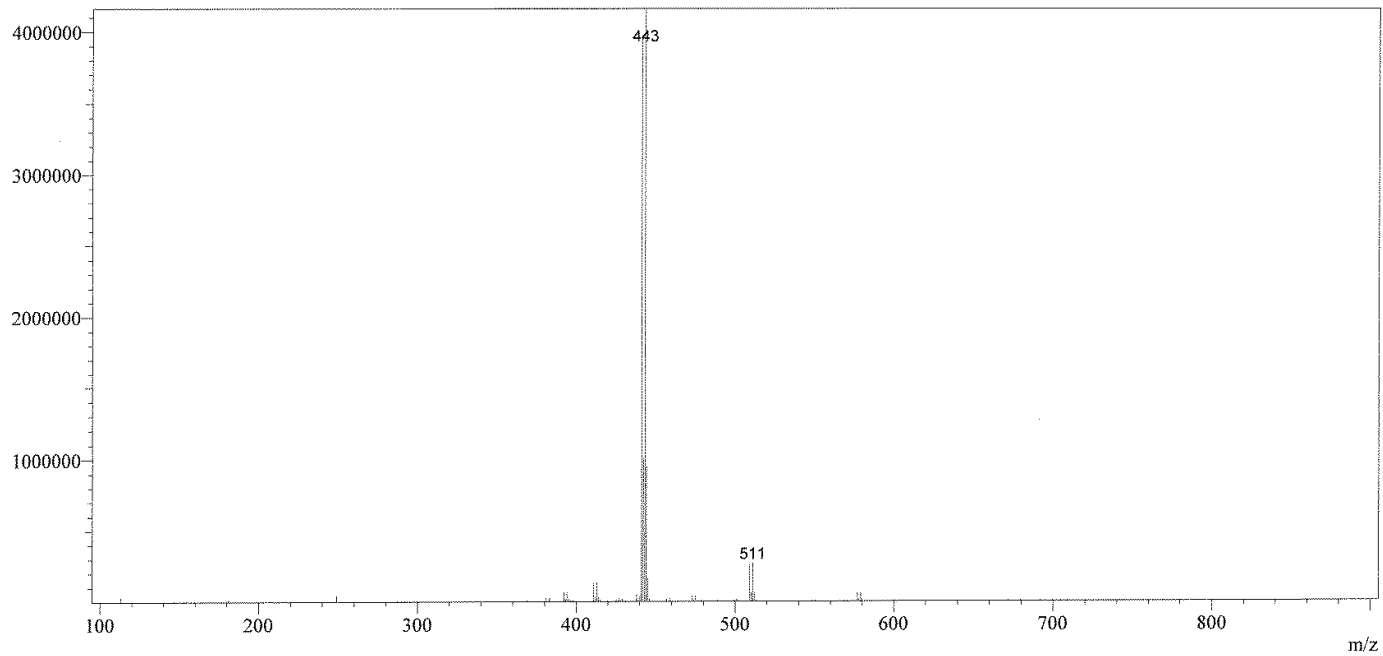
Acquired by : System Administrator  
Sample Name : SG-BCK-6-Br-2-Naphth-NIN-  
Data File : SG-BCK-2Naphth-NIN-3.lcd  
Method File : ESI-LCMS Method3.lcm  
Month-Day Acquired : 10/7/2015

Name	:	_____
Notebook #	:	_____
Date	:	_____



ESI-MS Spectrum

Peak # : 1, Retention Time : 3.183 min  
Base Peak m/z : 443, Base Peak Intensity : 41627134162713  
Polarity : Negative, Event : 1 - 2





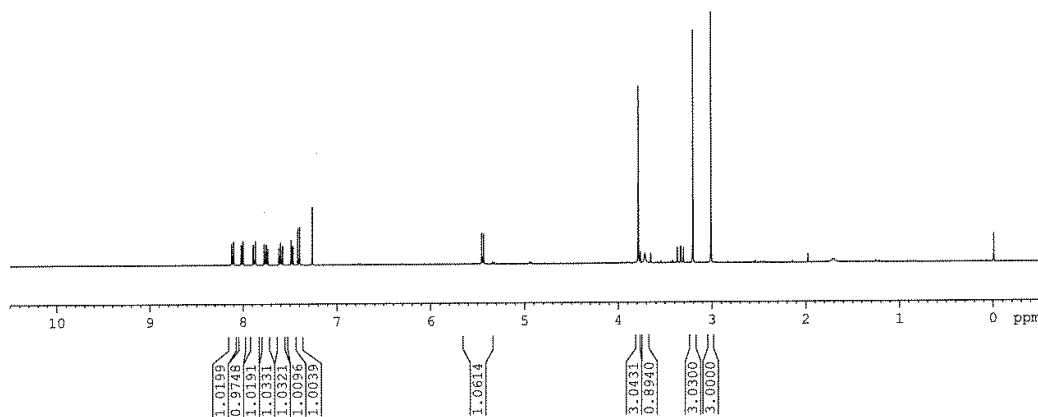
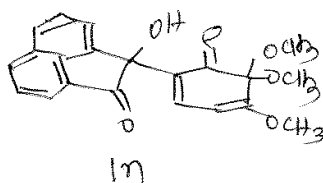
AMRI; SRC AV400  
location; 18



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

8.121  
8.101  
8.100  
8.019  
8.018  
8.002  
7.890  
7.890  
7.870  
7.773  
7.756  
7.735  
7.617  
7.599  
7.596  
7.579  
7.486  
7.485  
7.468  
7.467  
7.415  
7.396  
7.260  
5.457  
5.438

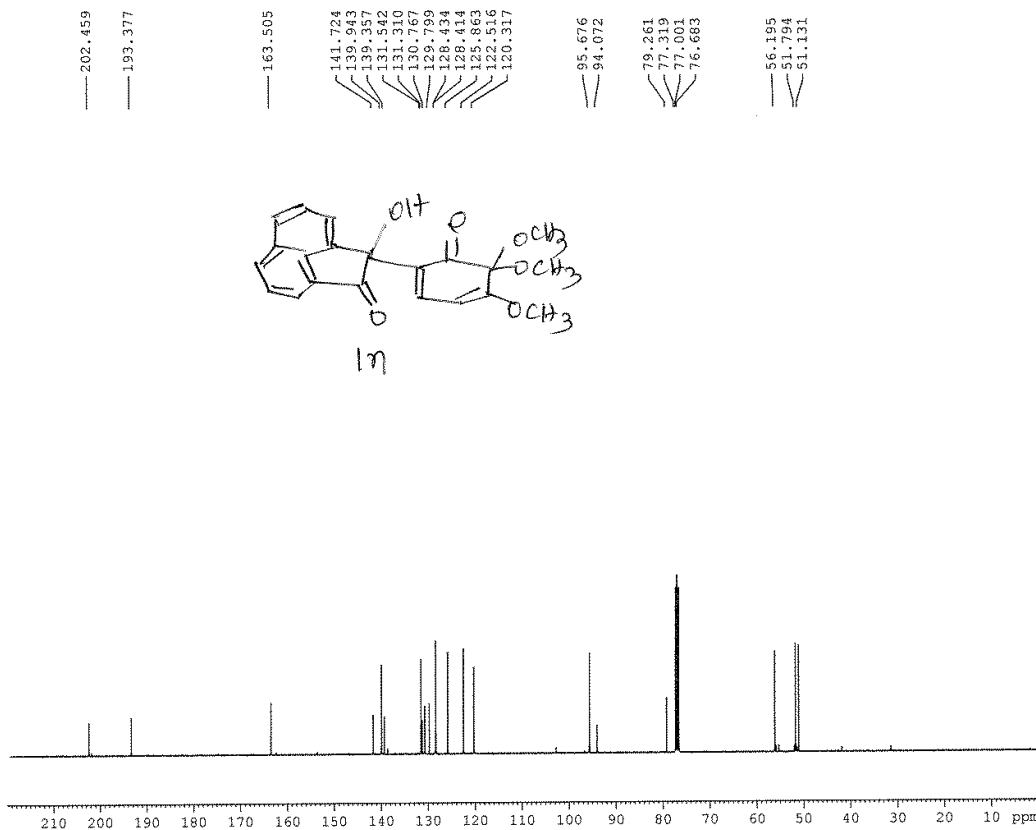
3.786  
3.205  
3.011



```

NAME SG-BCK-I-Acenaphth-Q-MAIN
EXPNO 10
PROCNO 1
Date_ 20150802
Time_ 4.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 71.8
DW 62.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.0000000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 1H
P1 10.70 usec
PL1 -2.00 dB
PL1W 14.33185768 W
SFO1 400.230985 MHz
SI 32768
SF 400.2300118 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
  
```

AMRI; SRC AV400  
location; 18



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

NAME SG-BCK-I-Acenaphth-Q-MAIN  
EXPNO 11  
PROCNO 1  
Date\_ 20150802  
Time 7.36  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 6200  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 80.6  
DW 20.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 0.5000000 sec  
D11 0.0300000 sec  
TED 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 8.60 usec  
PL1 -1.00 dB  
PL1W 44.58811569 W  
SFO1 100.6479769 MHz

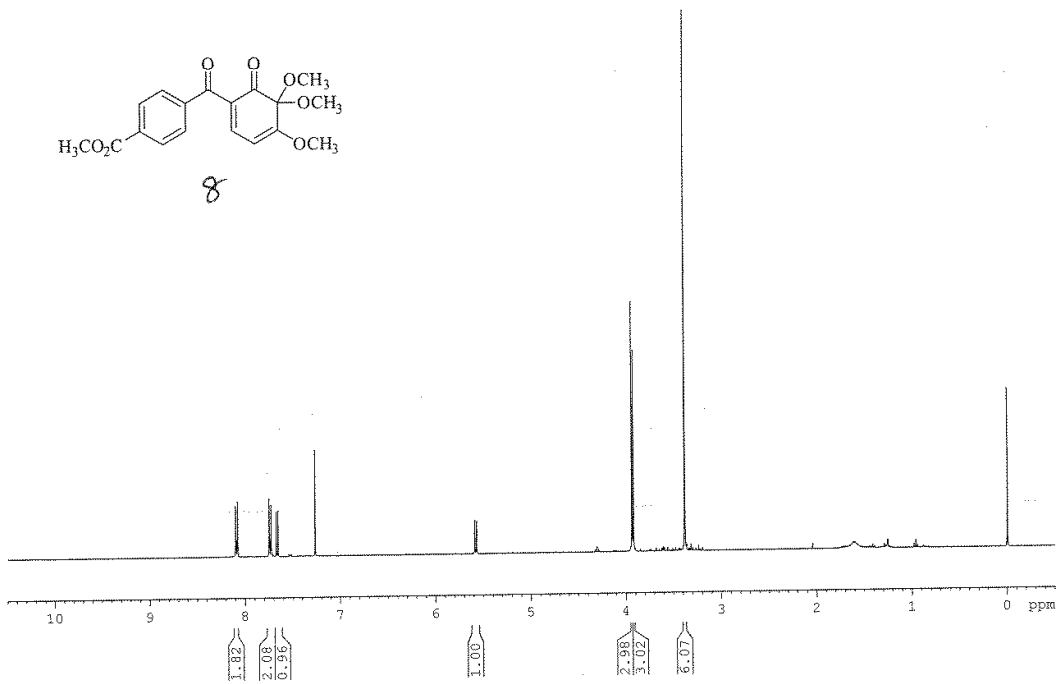
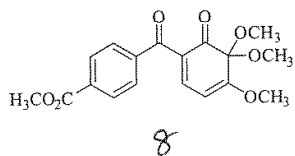
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -2.00 dB  
PL12 15.47 dB  
PL13 15.72 dB  
PL2W 14.33185768 W  
PL12W 0.25662708 W  
PL13W 0.24227159 W  
SFO2 400.2316009 MHz  
SI 32768  
SF 100.6379187 MHz  
WDW EM  
SFB 0  
LB 1.00 Hz  
GB 0  
FC 1.40

8.007  
8.002  
8.002  
8.075  
7.746  
7.742  
7.730  
7.725  
7.573  
7.554  
7.264

5.591  
5.572

3.940  
3.924

3.385



Current Data Parameters  
NAME SG-MKK-L-4-CO2Me-DMP  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20190726  
Time 16.53  
INSTRUM spect  
PROBHD 5 mm PARAC BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 228.1  
DW 62.400 usec  
DE 4.50 usec  
TE 300.0 K  
D1 1.0000000 sec  
TD0 1

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
NUC1 1H  
P1 10.40 usec  
PL1 -1.00 dB  
PL1W 19.34582710 W  
SFO1 400.1318542 MHz

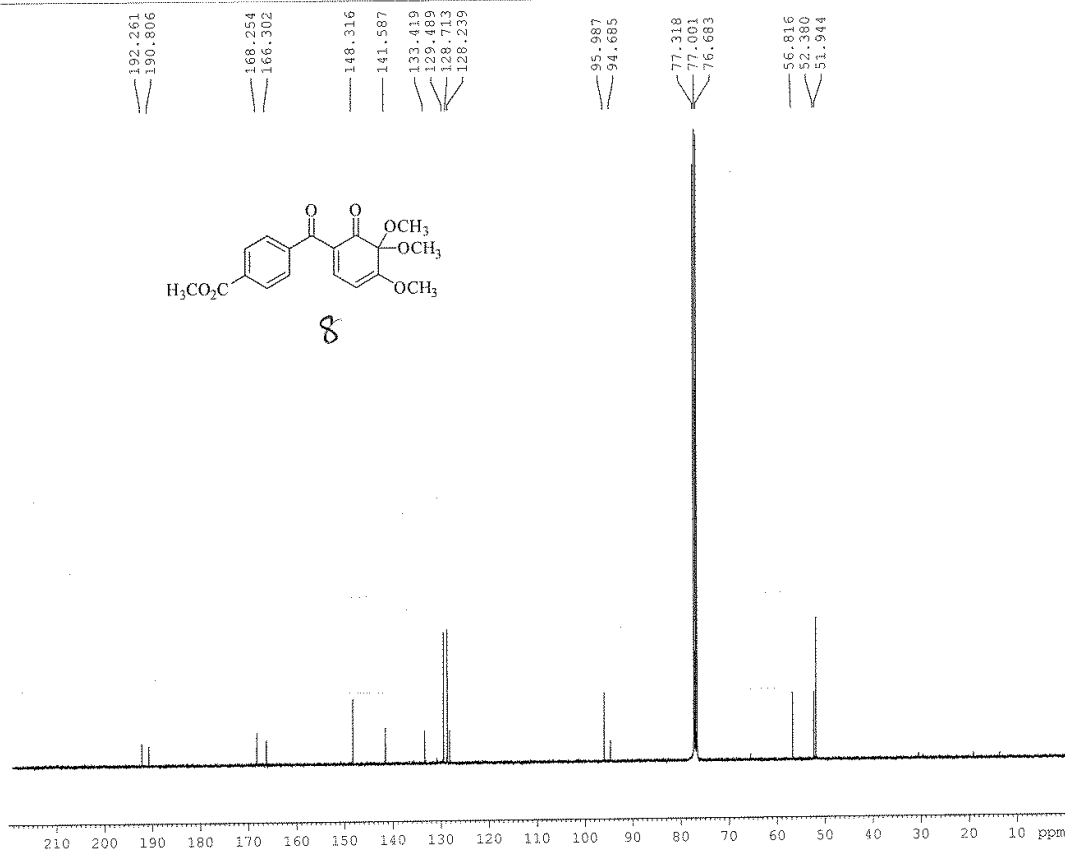
F2 - Processing parameters  
SI 32788  
SF 400.130078 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Name \_\_\_\_\_

Date \_\_\_\_\_

NB # \_\_\_\_\_

AMRI SRC  
location; 17



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

Current Data Parameters  
NAME SG-MKK-L-4-CO2Me-DMP  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150726  
Time 22.39  
INSTRUM spect  
PROBRD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 6000  
DS 4  
SWH 23980.814 Hz  
FIDRES 0.365918 Hz  
AQ 1.3664756 sec  
RG 14596.5  
RW 20.850 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 7.40 usec  
PL1 -4.00 dB  
PL1W 82.02445221 W  
SFO1 100.6228290 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPDZ 80.00 usec  
PL2 -3.00 dB  
PL2 14.72 dB  
PL3 15.06 dB  
PL2W 19.34582710 W  
PL2W 0.32702976 W  
PL3W 0.30240381 W  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 22166  
SF 100.6127751 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40