Electronic Supplementary Material (ESI) for RSC Advances.

One-pot synthesis and evaluation of novel 3-Aryl-6-ethoxycarbonyl-4-hydroxy-2H-pyran-2-one as potent cytotoxic agents

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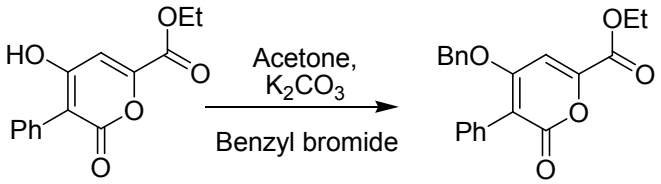
Synthesis of Ethyl 4-(benzyloxy)-6-oxo-5-phenyl-6H-pyran-2-carboxylate (10),

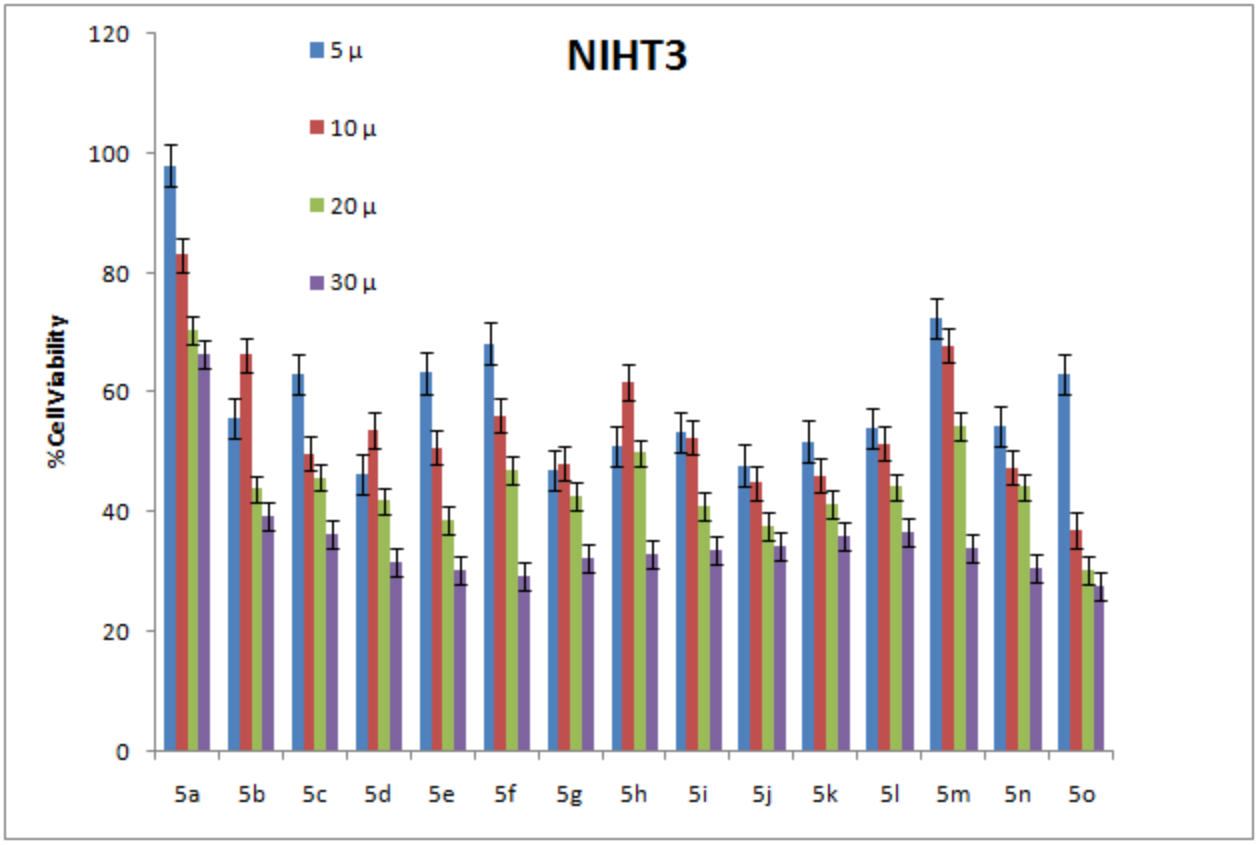
Procedure- To a solution of compound **5a** (1.0 g, 3.846 mmol) in acetone, potassium carbonate (1.1g, 7.6923 mmol) and benzyl bromide (0.91 mL, 7.6923 mmol) was added. Reaction mixture was refluxed for 3-4 h. After completion of reaction water (25 mL) was added to it which was then extracted with ethyl acetate (3 x 25 mL). Product was purified using 10 % ethyl acetate in n-hexane to give **10** as bright yellow solid.

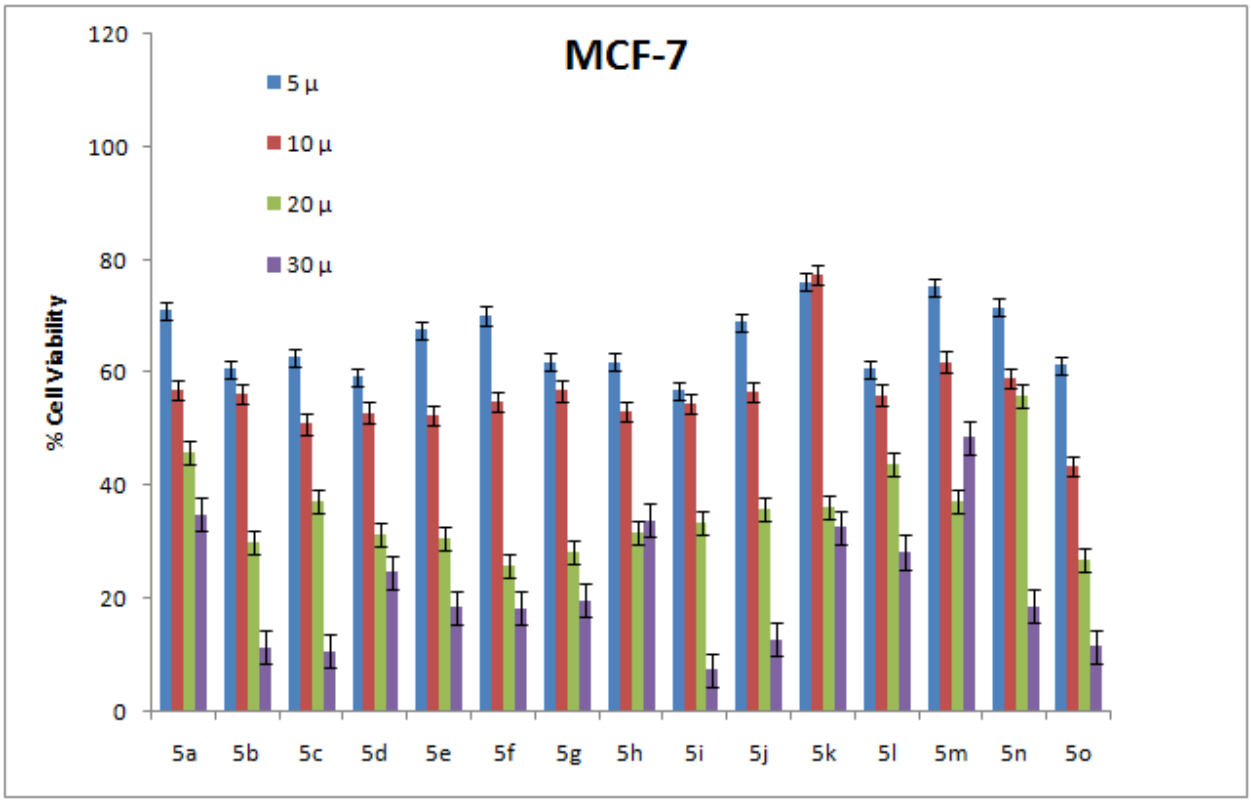


5a **10**

Bright yellow solid (**10**) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (m, 2H, Ar-H), 7.48 (m, 2H, Ar-H), 7.40 (m, 5H, Ar-H), 7.32 (m, 1H, Ar-H), 6.80 (s, 1H, C5-H), 5.73 (s, *J* = 7.12 Hz, 2H, -OCH_2Ph), 4.41 (q, 2H, -OCH_2), 1.42 (t, *J* = 7.12 Hz, 3H,-CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.9, 160.9, 146.2, 142.3, 135.7, 133.4, 130.6, 128.7, 128.7, 128.6, 127.8, 119.1, 112.5, 73.4, 61.7, 14.2; HRMS (ESI): *m/z* calculated for $C_{21}H_{17}O_5$ $[M-H]^-$: 349.1071, found: 349.1078.

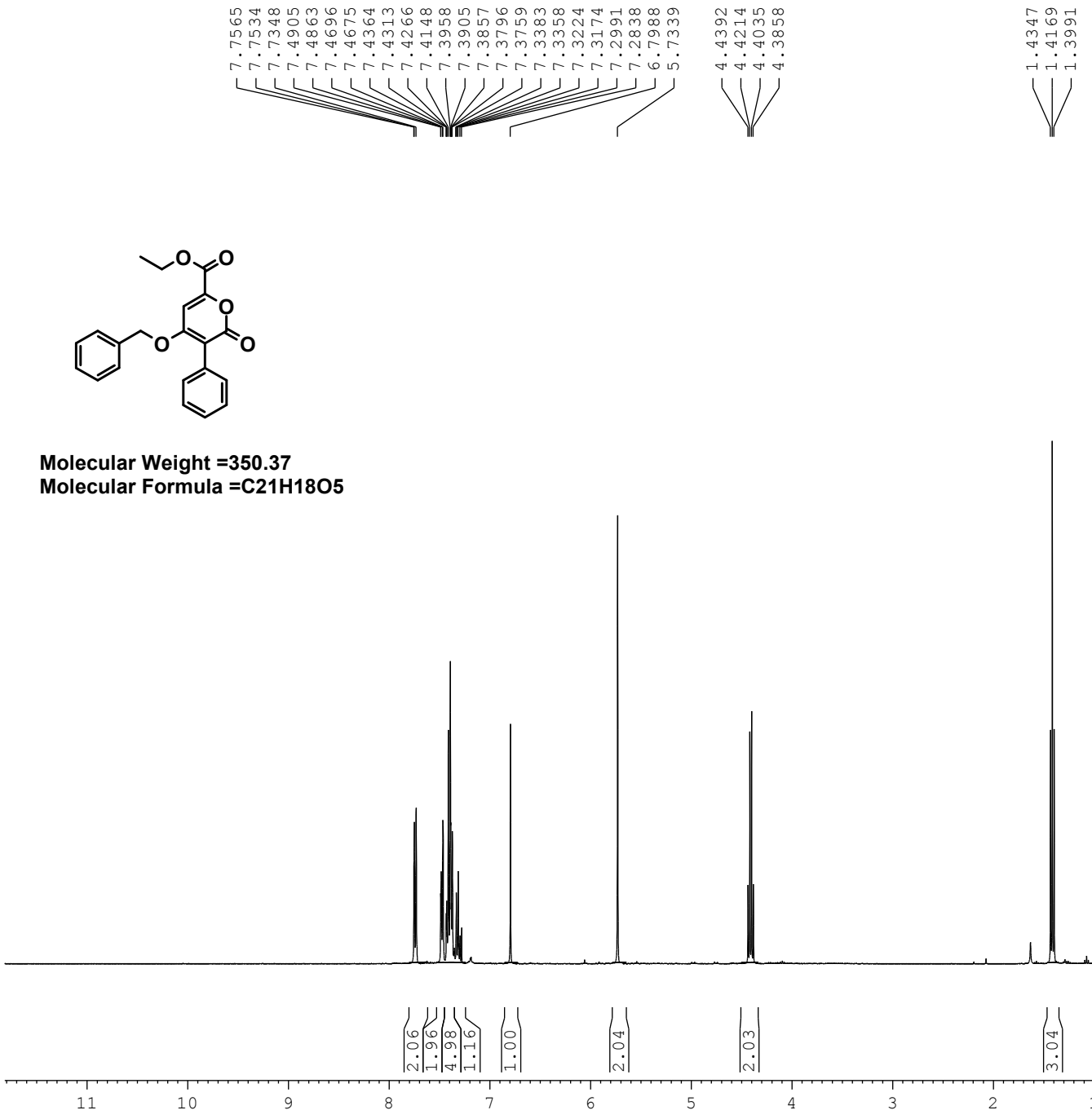
1. Dose response curves of compounds (5a-5o)


NIHT3
5 µ
10 µ
20 µ
30 µ
% Cell Viability
120
100
80
60
40
20
0
5a
5b
5c
5d
5e
5f
5g
5h
5i
5j
5k
5l
5m
5n
5o


MCF-7
5 µ
10 µ
20 µ
30 µ
% Cell Viability
120
100
80
60
40
20
0
5a
5b
5c
5d
5e
5f
5g
5h
5i
5j
5k
5l
5m
5n
5o

2. ^{1}H and ^{13}C data for 5a-5o.

GRD-104



Molecular Weight =350.37
Molecular Formula =C21H18O5

BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

Current Data Parameters	
NAME	Dec09-2013
EXPNO	550
PROCNO	1

F2 - Acquisition Parameters	
Date_	20131210
Time	10.08
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	2
SWH	12019.230 Hz
FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	228
DW	41.600 usec
DE	6.00 usec
TE	296.2 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========	
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P1	10.90 usec
PL1	-3.00 dB
SFO1	400.1324710 MHz

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

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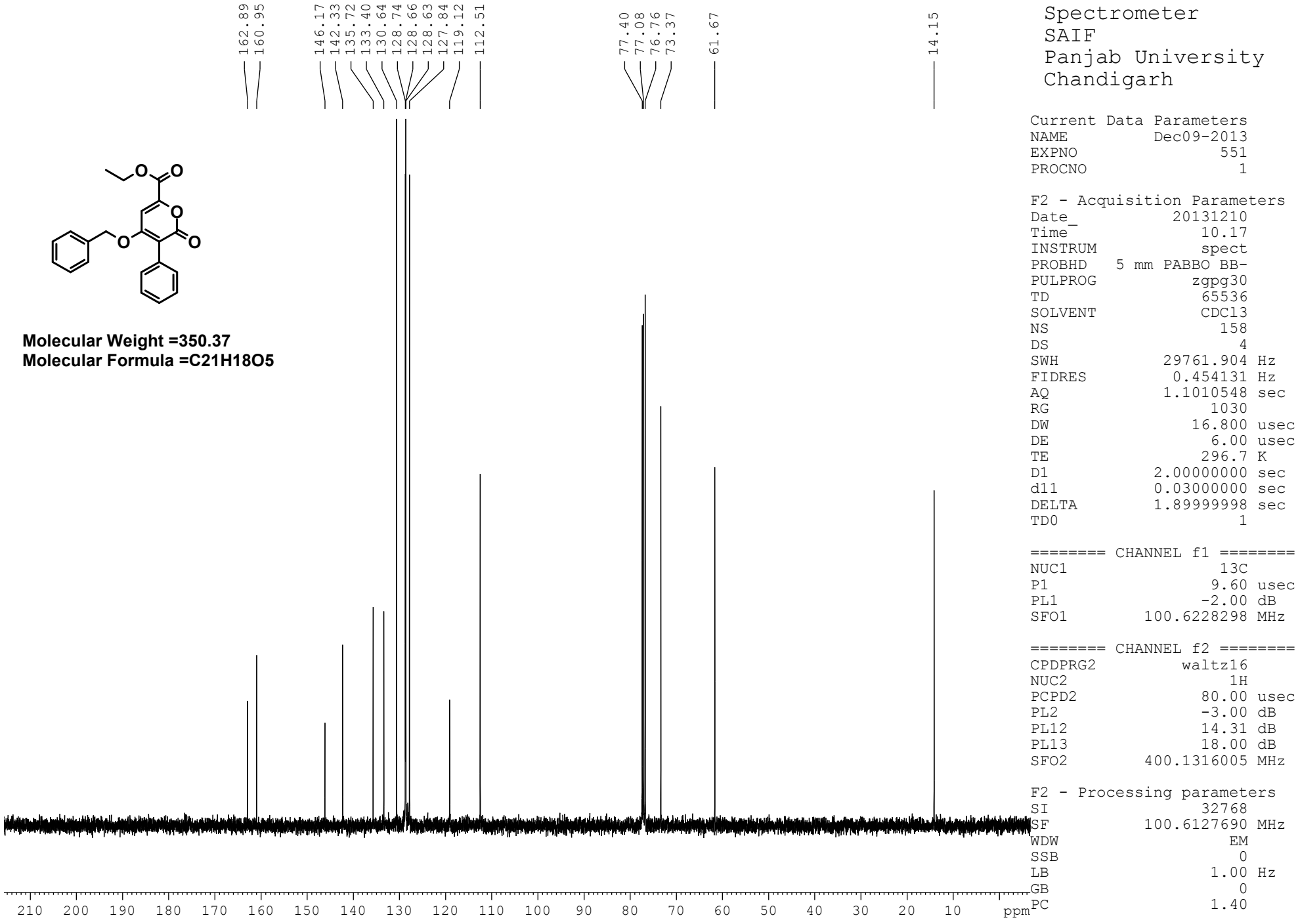
GRD-104



Molecular Weight =350.37
Molecular Formula =C21H18O5

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AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

Current Data Parameters	
NAME	Dec09-2013
EXPNO	551
PROCNO	1
F2 - Acquisition Parameters	
Date_	20131210
Time	10.17
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	158
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	1030
DW	16.800 usec
DE	6.00 usec
TE	296.7 K
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d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
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NUC1	13C
P1	9.60 usec
PL1	-2.00 dB
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	14.31 dB
PL13	18.00 dB
SFO2	400.1316005 MHz
F2 - Processing parameters	
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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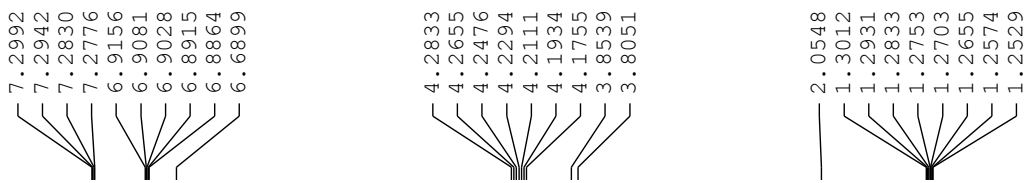
GRD-96



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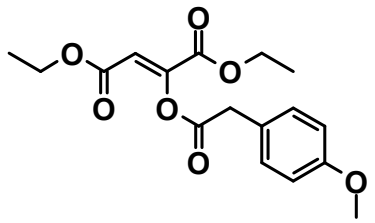


Molecular Formula =C17H20O7

Current Data Parameters

NAME	Aug01-2013
EXPNO	480
PROCNO	1

F2 - Acquisition Parameters

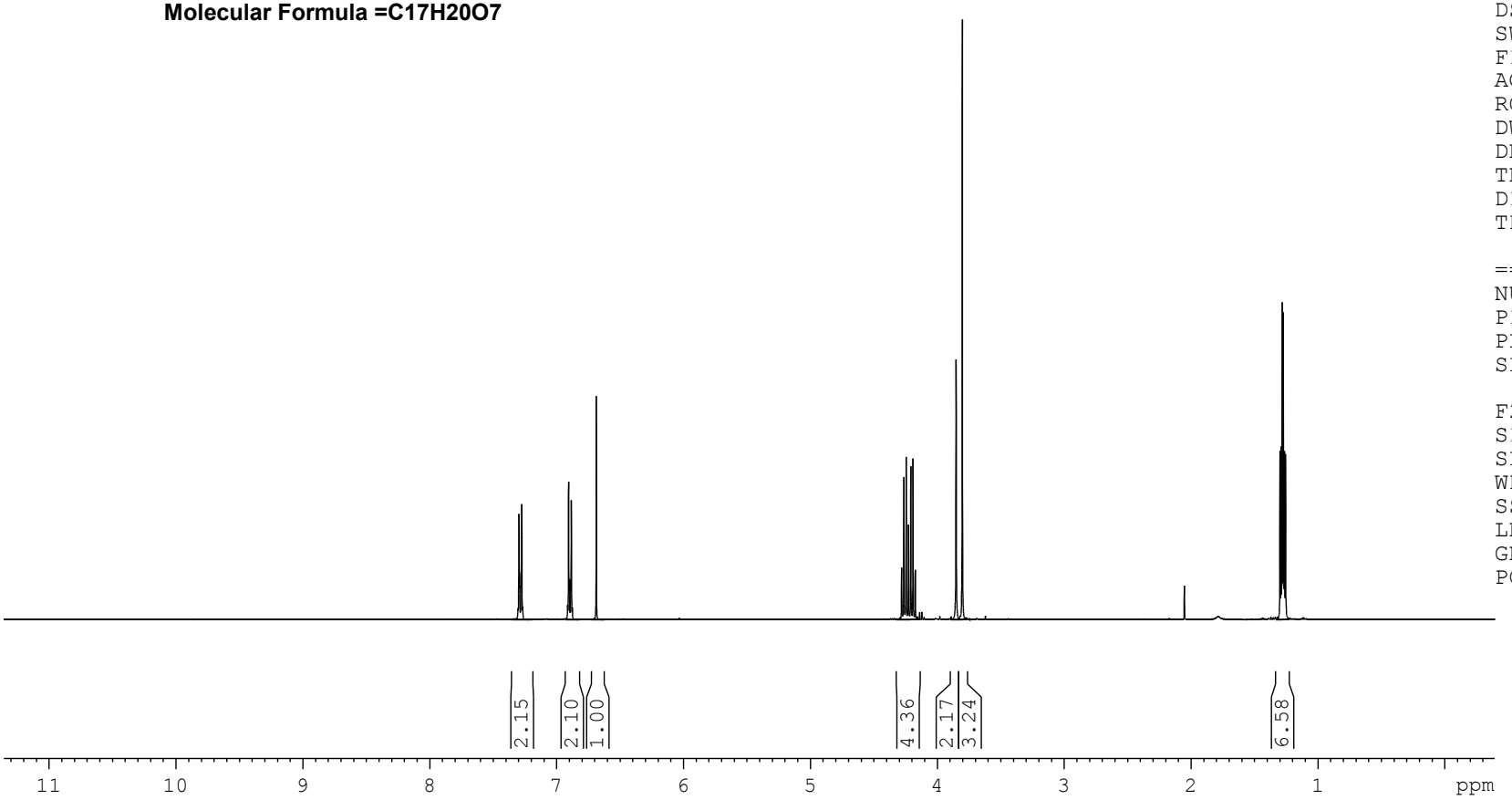
Date_	20130802
Time	11.53
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	12019.230 Hz
FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	90.5
DW	41.600 usec
DE	6.00 usec
TE	295.5 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	1H
P1	10.90 usec
PL1	-3.00 dB
SFO1	400.1324710 MHz

F2 - Processing parameters

SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



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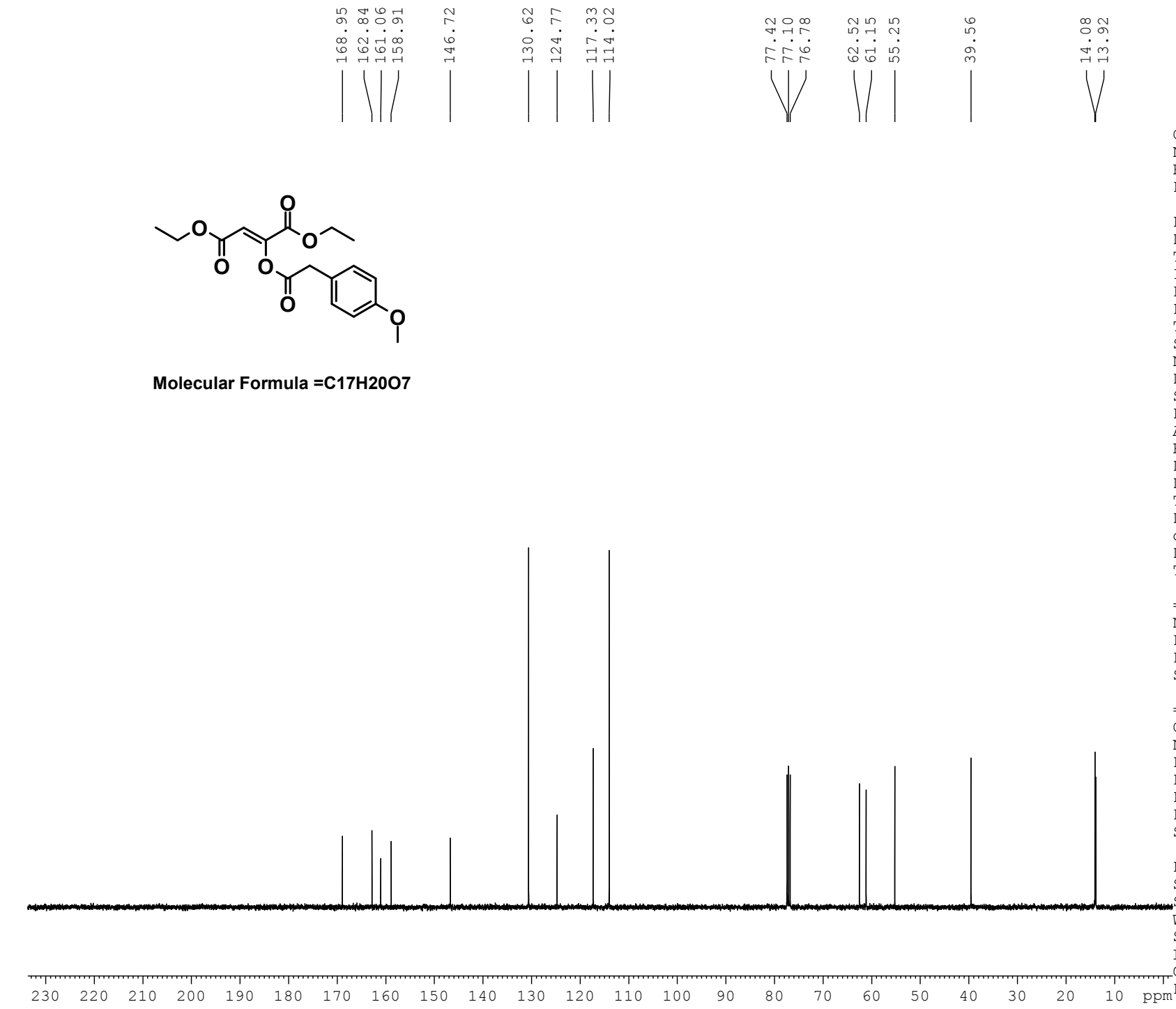

Molecular Formula =C17H20O7

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Current Data Parameters	
NAME	Aug01-2013
EXPNO	481
PROCNO	1
F2 - Acquisition Parameters	
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Time	12.01
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	88
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	36
DW	16.800 usec
DE	6.00 usec
TE	296.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.60 usec
PL1	-2.00 dB
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	14.31 dB
PL13	18.00 dB
SFO2	400.1316005 MHz
F2 - Processing parameters	
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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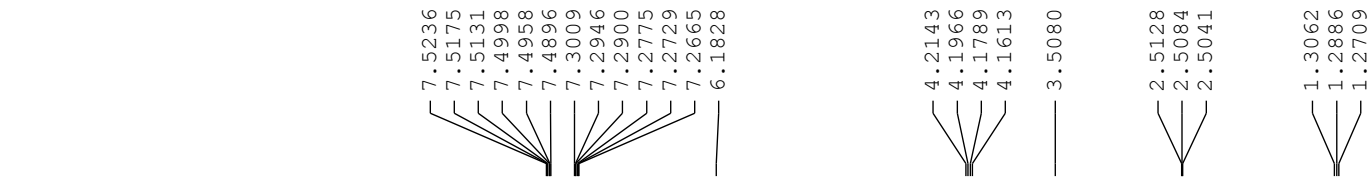

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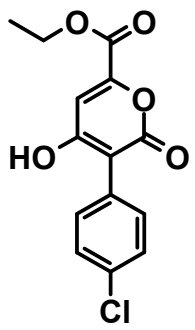

Molecular Weight =294.69
Molecular Formula =C14H11ClO5

Current Data Parameters	
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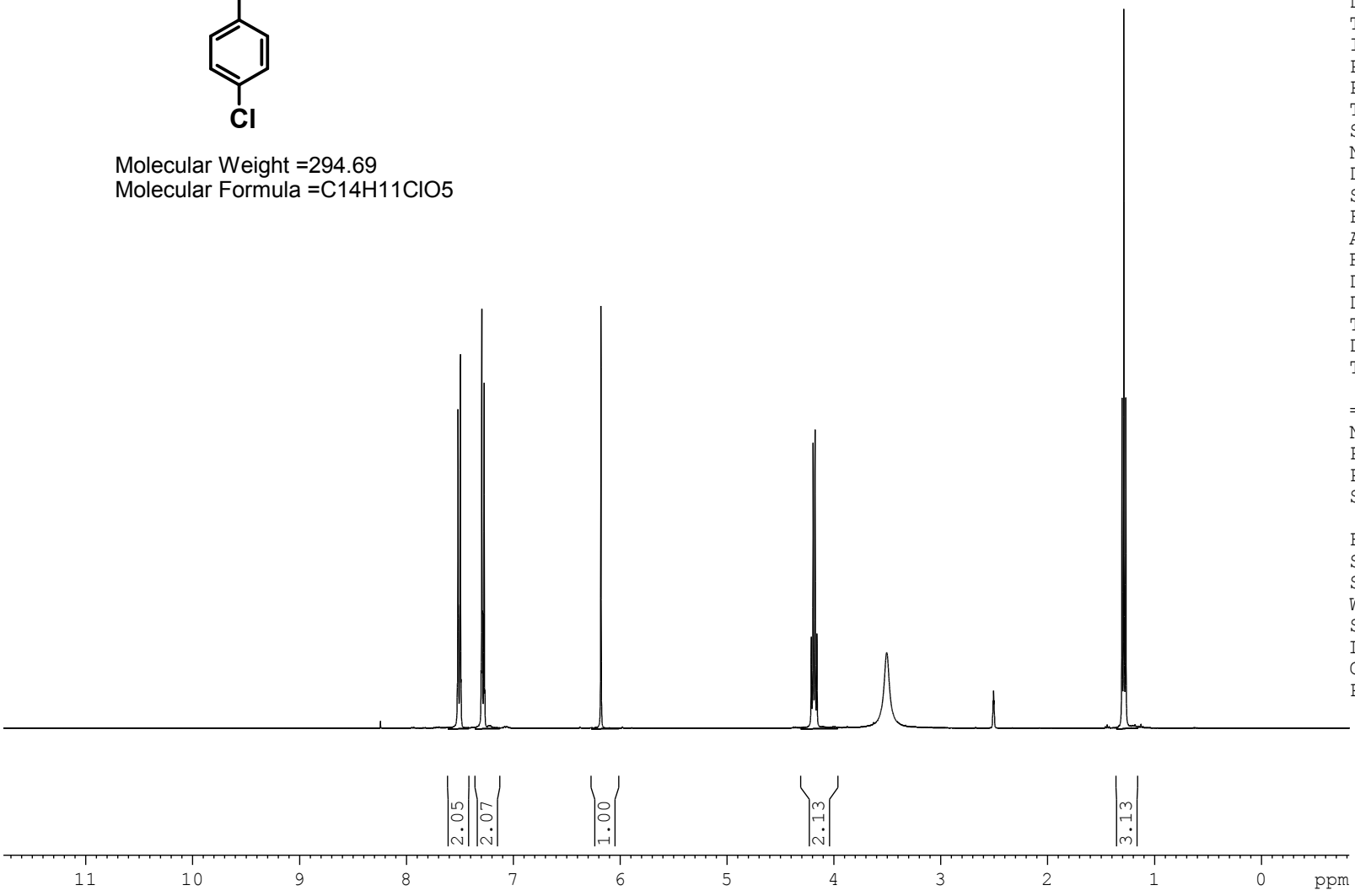
EXPNO	190
PROCNO	1

F2 - Acquisition Parameters	
Date_	20130917
Time	11.02
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	8
DS	2
SWH	12019.230 Hz
FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	128
DW	41.600 usec
DE	6.00 usec
TE	295.1 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========	
NUC1	1H
P1	10.90 usec
PL1	-3.00 dB
SFO1	400.1324710 MHz

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



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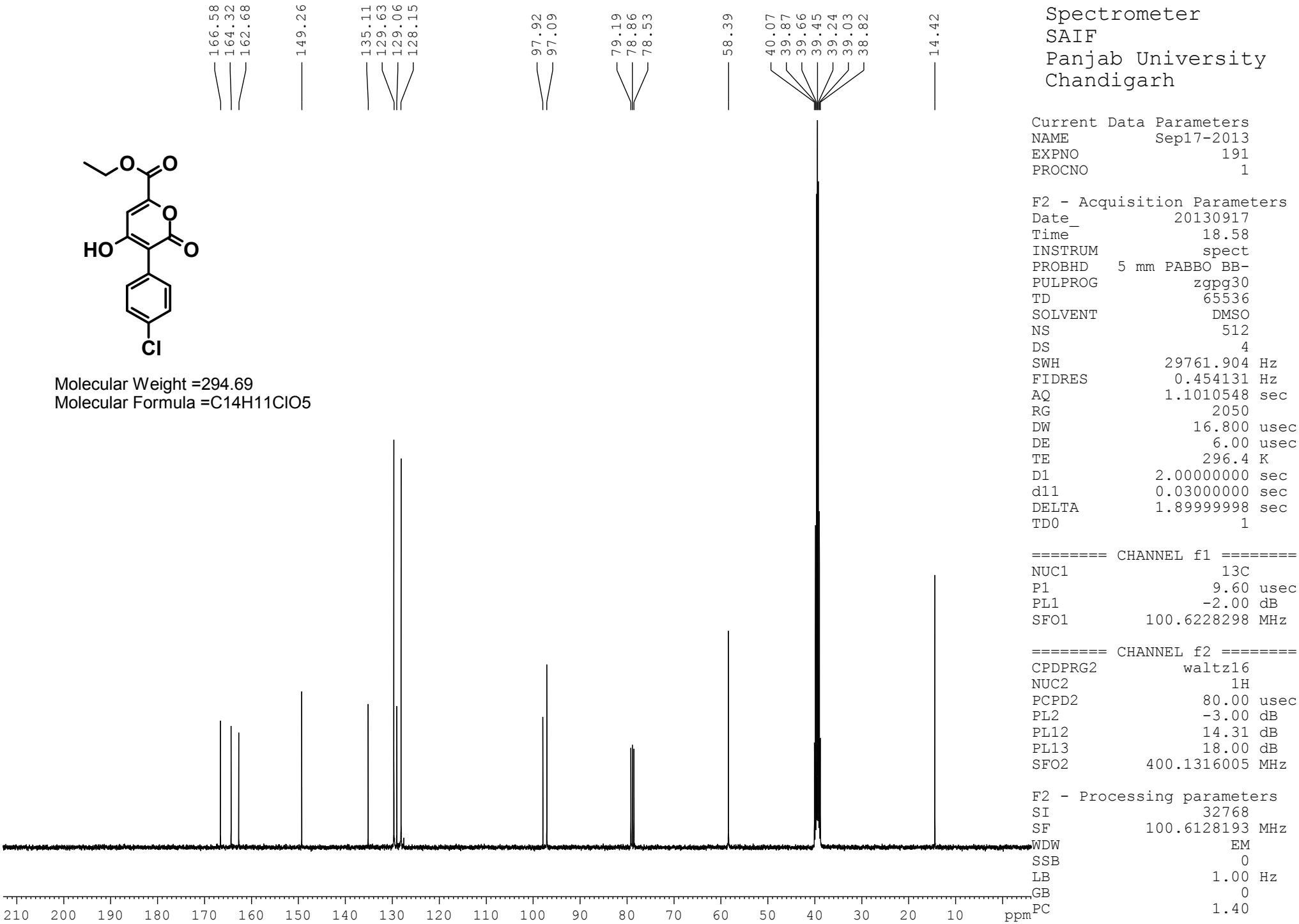

Molecular Weight =294.69
Molecular Formula =C14H11ClO5

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Current Data Parameters	
NAME	Sep17-2013
EXPNO	191
PROCNO	1

F2 - Acquisition Parameters	
Date_	20130917
Time	18.58
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	512
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	2050
DW	16.800 usec
DE	6.00 usec
TE	296.4 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

======== CHANNEL f1 ========	
NUC1	13C
P1	9.60 usec
PL1	-2.00 dB
SFO1	100.6228298 MHz

======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	14.31 dB
PL13	18.00 dB
SFO2	400.1316005 MHz

F2 - Processing parameters	
SI	32768
SF	100.6128193 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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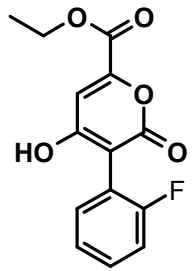
GRD100 I



Molecular Weight =278.24
Molecular Formula =C14H11FO5

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Current Data Parameters	
NAME	Jan01-2014
EXPNO	40
PROCNO	1
F2 - Acquisition Parameters	
Date_	20140101
Time	10.59
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	8
DS	2
SWH	12019.230 Hz
FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	512
DW	41.600 usec
DE	6.00 usec
TE	294.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.90 usec
PL1	-3.00 dB
SFO1	400.1324710 MHz
F2 - Processing parameters	
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

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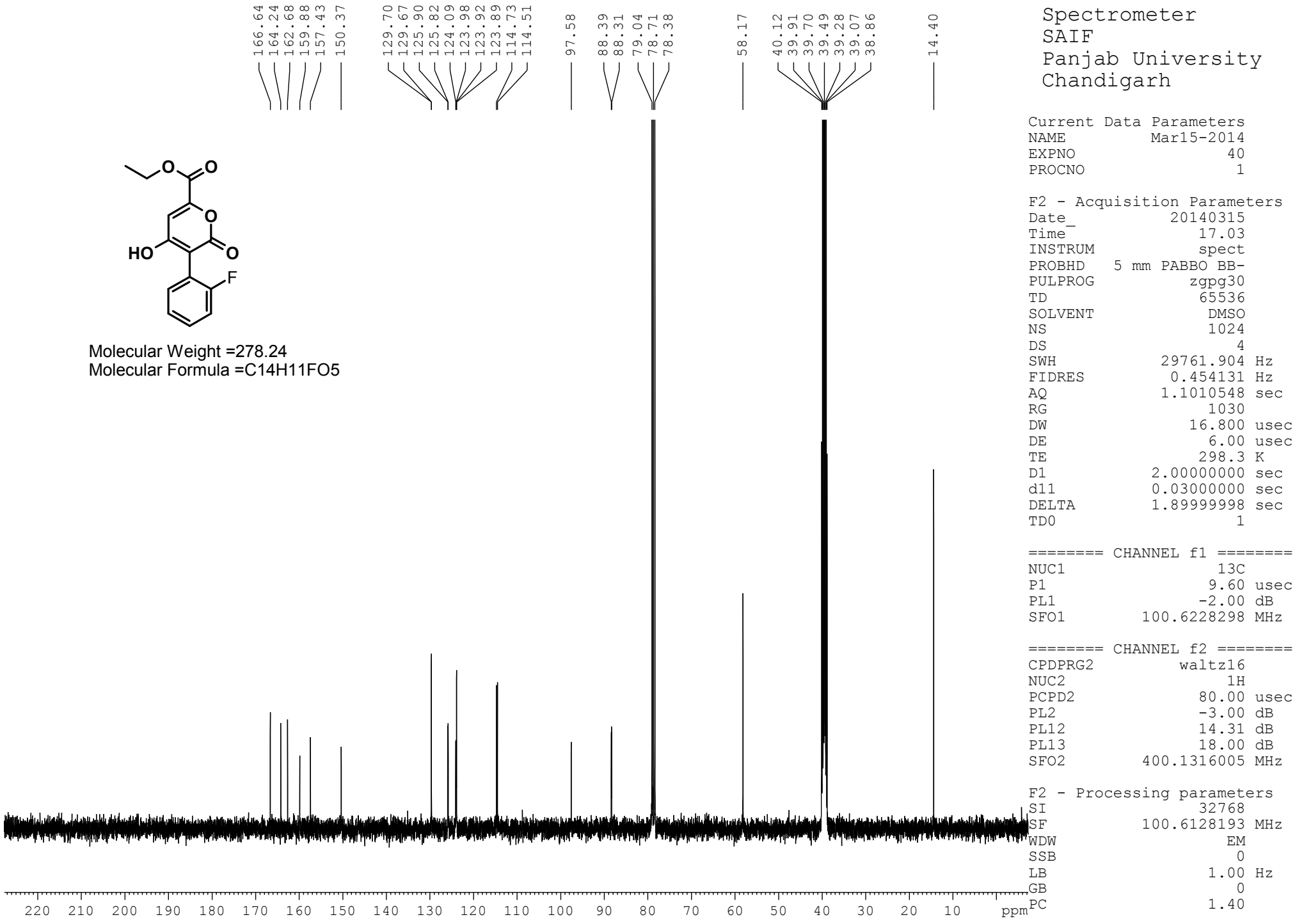
GRD100I



Molecular Weight =278.24
Molecular Formula =C14H11FO5

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Current Data Parameters	
NAME	Mar15-2014
EXPNO	40
PROCNO	1
F2 - Acquisition Parameters	
Date_	20140315
Time	17.03
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PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	1024
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	1030
DW	16.800 usec
DE	6.00 usec
TE	298.3 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.60 usec
PL1	-2.00 dB
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	14.31 dB
PL13	18.00 dB
SFO2	400.1316005 MHz
F2 - Processing parameters	
SI	32768
SF	100.6128193 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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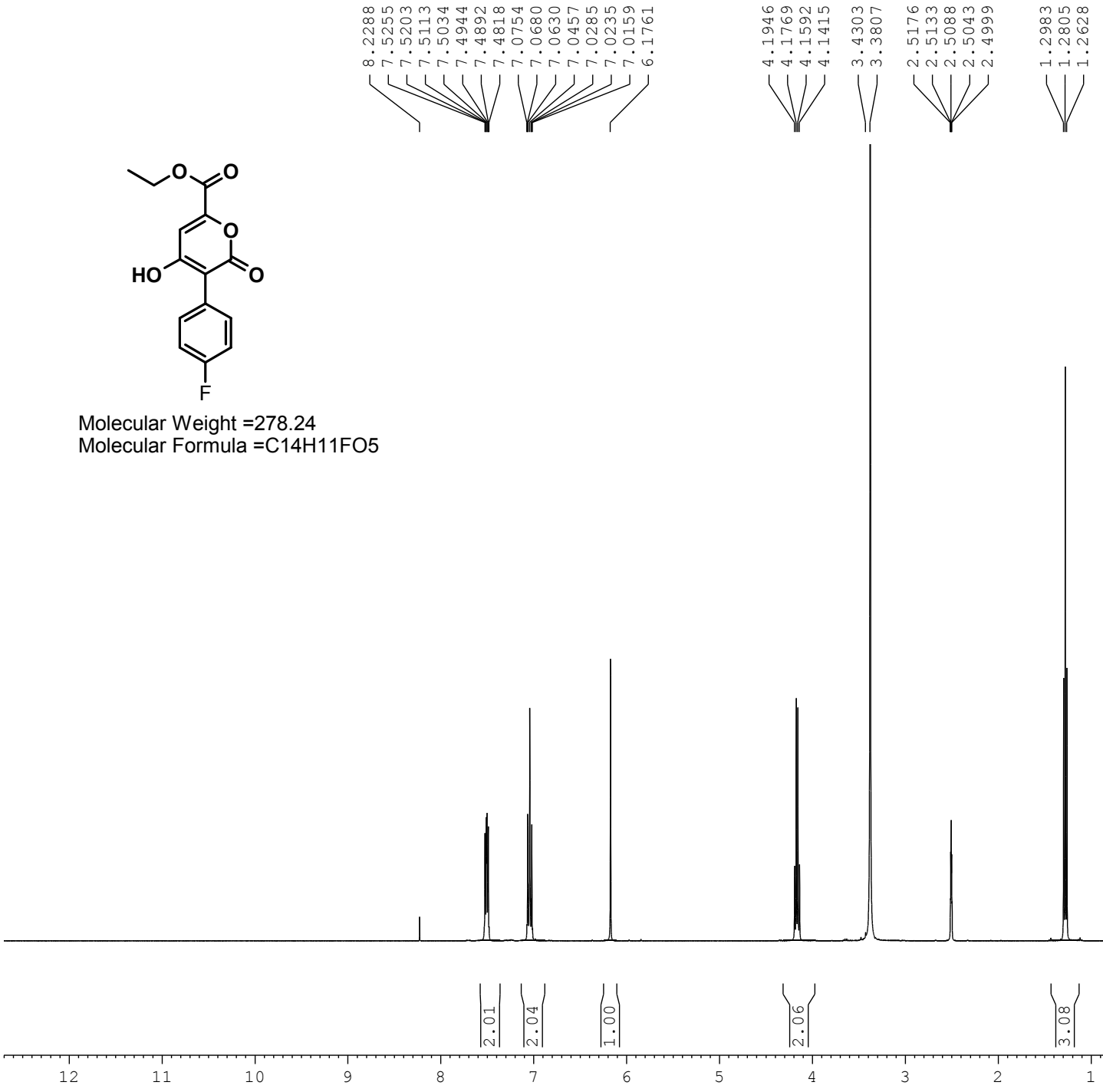
GRD100 J



Molecular Weight =278.24
Molecular Formula =C14H11FO5

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Current Data Parameters	
NAME	Jan01-2014
EXPNO	50
PROCNO	1

F2 - Acquisition Parameters	
Date_	20140101
Time	11.04
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	8
DS	2
SWH	12019.230 Hz
FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	256
DW	41.600 usec
DE	6.00 usec
TE	294.2 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========	
NUC1	1H
P1	10.90 usec
PL1	-3.00 dB
SFO1	400.1324710 MHz

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

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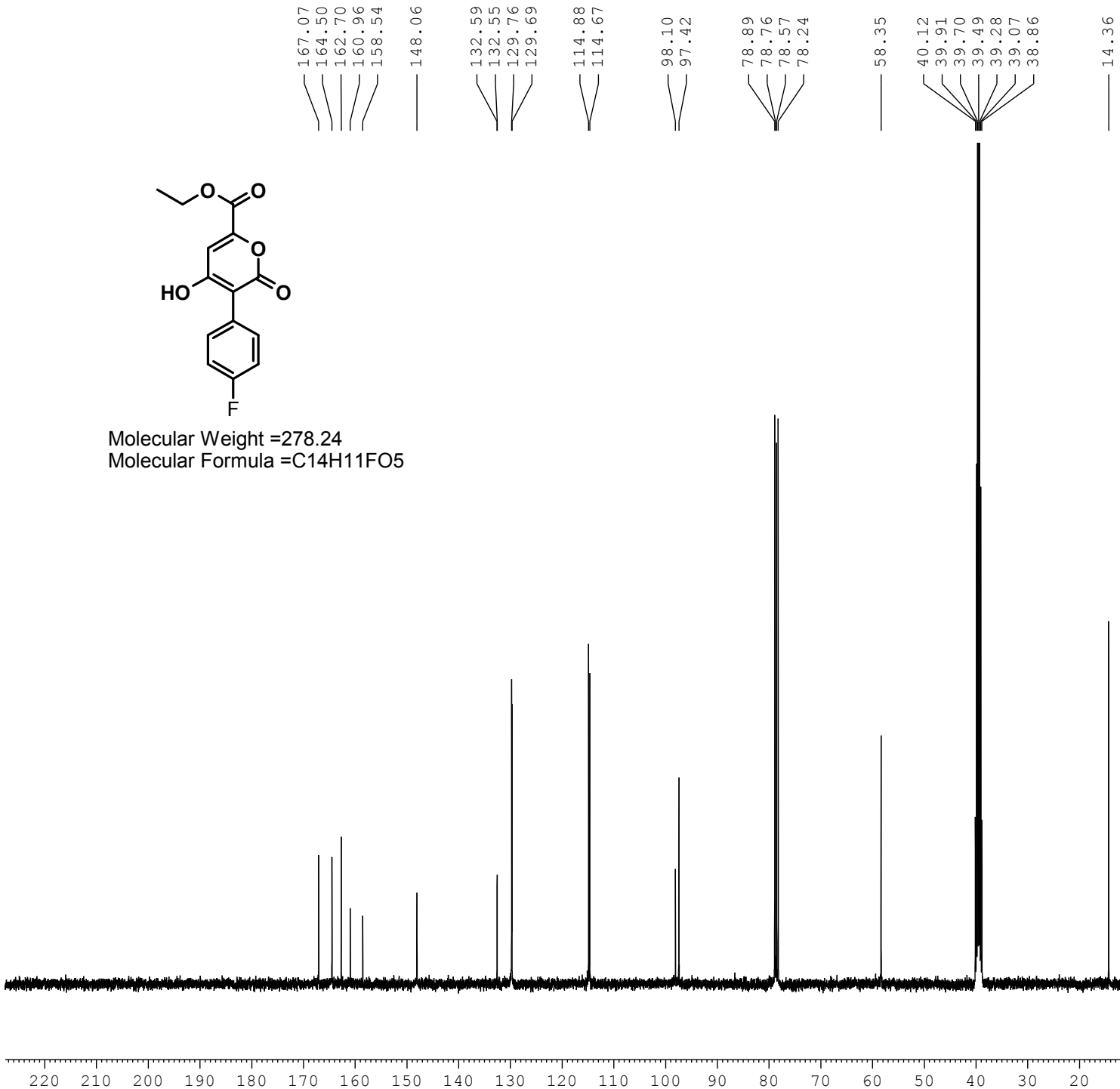

Molecular Weight =278.24
Molecular Formula =C14H11FO5

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Current Data Parameters	
NAME	Mar15-2014
EXPNO	50
PROCNO	1
F2 - Acquisition Parameters	
Date_	20140315
Time	18.03
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	1024
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	1820
DW	16.800 usec
DE	6.00 usec
TE	298.4 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.60 usec
PL1	-2.00 dB
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	14.31 dB
PL13	18.00 dB
SFO2	400.1316005 MHz
F2 - Processing parameters	
SI	32768
SF	100.6128193 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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GRD-100C

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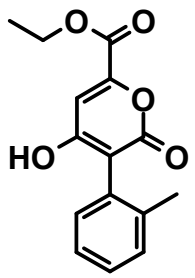

Molecular Weight =274.28
Molecular Formula =C15H14O5

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EXPNO 80
PROCNO 1

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Time 13.38
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 456
DW 41.600 usec
DE 6.00 usec
TE 297.1 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

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

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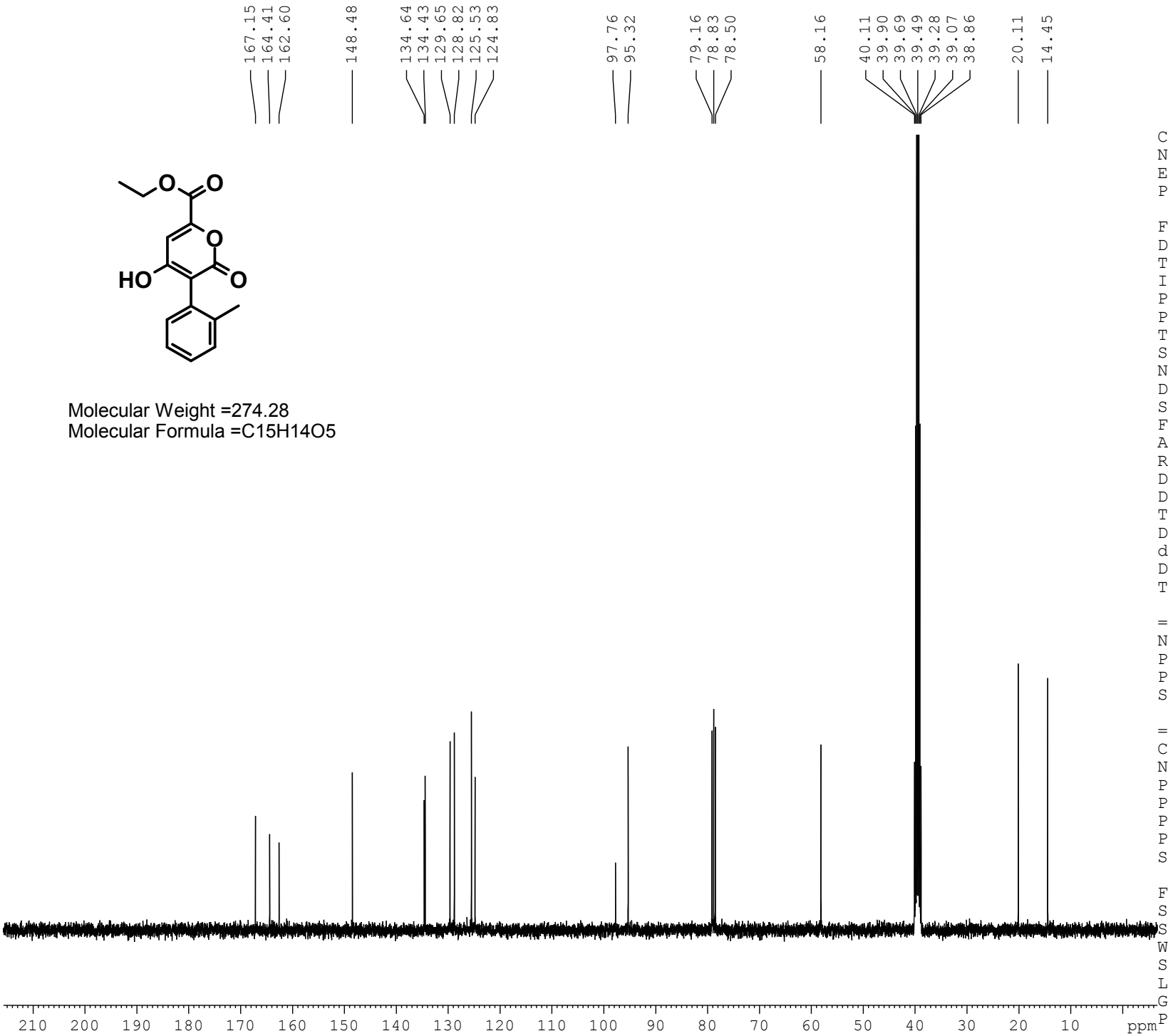
GRD-100C



Molecular Weight =274.28
Molecular Formula =C15H14O5

BRUKER
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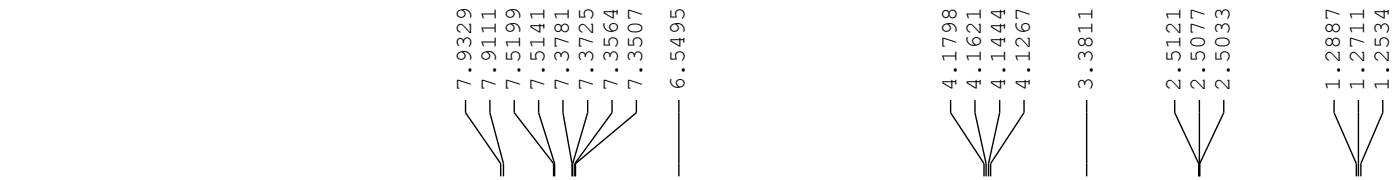
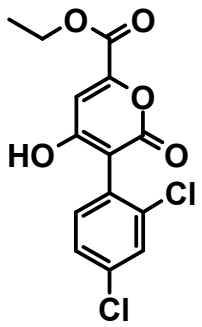
Spectrometer
SAIF
Panjab University
Chandigarh

Current Data Parameters	
NAME	Dec09-2013
EXPNO	580
PROCNO	1
F2 - Acquisition Parameters	
Date_	20131210
Time	10.50
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	378
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	2050
DW	16.800 usec
DE	6.00 usec
TE	296.7 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.60 usec
PL1	-2.00 dB
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	14.31 dB
PL13	18.00 dB
SFO2	400.1316005 MHz
F2 - Processing parameters	
SI	32768
SF	100.6128193 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

avtar_saifpu@yahoo.co.in

GRD-100D





Molecular Weight =329.14
Molecular Formula =C14H10Cl2O5

BRUKER
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Current Data Parameters	
NAME	Sep17-2013
EXPNO	220
PROCNO	1

F2 - Acquisition Parameters	
Date_	20130917
Time	11.17
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	8
DS	2
SWH	12019.230 Hz
FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	228
DW	41.600 usec
DE	6.00 usec
TE	295.2 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========	
NUC1	1H
P1	10.90 usec
PL1	-3.00 dB
SFO1	400.1324710 MHz

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

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GRD-100D

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166.07
164.10
162.89
151.47
133.00
131.48
130.81
129.01
128.55
127.15
97.15
91.68
58.26
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39.87
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39.45
39.25
39.04
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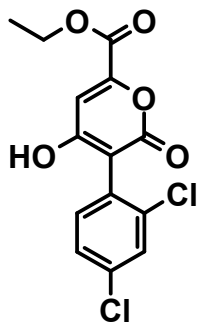
14.47



Molecular Weight =329.14
Molecular Formula =C14H10Cl2O5

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Current Data Parameters
NAME          Sep17-2013
EXPNO                221
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130917
Time_              19.20
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT             DMSO
NS                    512
DS                      4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010548 sec
RG                   1030
DW                16.800 usec
DE                 6.00 usec
TE                296.4 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                  9.60 usec
PL1                -2.00 dB
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -3.00 dB
PL12               14.31 dB
PL13               18.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6128193 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

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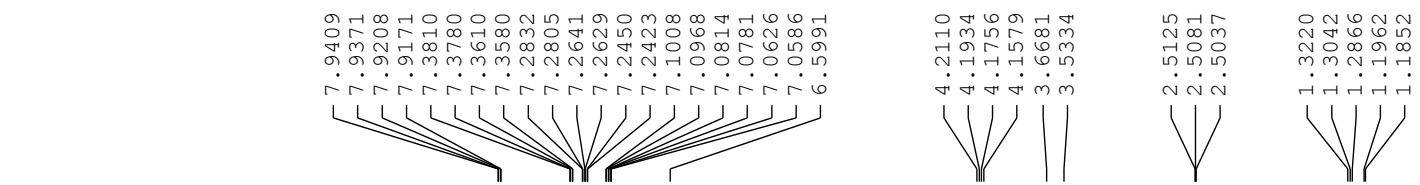
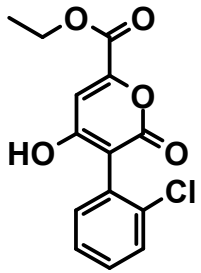
GRD-100E





Molecular Weight =294.69
Molecular Formula =C14H11ClO5

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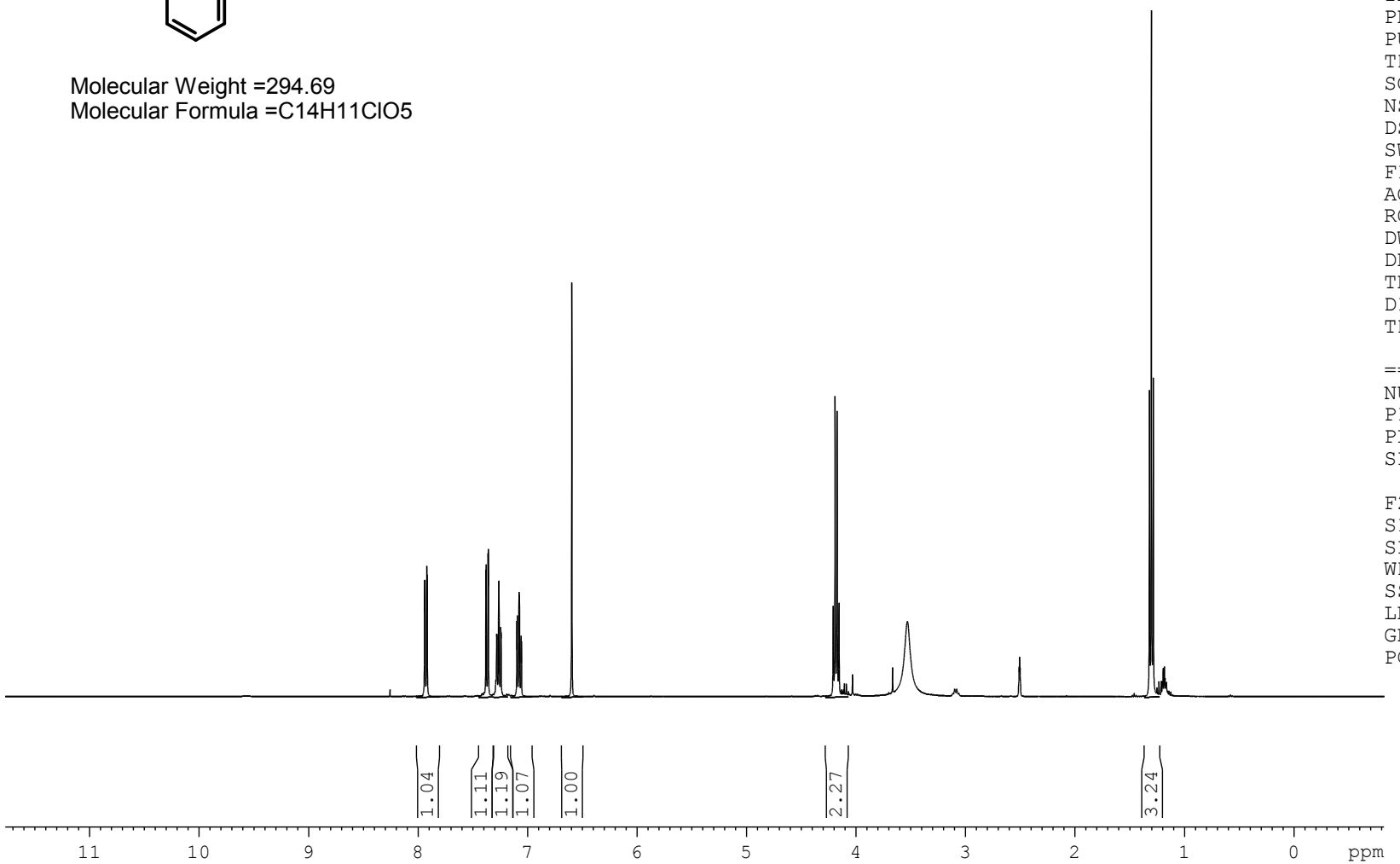
Current Data Parameters	
NAME	Sep17-2013
EXPNO	230
PROCNO	1

F2 - Acquisition Parameters	
Date_	20130917
Time	11.22
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	8
DS	2
SWH	12019.230 Hz
FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	128
DW	41.600 usec
DE	6.00 usec
TE	295.2 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========	
NUC1	1H
P1	10.90 usec
PL1	-3.00 dB
SFO1	400.1324710 MHz

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



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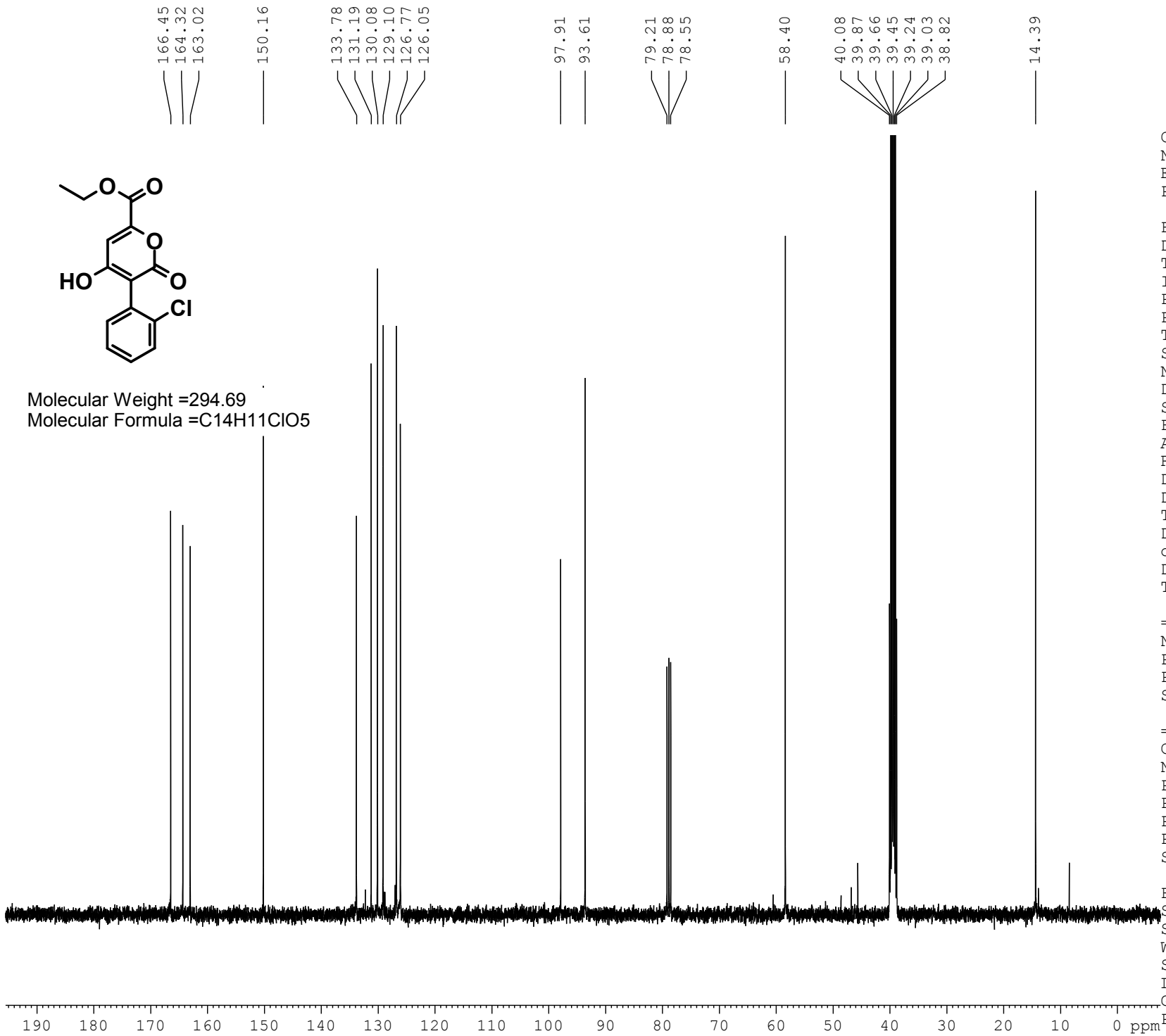
GRD-100E



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Current Data Parameters	
NAME	Sep17-2013
EXPNO	231
PROCNO	1
F2 - Acquisition Parameters	
Date_	20130917
Time	20.09
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	512
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	1030
DW	16.800 usec
DE	6.00 usec
TE	296.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.60 usec
PL1	-2.00 dB
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	14.31 dB
PL13	18.00 dB
SFO2	400.1316005 MHz
F2 - Processing parameters	
SI	32768
SF	100.6128193 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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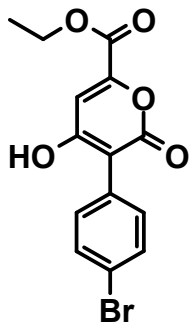
GRD-100F



Molecular Weight =339.14
Molecular Formula =C14H11BrO5

BRUKER
AVANCE II 400 NMR
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Current Data Parameters	
NAME	Sep17-2013
EXPNO	240
PROCNO	1

F2 - Acquisition Parameters	
Date_	20130917
Time	11.27
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	8
DS	2
SWH	12019.230 Hz
FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	144
DW	41.600 usec
DE	6.00 usec
TE	295.2 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========	
NUC1	1H
P1	10.90 usec
PL1	-3.00 dB
SFO1	400.1324710 MHz

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

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GRD-100F

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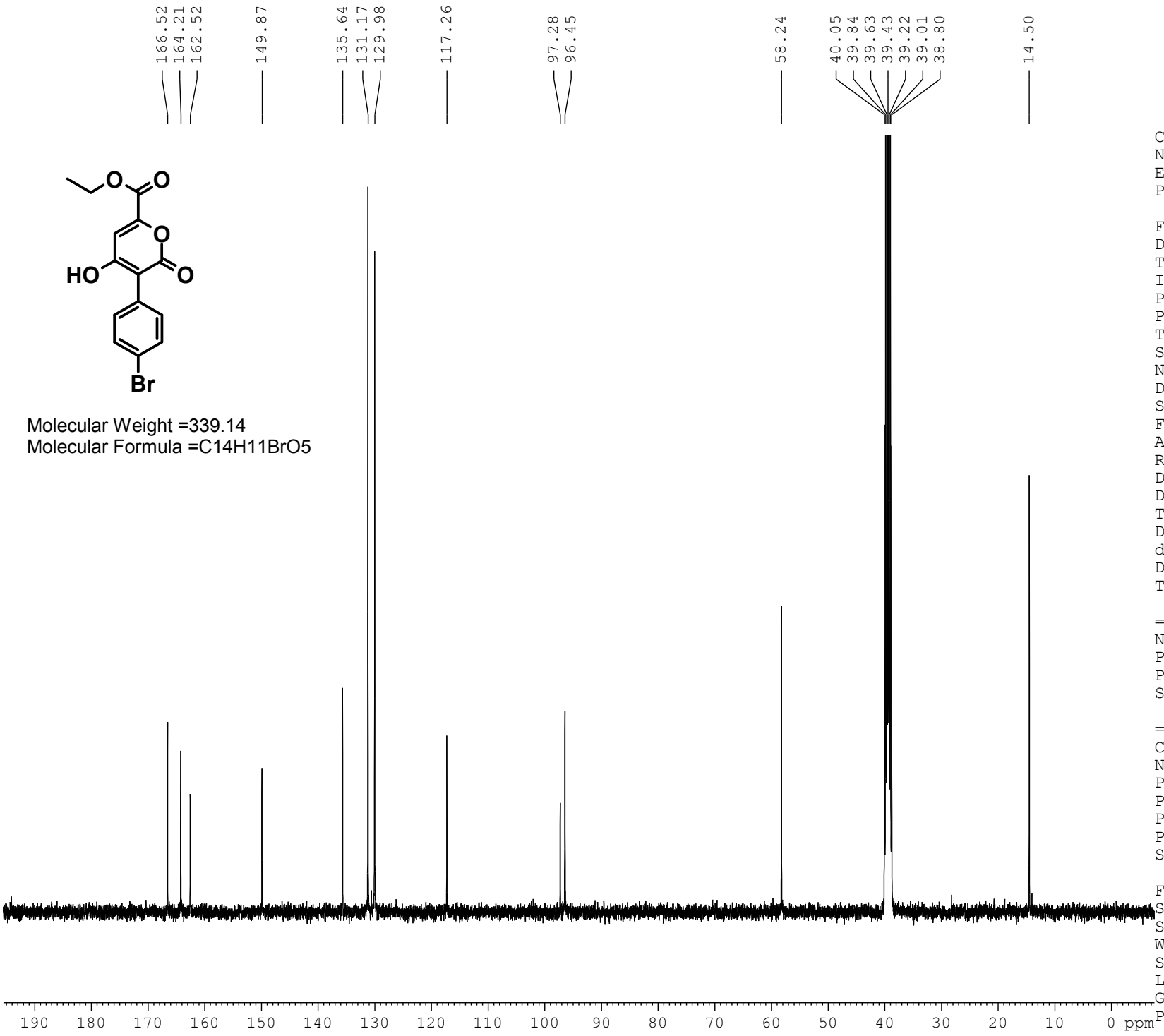

Molecular Weight =339.14
Molecular Formula =C14H11BrO5

Current Data Parameters	
NAME	Sep17-2013
EXPNO	241
PROCNO	1
F2 - Acquisition Parameters	
Date_	20130917
Time	20.41
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	512
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	1030
DW	16.800 usec
DE	6.00 usec
TE	295.9 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.60 usec
PL1	-2.00 dB
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	14.31 dB
PL13	18.00 dB
SFO2	400.1316005 MHz
F2 - Processing parameters	
SI	32768
SF	100.6128193 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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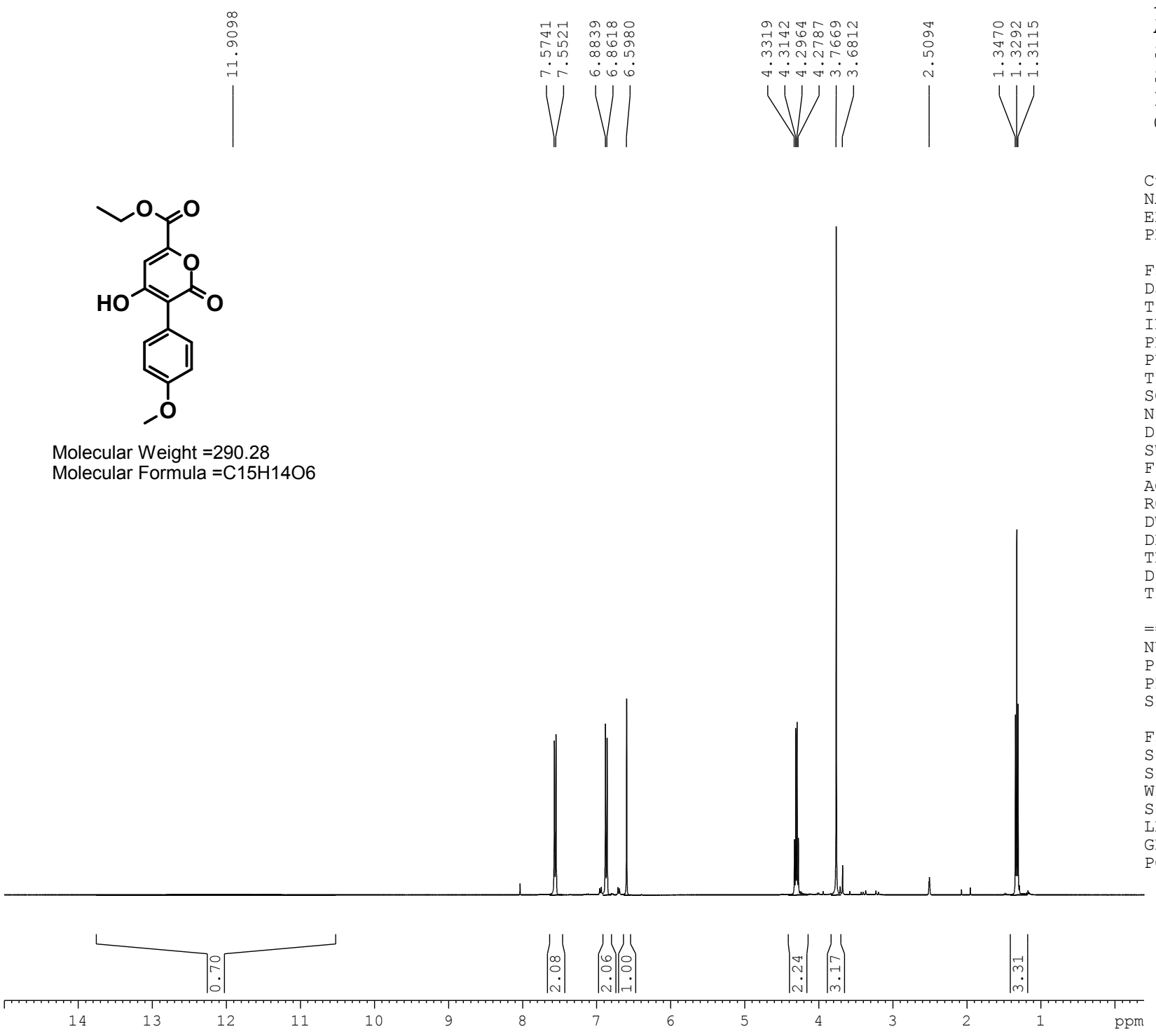
GRD-97



Molecular Weight =290.28
Molecular Formula =C15H14O6

BRUKER
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Spectrometer
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Current Data Parameters	
NAME	Aug01-2013
EXPNO	470
PROCNO	1
F2 - Acquisition Parameters	
Date_	20130802
Time	11.34
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	12019.230 Hz
FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	181
DW	41.600 usec
DE	6.00 usec
TE	295.5 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.90 usec
PL1	-3.00 dB
SFO1	400.1324710 MHz
F2 - Processing parameters	
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

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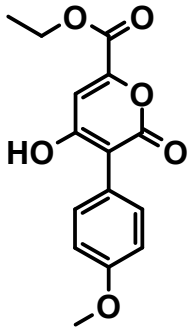
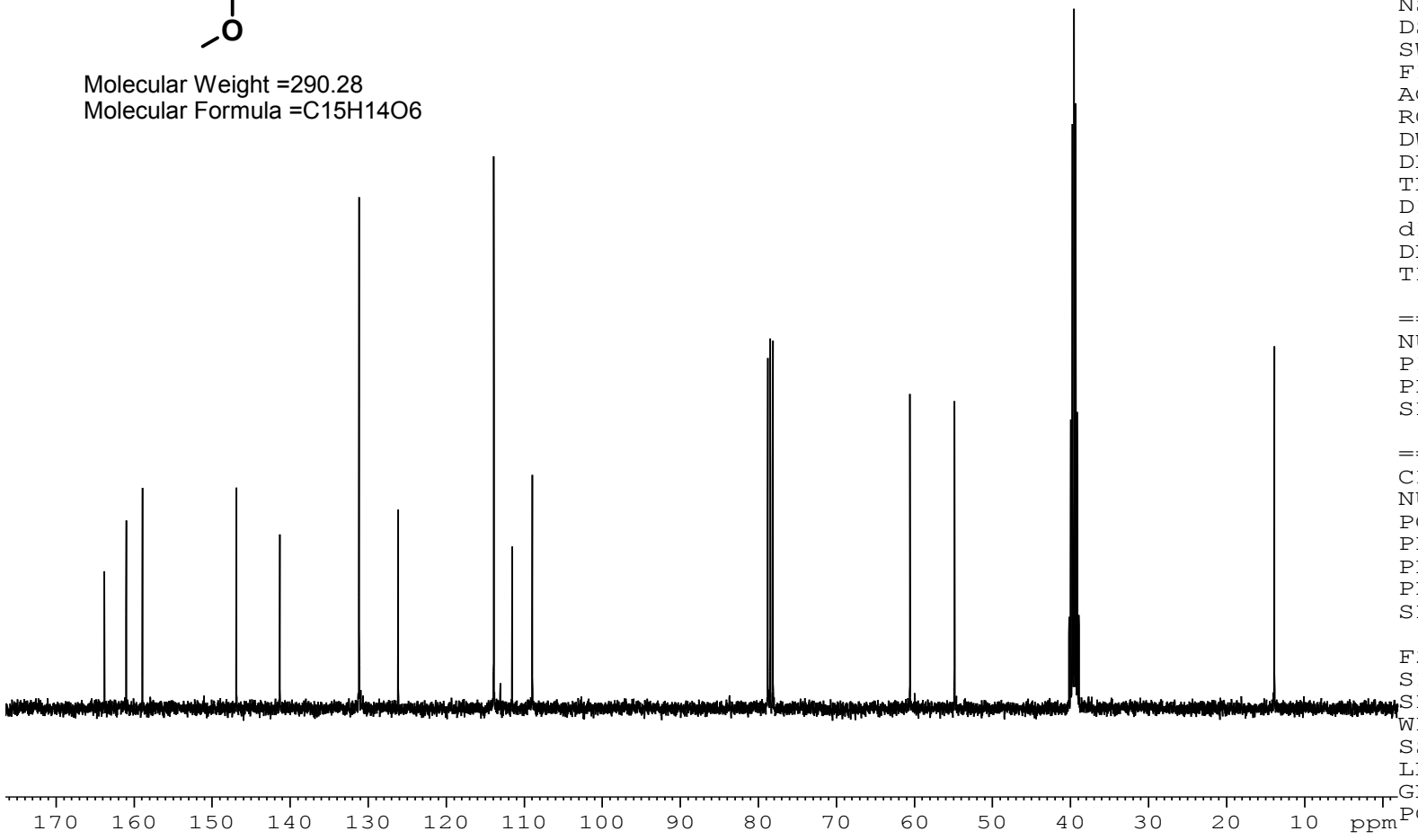


Molecular Weight =290.28
Molecular Formula =C15H14O6



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Current Data Parameters	
NAME	Aug01-2013
EXPNO	471
PROCNO	1
F2 - Acquisition Parameters	
Date_	20130802
Time	11.47
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	192
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	1030
DW	16.800 usec
DE	6.00 usec
TE	296.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.60 usec
PL1	-2.00 dB
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	14.31 dB
PL13	18.00 dB
SFO2	400.1316005 MHz
F2 - Processing parameters	
SI	32768
SF	100.6128193 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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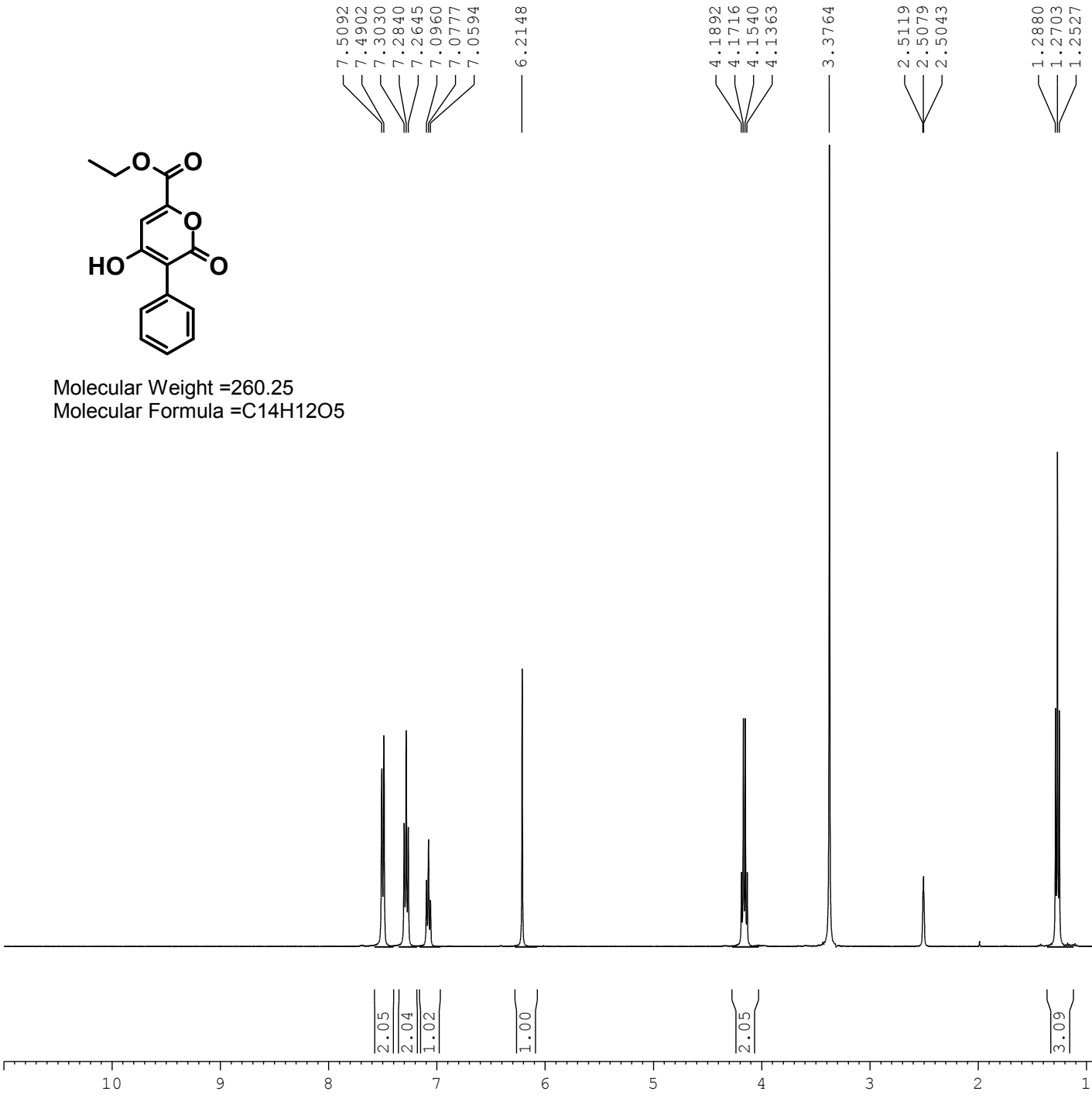
GRD-100G



Molecular Weight =260.25
Molecular Formula =C14H12O5

BRUKER
AVANCE II 400 NMR
Spectrometer
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Current Data Parameters	
NAME	Oct03-2013
EXPNO	90
PROCNO	1
F2 - Acquisition Parameters	
Date_	20131003
Time	13.43
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	8
DS	2
SWH	12019.230 Hz
FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	456
DW	41.600 usec
DE	6.00 usec
TE	297.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.90 usec
PL1	-3.00 dB
SFO1	400.1324710 MHz
F2 - Processing parameters	
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

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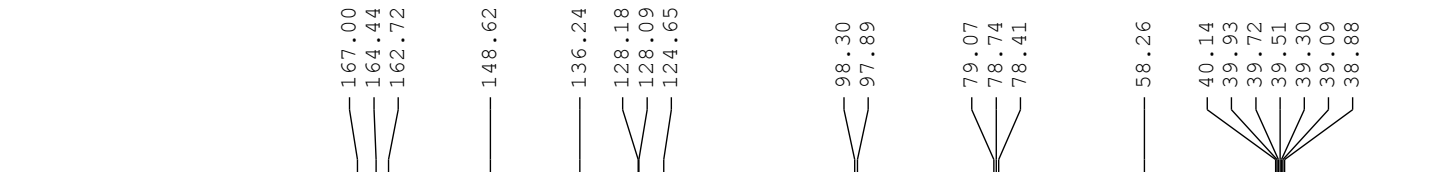
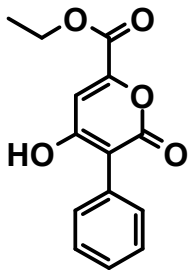
GRD-100G





Molecular Weight =260.25
Molecular Formula =C14H12O5

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Current Data Parameters	
NAME	Dec09-2013
EXPNO	590
PROCNO	1

F2 - Acquisition Parameters	
Date_	20131210
Time	11.13
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	228
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	2050
DW	16.800 usec
DE	6.00 usec
TE	296.8 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

======== CHANNEL f1 ========	
NUC1	13C
P1	9.60 usec
PL1	-2.00 dB
SFO1	100.6228298 MHz

======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	14.31 dB
PL13	18.00 dB
SFO2	400.1316005 MHz

F2 - Processing parameters	
SI	32768
SF	100.6128193 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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GRD-100P

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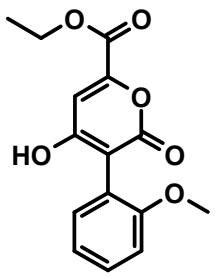

Molecular Weight =290.28
Molecular Formula =C15H14O6

Current Data Parameters
NAME Apr22-2014-Administrator
EXPNO 260
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140423
Time 5.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 2050
DW 16.800 usec
DE 6.00 usec
TE 300.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

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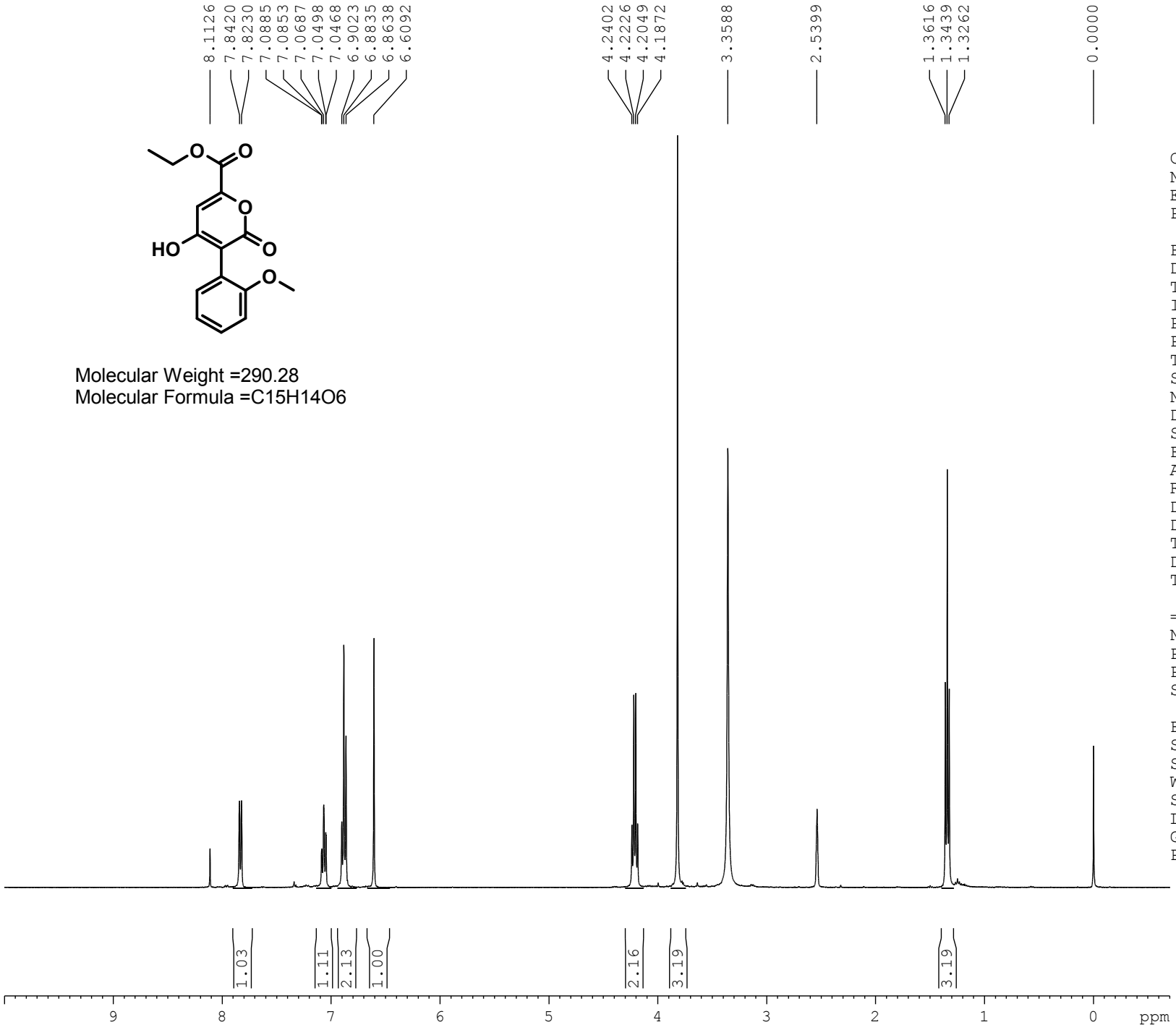
GRD100P



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Current Data Parameters	
NAME	Feb21-2014
EXPNO	150
PROCNO	1

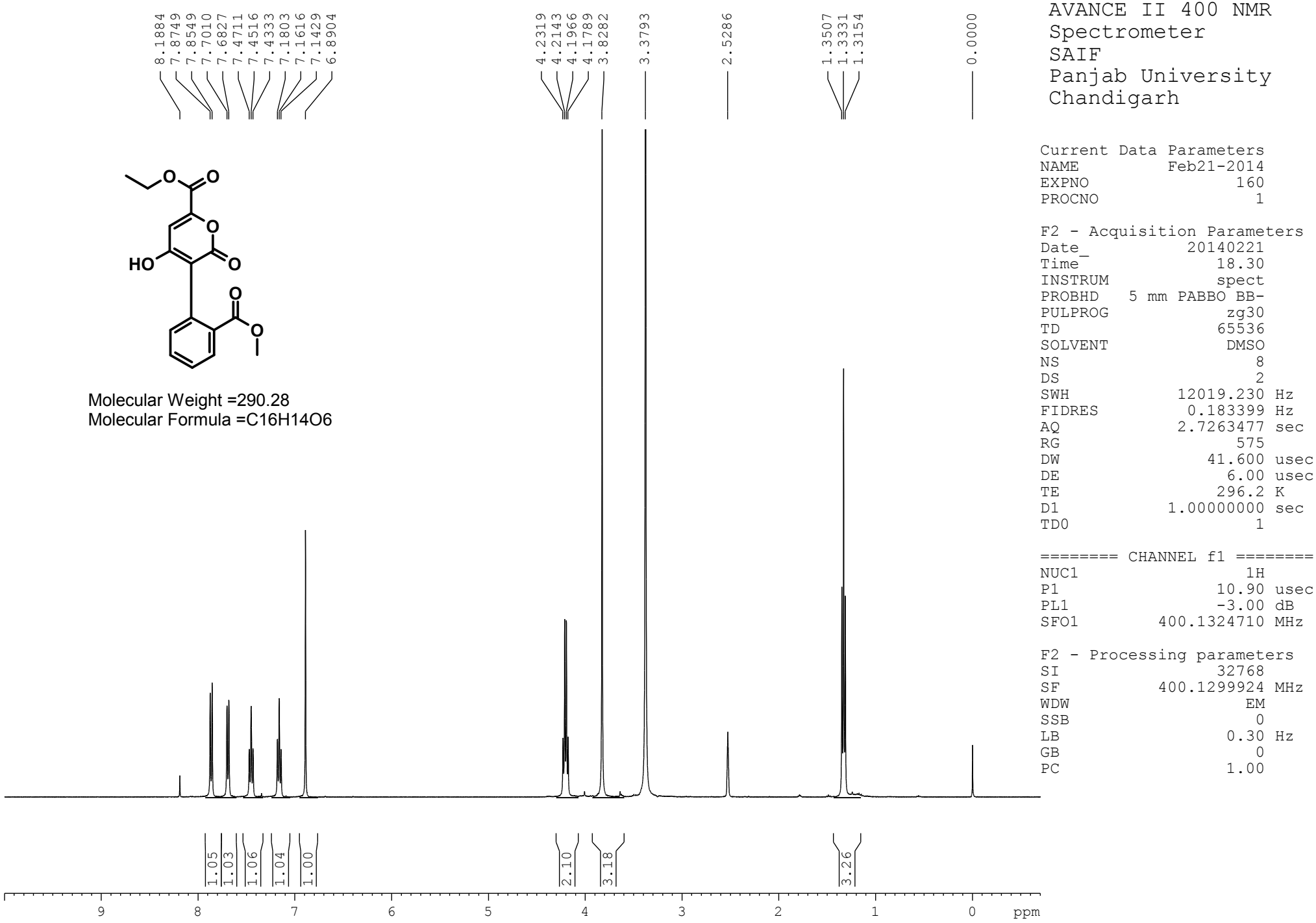
F2 - Acquisition Parameters	
Date_	20140221
Time	18.25
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	8
DS	2
SWH	12019.230 Hz
FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	322
DW	41.600 usec
DE	6.00 usec
TE	296.2 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========	
NUC1	1H
P1	10.90 usec
PL1	-3.00 dB
SFO1	400.1324710 MHz

F2 - Processing parameters	
SI	32768
SF	400.1299881 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

avtar saifpu@yahoo.co.in

GRD100Q



Molecular Weight =290.28
Molecular Formula =C16H14O6

BRUKER
AVANCE II 400 NMR
Spectrometer
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Chandigarh

Current Data Parameters	
NAME	Feb21-2014
EXPNO	160
PROCNO	1

F2 - Acquisition Parameters	
Date_	20140221
Time	18.30
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	8
DS	2
SWH	12019.230 Hz
FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	575
DW	41.600 usec
DE	6.00 usec
TE	296.2 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========	
NUC1	1H
P1	10.90 usec
PL1	-3.00 dB
SFO1	400.1324710 MHz

F2 - Processing parameters	
SI	32768
SF	400.1299924 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

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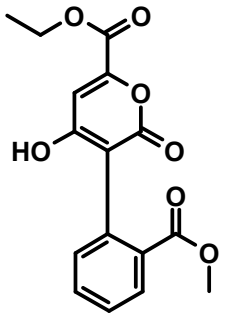
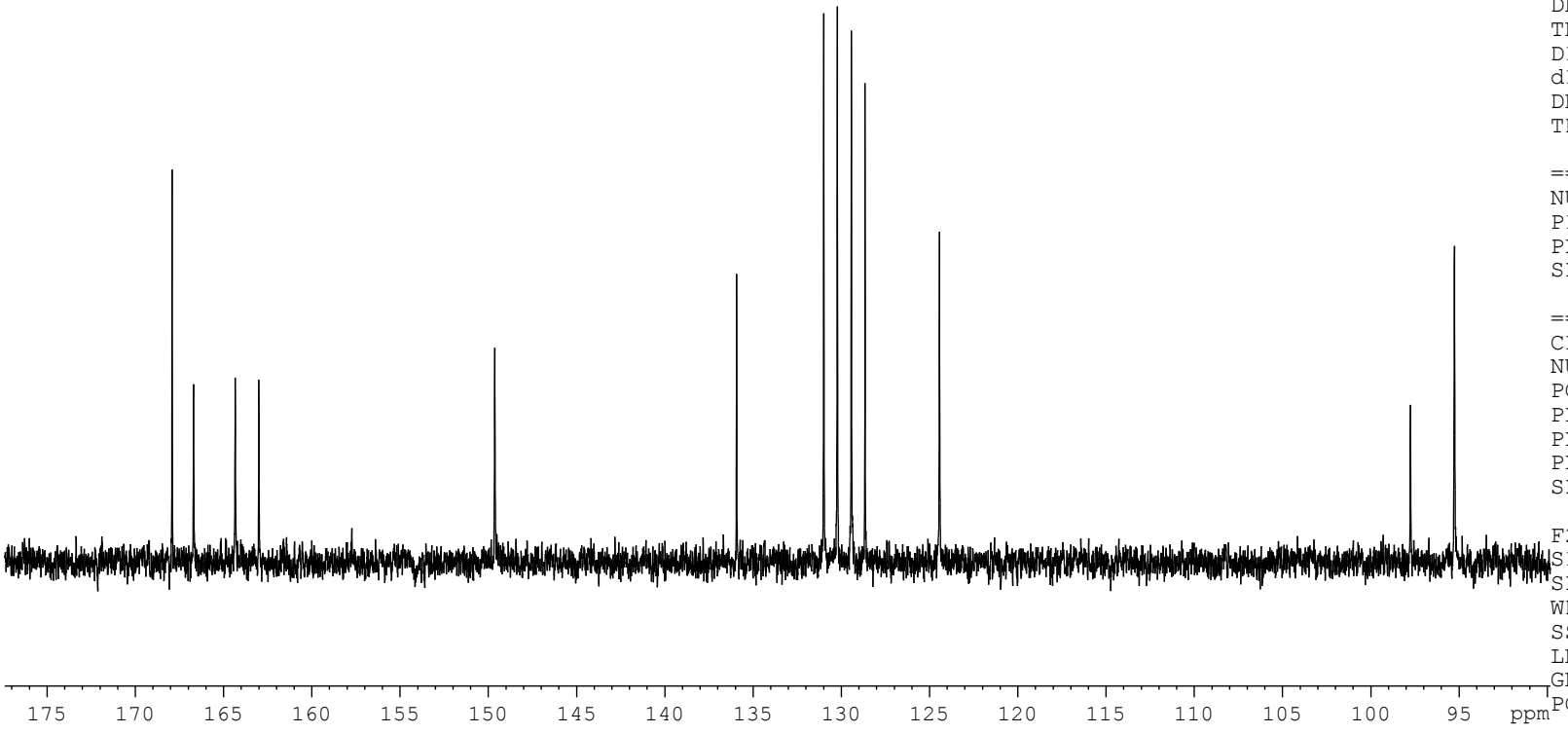
GRD100Q

167.93
166.69
164.33
162.99
149.62
135.94
131.00
130.23
129.43
128.66
124.44
97.75
95.28



Molecular Weight =290.28
Molecular Formula =C16H14O6



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AVANCE II 400 NMR
Spectrometer
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Current Data Parameters
NAME Mar15-2014
EXPNO 110
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140315
Time 22.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 1030
DW 16.800 usec
DE 6.00 usec
TE 298.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

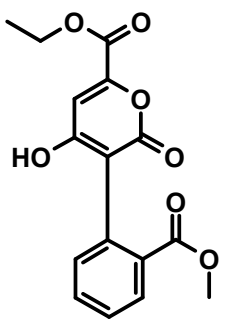
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

avtar saifpu@yahoo.co.in

GRD100Q

BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh



Molecular Weight =290.28
Molecular Formula =C16H14O6

Current Data Parameters
NAME Mar15-2014
EXPNO 110
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140315
Time 22.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 1030
DW 16.800 usec
DE 6.00 usec
TE 298.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

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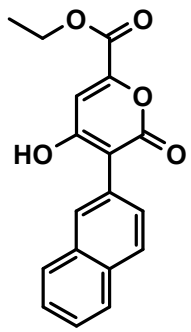
avtar_saifpu@yahoo.co.in



Molecular Weight =310.31
Molecular Formula =C18H14O5

GRD100N

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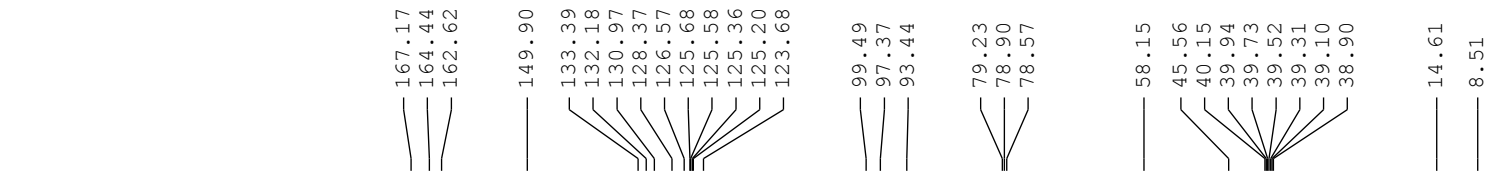

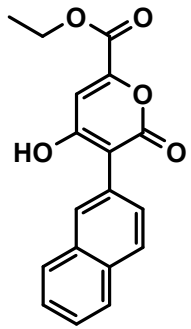

Molecular Weight =310.31
Molecular Formula =C18H14O5

Current Data Parameters
NAME Mar15-2014
EXPNO 90
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140315
Time 20.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 36
DW 16.800 usec
DE 6.00 usec
TE 298.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

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GRD100 M

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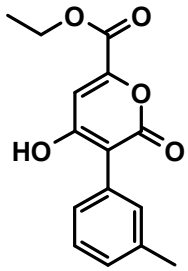
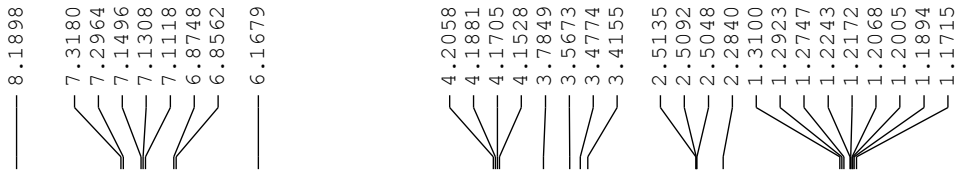
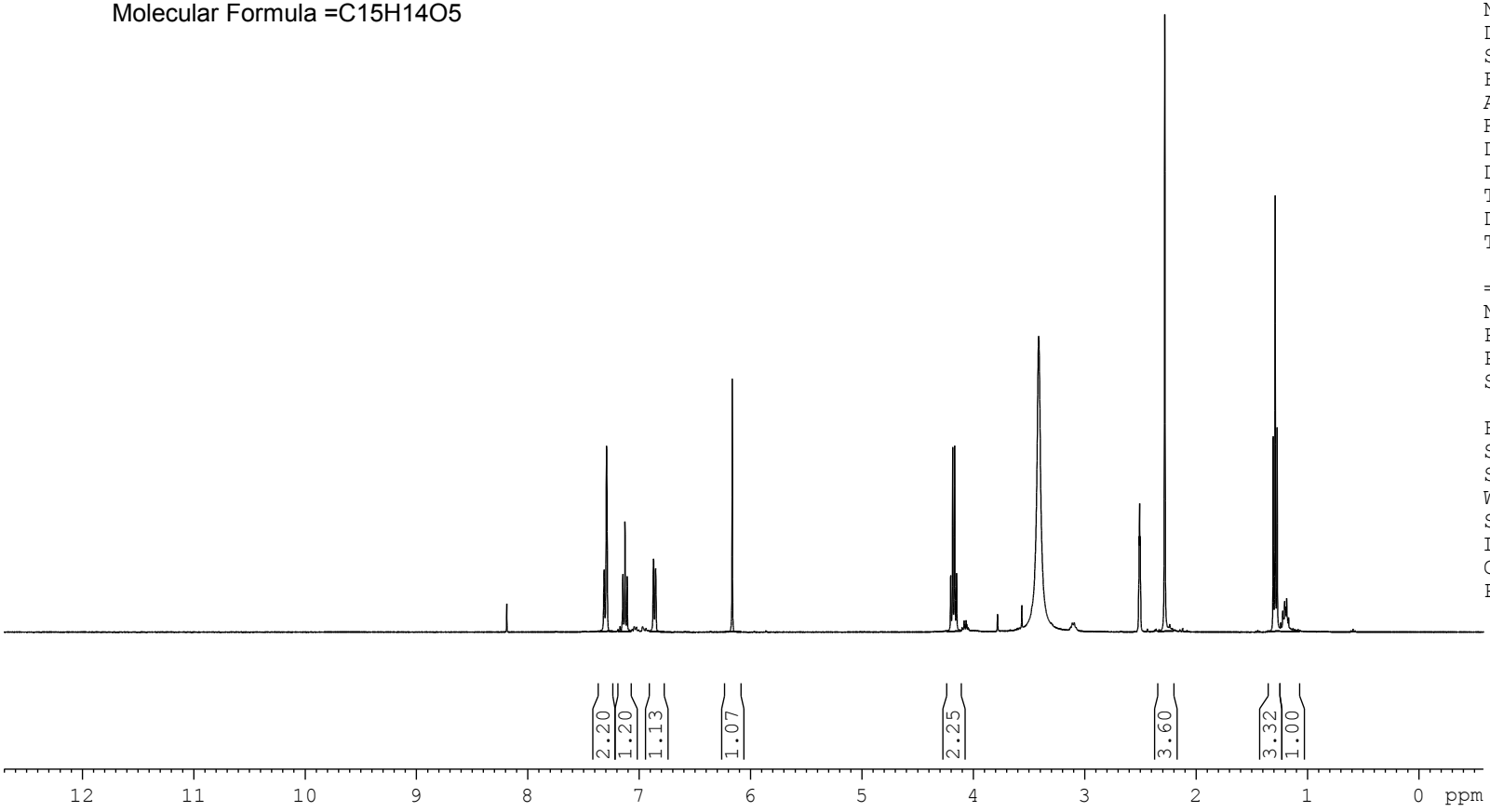


Molecular Weight =274.28
Molecular Formula =C15H14O5





Current Data Parameters
NAME Jan01-2014
EXPNO 80
PROCNO 1

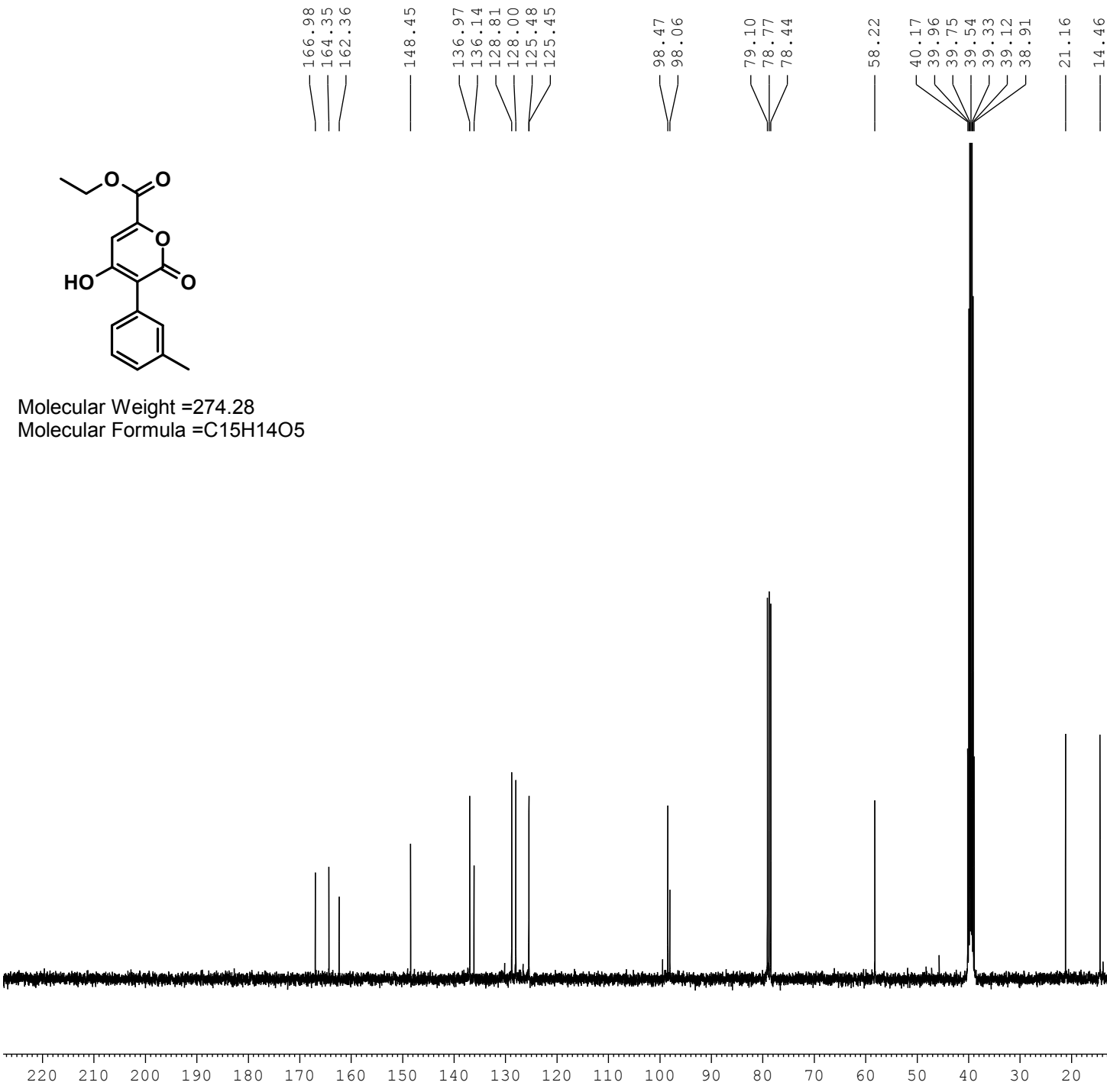
F2 - Acquisition Parameters
Date_ 20140101
Time 11.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 228
DW 41.600 usec
DE 6.00 usec
TE 294.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

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

avtar saifpu@yahoo.co.in

GRD100M



Molecular Weight =274.28
Molecular Formula =C15H14O5

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Current Data Parameters	
NAME	Mar15-2014
EXPNO	80
PROCNO	1
F2 - Acquisition Parameters	
Date_	20140315
Time	20.27
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	512
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	36
DW	16.800 usec
DE	6.00 usec
TE	298.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.60 usec
PL1	-2.00 dB
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	14.31 dB
PL13	18.00 dB
SFO2	400.1316005 MHz
F2 - Processing parameters	
SI	32768
SF	100.6128193 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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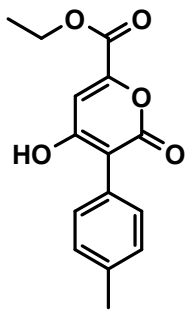
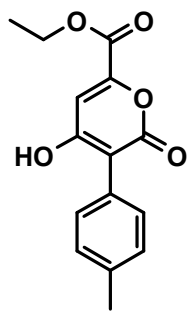


Molecular Weight =274.28
Molecular Formula =C15H14O5

GRD100K



Molecular Weight =274.28
Molecular Formula =C15H14O5

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Current Data Parameters	
NAME	Mar15-2014
EXPNO	60
PROCNO	1
F2 - Acquisition Parameters	
Date_	20140315
Time	19.22
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	512
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	36
DW	16.800 usec
DE	6.00 usec
TE	298.3 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.60 usec
PL1	-2.00 dB
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	14.31 dB
PL13	18.00 dB
SFO2	400.1316005 MHz
F2 - Processing parameters	
SI	32768
SF	100.6128193 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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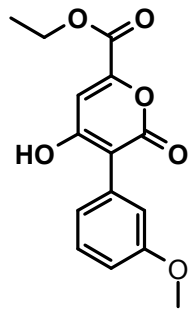
GRD100 L



Molecular Weight =290.28
Molecular Formula =C15H14O6

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Current Data Parameters	
NAME	Jan01-2014
EXPNO	70
PROCNO	1

F2 - Acquisition Parameters	
Date_	20140101
Time	11.14
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	8
DS	2
SWH	12019.230 Hz
FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	228
DW	41.600 usec
DE	6.00 usec
TE	294.2 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========	
NUC1	1H
P1	10.90 usec
PL1	-3.00 dB
SFO1	400.1324710 MHz

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

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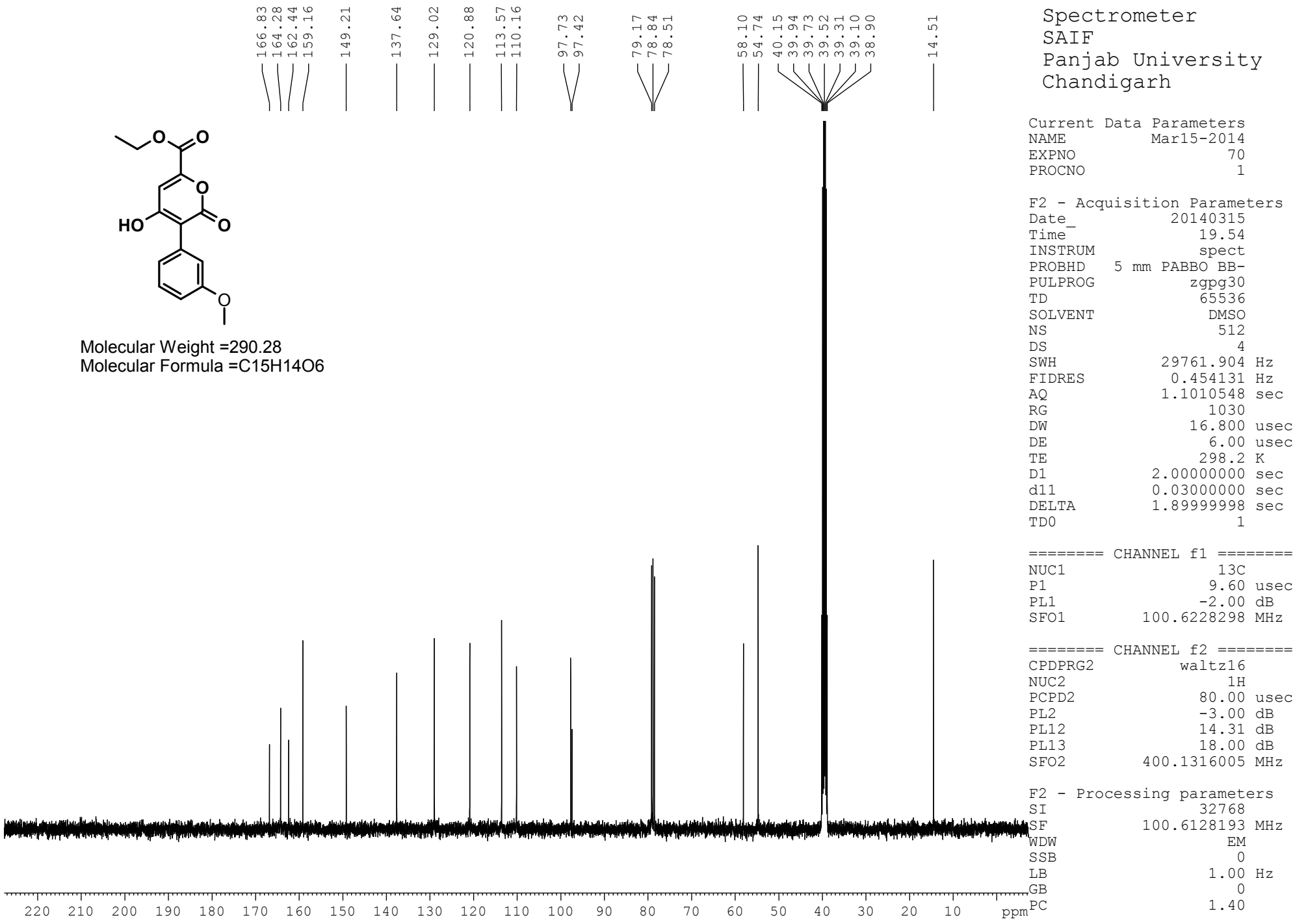
GRD100L



Molecular Weight =290.28
Molecular Formula =C15H14O6

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Spectrometer
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Current Data Parameters	
NAME	Mar15-2014
EXPNO	70
PROCNO	1
F2 - Acquisition Parameters	
Date_	20140315
Time	19.54
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	512
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	1030
DW	16.800 usec
DE	6.00 usec
TE	298.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.60 usec
PL1	-2.00 dB
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	14.31 dB
PL13	18.00 dB
SFO2	400.1316005 MHz
F2 - Processing parameters	
SI	32768
SF	100.6128193 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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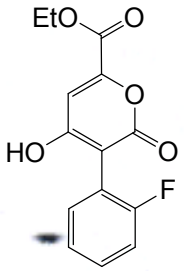
Elemental Composition Report



Molecular Formula =C14H11FO5

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

21 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

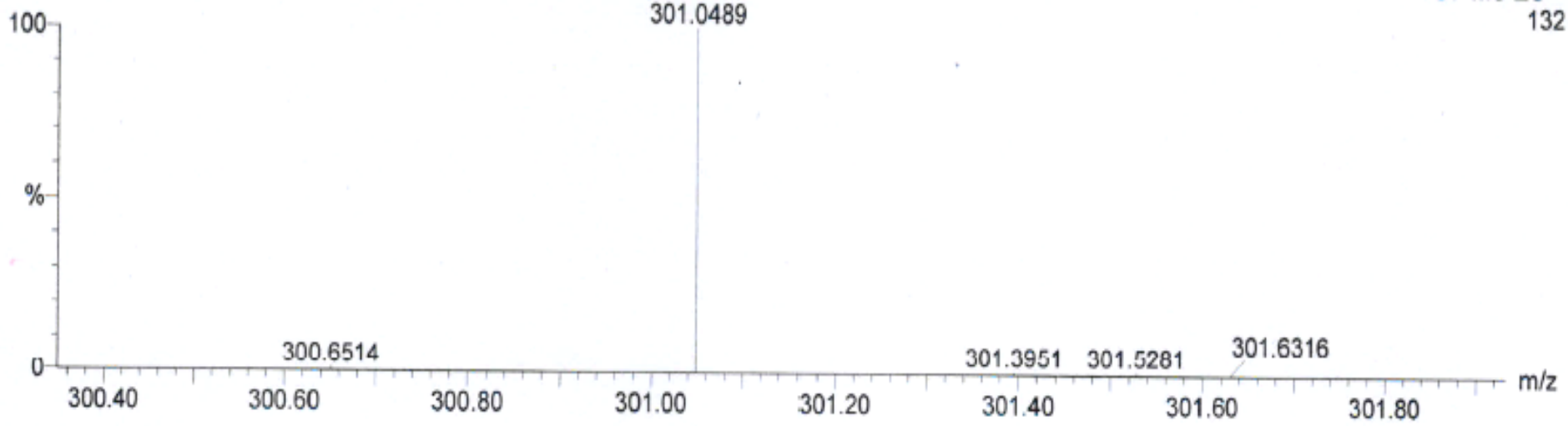
Elements Used:

C: 0-14 H: 0-11 O: 0-5 F: 0-1 Na: 0-1

EXT-GRD100I DEPARTMENT OF CHEMISTRY IITM 16:51:2823-Aug-2014

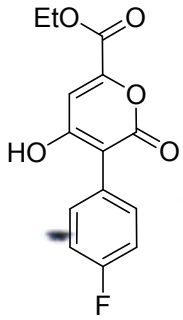
EXT-GRD100I 96 (0.974) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x4.00) TOF MS ES+

132



Minimum:				-1.5	
Maximum:		5.0	10.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	Formula
301.0489	301.0488	0.1	0.3	8.5	C14 H11 O5 F Na

Elemental Composition Report



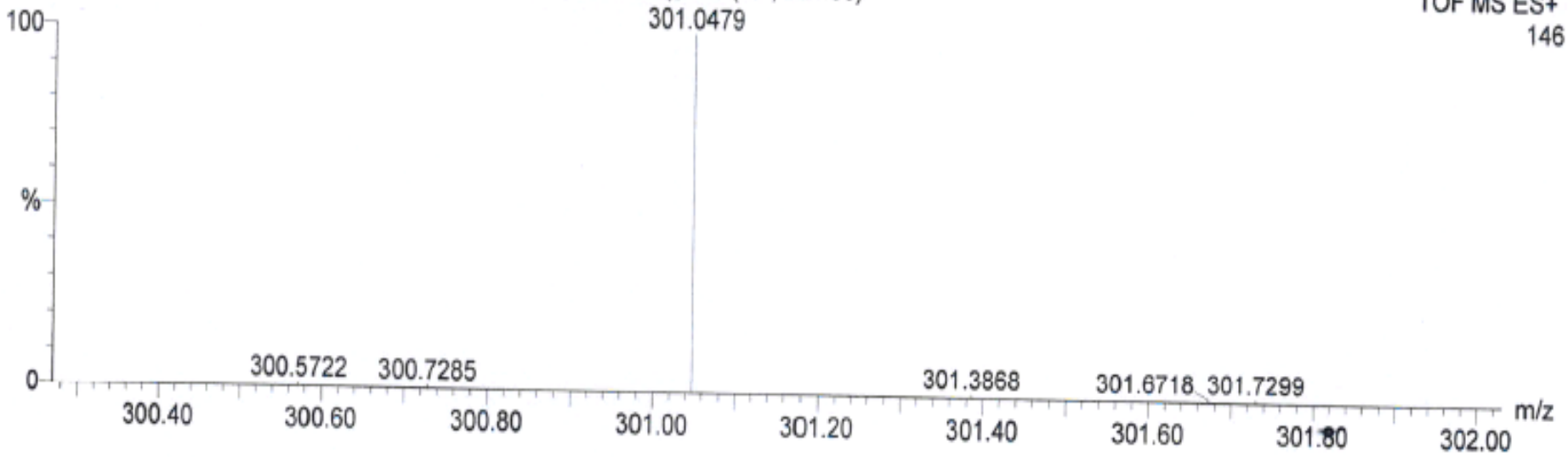
Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Selected filters: None

Molecular Formula =C14H11FO5

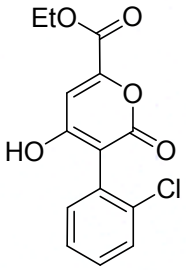
Monoisotopic Mass, Odd and Even Electron Ions
21 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-14 H: 0-11 O: 0-5 F: 0-1 Na: 0-1

EXT-GRD100J
DEPARTMENT OF CHEMISTRY IITM
EXT-GRD100J 7 (0.071) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x4.00)
16:54:4223-Aug-2014
TOF MS ES+
146



Minimum:				-1.5	
Maximum:		5.0	10.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	Formula
301.0479	301.0488	-0.9	-3.0	8.5	C14 H11 O5 F Na

Elemental Composition Report



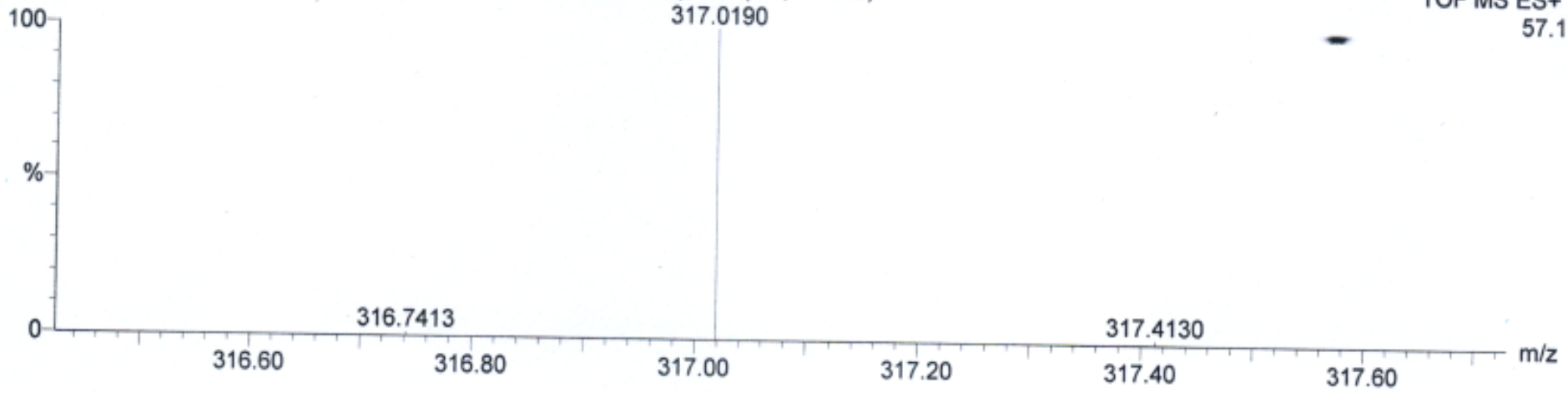
Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Selected filters: None

$C_{14}H_{11}ClO_5$

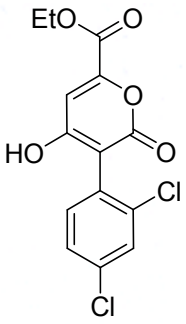
Monoisotopic Mass, Odd and Even Electron Ions
22 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-14 H: 0-11 O: 0-5 Na: 0-1 Cl: 0-1

EXT-GRD100E
DEPARTMENT OF CHEMISTRY IITM
EXT_GRD100E 2 (0.021) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x4.00)
16:28:5323-Aug-2014
TOF MS ES+
57.1



Minimum:				-1.5	
Maximum:		5.0	10.0	50.0	
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**Formula**
317.0190	317.0193	-0.3	-0.9	8.5	C14 H11 O5 Na Cl

Elemental Composition Report



$C_{14}H_{10}Cl_2O_5$

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

17 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

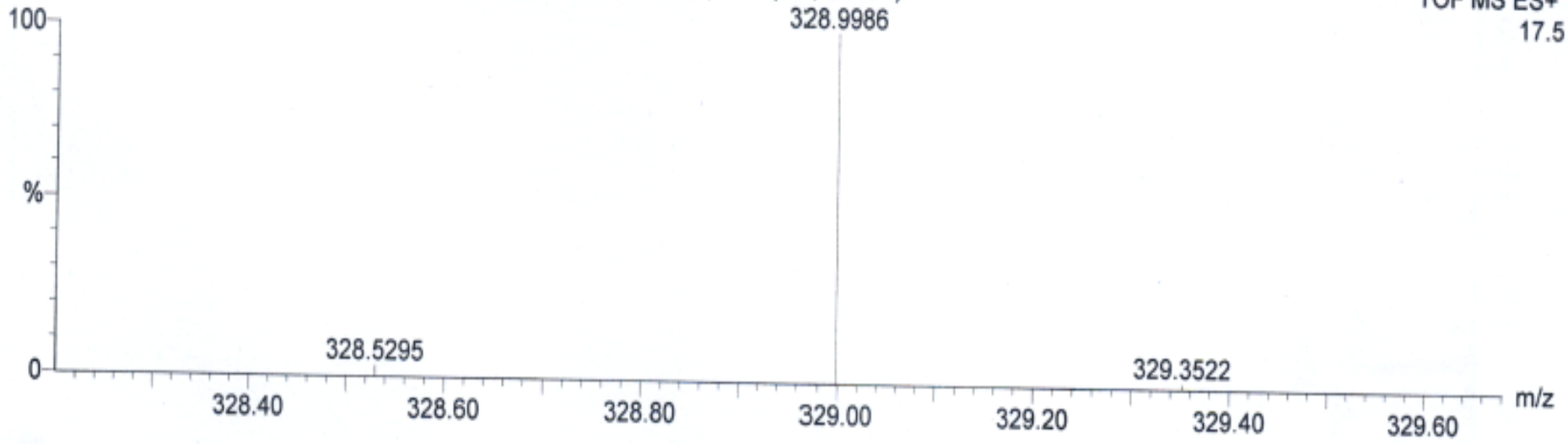
Elements Used:

C: 0-14 H: 0-11 O: 0-5 Cl: 0-2

EXT-GRD-100D DEPARTMENT OF CHEMISTRY IITM

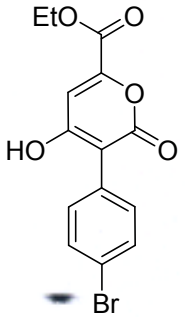
EXT-GRD-100D 190 (1.945) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x4.00)

16:58:4819-Aug-2014
TOF MS ES+
17.5



Minimum:				-1.5	
Maximum:		5.0	10.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	Formula
328.9986	328.9984	0.2	0.6	8.5	C14 H11 O5 Cl2

Elemental Composition Report



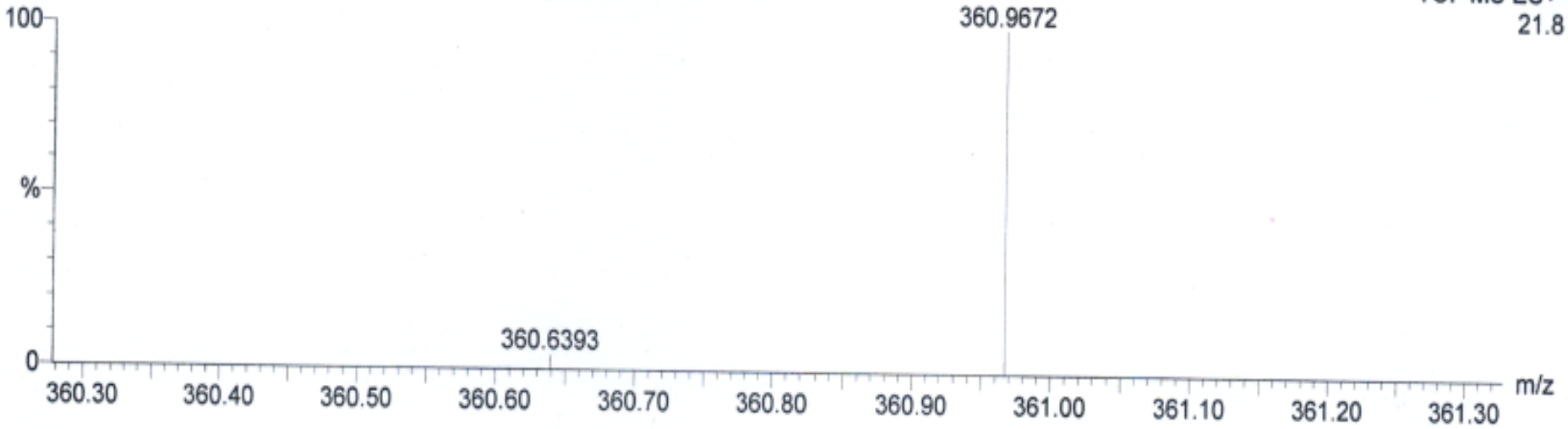
$C_{14}H_{11}BrO_5$

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Selected filters: None

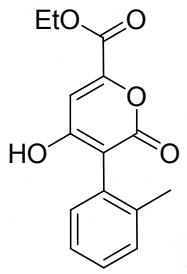
Monoisotopic Mass, Odd and Even Electron Ions
22 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-14 H: 0-11 O: 0-5 Na: 0-1 Br: 0-1

EXT-GRD100F DEPARTMENT OF CHEMISTRY IITM 16:40:2523-Aug-2014
EXT_GRD100F 12 (0.121) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x4.00) TOF MS ES+
21.8



Minimum:				-1.5	
Maximum:		5.0	10.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	Formula
360.9672	360.9688	-1.6	-4.4	8.5	C14 H11 O5 Na Br

Elemental Composition Report



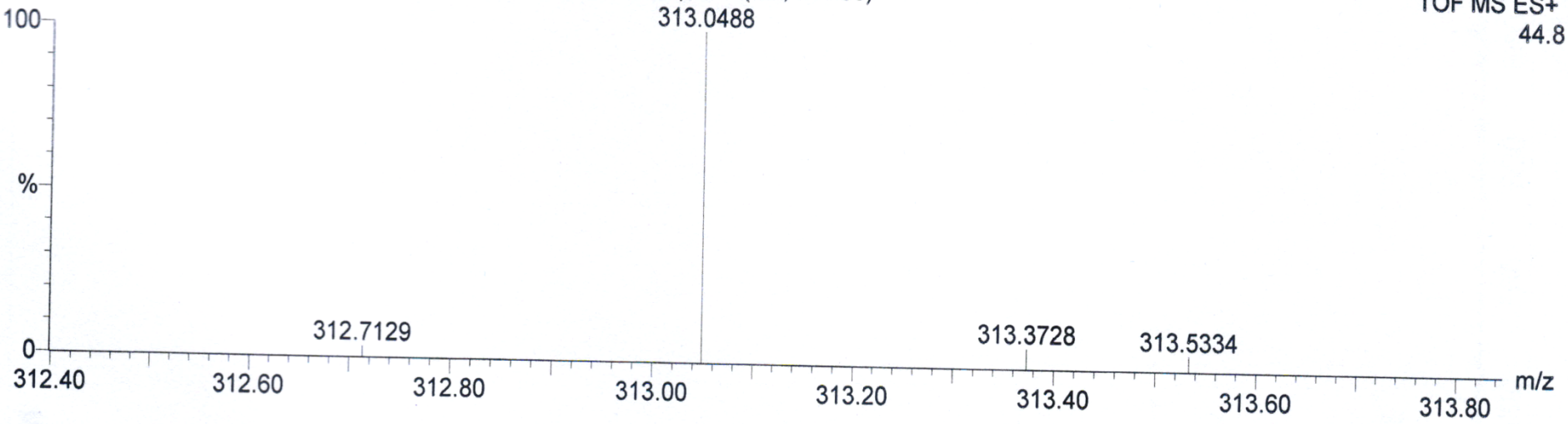
$C_{15}H_{14}O_5$

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Selected filters: None

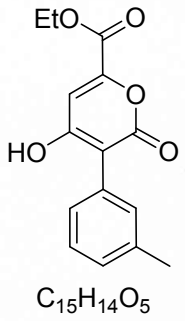
Monoisotopic Mass, Odd and Even Electron Ions
11 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-15 H: 0-14 O: 0-5 K: 0-1

EXT-GRD-100C
DEPARTMENT OF CHEMISTRY IITM
EXT-GRD-100C 1 (0.010) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x4.00)
16:49:3719-Aug-2014
TOF MS ES+
44.8



Minimum:				-1.5	
Maximum:		5.0	10.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	Formula
313.0488	313.0478	1.0	3.2	8.5	C15 H14 O5 K

Elemental Composition Report

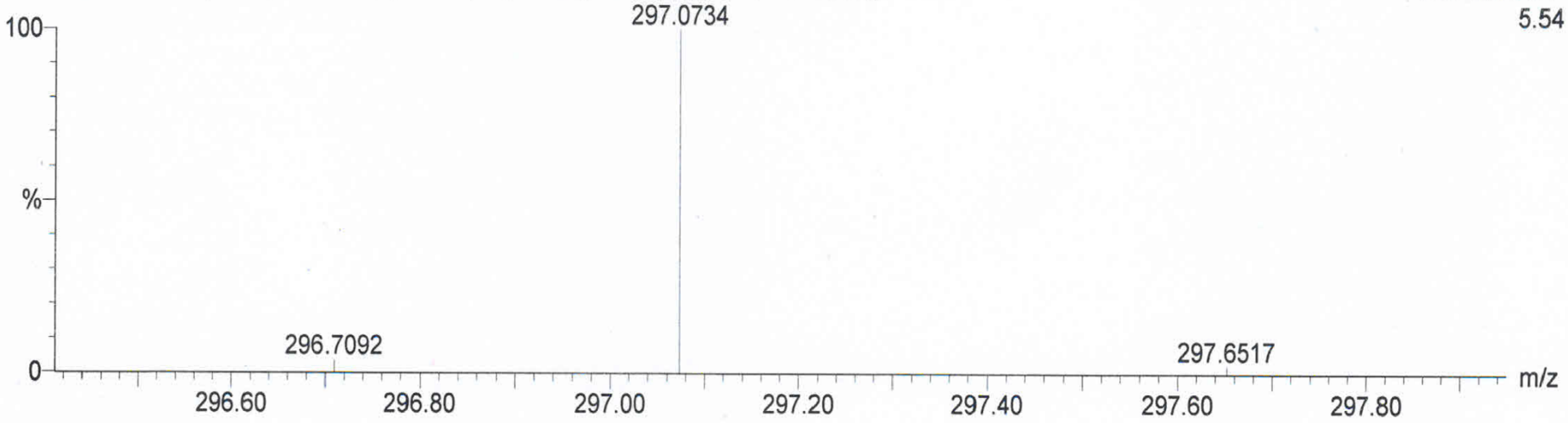


Single Mass Analysis

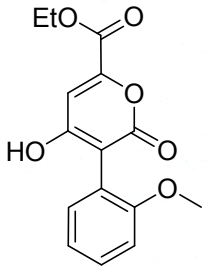
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
10 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-15 H: 0-15 O: 0-5 Na: 0-1

EXT-GRD100M DEPARTMENT OF CHEMISTRY IITM 17:02:4308-Aug-2014
EXT-GRD100M 10 (0.103) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x4.00) TOF MS ES+
5.54



Minimum:				-1.5	
Maximum:		5.0	10.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	Formula
297.0734	297.0739	-0.5	-1.7	8.5	C15 H14 O5 Na



$C_{15}H_{14}O_6$

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-15 H: 0-14 O: 0-6 K: 0-1

EXT-GRD-100P

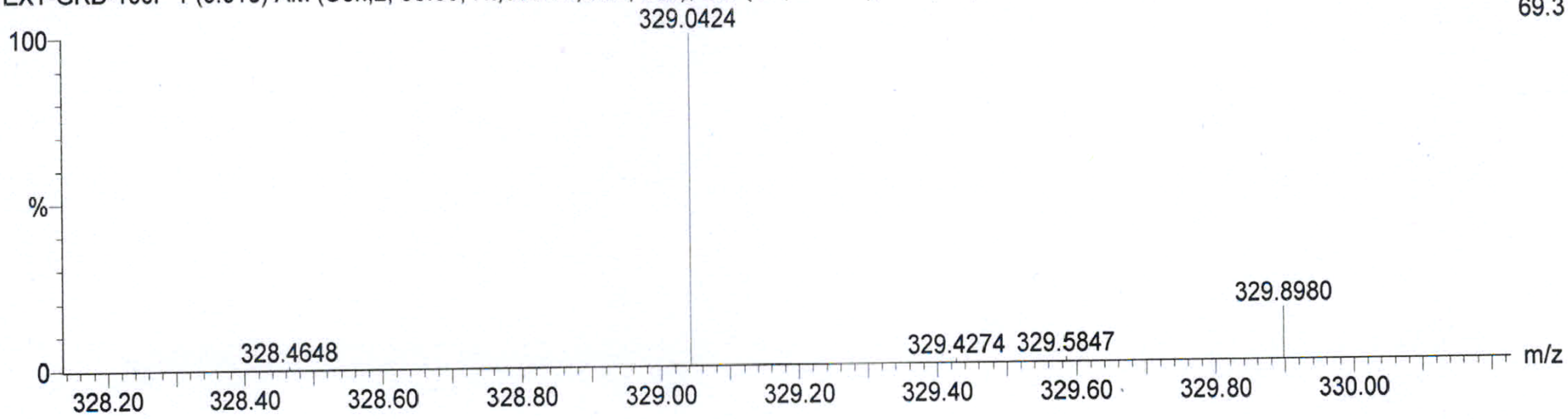
DEPARTMENT OF CHEMISTRY IITM

17:33:2013-Aug-2014

EXT-GRD-100P 1 (0.010) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x4.00); Cm (1:2)

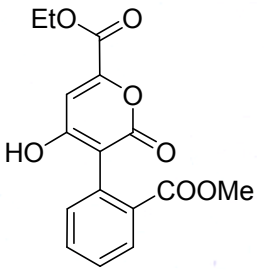
TOF MS ES+

69.3



Minimum:				-1.5	
Maximum:		5.0	10.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	Formula
329.0424	329.0427	-0.3	-0.9	8.5	C15 H14 O6 K

Elemental Composition Report



$C_{16}H_{14}O_7$

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

14 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

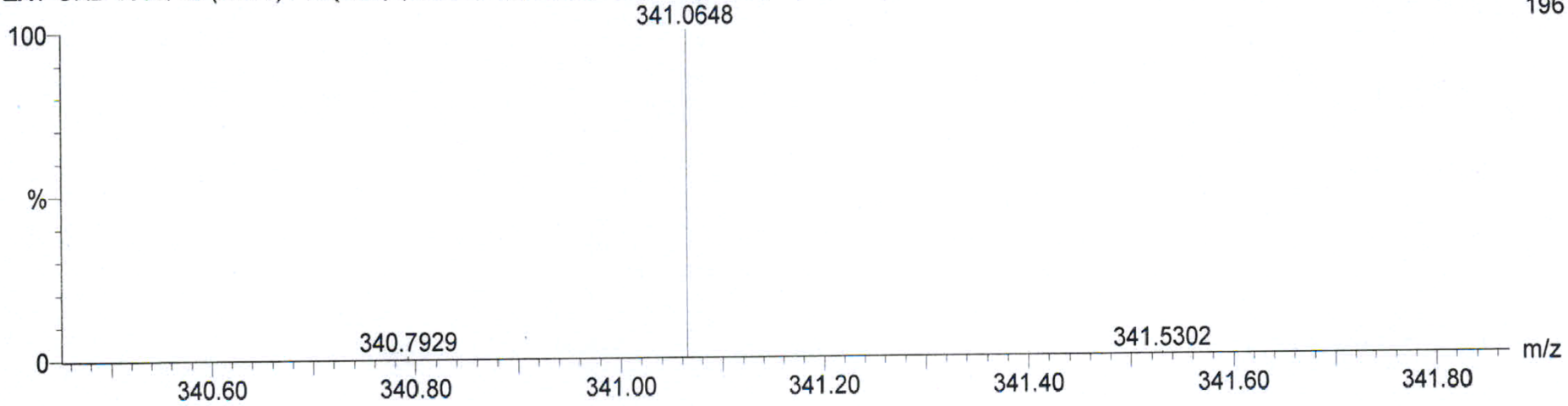
Elements Used:

C: 0-16 H: 0-14 O: 0-7 Na: 0-1

EXT-GRD-100Q DEPARTMENT OF CHEMISTRY IITM 17:37:3613-Aug-2014

EXT-GRD-100Q 38 (0.389) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x4.00) TOF MS ES+

196



Minimum:				-1.5	
Maximum:		5.0	10.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	Formula
341.0648	341.0637	1.1	3.2	9.5	C16 H14 O7 Na