

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

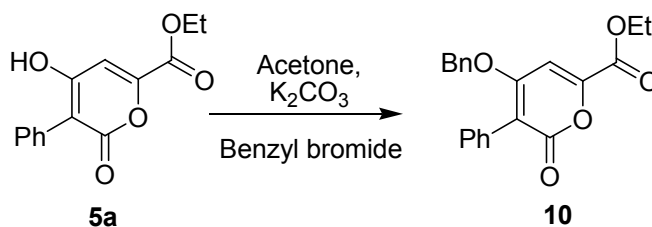
Ganesh Raosaheb Dhage^a, Shankar Thopate^{*a}, Shefali Ramteke^b, Prasad Kulkarni^b,

^aDepartment of Chemistry, Prof. John Barnabas Post Graduate School of Biological Studies, Ahmednagar College, Ahmednagar, Ahmednagar-414001, India.

^bBiometry and Nutrition Group, Agharkar Research Institute, Pune-411004, India.

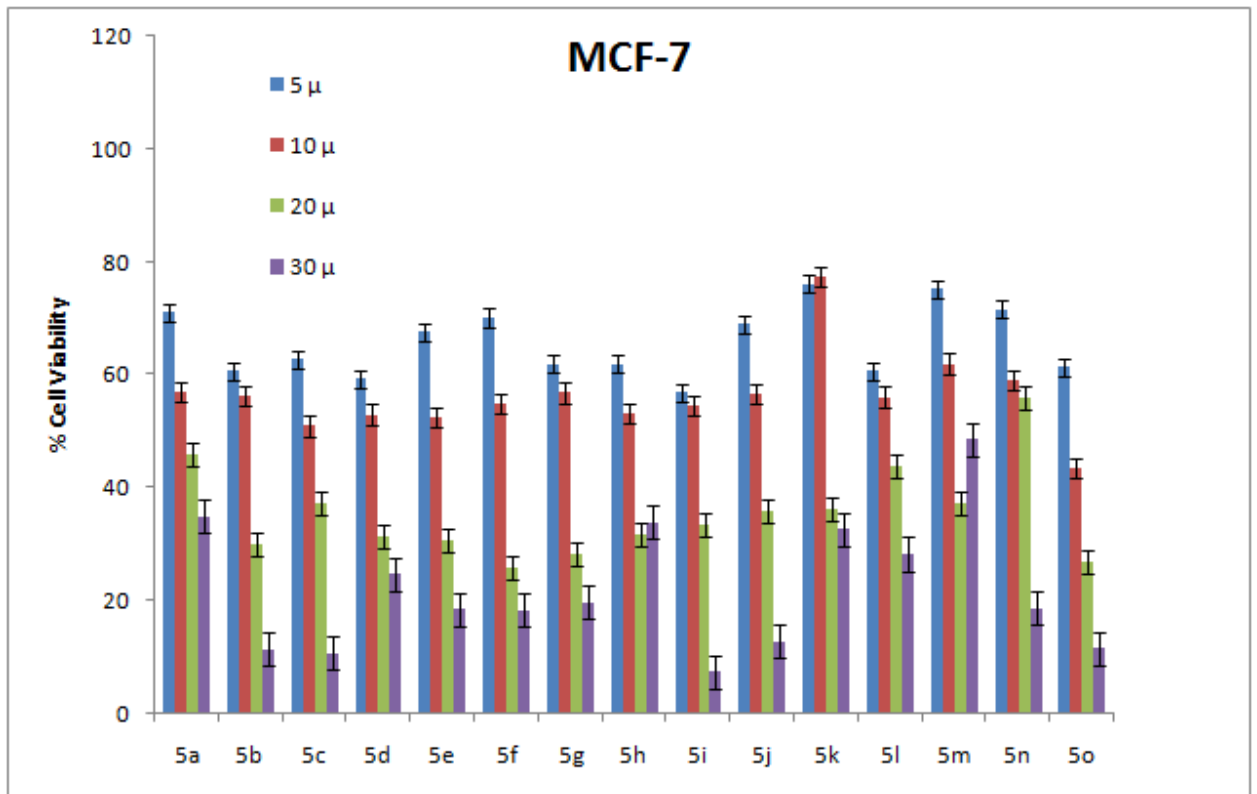
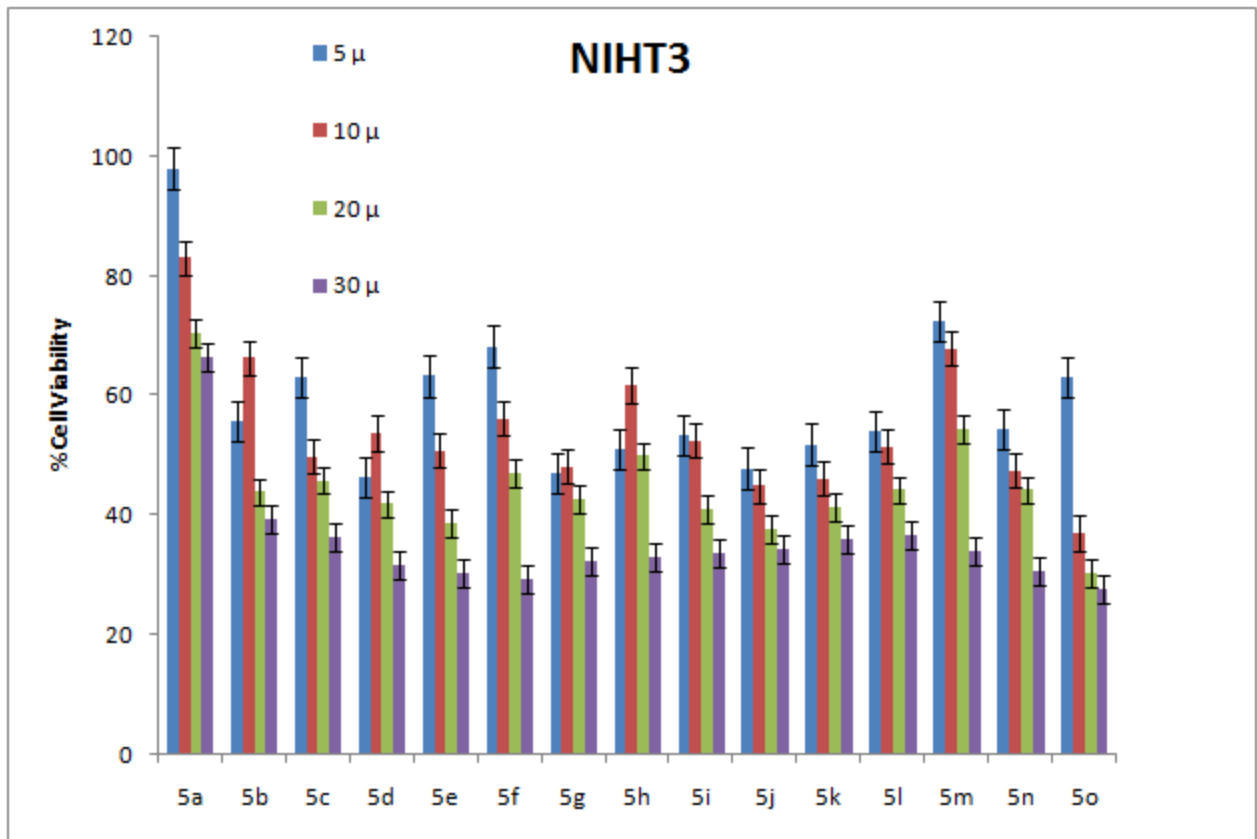
Synthesis of Ethyl 4-(benzyloxy)-6-oxo-5-phenyl-6H-pyran-2-carboxylate (**10**),

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 hexane to give **10** as bright yellow solid.



Bright yellow solid (**10**) ¹H NMR (400 MHz, CDCl₃) 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, -OCH₂Ph), 4.41 (q, 2H, -OCH₂), 1.42 (t, *J* = 7.12 Hz, 3H, -CH₃); ¹³C NMR (100 MHz, CDCl₃) 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 C₂₁H₁₇O₅ [M-H]⁻: 349.1071, found: 349.1078.

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



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

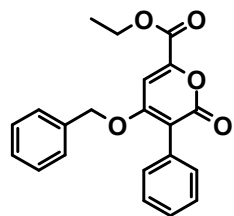
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 Panjab University
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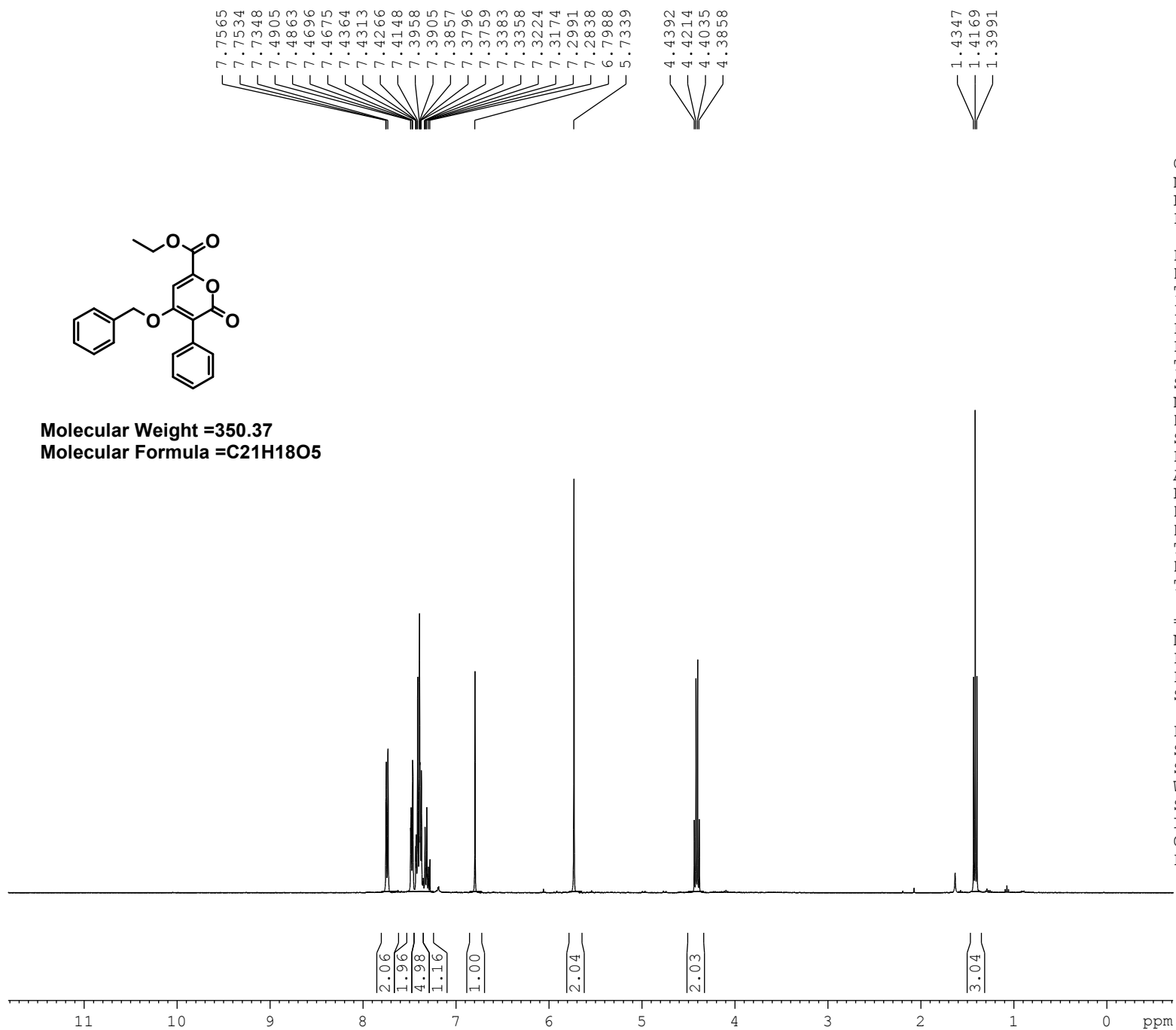
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 DE 6.00 usec
 TE 296.2 K
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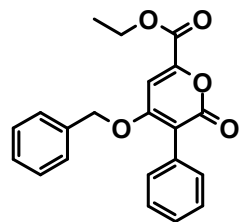
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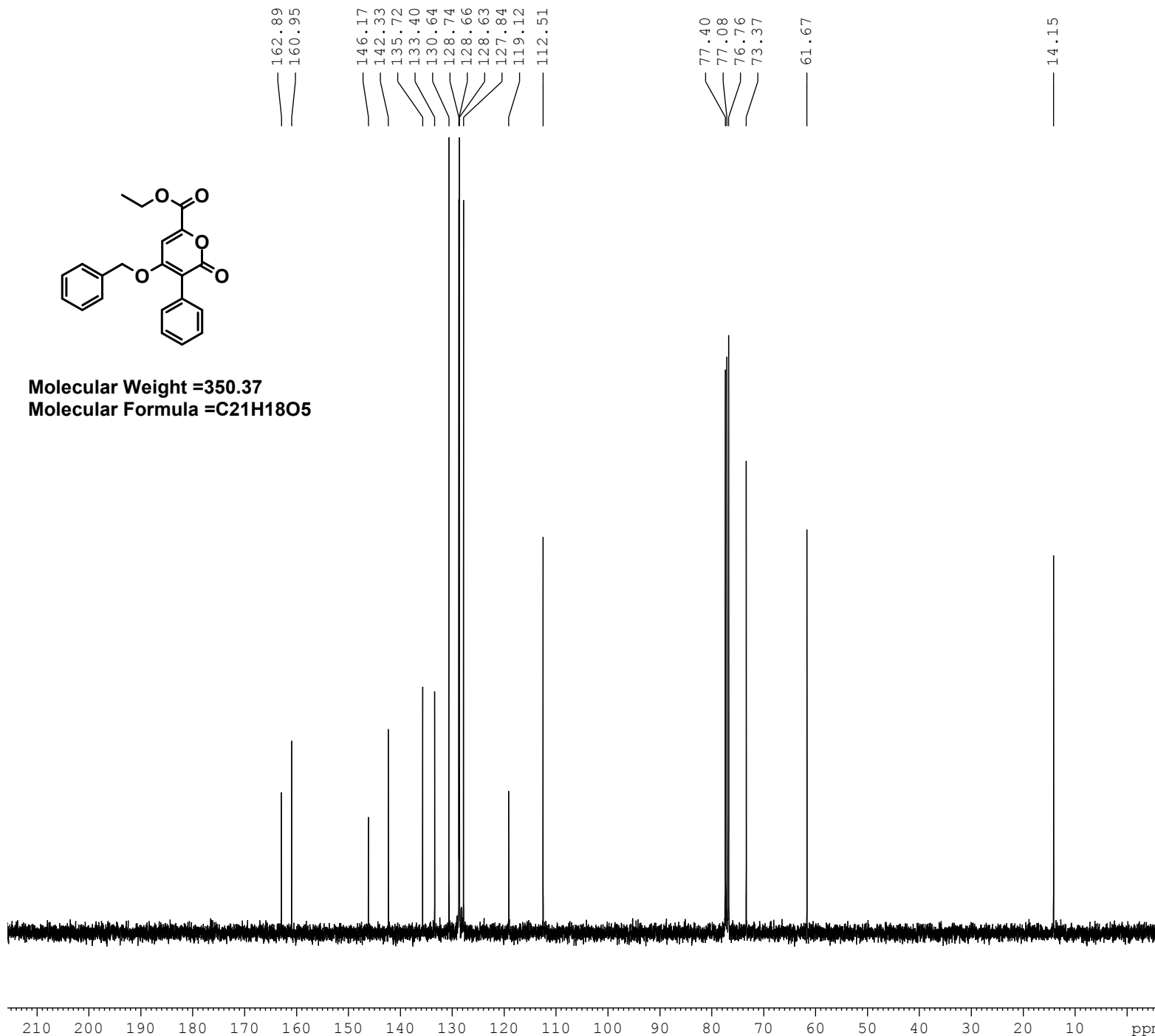
Molecular Weight =350.37
 Molecular Formula =C₂₁H₁₈O₅



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Molecular Weight =350.37
 Molecular Formula =C₂₁H₁₈O₅



Current Data Parameters
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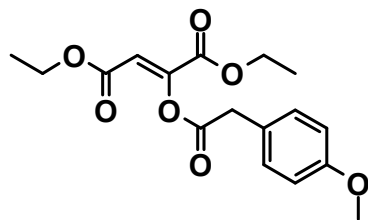
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 TD0 1

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Molecular Formula =C₁₇H₂₀O₇

7.2992
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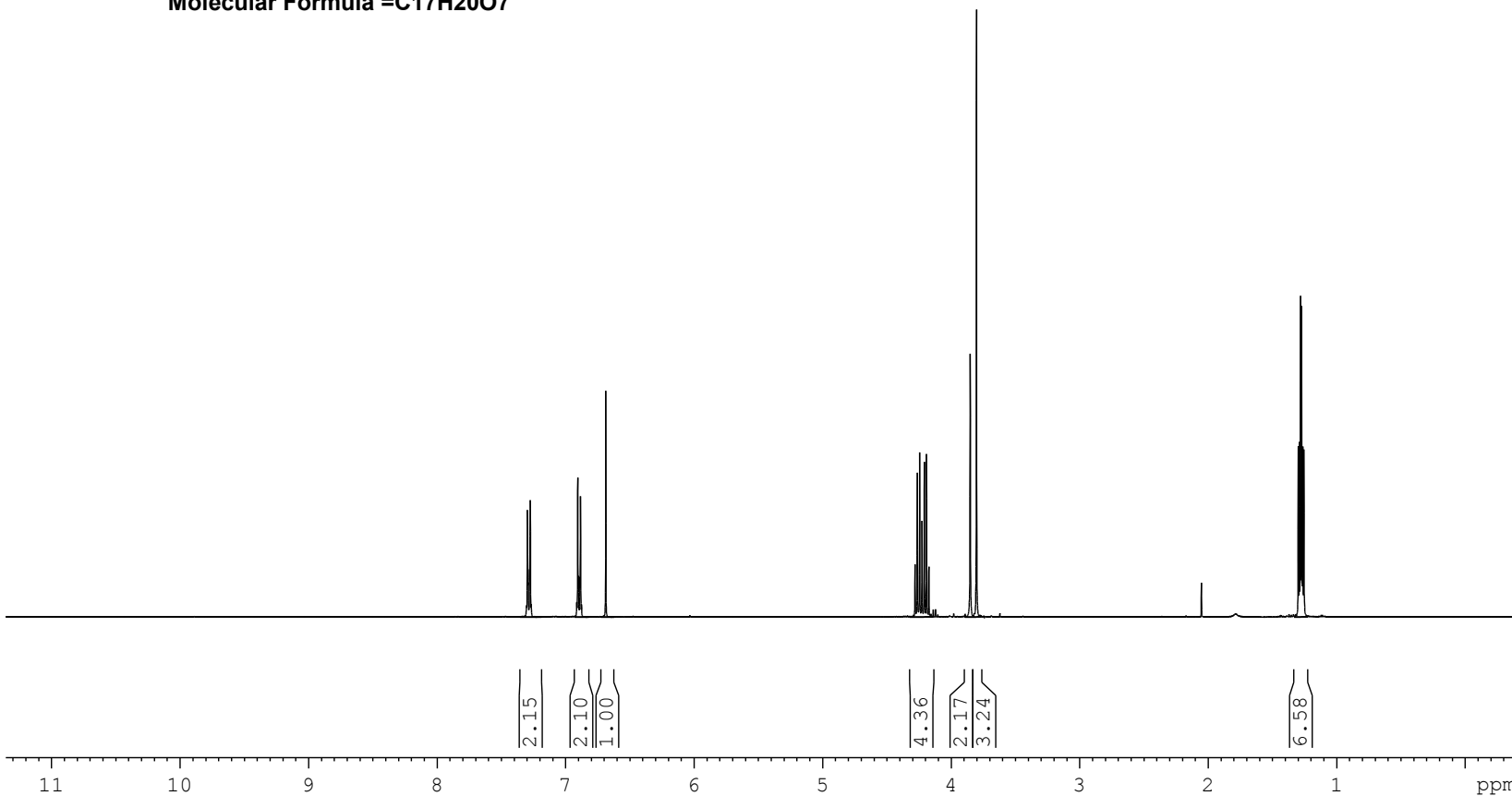
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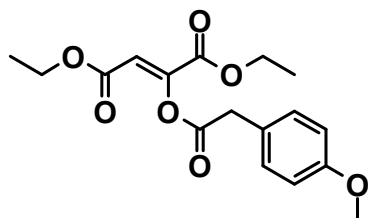
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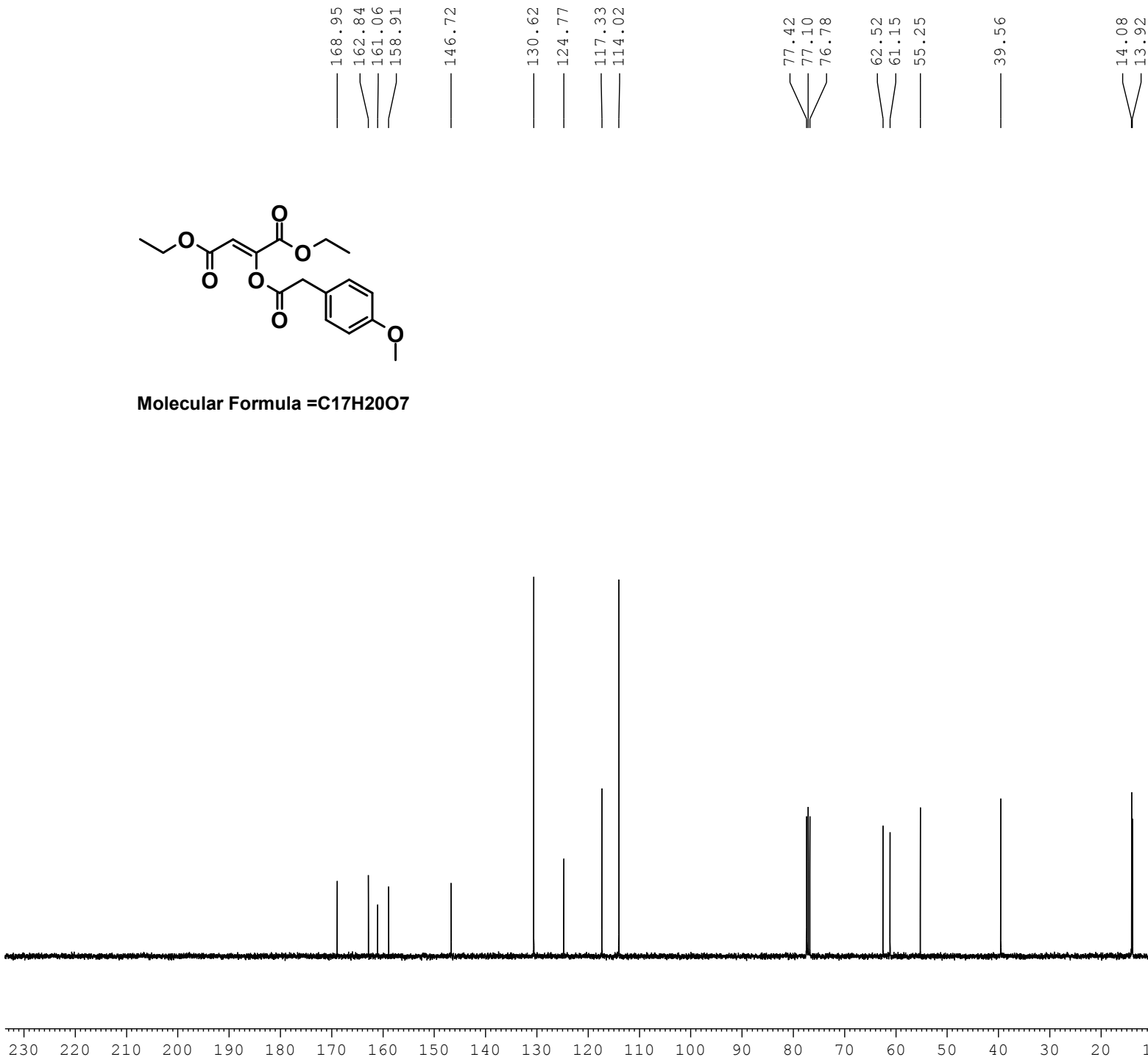
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==== CHANNEL f2 =====
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 PCPD2 80.00 usec
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 PL12 14.31 dB
 PL13 18.00 dB
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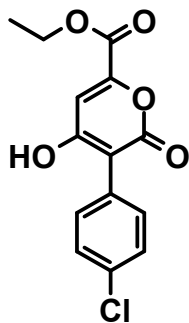
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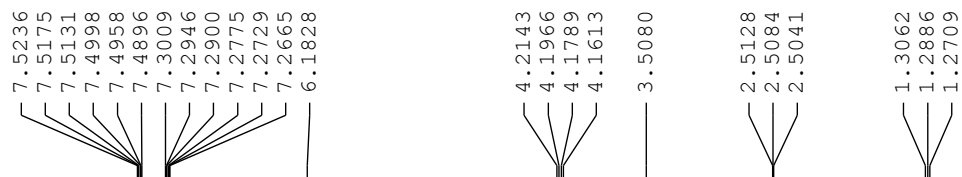
Molecular Formula =C₁₇H₂₀O₇



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Molecular Weight =294.69
 Molecular Formula =C₁₄H₁₁ClO₅

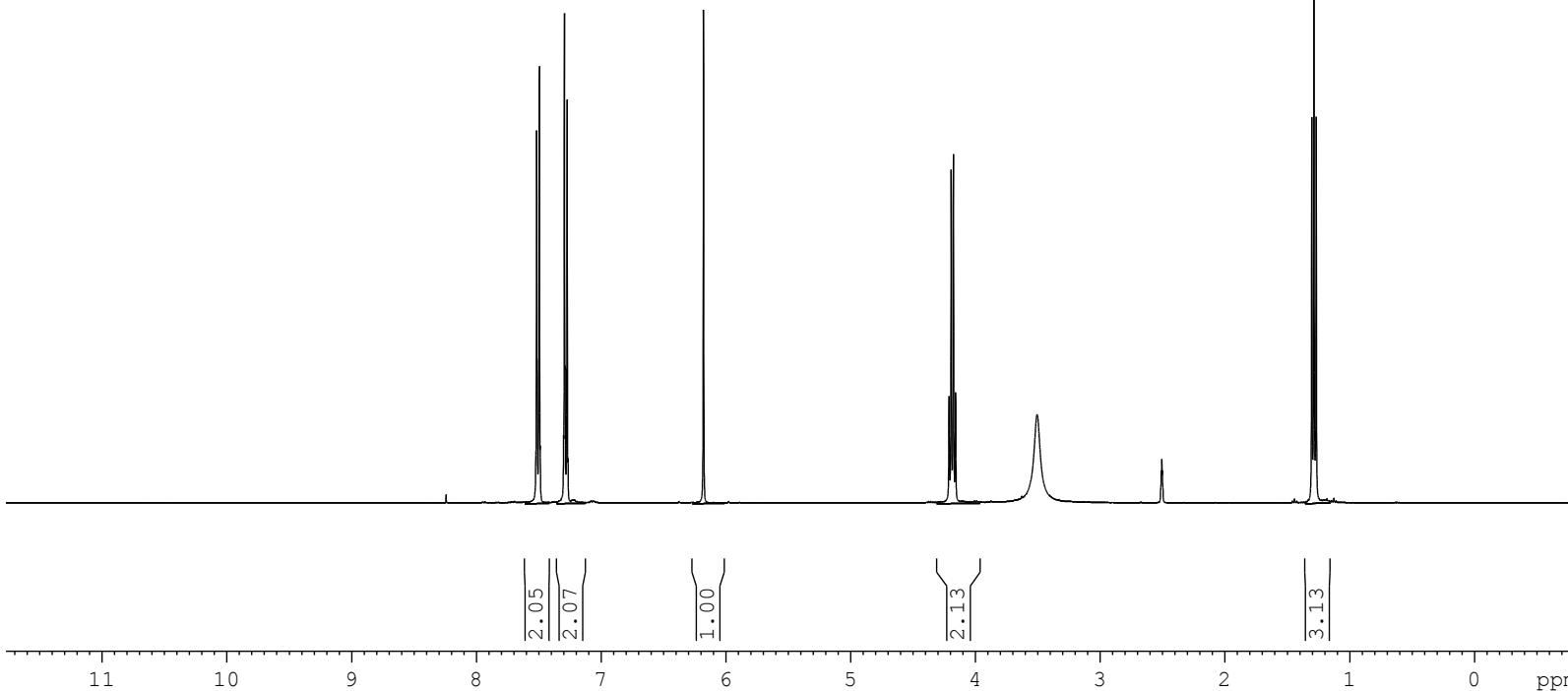


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 SOLVENT DMSO
 NS 8
 DS 2
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 FIDRES 0.183399 Hz
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 DE 6.00 usec
 TE 295.1 K
 D1 1.00000000 sec
 TD0 1

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 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
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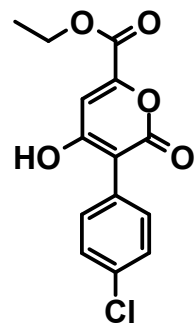
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 FIDRES 0.454131 Hz
 AQ 1.1010548 sec
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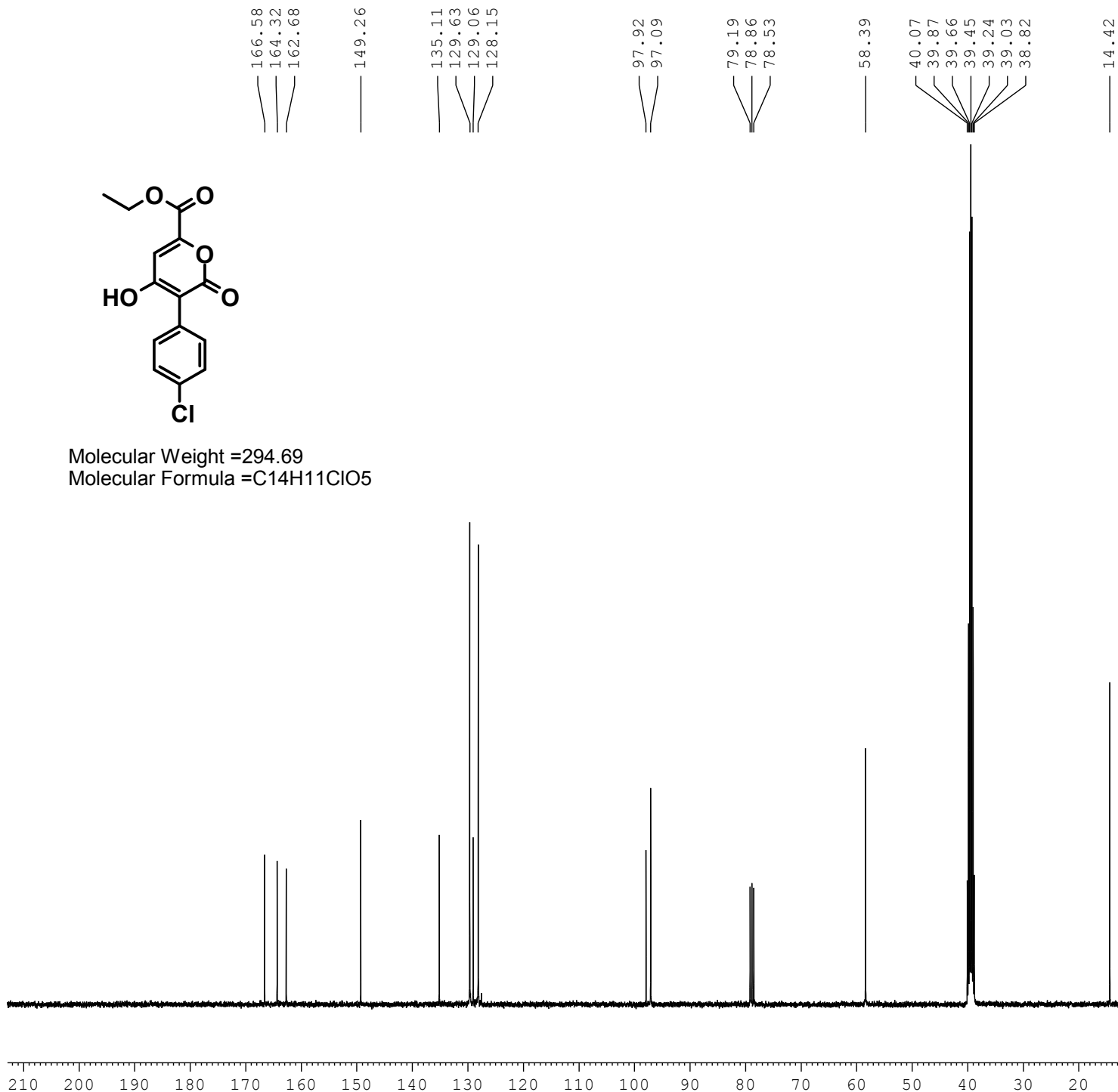
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==== CHANNEL f2 =====
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 PCPD2 80.00 usec
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 PL12 14.31 dB
 PL13 18.00 dB
 SFO2 400.1316005 MHz

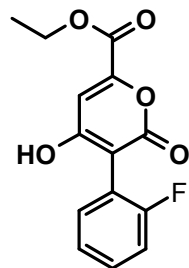
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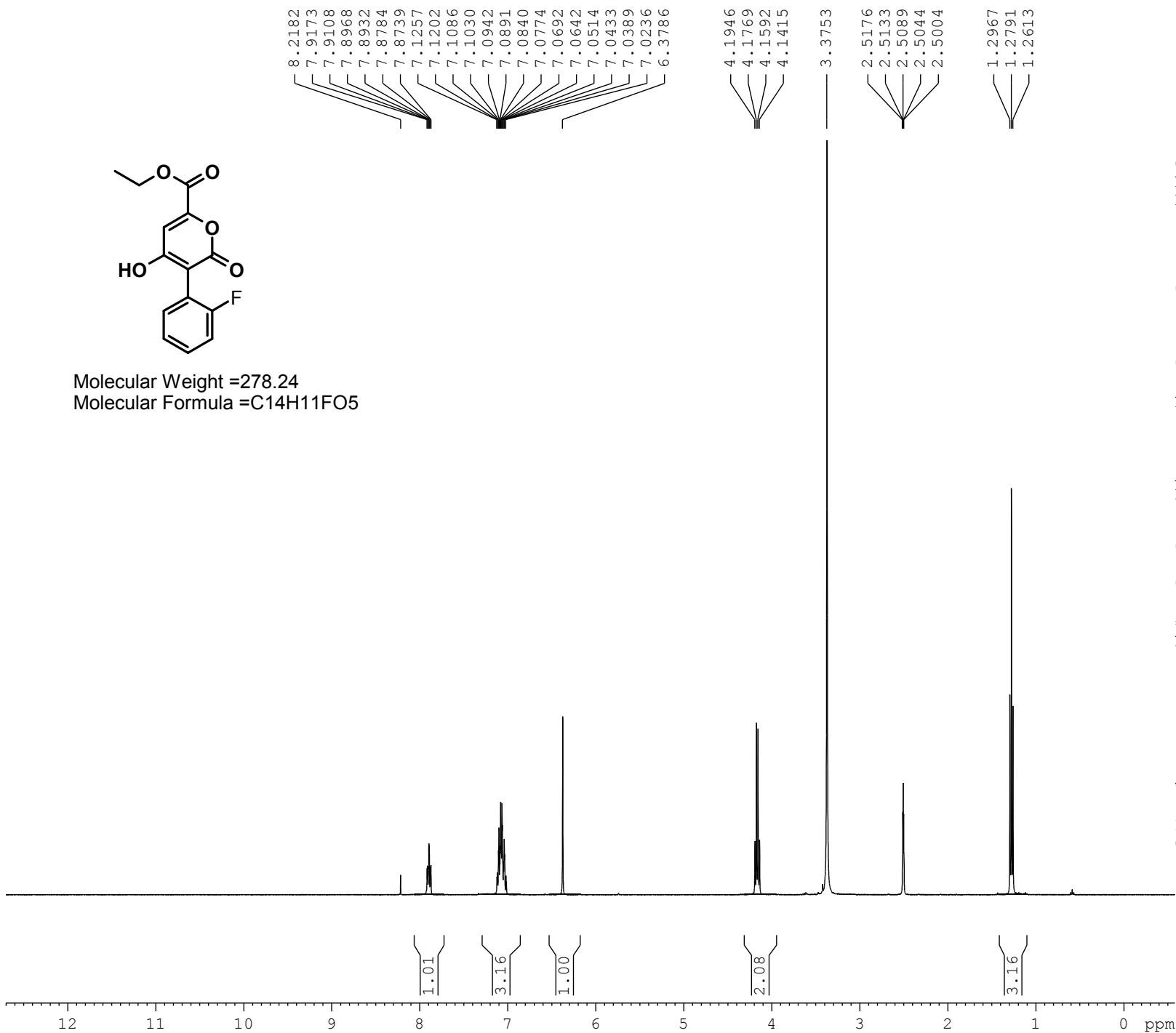
Molecular Weight =294.69
 Molecular Formula =C₁₄H₁₁ClO₅



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Molecular Weight =278.24
 Molecular Formula =C₁₄H₁₁FO₅



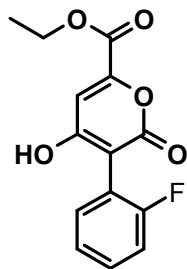
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 NS 8
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 FIDRES 0.183399 Hz
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 TE 294.2 K
 D1 1.00000000 sec
 TD0 1

==== 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
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 PC 1.00

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Molecular Weight =278.24
 Molecular Formula =C₁₄H₁₁FO₅



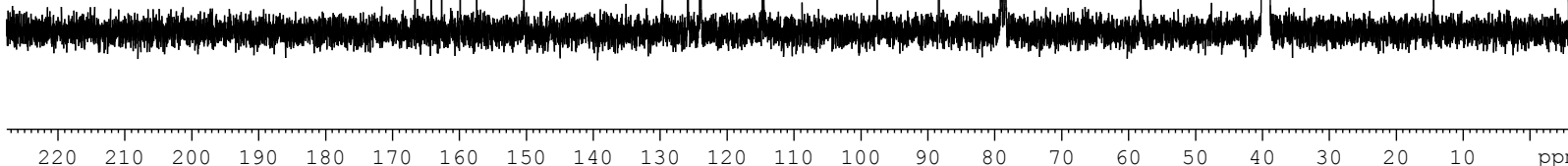
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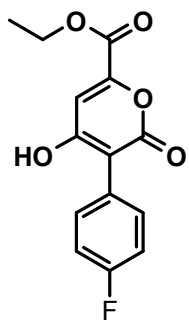
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 PL1 -2.00 dB
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==== CHANNEL f2 =====
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 NUC2 1H
 PCPD2 80.00 usec
 PL2 -3.00 dB
 PL12 14.31 dB
 PL13 18.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
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 LB 1.00 Hz
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 PC 1.40



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Molecular Weight =278.24
 Molecular Formula =C₁₄H₁₁FO₅

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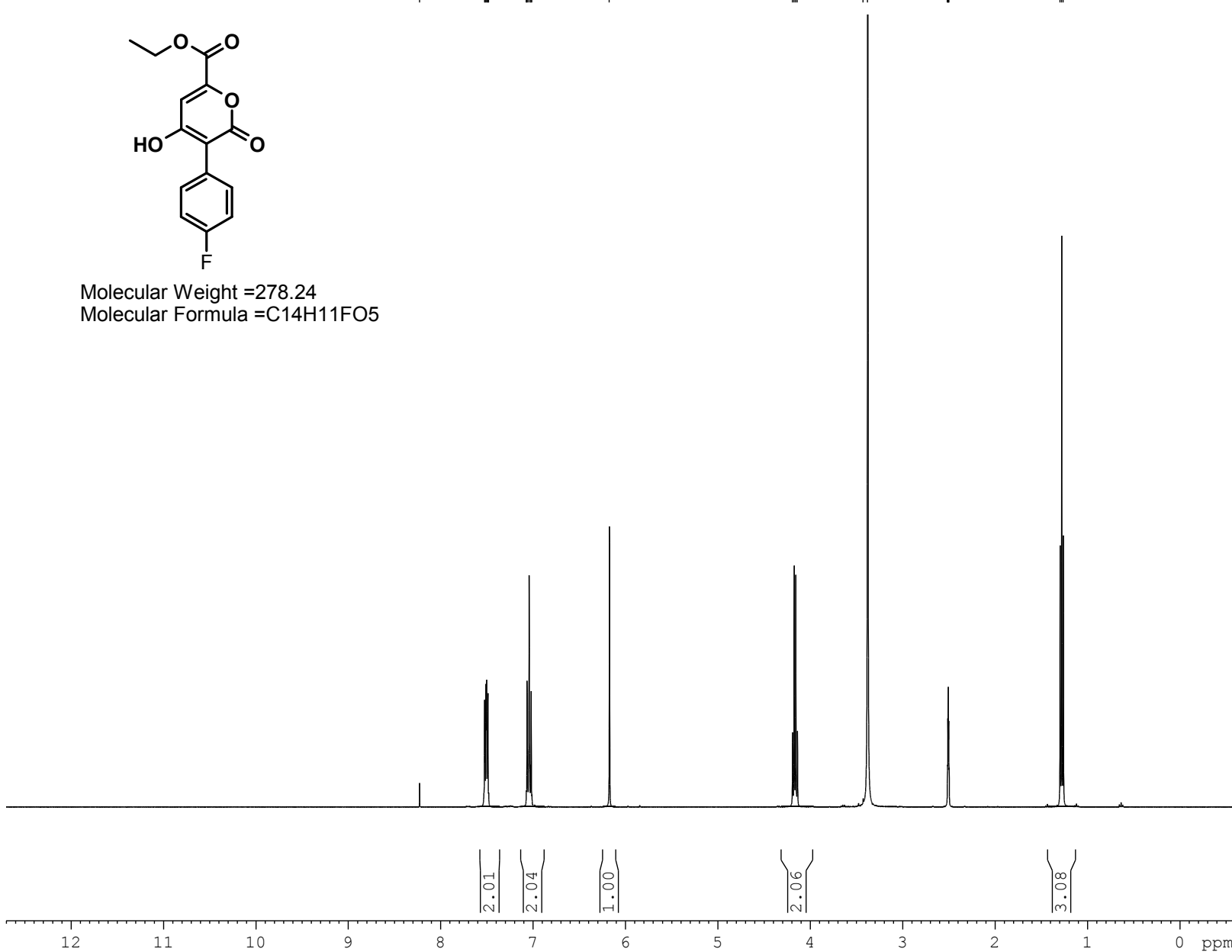
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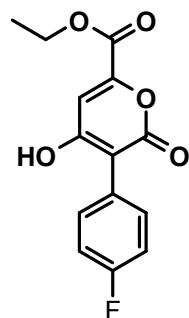
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===== CHANNEL f1 =====
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 SFO1 400.1324710 MHz

F2 - Processing parameters
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Molecular Weight =278.24
 Molecular Formula =C₁₄H₁₁FO₅

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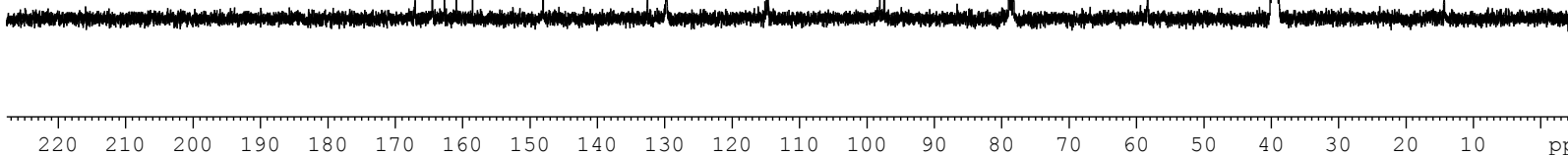
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 FIDRES 0.454131 Hz
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 DW 16.800 usec
 DE 6.00 usec
 TE 298.4 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.89999998 sec
 TD0 1

==== 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
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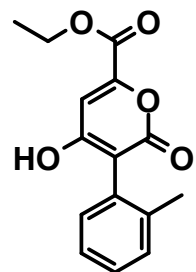
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Current Data Parameters
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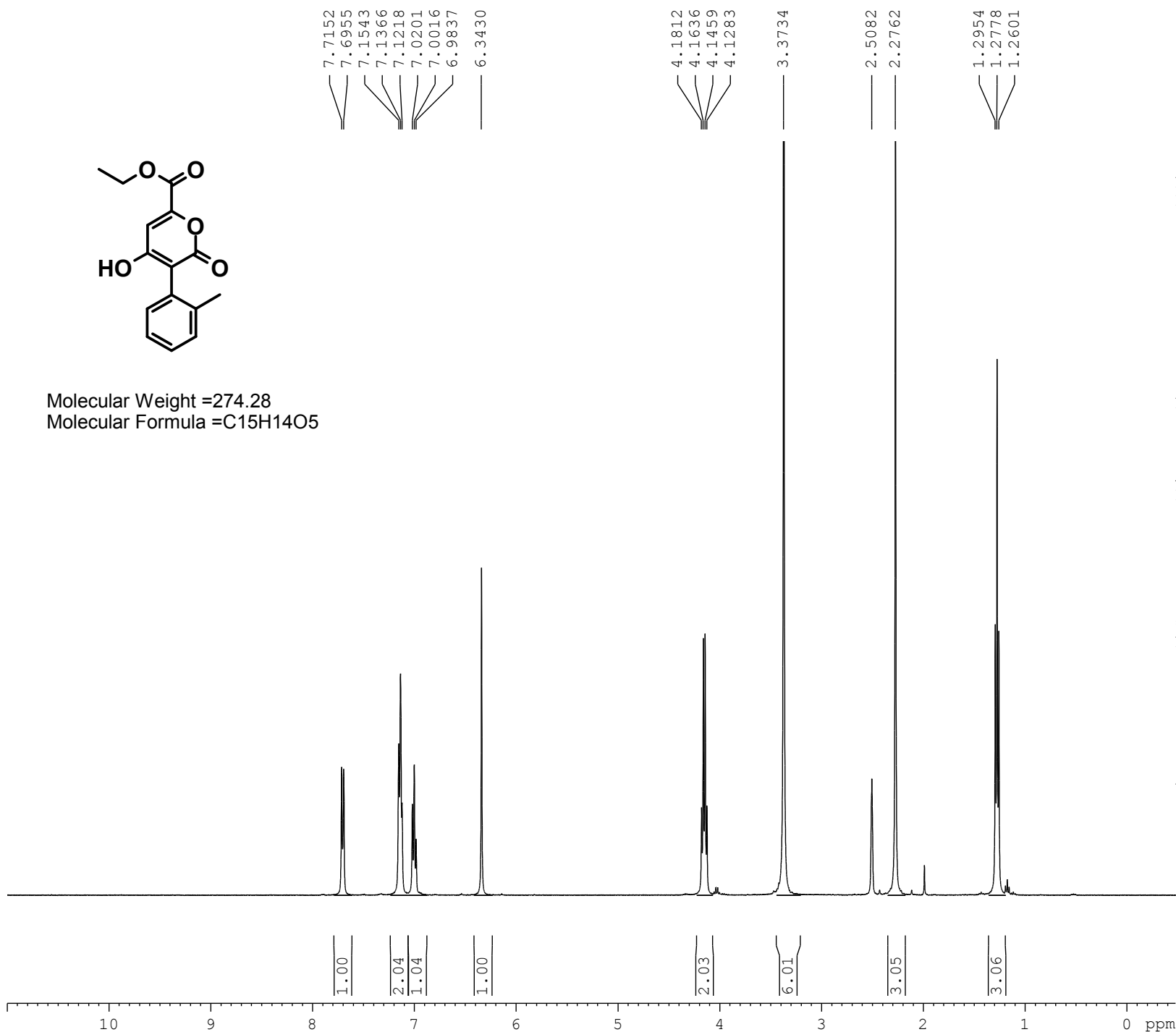
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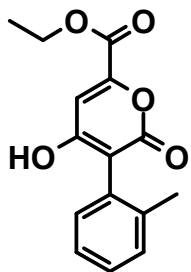
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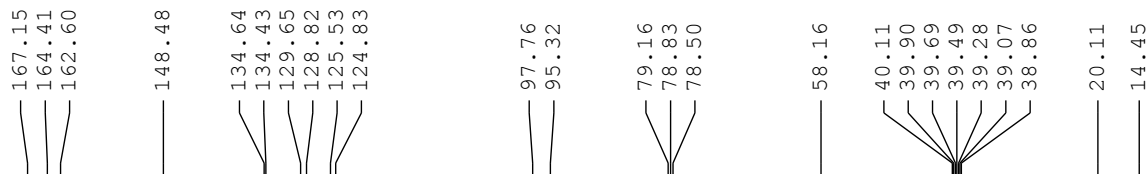


Molecular Weight =274.28
 Molecular Formula =C₁₅H₁₄O₅





Molecular Weight =274.28
 Molecular Formula =C₁₅H₁₄O₅



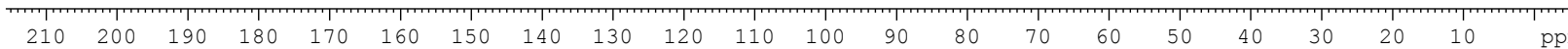
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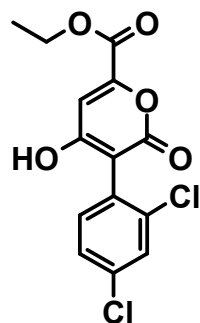
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==== CHANNEL f2 =====
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 NUC2 1H
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 PL2 -3.00 dB
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 PL13 18.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
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 PC 1.40



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Molecular Weight = 329.14
 Molecular Formula = C₁₄H₁₀Cl₂O₅

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3.3811

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 2.5033

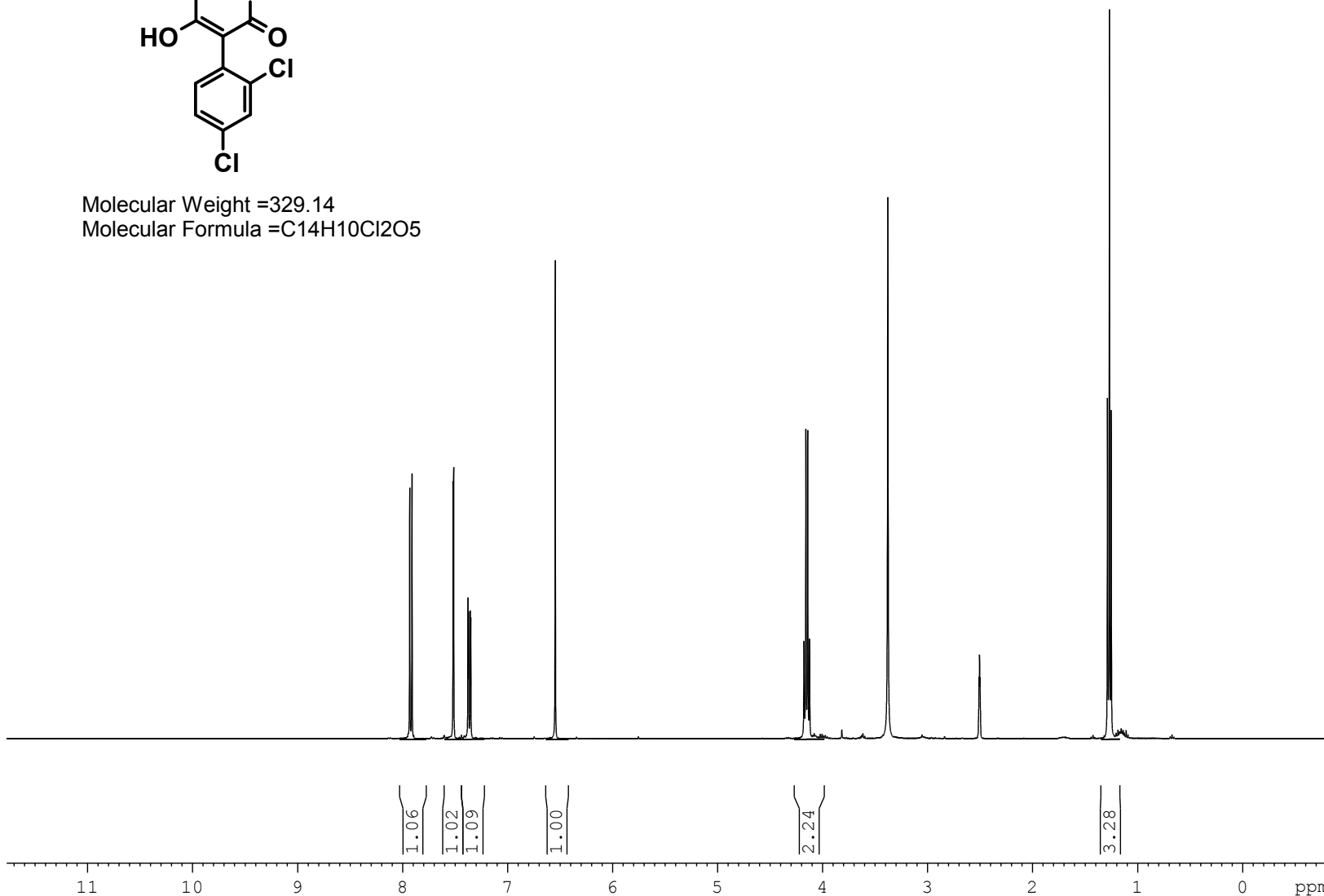
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 1.2711
 1.2534

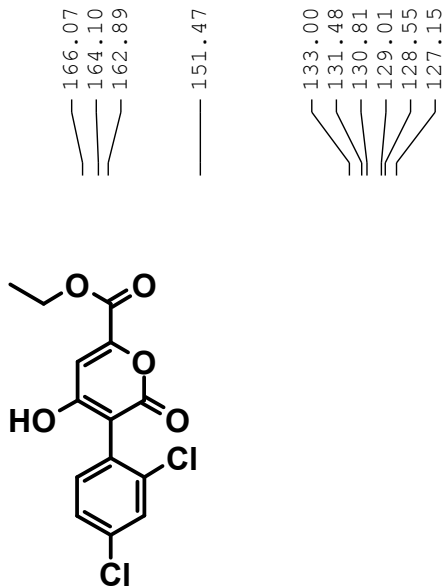
Current Data Parameters
 NAME Sep17-2013
 EXPNO 220
 PROCNO 1

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

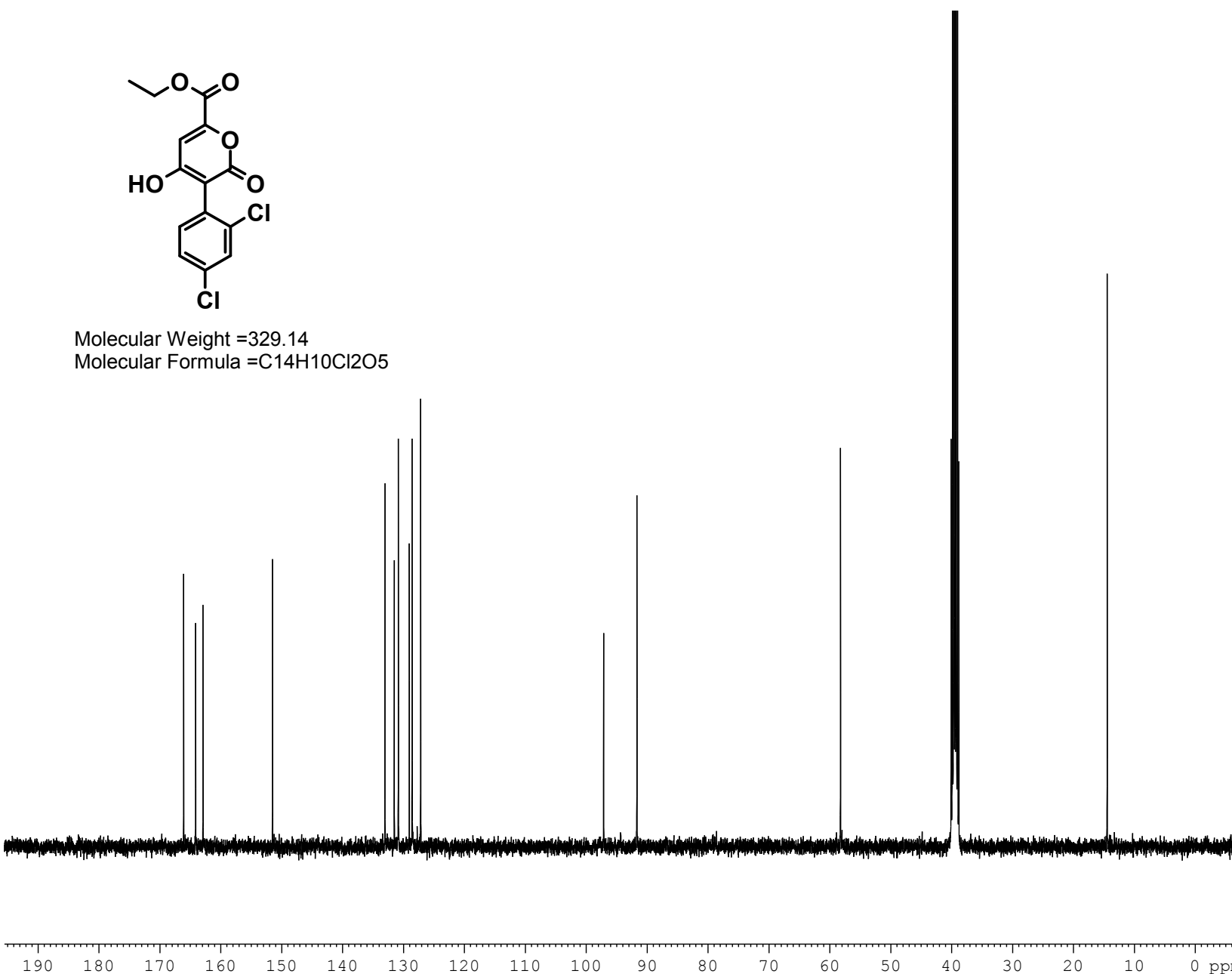
F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





Molecular Weight = 329.14
 Molecular Formula = C₁₄H₁₀Cl₂O₅

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
 40.08
 39.87
 39.66
 39.45
 39.25
 39.04
 38.83
 14.47



Current Data Parameters
 NAME Sep17-2013
 EXPNO 221
 PROCNO 1

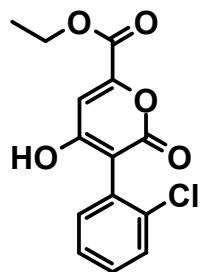
F2 - Acquisition Parameters
 Date_ 20130917
 Time_ 19.20
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 512
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010548 sec
 RG 1030
 DW 16.800 usec
 DE 6.00 usec
 TE 296.4 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA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

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

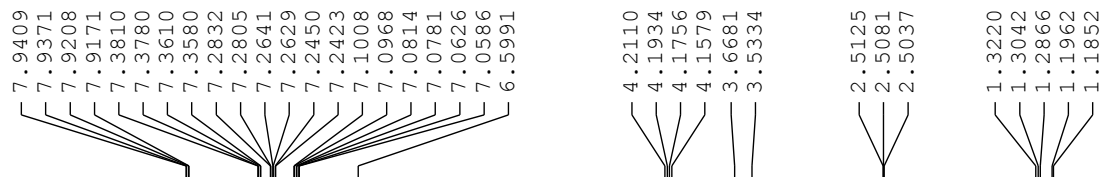
==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -3.00 dB
 PL12 14.31 dB
 PL13 18.00 dB
 SFO2 400.1316005 MHz

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

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Molecular Weight =294.69
 Molecular Formula =C₁₄H₁₁ClO₅

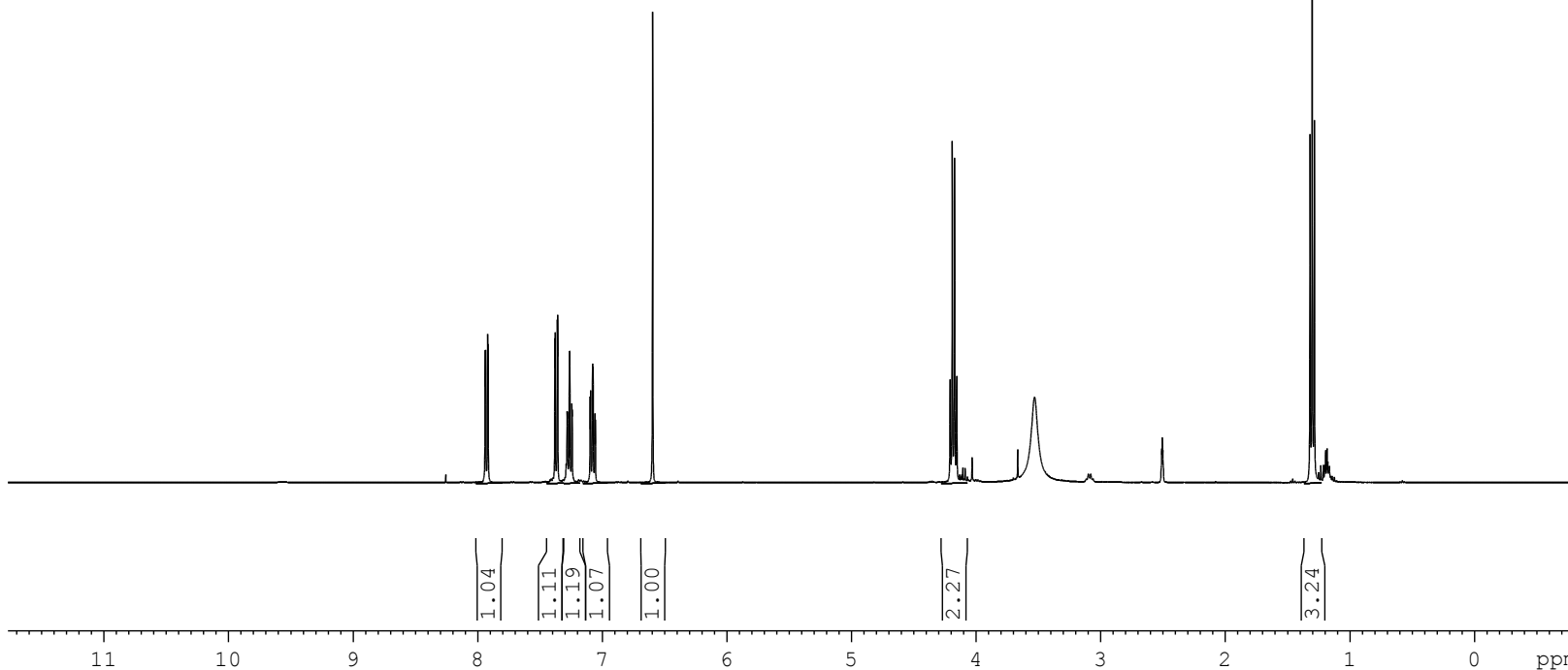


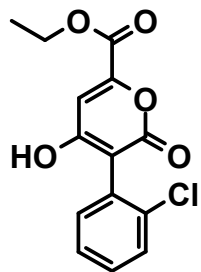
Current Data Parameters
 NAME Sep17-2013
 EXPNO 230
 PROCNO 1

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





Molecular Weight =294.69
 Molecular Formula =C₁₄H₁₁ClO₅

166.45
 164.32
 163.02
 150.16
 133.78
 131.19
 130.08
 129.10
 126.77
 126.05
 97.91
 93.61
 79.21
 78.88
 78.55
 58.40
 40.08
 39.87
 39.66
 39.45
 39.24
 39.03
 38.82
 14.39

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

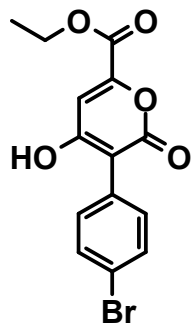
==== CHANNEL f1 =====
 NUC1 13C
 P1 9.60 usec
 PL1 -2.00 dB
 SFO1 100.6228298 MHz

==== 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

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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Molecular Weight = 339.14
 Molecular Formula = C₁₄H₁₁BrO₅

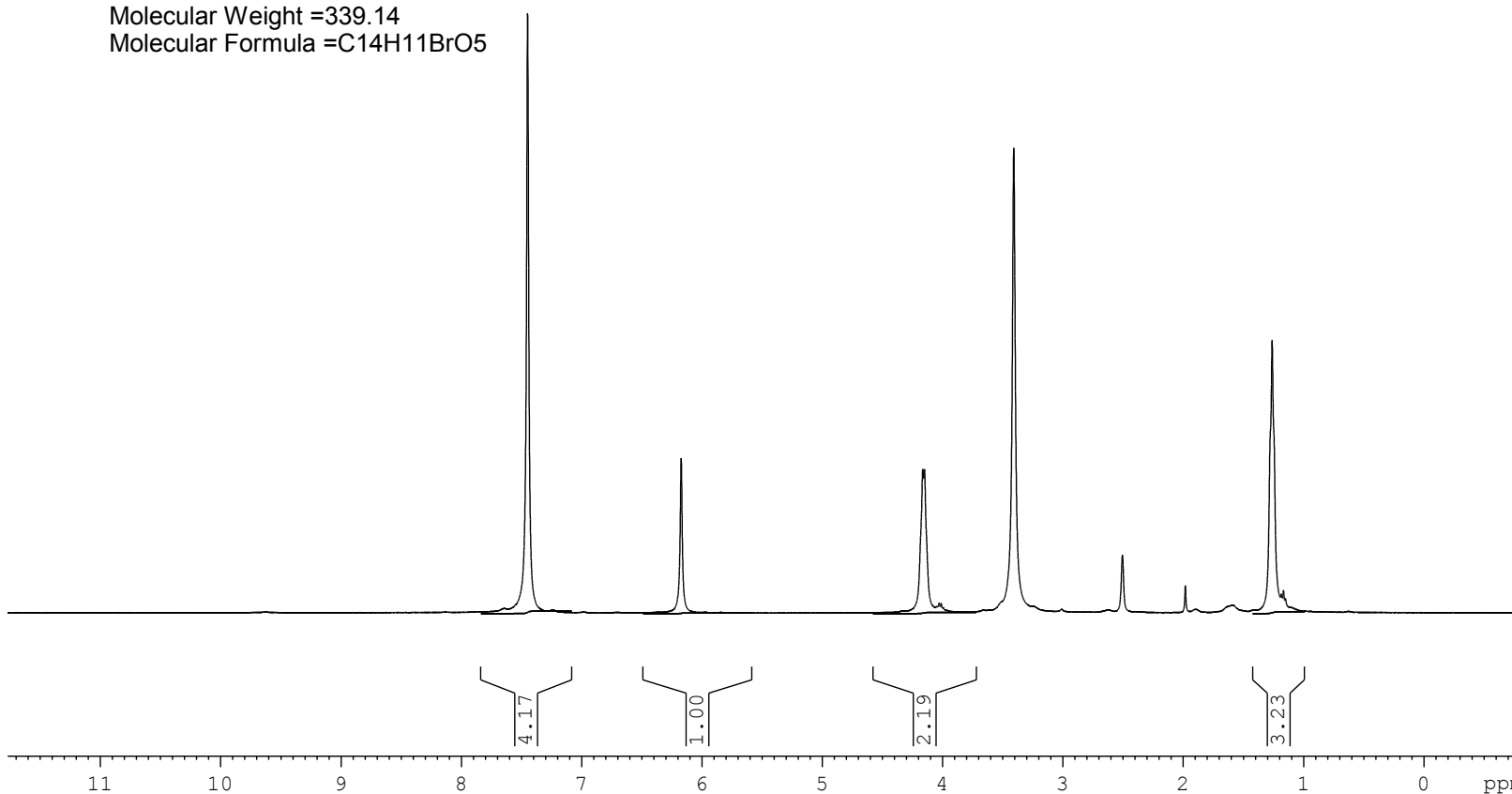
7.4494
 6.1755
 4.1677
 4.1529
 3.4106
 2.5080
 1.9849
 1.2634
 1.1691

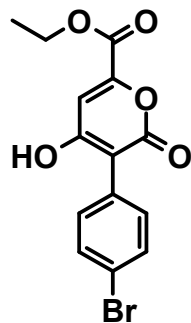
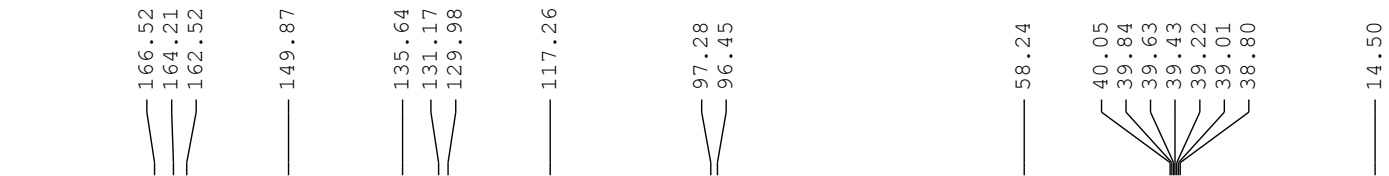
Current Data Parameters
 NAME Sep17-2013
 EXPNO 240
 PROCNO 1

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





Molecular Weight = 339.14
 Molecular Formula = C₁₄H₁₁BrO₅

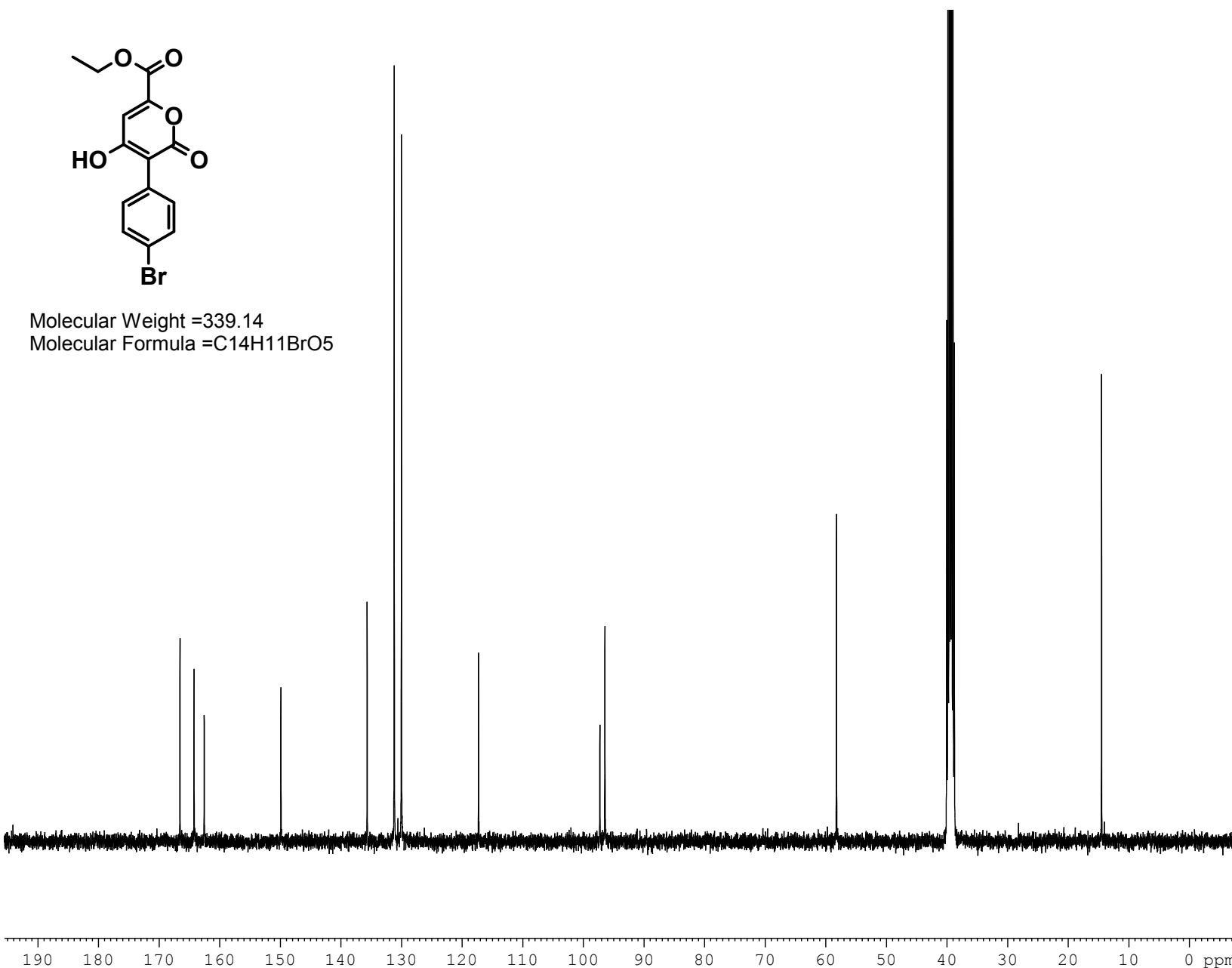
Current Data Parameters
 NAME Sep17-2013
 EXPNO 241
 PROCNO 1

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



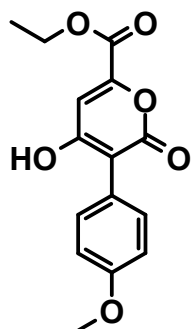
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Current Data Parameters
 NAME Aug01-2013
 EXPNO 470
 PROCNO 1

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 1.0000000 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 400.130000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Molecular Weight =290.28
 Molecular Formula =C₁₅H₁₄O₆

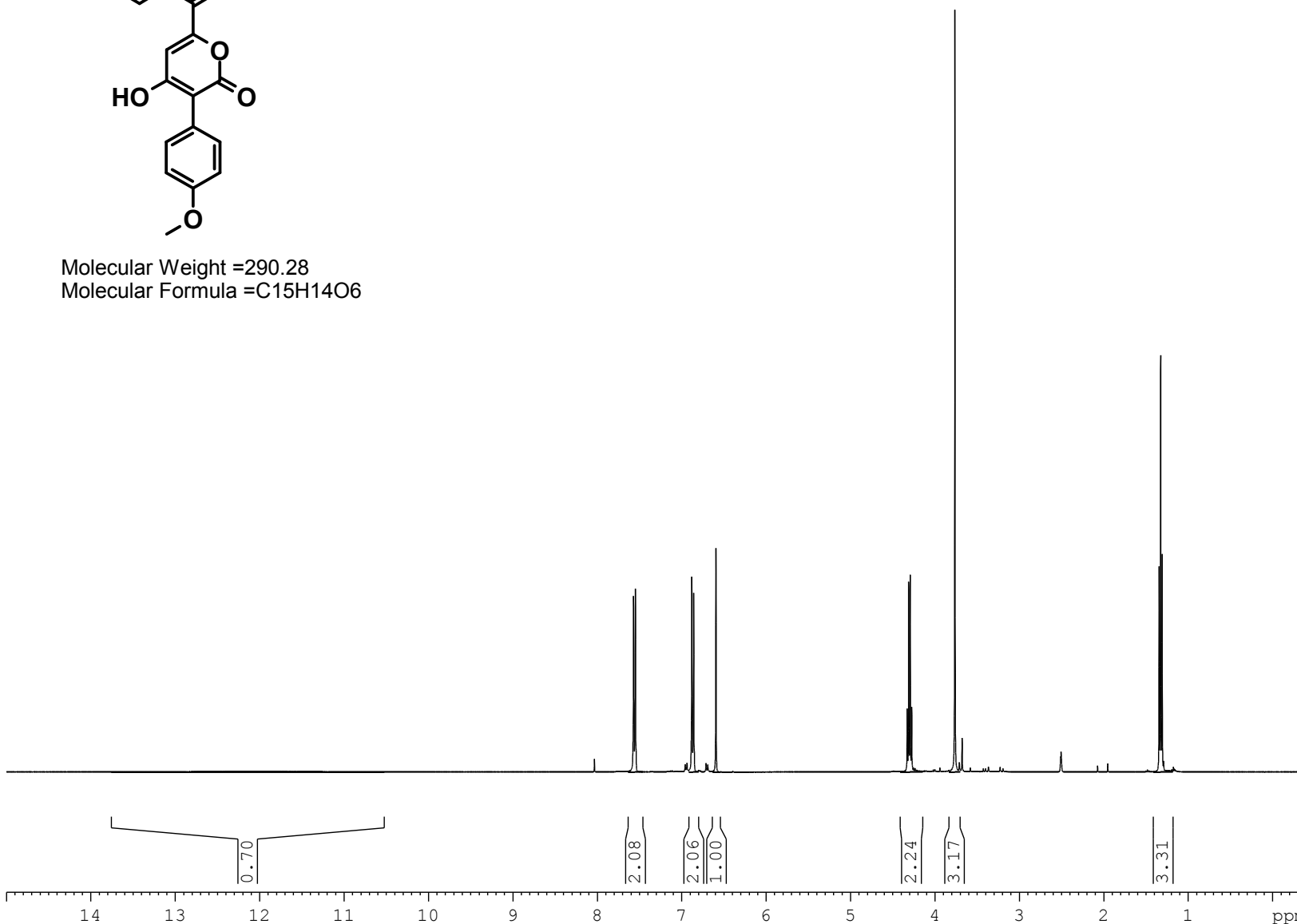
11.9098

7.5741
7.5521
6.8839
6.8618
6.5980

4.3319
4.3142
4.2964
4.2787
3.7669
3.6812

2.5094

1.3470
1.3292
1.3115



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Current Data Parameters
 NAME Aug01-2013
 EXPNO 471
 PROCNO 1

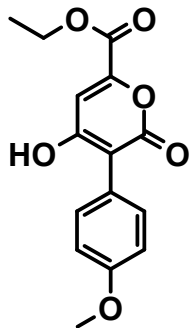
F2 - Acquisition Parameters
 Date_ 20130802
 Time_ 11.47
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 192
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010548 sec
 RG 1030
 DW 16.800 used
 DE 6.00 used
 TE 296.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

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

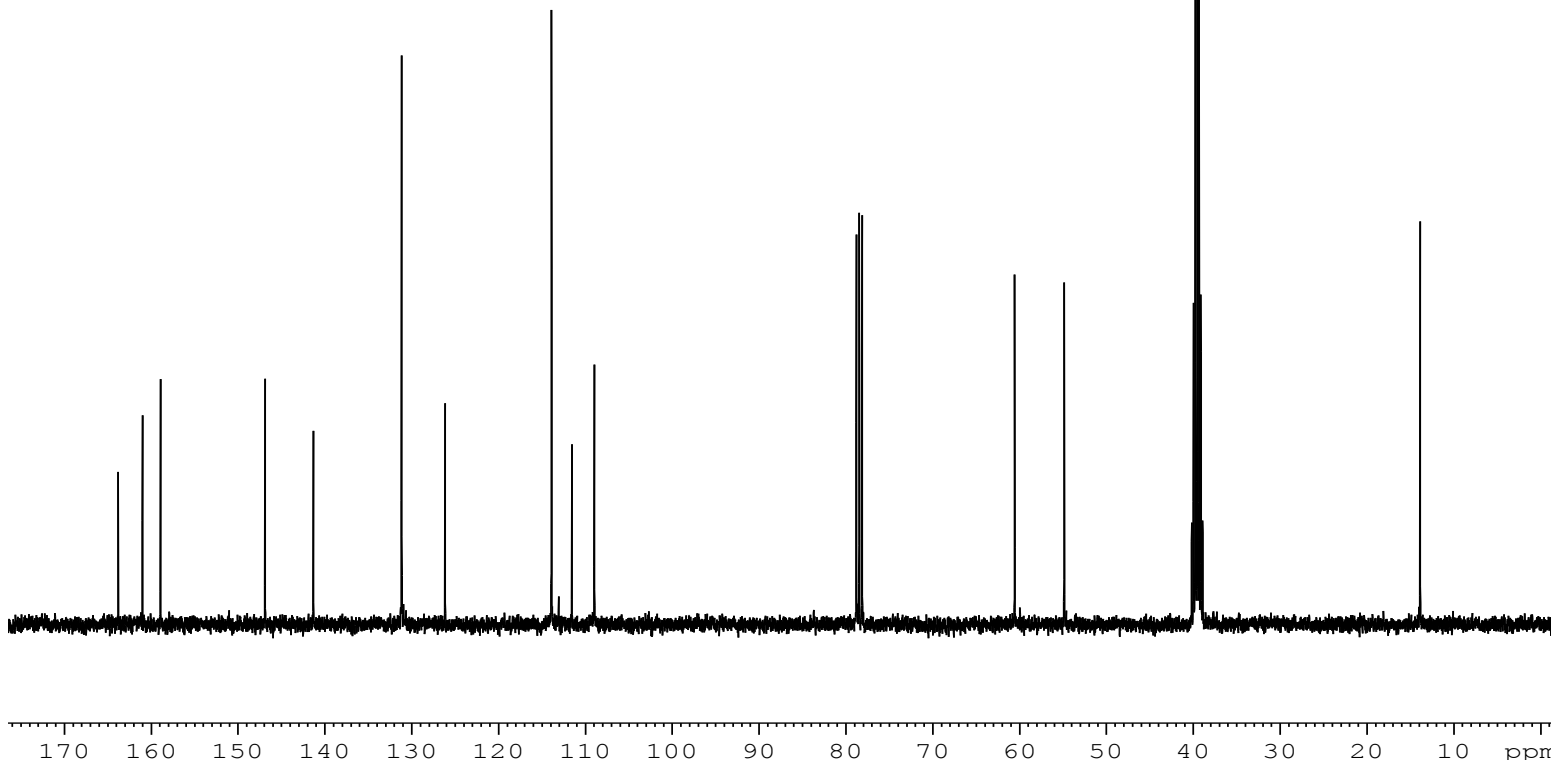
==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 used
 PL2 -3.00 dB
 PL12 14.31 dB
 PL13 18.00 dB
 SFO2 400.1316005 MHz

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

163.81
 161.01
 158.93
 146.90
 141.33
 131.17
 126.15
 113.90
 111.56
 108.98
 78.80
 78.47
 78.15
 60.57
 54.87
 40.17
 39.96
 39.76
 39.55
 39.34
 39.13
 38.92
 13.93

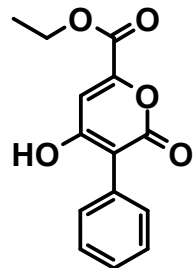


Molecular Weight =290.28
 Molecular Formula =C15H14O6

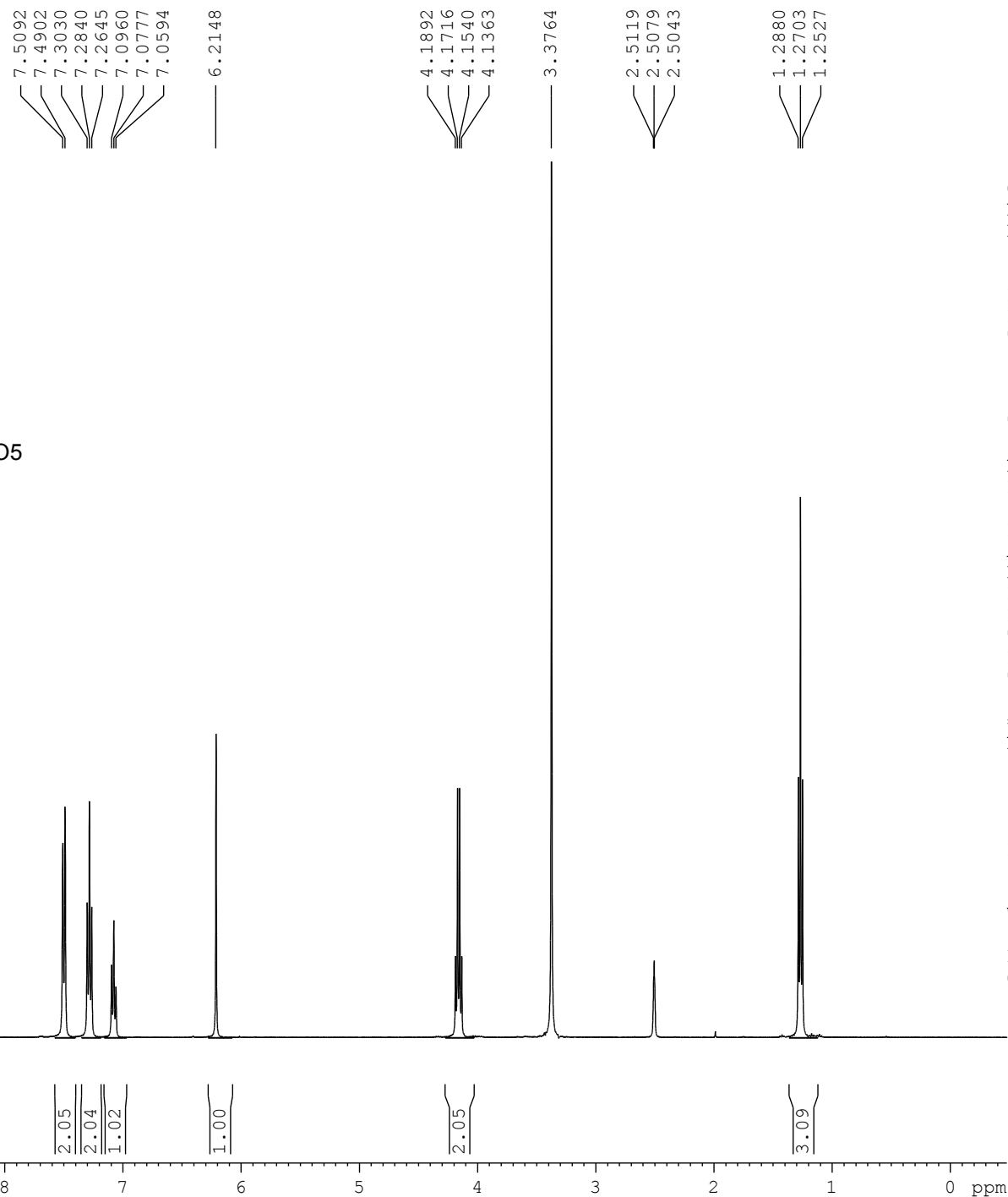


avtar saifpu@yahoo.co.in

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Molecular Weight =260.25
 Molecular Formula =C₁₄H₁₂O₅



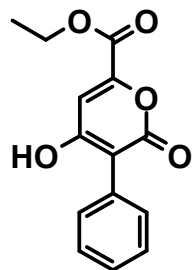
Current Data Parameters
 NAME Oct03-2013
 EXPNO 90
 PROCNO 1

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

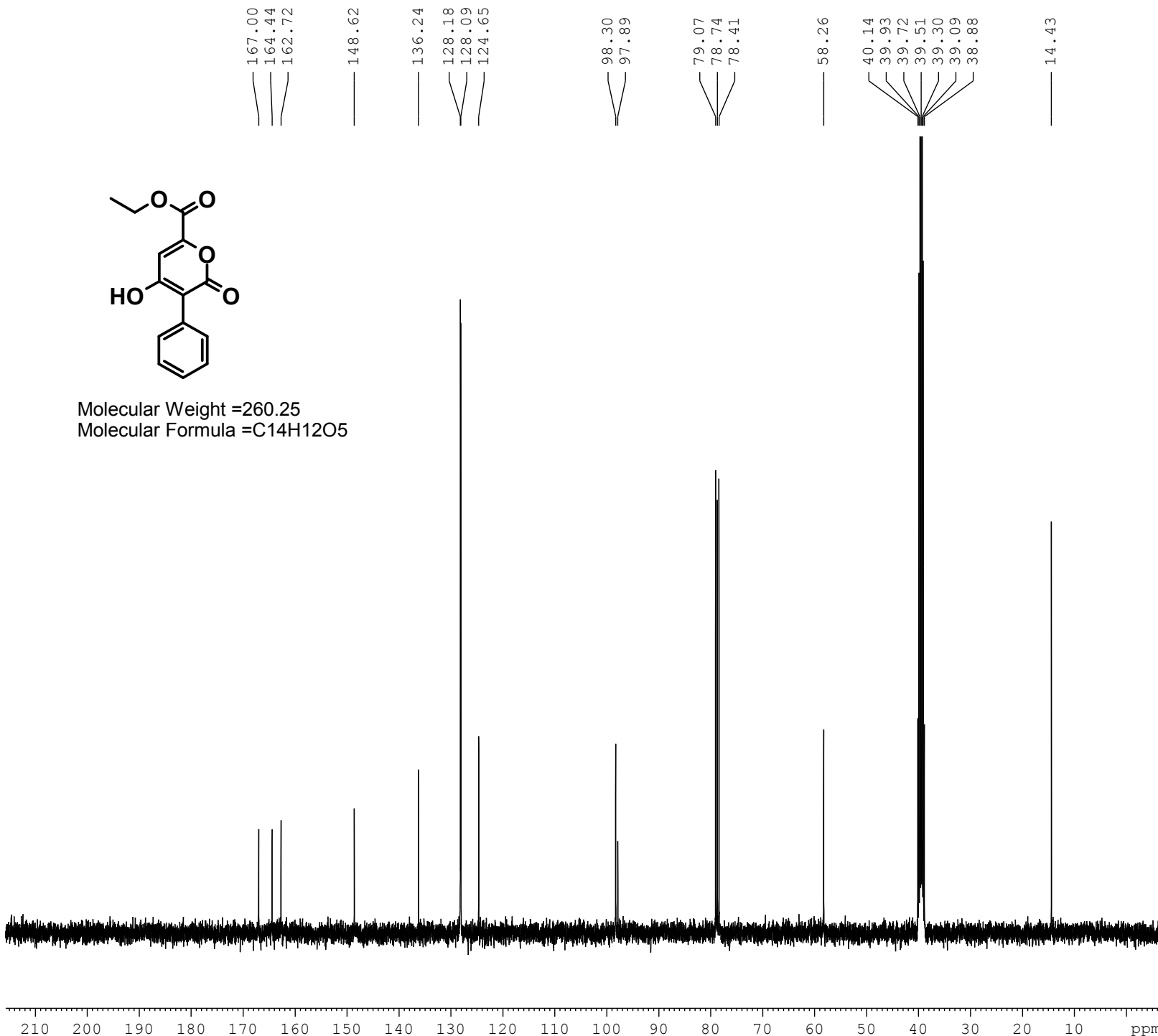
===== CHANNEL f1 =====
 NUC1 1H
 P1 10.90 usec
 PL1 -3.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.130000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

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Molecular Weight =260.25
 Molecular Formula =C₁₄H₁₂O₅



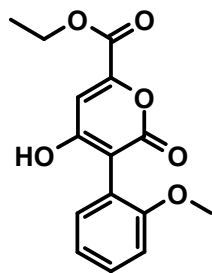
Current Data Parameters
 NAME Dec09-2013
 EXPNO 590
 PROCNO 1

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 2.0000000 sec
 d11 0.0300000 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



Molecular Weight =290.28
 Molecular Formula =C₁₅H₁₄O₆

167.21
 164.44
 162.60
 155.49
 148.33
 129.28
 125.86
 124.94
 120.20
 110.45
 98.10
 91.94
 79.13
 78.80
 78.47
 58.14
 55.31
 40.19
 39.98
 39.77
 39.57
 39.36
 39.15
 38.94
 14.38

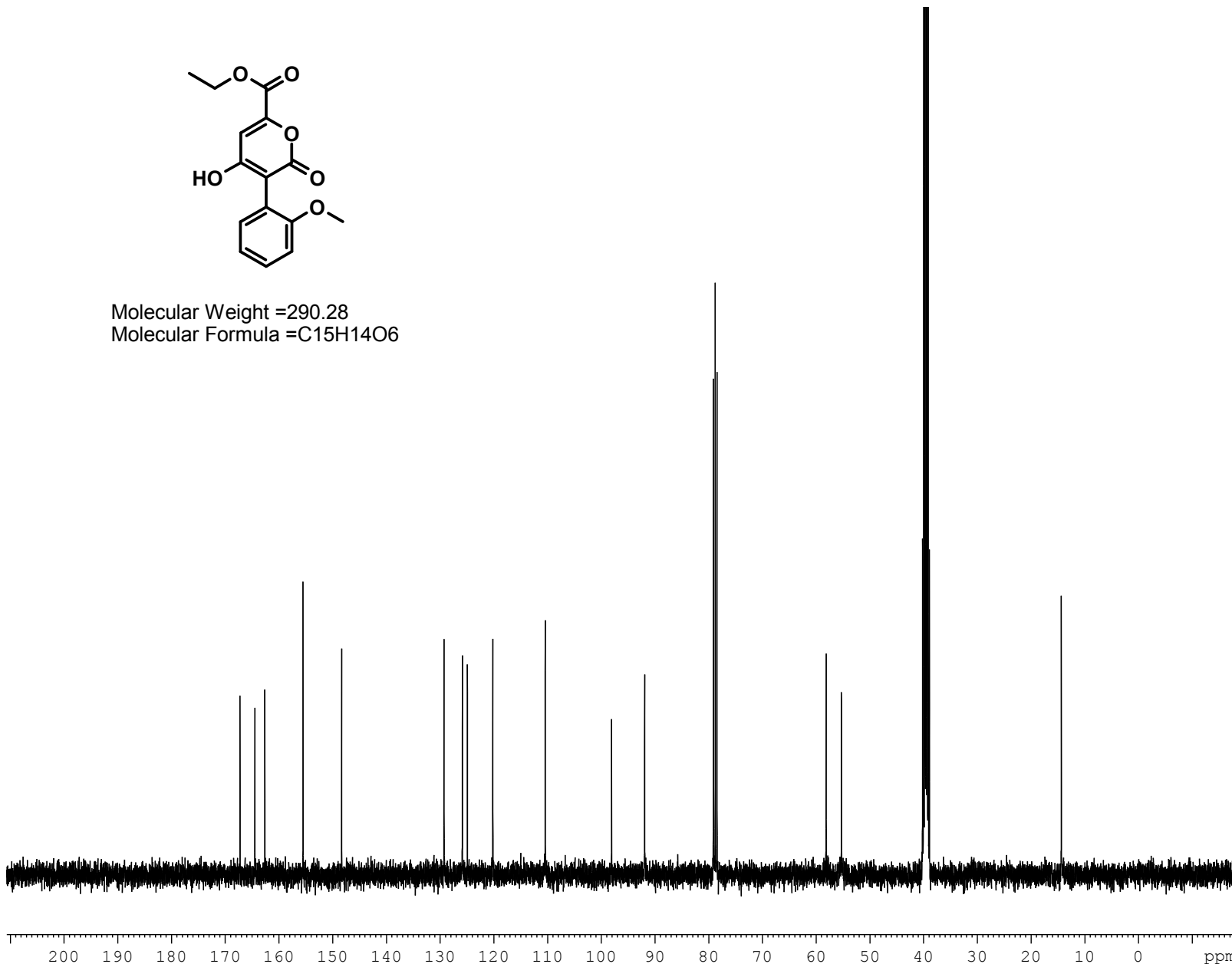
Current Data Parameters
 NAME Apr22-2014-Administrator
 EXPNO 260
 PROCNO 1

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

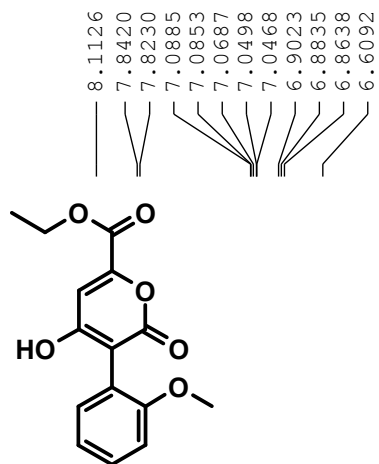
==== CHANNEL f1 =====
 NUC1 13C
 P1 9.60 usec
 PL1 -2.00 dB
 SFO1 100.6228298 MHz

==== 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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Molecular Weight = 290.28
 Molecular Formula = C₁₅H₁₄O₆

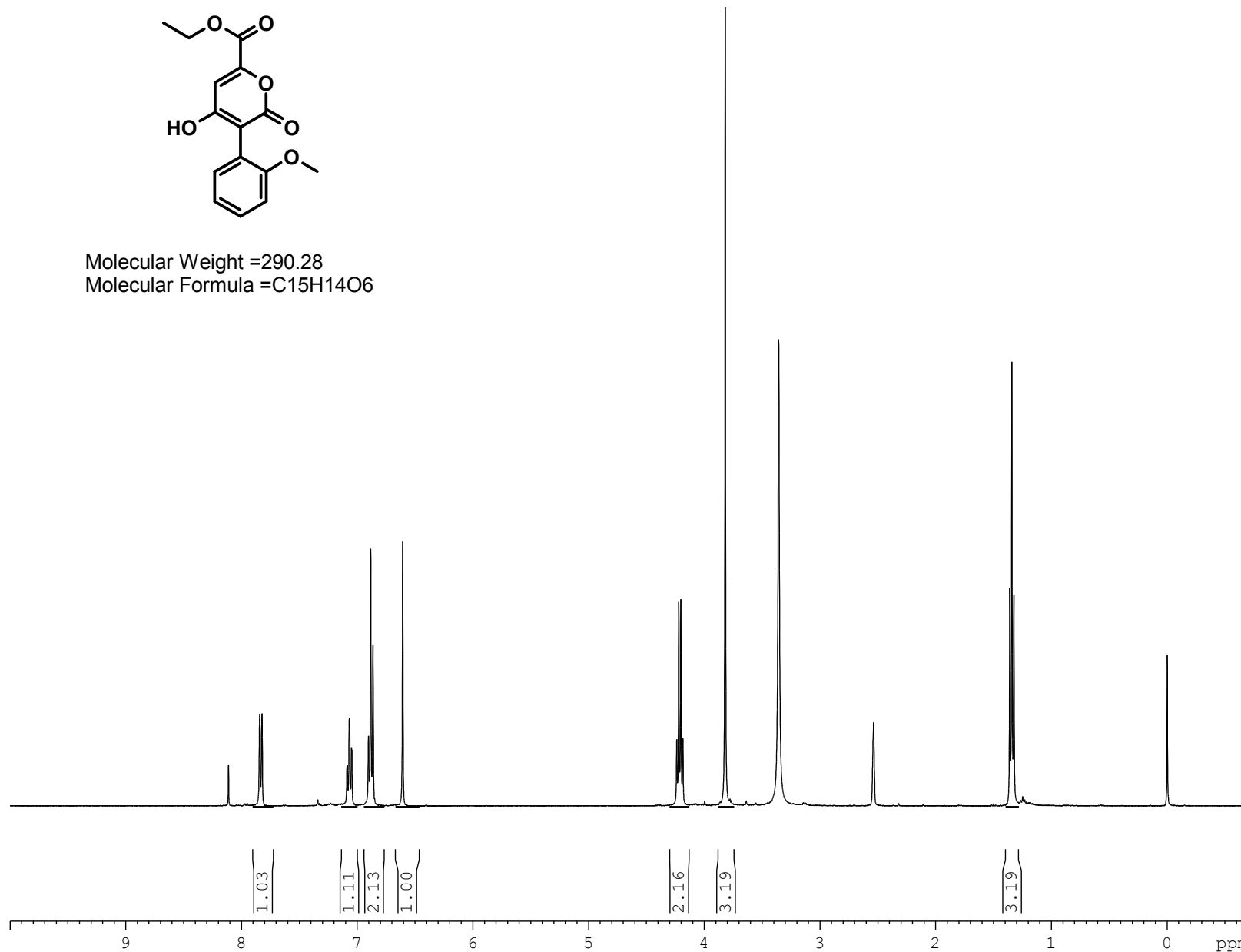
8.1126
 7.8420
 7.8230
 7.0885
 7.0853
 7.0687
 7.0498
 7.0468
 6.9023
 6.8835
 6.8638
 6.6092
 4.2402
 4.2226
 4.2049
 4.1872
 3.3588
 2.5399
 1.3616
 1.3439
 1.3262
 0.0000

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

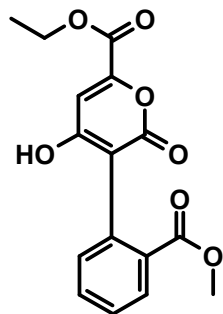
F2 - Processing parameters
 SI 32768
 SF 400.1299881 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



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8.1884
 7.8749
 7.8549
 7.7010
 7.6827
 7.4711
 7.4516
 7.4333
 7.1803
 7.1616
 7.1429
 6.8904

4.2319
 4.2143
 4.1966
 4.1789
 3.8282
 3.3793
 2.5286
 1.3507
 1.3331
 1.3154
 0.0000



Molecular Weight =290.28
 Molecular Formula =C₁₆H₁₄O₆

Current Data Parameters
 NAME Feb21-2014
 EXPNO 160
 PROCNO 1

F2 - Acquisition Parameters

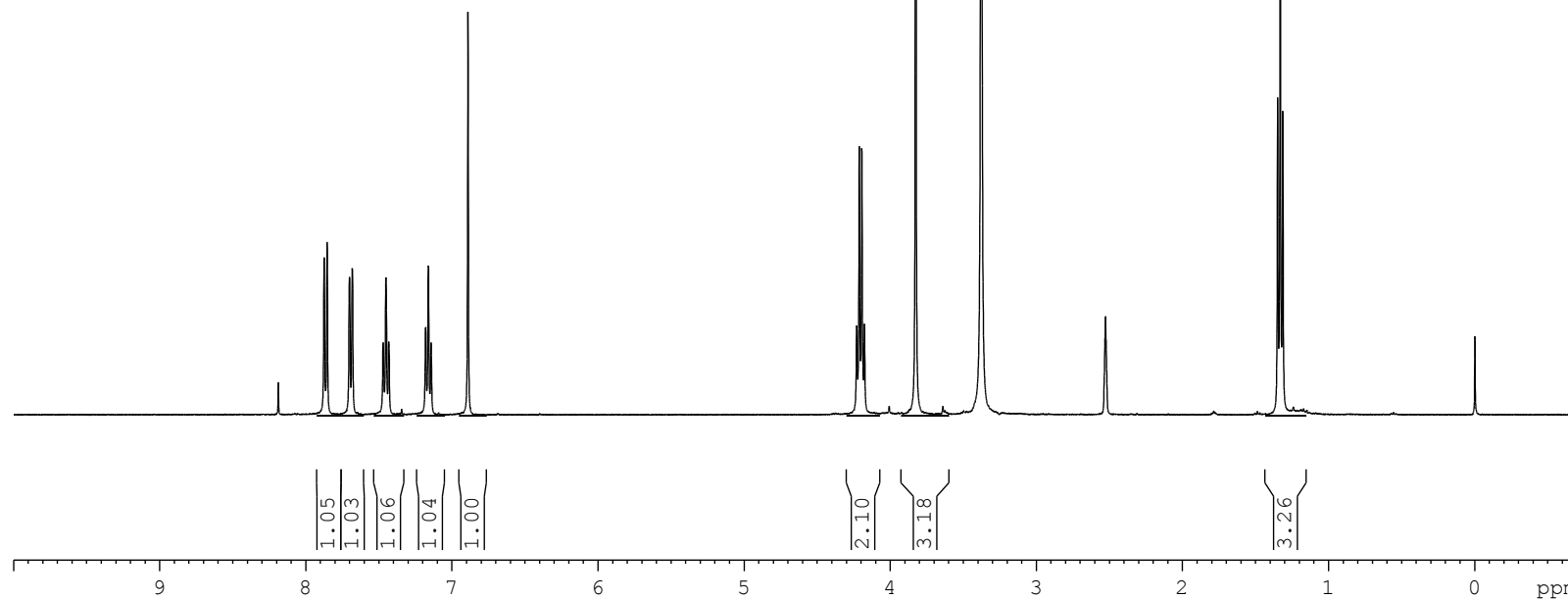
Date_ 20140221
 Time 18.30
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7263477 sec
 RG 575
 DW 41.600 usec
 DE 6.00 usec
 TE 296.2 K
 D1 1.0000000 sec
 TDO 1

===== 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



GRD100Q

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167.93
166.69
164.33
162.99

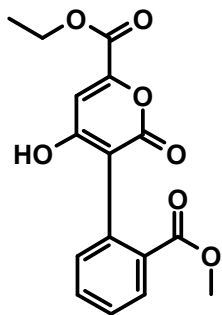
149.62

135.94

131.00
130.23
129.43
128.66

124.44

97.75
95.28



Molecular Weight =290.28
Molecular Formula =C16H14O6

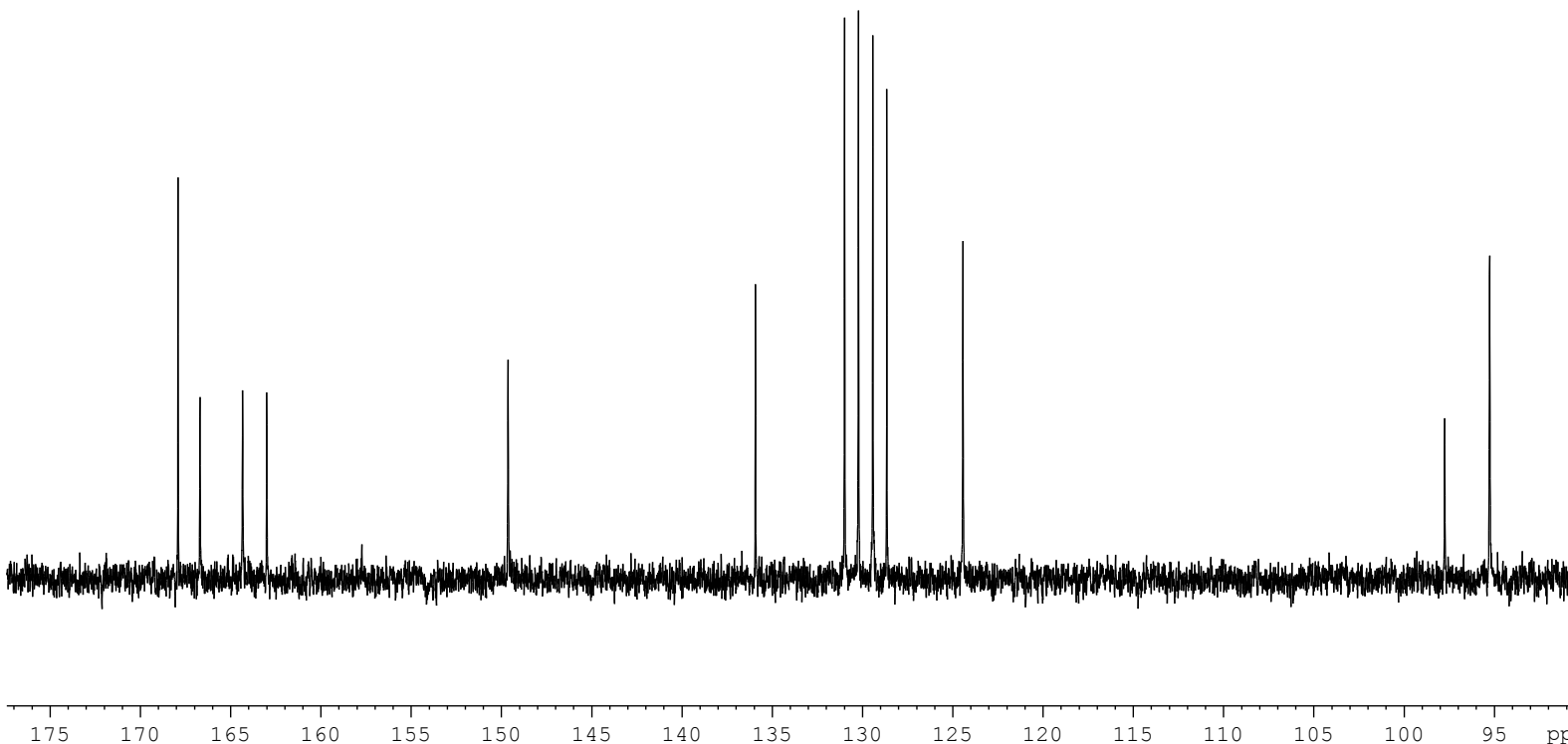
Current Data Parameters
NAME Mar15-2014
EXPNO 110
PROCNO 1

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

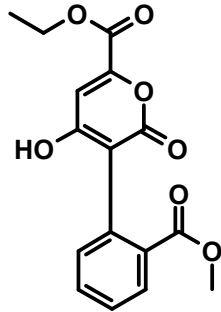


avtar_saifpu@yahoo.co.in

GRD100Q

BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

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
79.18
78.85
78.52
58.22
51.70
40.12
39.91
39.71
39.50
39.29
39.08
38.87
14.40



Molecular Weight =290.28
Molecular Formula =C16H14O6

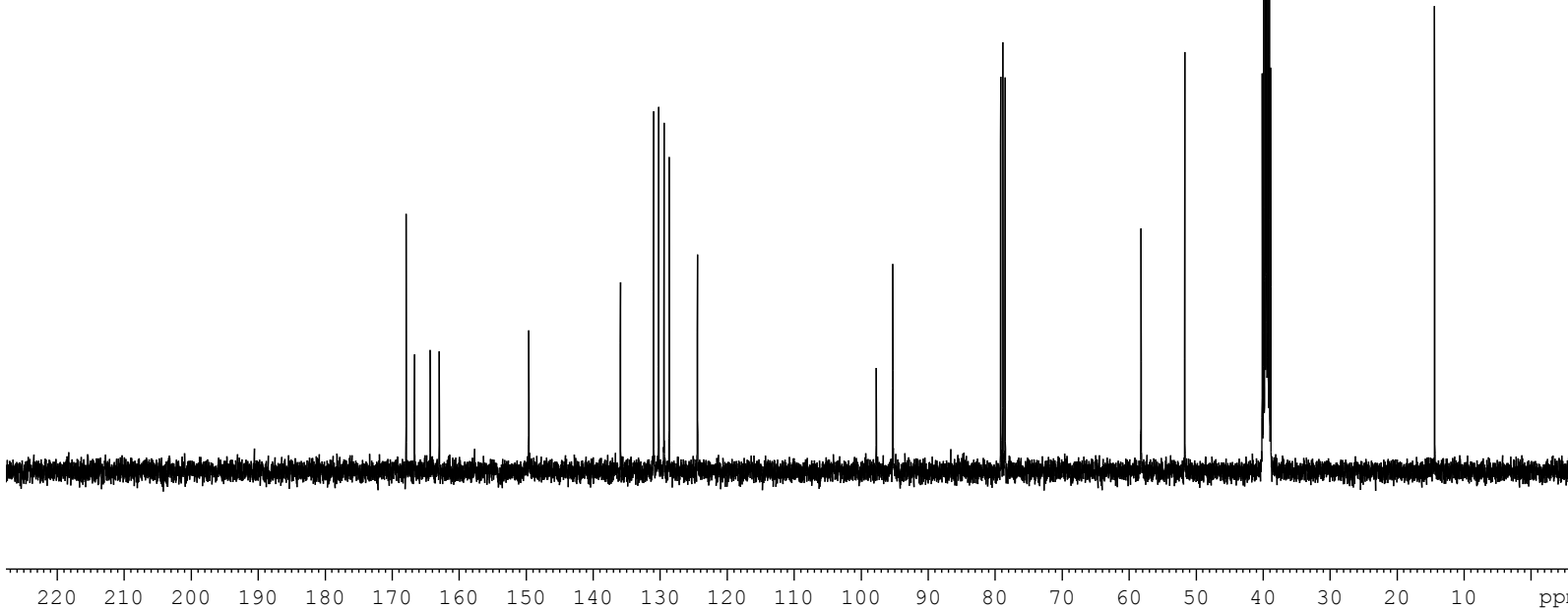
Current Data Parameters
NAME Mar15-2014
EXPNO 110
PROCNO 1

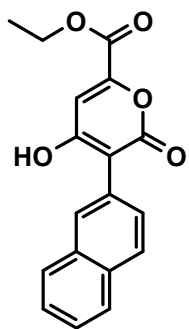
F2 - Acquisition Parameters
Date_ 20140315
Time_ 22.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 1030
DW 16.800 usec
DE 6.00 usec
TE 298.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0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

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

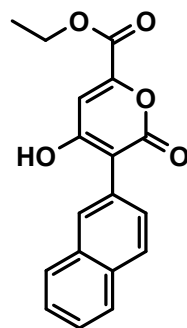
==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz

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

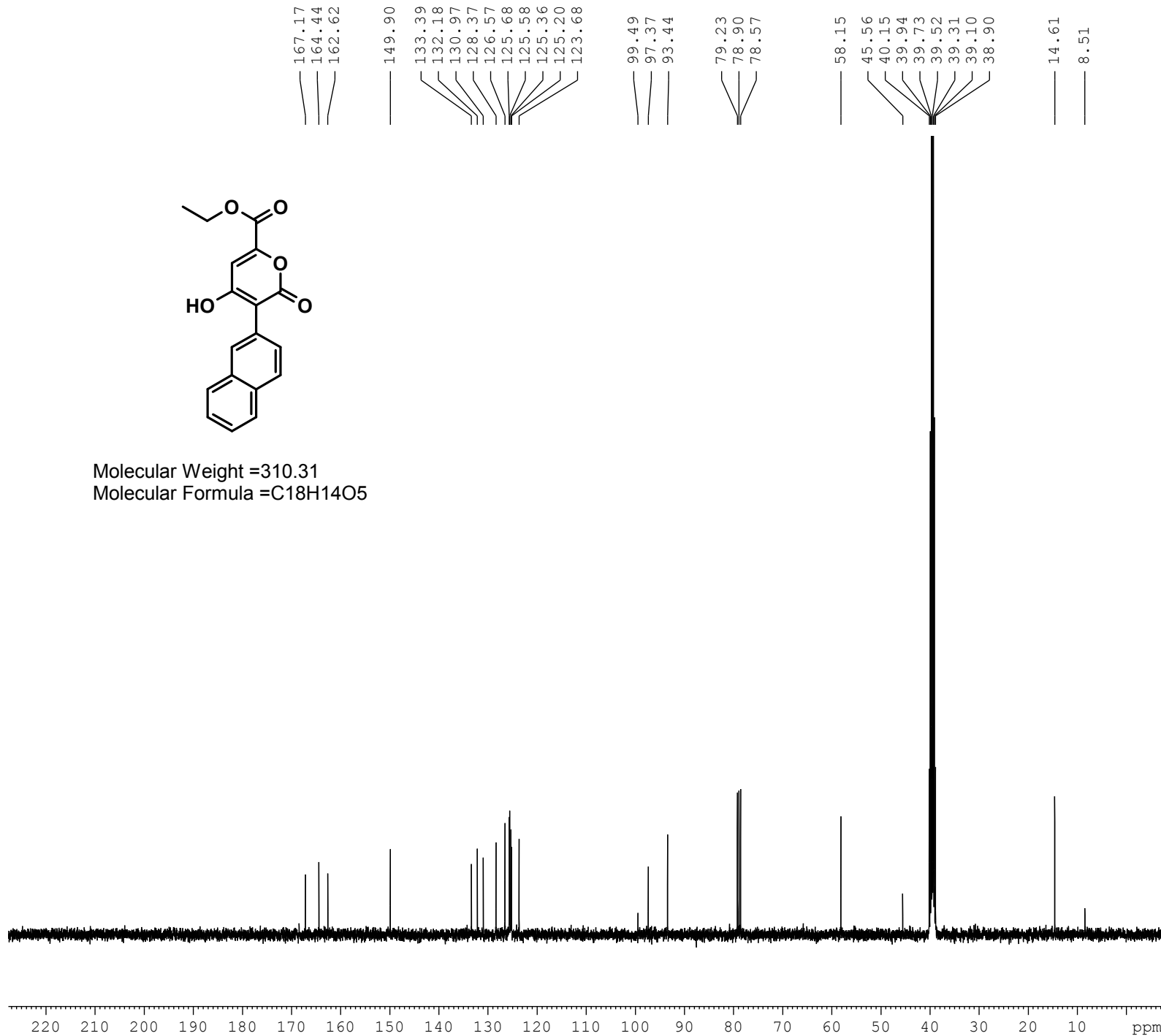




Molecular Weight =310.31
Molecular Formula =C₁₈H₁₄O₅



Molecular Weight = 310.31
 Molecular Formula = C₁₈H₁₄O₅



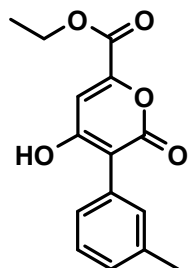
Current Data Parameters
 NAME Mar15-2014
 EXPNO 90
 PROCNO 1

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

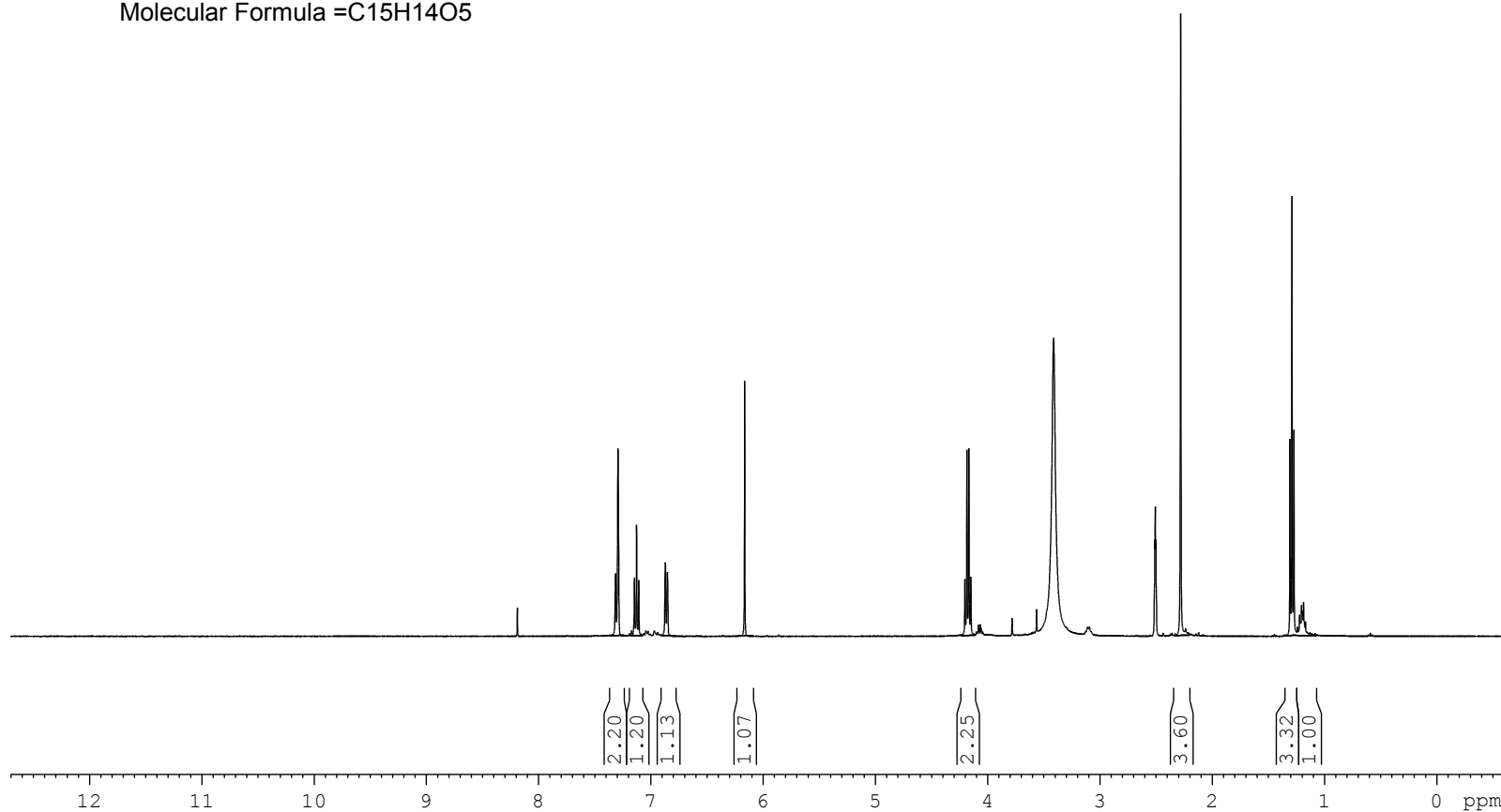
==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -3.00 dB
 PL12 14.31 dB
 PL13 18.00 dB
 SFO2 400.1316005 MHz

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



Molecular Weight =274.28
Molecular Formula =C₁₅H₁₄O₅

8.1898
7.3180
7.2964
7.1496
7.1308
7.1118
6.8748
6.8562
6.1679
4.2058
4.1881
4.1705
4.1528
3.7849
3.5673
3.4774
3.4155
2.5135
2.5092
2.5048
2.2840
1.3100
1.2923
1.2747
1.2243
1.2172
1.2068
1.2005
1.1894
1.1715



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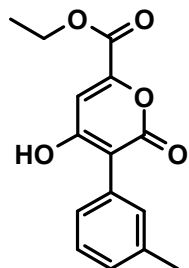
Current Data Parameters
NAME Jan01-2014
EXPNO 80
PROCNO 1

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

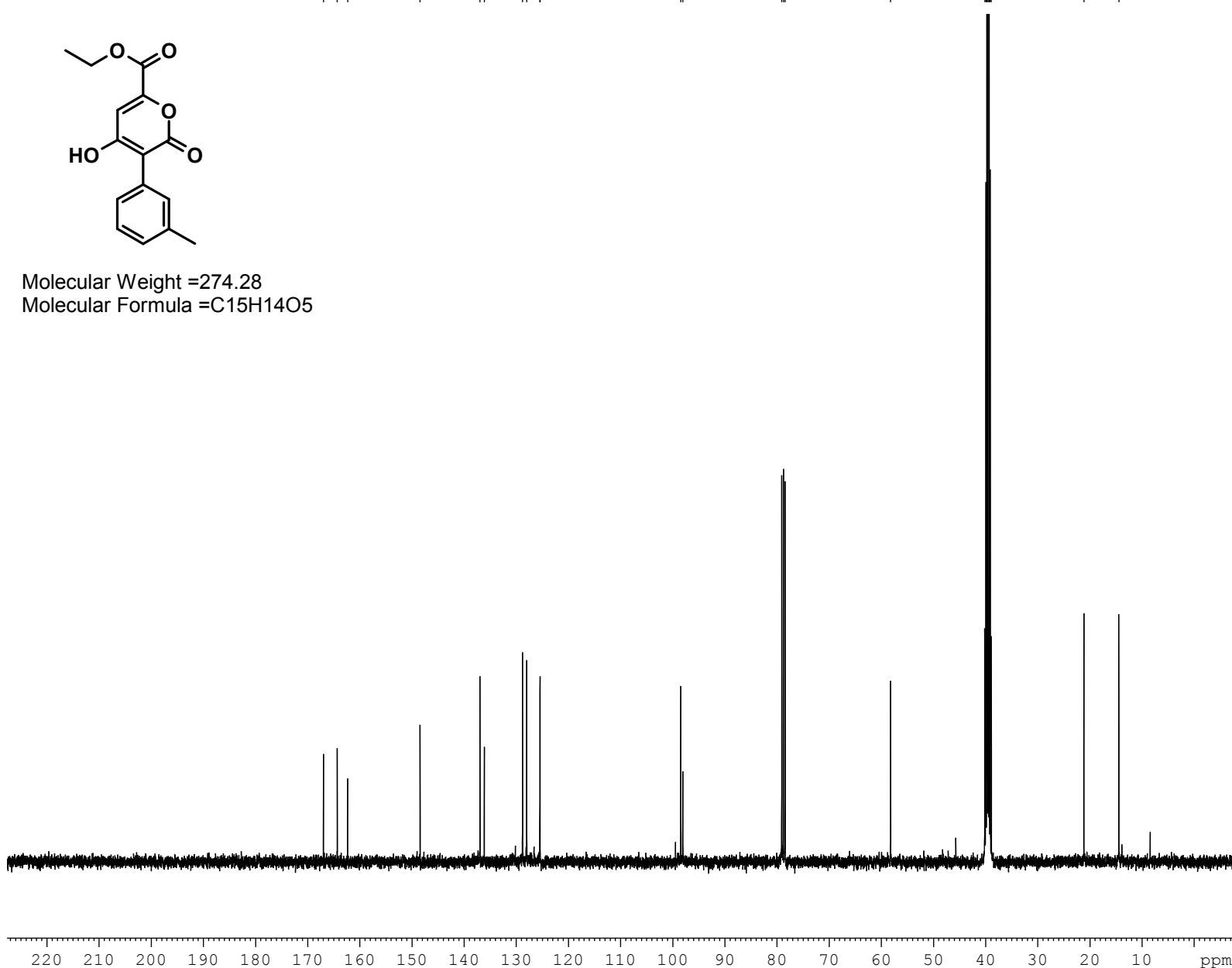
F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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 AVANCE II 400 NMR
 Spectrometer
 SAIF
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Molecular Weight =274.28
 Molecular Formula =C₁₅H₁₄O₅

166.98
 164.35
 162.36
 148.45
 136.97
 136.14
 128.81
 128.00
 125.48
 125.45
 98.47
 98.06
 79.10
 78.77
 78.44
 58.22
 40.17
 39.96
 39.75
 39.54
 39.33
 39.12
 38.91
 21.16
 14.46



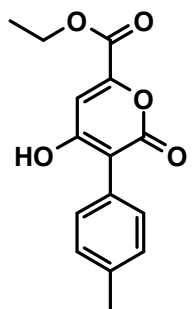
Current Data Parameters
 NAME Mar15-2014
 EXPNO 80
 PROCNO 1

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 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.89999998 sec
 TD0 1

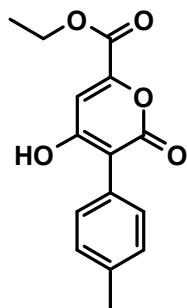
==== CHANNEL f1 =====
 NUC1 13C
 P1 9.60 usec
 PL1 -2.00 dB
 SFO1 100.6228298 MHz

==== 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

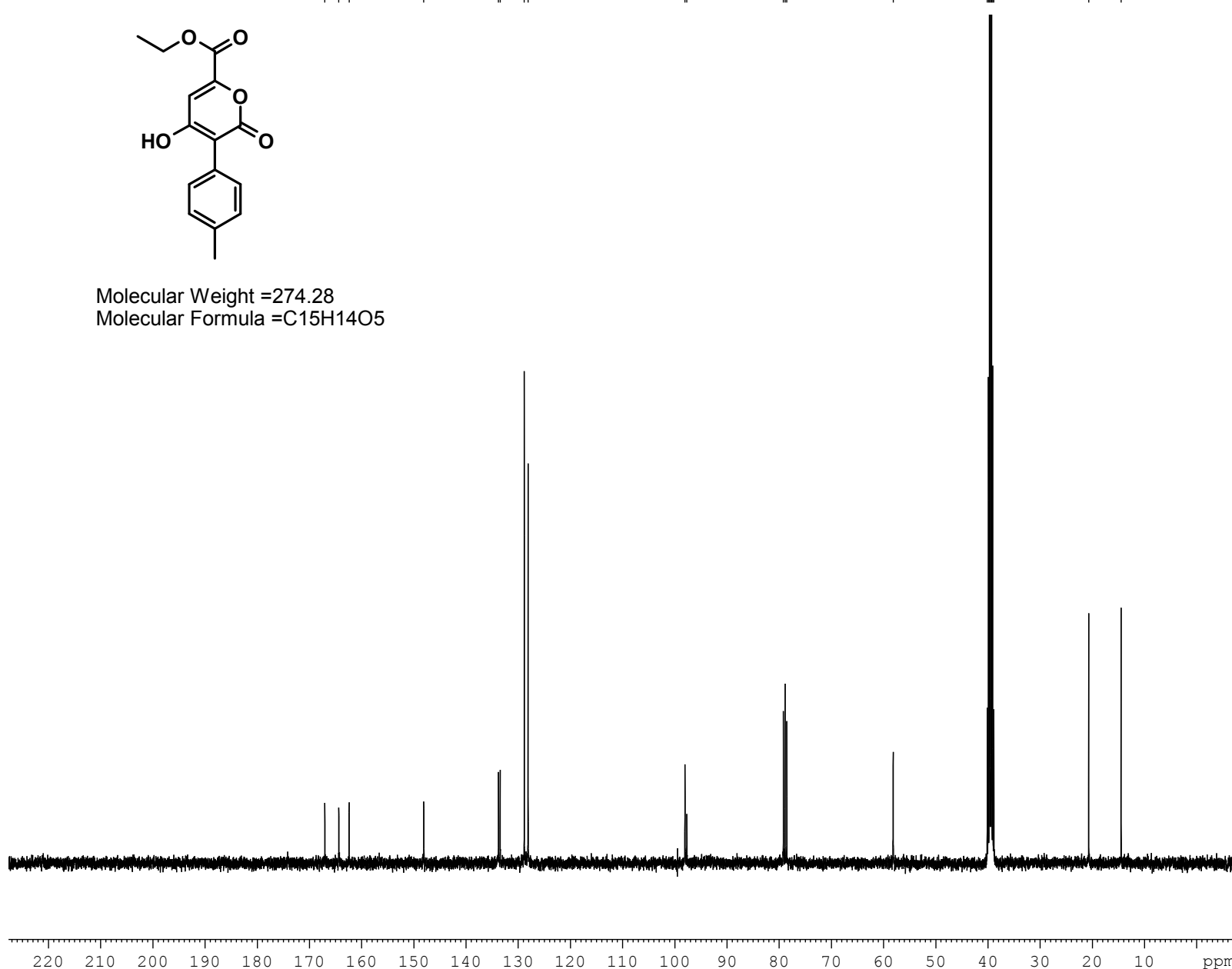


Molecular Weight =274.28
Molecular Formula =C₁₅H₁₄O₅



Molecular Weight =274.28
 Molecular Formula =C₁₅H₁₄O₅

167.06
 164.38
 162.41
 148.10
 133.79
 133.46
 128.84
 128.11
 98.05
 97.70
 79.20
 78.87
 78.54
 58.16
 40.13
 39.92
 39.71
 39.50
 39.29
 39.08
 38.87
 20.69
 14.48



Current Data Parameters
 NAME Mar15-2014
 EXPNO 60
 PROCNO 1

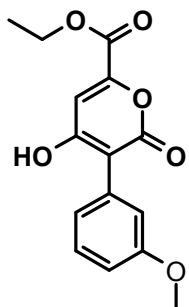
F2 - Acquisition Parameters
 Date_ 20140315
 Time 19.22
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 512
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010548 sec
 RG 36
 DW 16.800 usec
 DE 6.00 usec
 TE 298.3 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 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 =290.28
 Molecular Formula =C₁₅H₁₄O₆

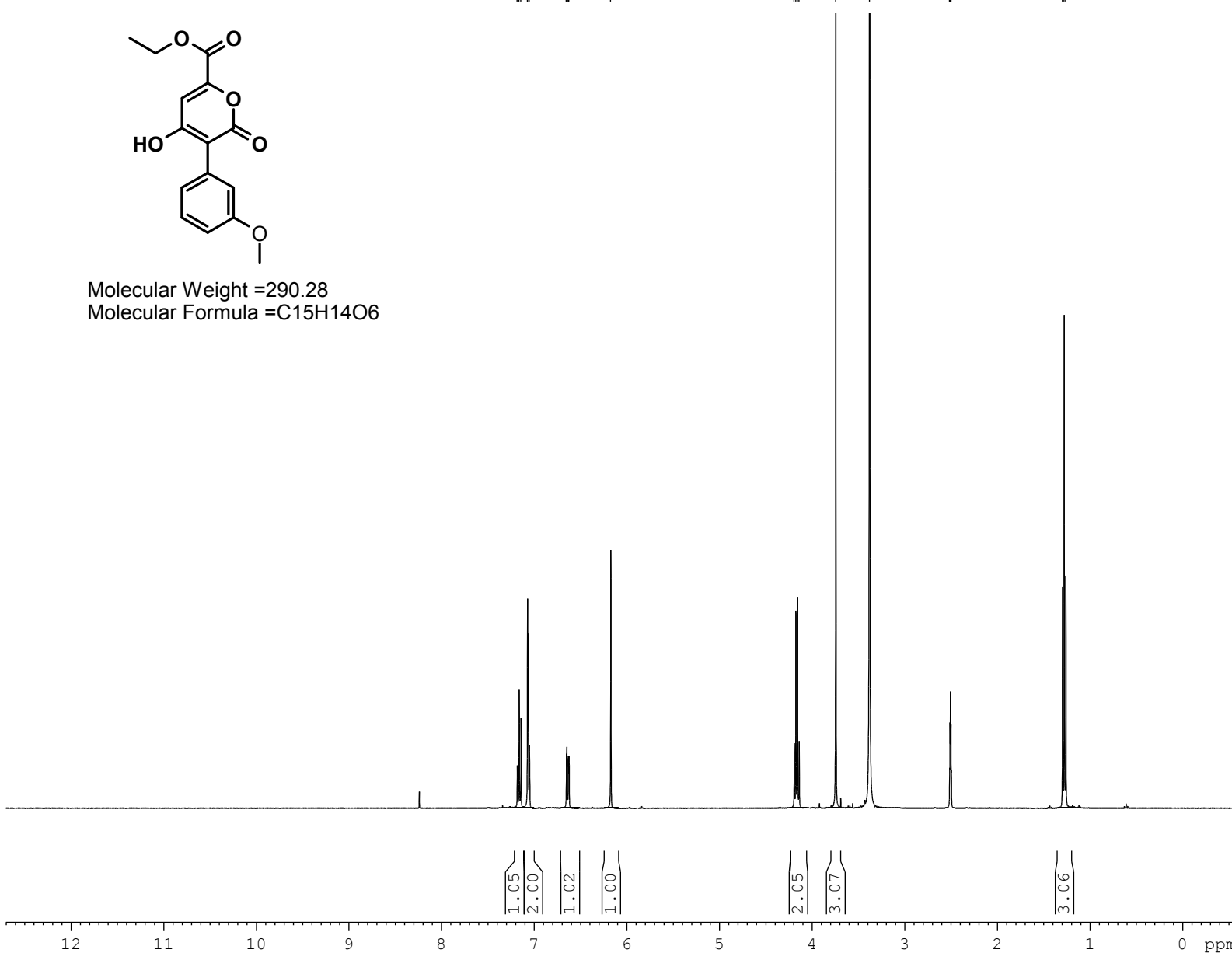
7.1861
 7.1656
 7.1453
 7.0750
 7.0713
 7.0547
 6.6549
 6.6508
 6.6463
 6.6343
 6.6330
 6.6281
 6.1762
 4.1952
 4.1775
 4.1598
 4.1421
 3.7470
 3.3824
 2.5176
 2.5132
 2.5087
 2.5042
 2.4998
 1.2982
 1.2804
 1.2628

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

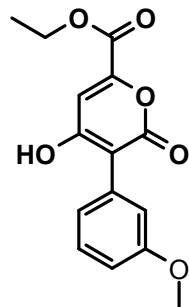
==== CHANNEL f1 =====
 NUC1 1H
 P1 10.90 usec
 PL1 -3.00 dB
 SFO1 400.1324710 MHz

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



GRD100L

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Molecular Weight =290.28
Molecular Formula =C₁₅H₁₄O₆

166.83
164.28
162.44
159.16
149.21
137.64
129.02
120.88
113.57
110.16
97.73
97.42
79.17
78.84
78.51
58.10
54.74
40.15
39.94
39.73
39.52
39.31
39.10
38.90
14.51

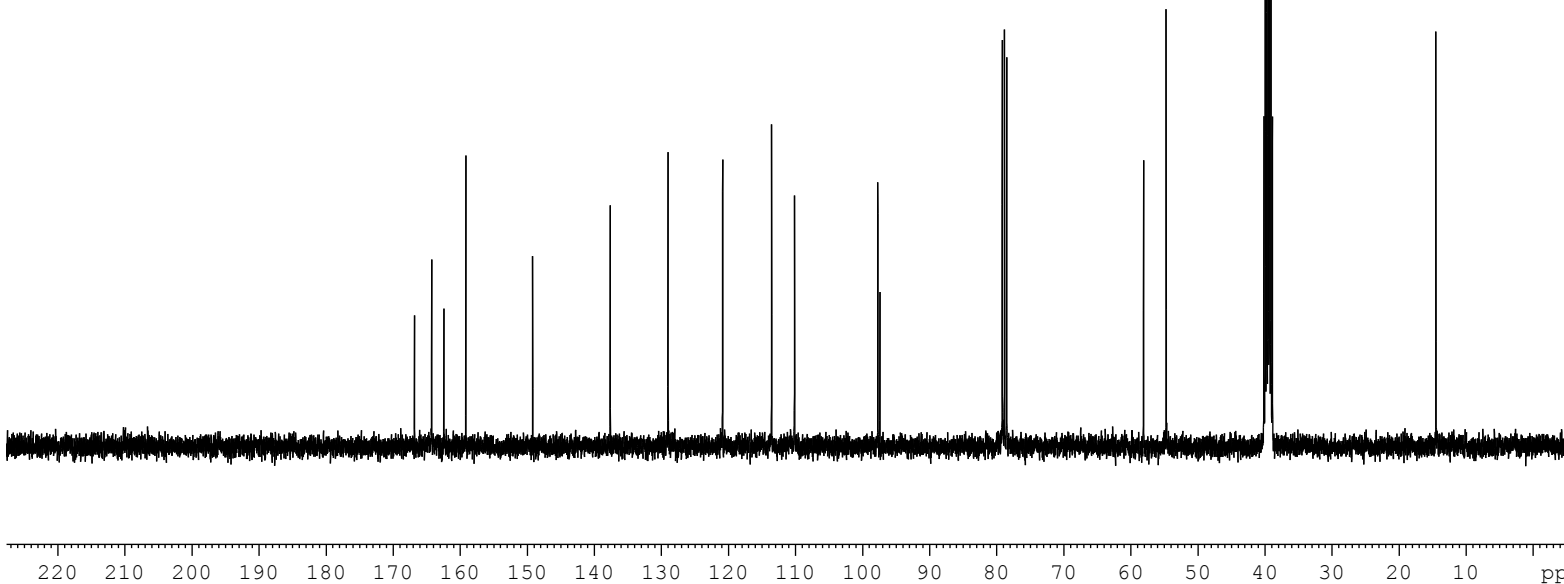
Current Data Parameters
NAME Mar15-2014
EXPNO 70
PROCNO 1

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



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

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

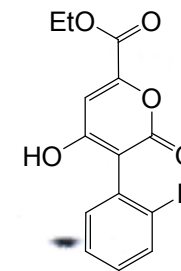
Elements Used:

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

EXT-GRD100I

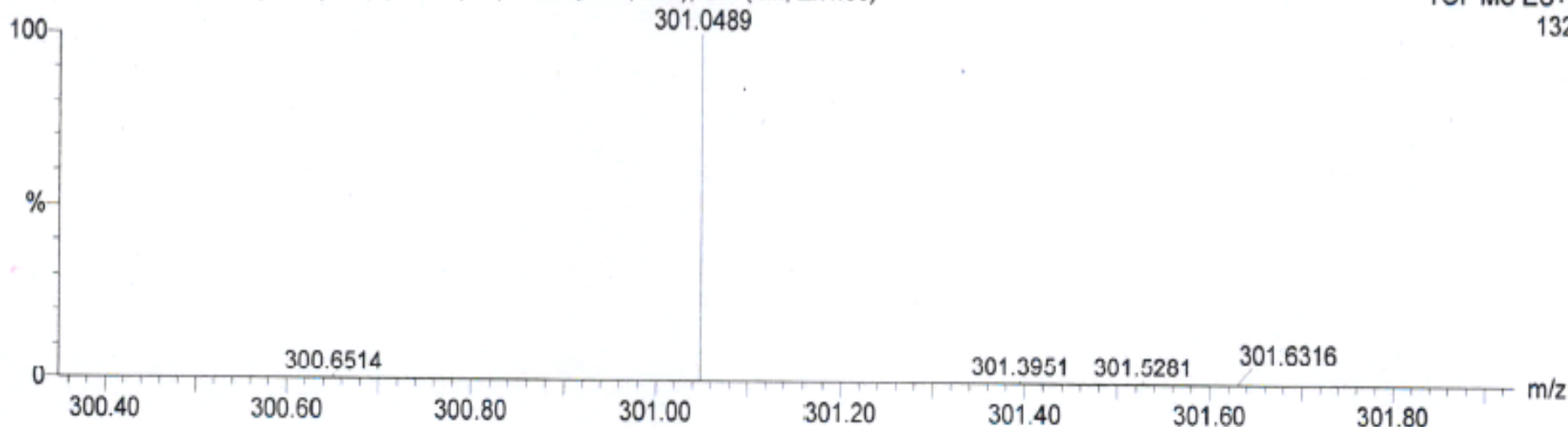
DEPARTMENT OF CHEMISTRY IITM

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



Molecular Formula =C₁₄H₁₁FO₅

16:51:2823-Aug-2014
TOF MS ES+
132



Minimum: -1.5
Maximum: 5.0 10.0 50.0

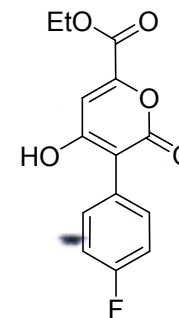
Mass	Calc. Mass	mDa	PPM	DBE	Formula
301.0489	301.0488	0.1	0.3	8.5	C ₁₄ H ₁₁ O ₅ F Na

Elemental Composition Report

Single Mass Analysis

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

Selected filters: None



Page 1

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

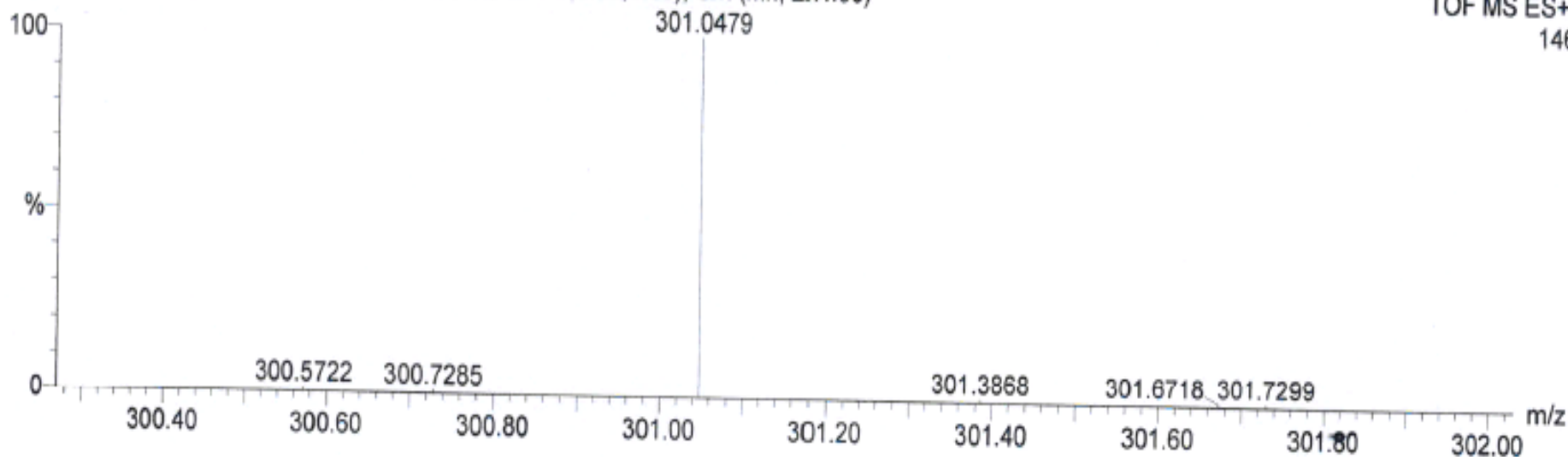
DEPARTMENT OF CHEMISTRY IITM

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:

Maximum:

-1.5

5.0

10.0

50.0

Mass	Calc. Mass	mDa	PPM	DBE	Formula
------	------------	-----	-----	-----	---------

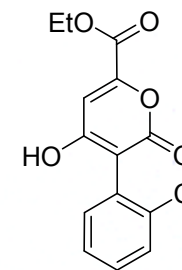
301.0479	301.0488	-0.9	-3.0	8.5	C ₁₄ H ₁₁ O ₅ F Na
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Elemental Composition Report

Single Mass Analysis

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

Selected filters: None



Page 1

C₁₄H₁₁ClO₅

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

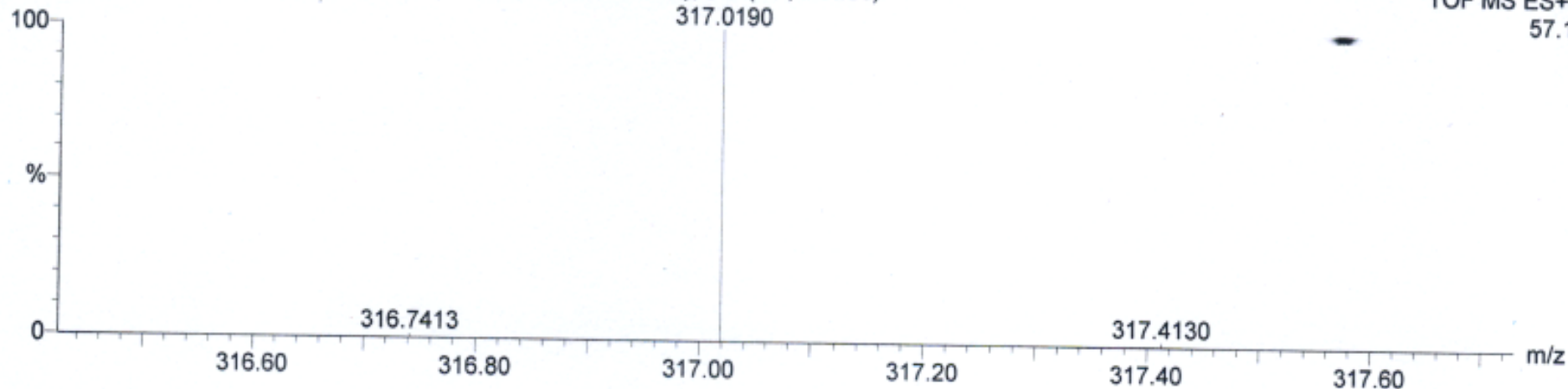
DEPARTMENT OF CHEMISTRY IITM

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:

Maximum:

5.0 10.0 -1.5
50.0

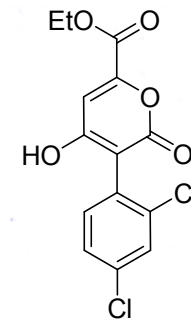
Mass	Calc. Mass	mDa	PPM	DBE	Formula
317.0190	317.0193	-0.3	-0.9	8.5	C14 H11 O5 Na Cl

Elemental Composition Report

Single Mass Analysis

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

Selected filters: None



C₁₄H₁₀Cl₂O₅

Page 1

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

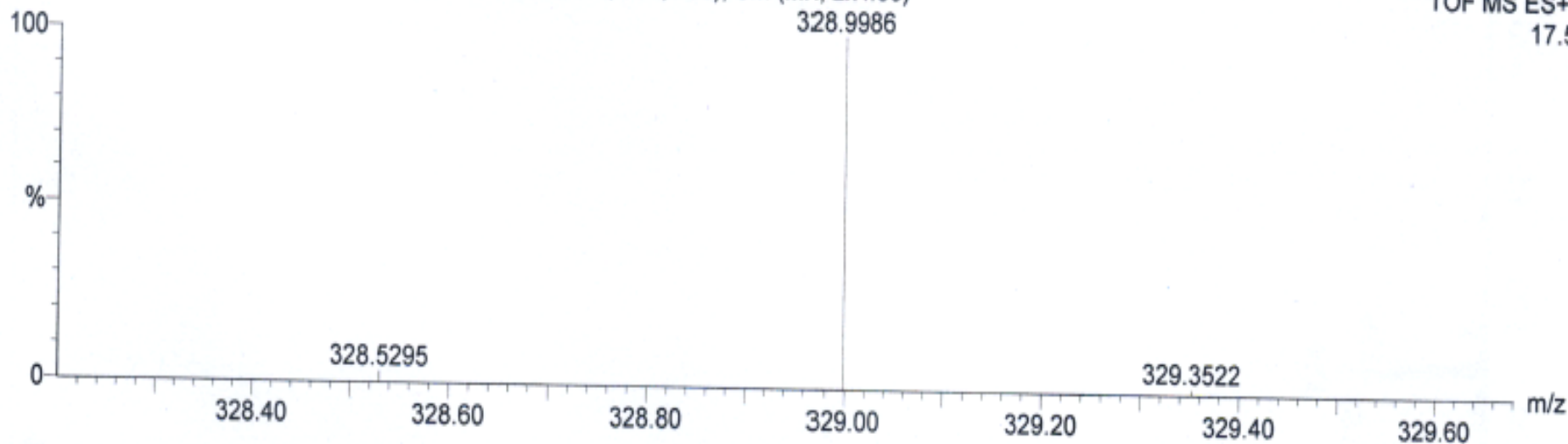
DEPARTMENT OF CHEMISTRY IITM

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:

Maximum:

Mass

Calc. Mass

mDa

PPM

DBE

Formula

328.9986

328.9984

0.2

0.6

8.5

C14 H11 O5 Cl2

-1.5

5.0

10.0

50.0

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

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

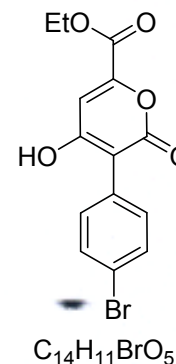
Elements Used:

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

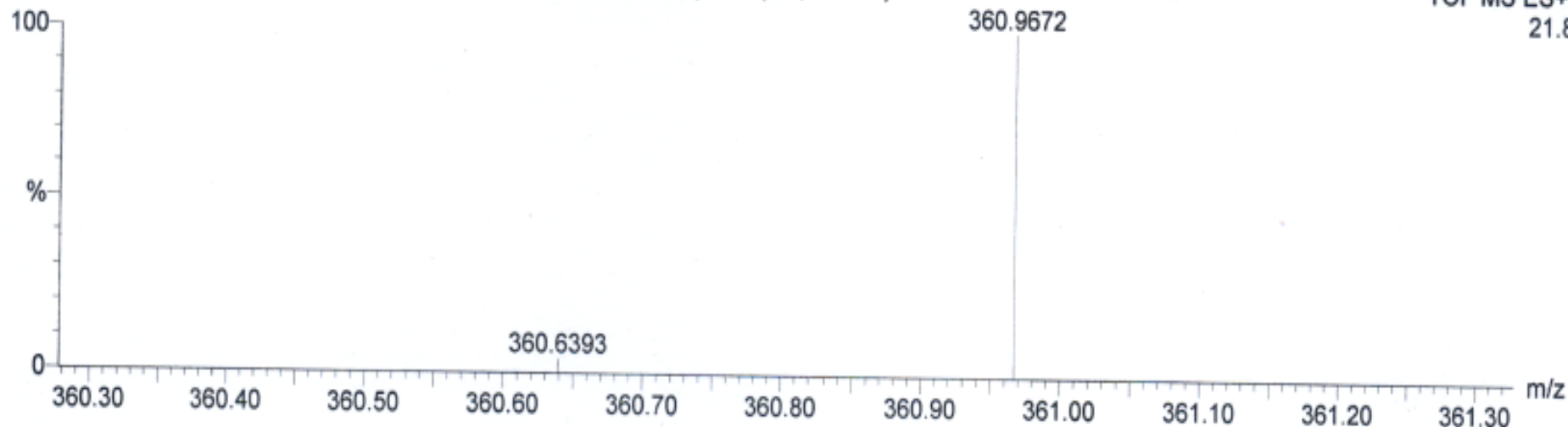
EXT-GRD100F

DEPARTMENT OF CHEMISTRY IITM

EXT_GRD100F 12 (0.121) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x4.00)



Page 1



16:40:2523-Aug-2014
TOF MS ES+
21.8

Minimum:

Maximum:

5.0 10.0 -1.5 50.0

Mass	Calc. Mass	mDa	PPM	DBE	Formula
------	------------	-----	-----	-----	---------

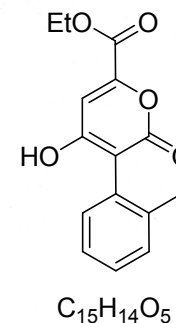
360.9672	360.9688	-1.6	-4.4	8.5	C14 H11 O5 Na Br
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Elemental Composition Report

Single Mass Analysis

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

Selected filters: None



Page 1

Monoisotopic Mass, Odd and Even Electron Ions

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

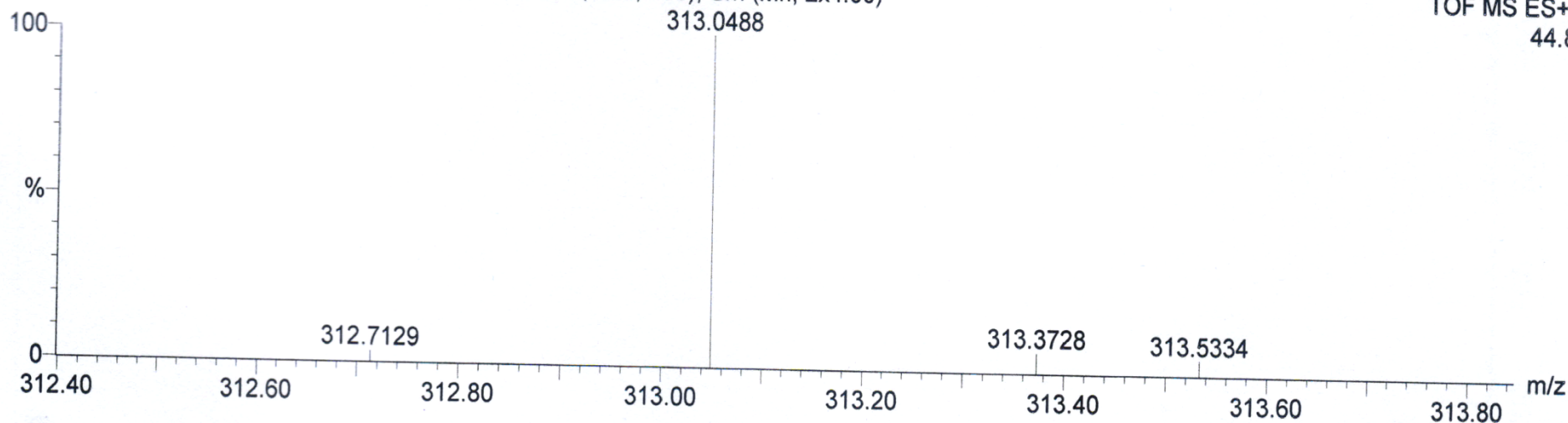
Elements Used:

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:

Maximum:

5.0 10.0 -1.5 50.0

Mass	Calc. Mass	mDa	PPM	DBE	Formula
------	------------	-----	-----	-----	---------

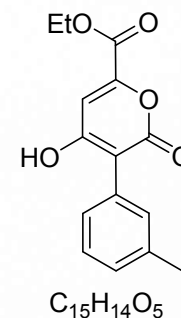
313.0488	313.0478	1.0	3.2	8.5	C15 H14 O5 K
----------	----------	-----	-----	-----	--------------

Elemental Composition Report

Single Mass Analysis

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

Selected filters: None



Page 1

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

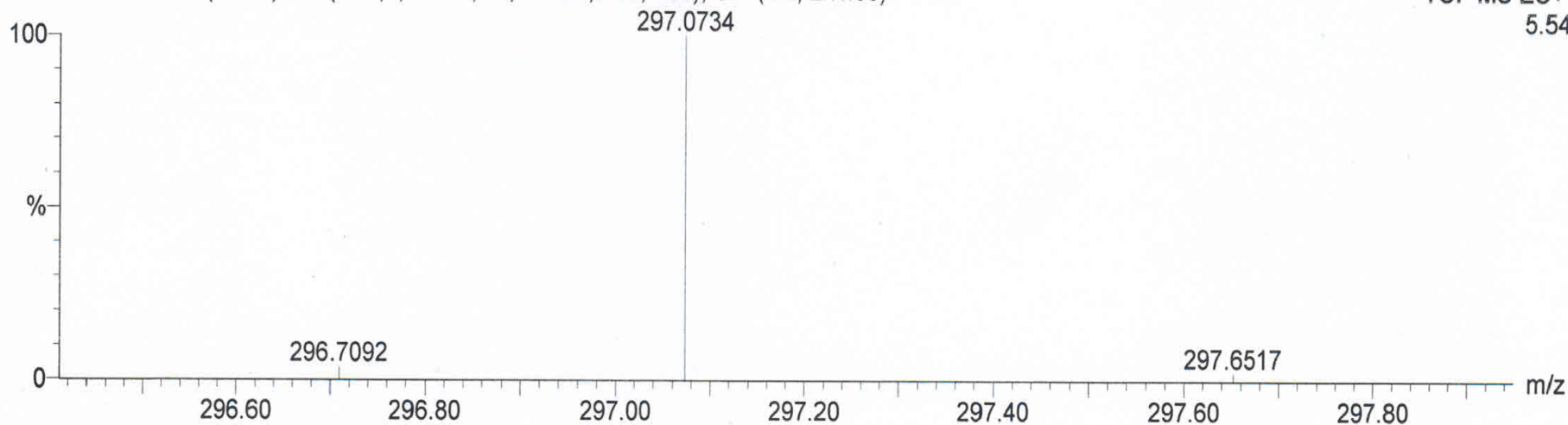
DEPARTMENT OF CHEMISTRY IITM

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:

Maximum:

5.0

10.0

-1.5

50.0

Mass	Calc. Mass	mDa	PPM	DBE	Formula
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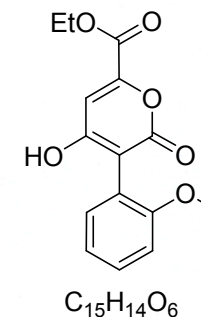
297.0734	297.0739	-0.5	-1.7	8.5	C15 H14 O5 Na
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Elemental Composition Report

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

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)

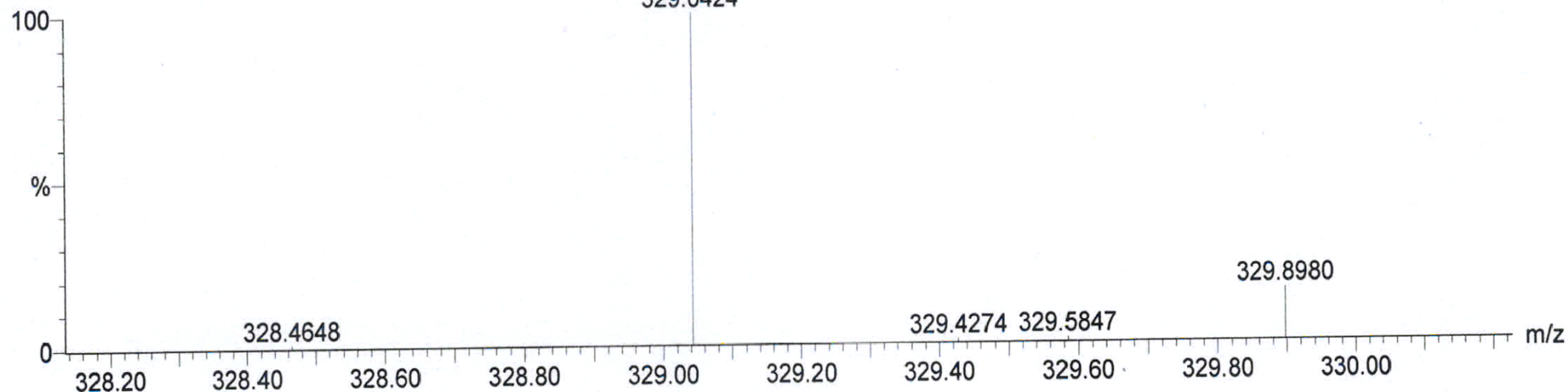
DEPARTMENT OF CHEMISTRY IITM

17:33:2013-Aug-2014

TOF MS ES+

69.3

329.0424



Minimum: -1.5
Maximum: 5.0 10.0 50.0

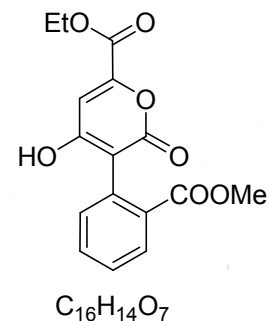
Mass	Calc. Mass	mDa	PPM	DBE	Formula
329.0424	329.0427	-0.3	-0.9	8.5	C15 H14 O6 K

Elemental Composition Report

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

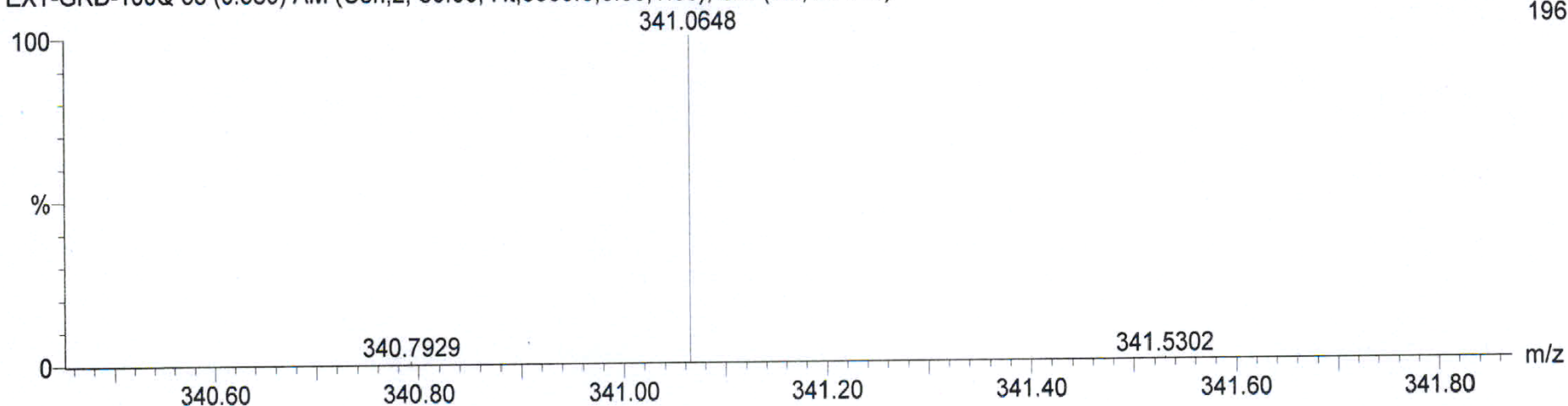
EXT-GRD-100Q 38 (0.389) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x4.00)

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17:37:3613-Aug-2014

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