

Supplementary Material

Metal-free approach for one-pot synthesis of 3-aryl-furo[3,2-c]coumarins

Mrugesh Patel¹, Paranjay Parikh¹, Jignesh Timaniya,¹ and Kaushal Patel^{1*}

¹ Department of Advanced Organic Chemistry, P. D. Patel Institute of Applied Sciences,
Charotar University of Science and Technology, Gujarat 388421, India.

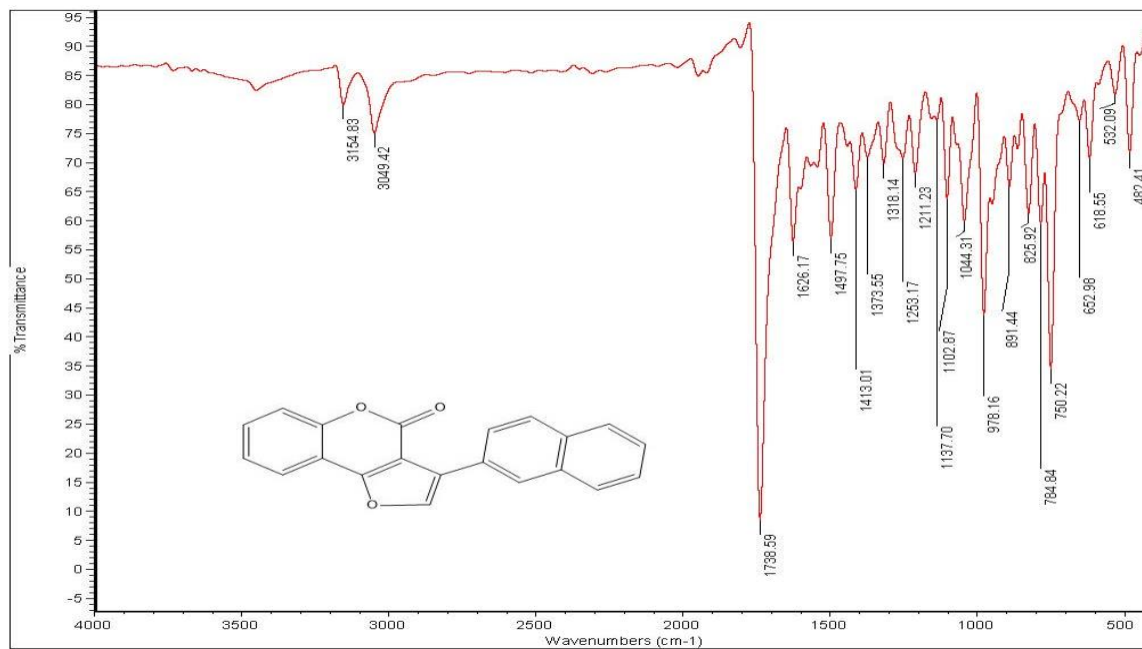
Email: kaus_chem@yahoo.com

Table of Contents

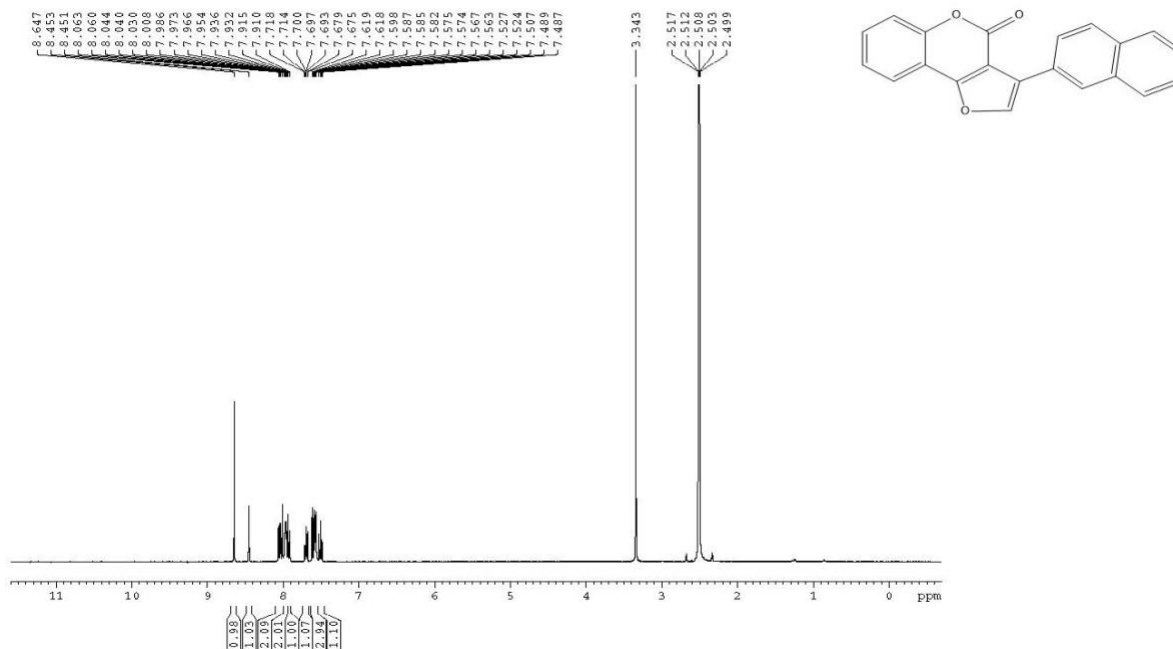
1. I.R. Spectra, ¹ H NMR, ¹³ C NMR, DEPT-90 and Mass spectra figures for 2a-2d	S2
2. I.R. Spectra, ¹ H NMR, ¹³ C NMR, DEPT-90 and Mass spectra figures for 3a-3d	S20
3. I.R. Spectra, ¹ H NMR, ¹³ C NMR, DEPT-90 and Mass spectra figures for 4a-4d	S37

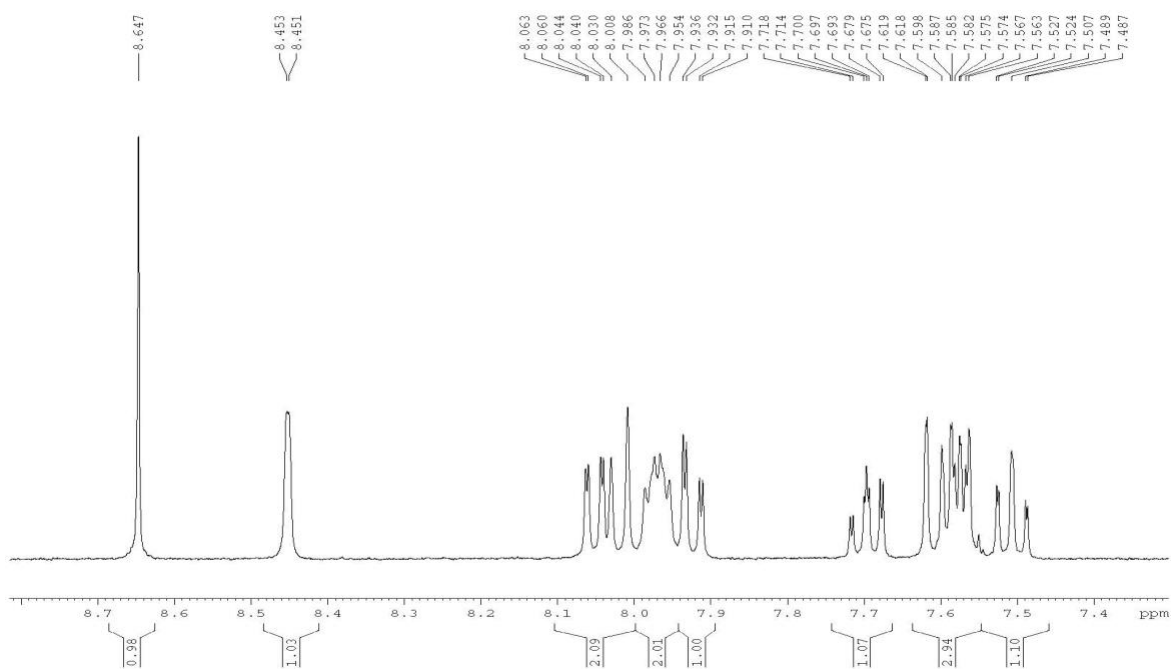
Compound 2a

Infrared Spectra

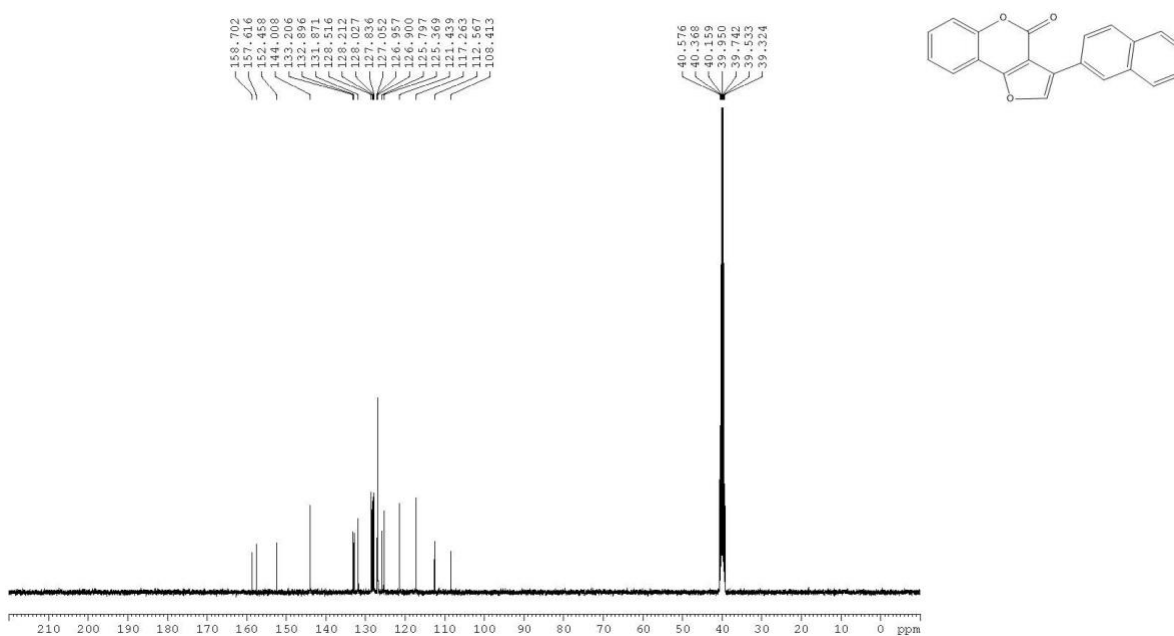


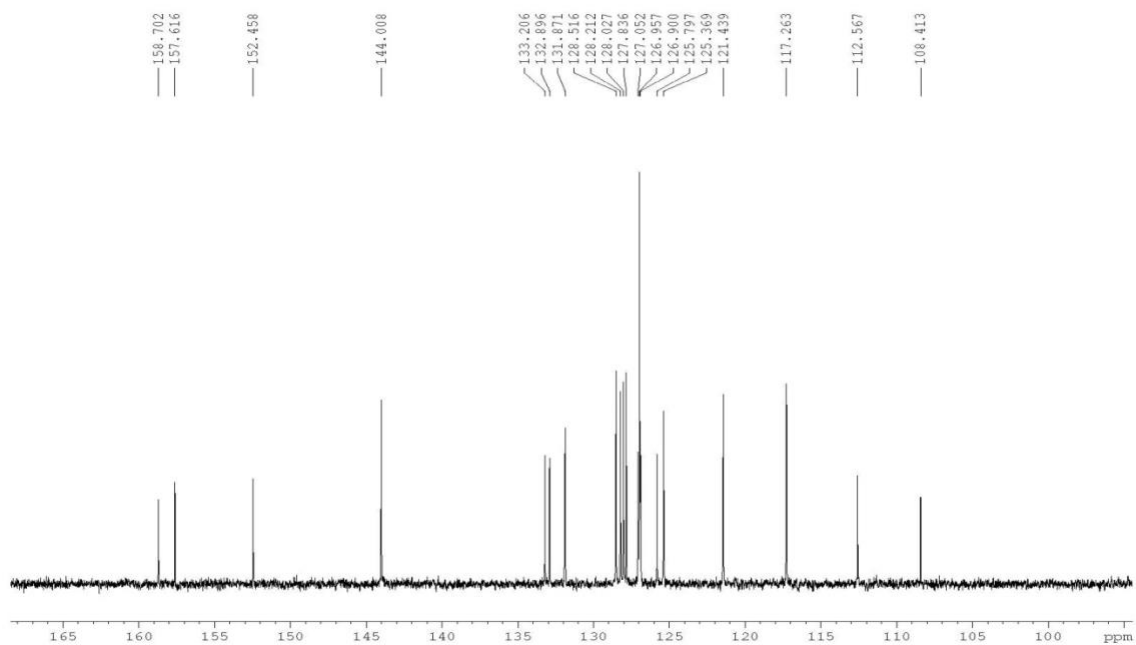
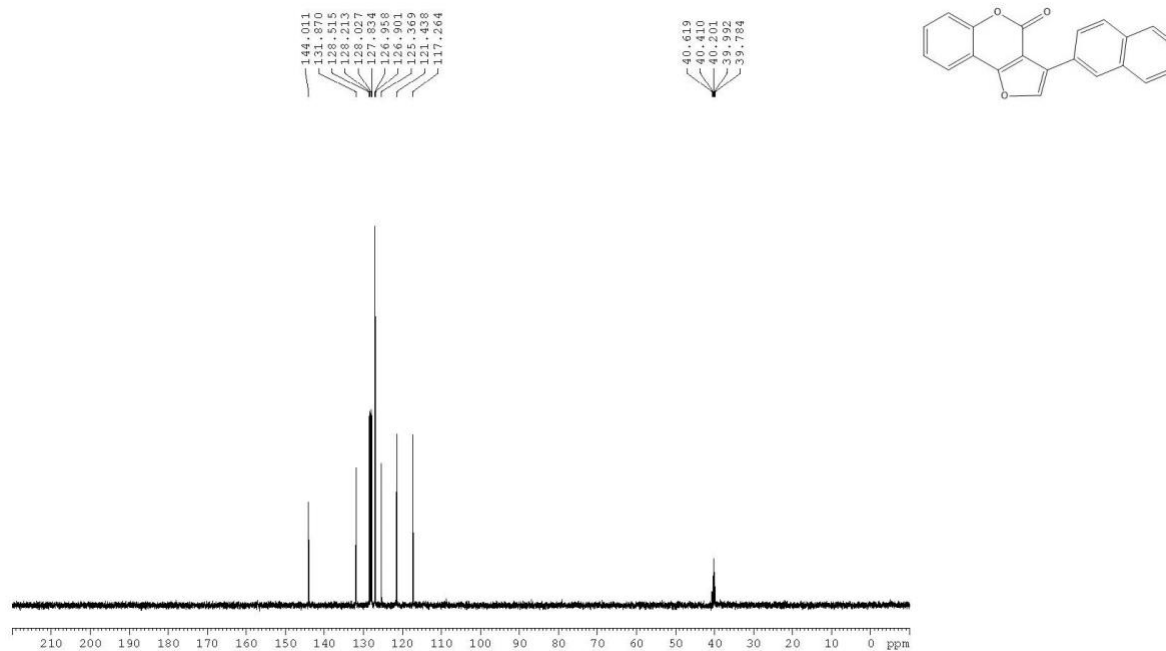
Compound 2a

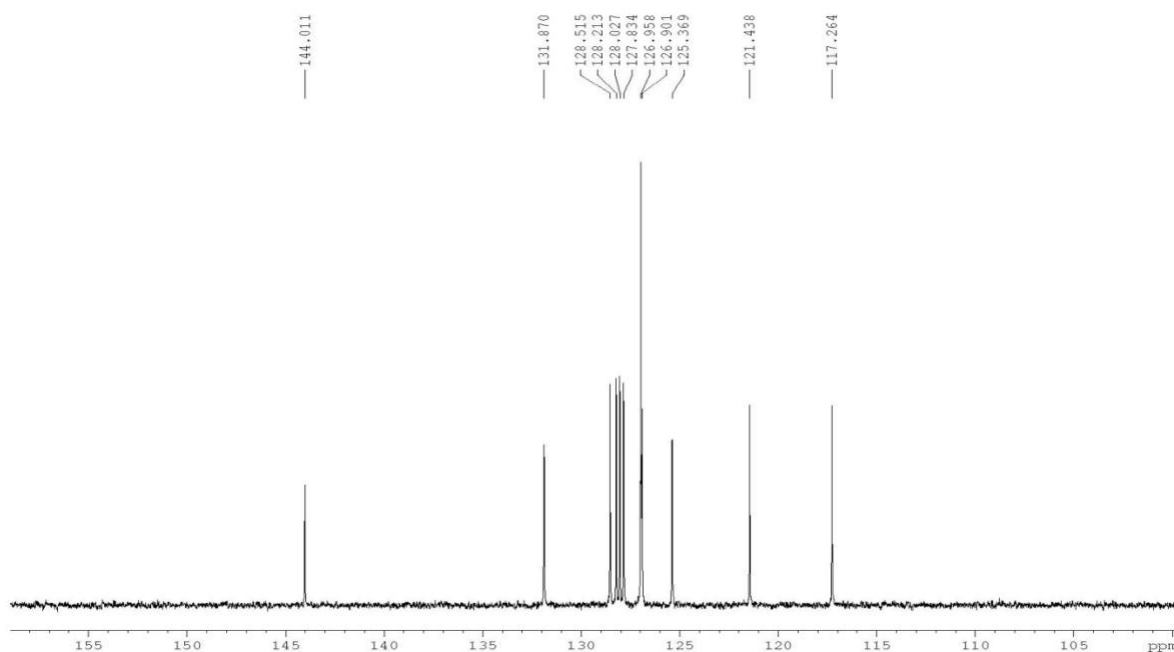
¹H NMR spectra



Compound 2a

¹³C NMR spectra

**Compound 2a****DEPT-90 spectra**



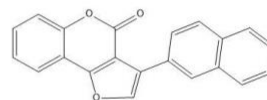
Compound 2a

Mass spectra

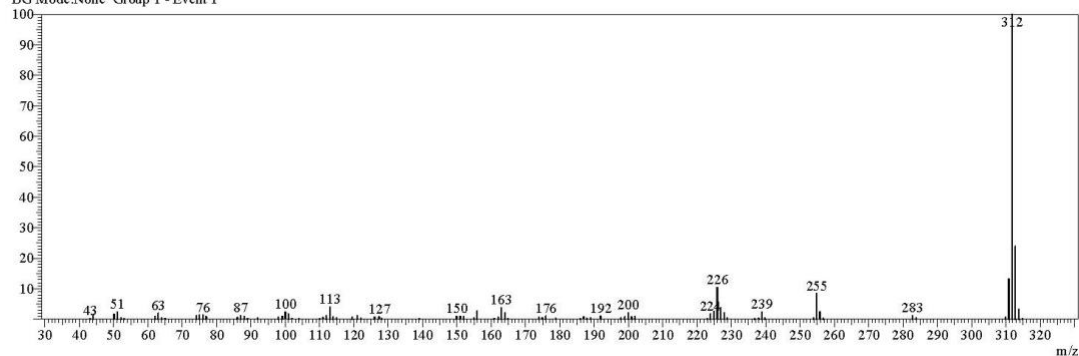
DEPARTMENT OF CHEMISTRY
(DST-FIST Funded & UGC-SAP Sponsored)
SAURASHTRA UNIVERSITY
RAJKOT-360005

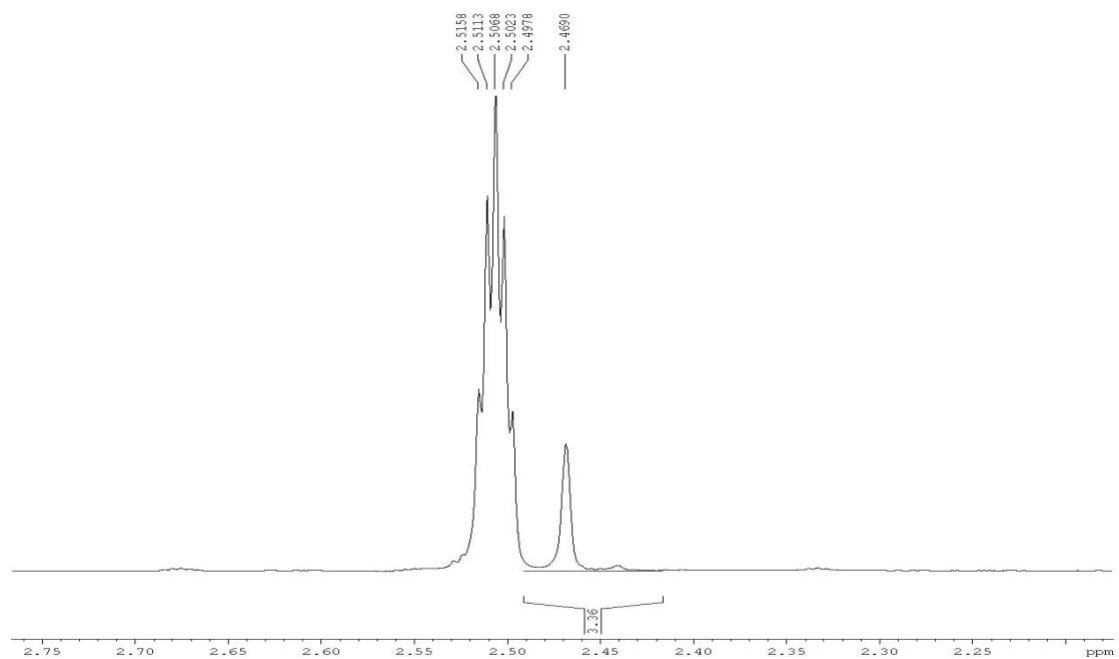
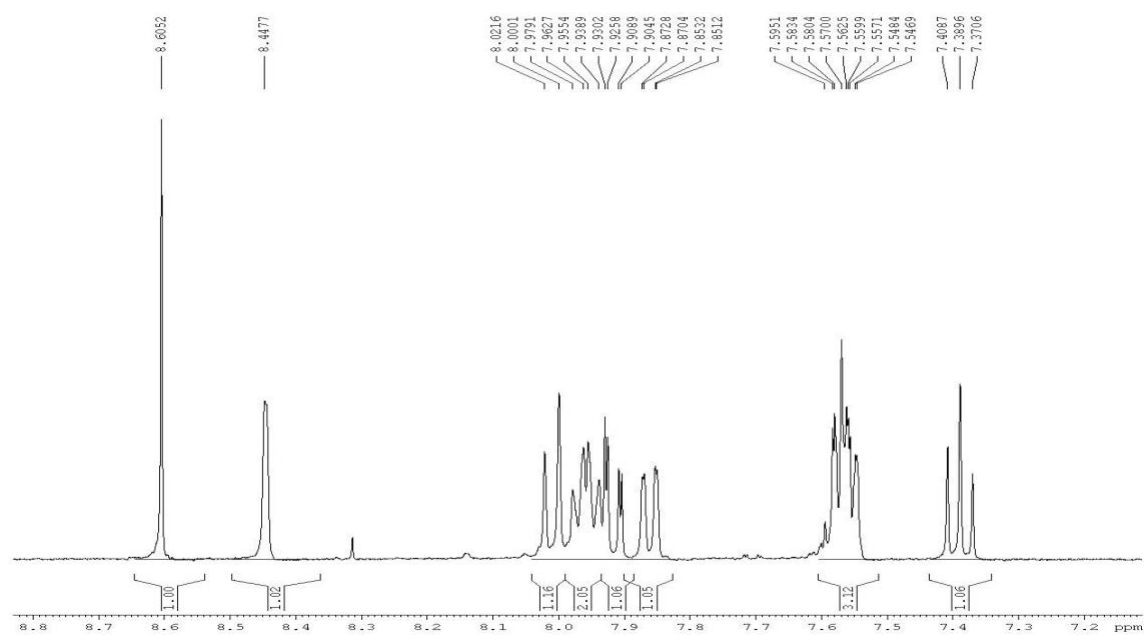
Sample Information

Analyzed by : BHOLA GAURAV
Analyzed : 2/3/2015 4:07:51 PM
Sample Name : M-8
Sample ID : M-8
Data File : D:\OUT OF DEPRKAUSHAL PATEL\M-8.apd
Tuning File : C:\GCMS\software\System\Tune\1020215_F1.MS.gcf

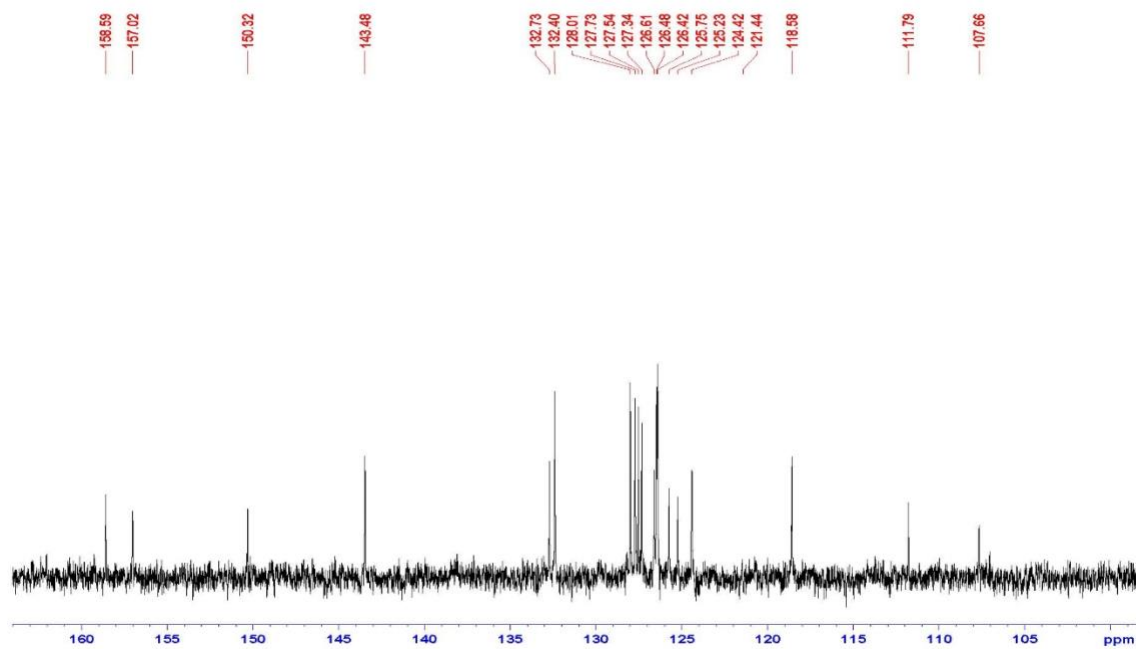
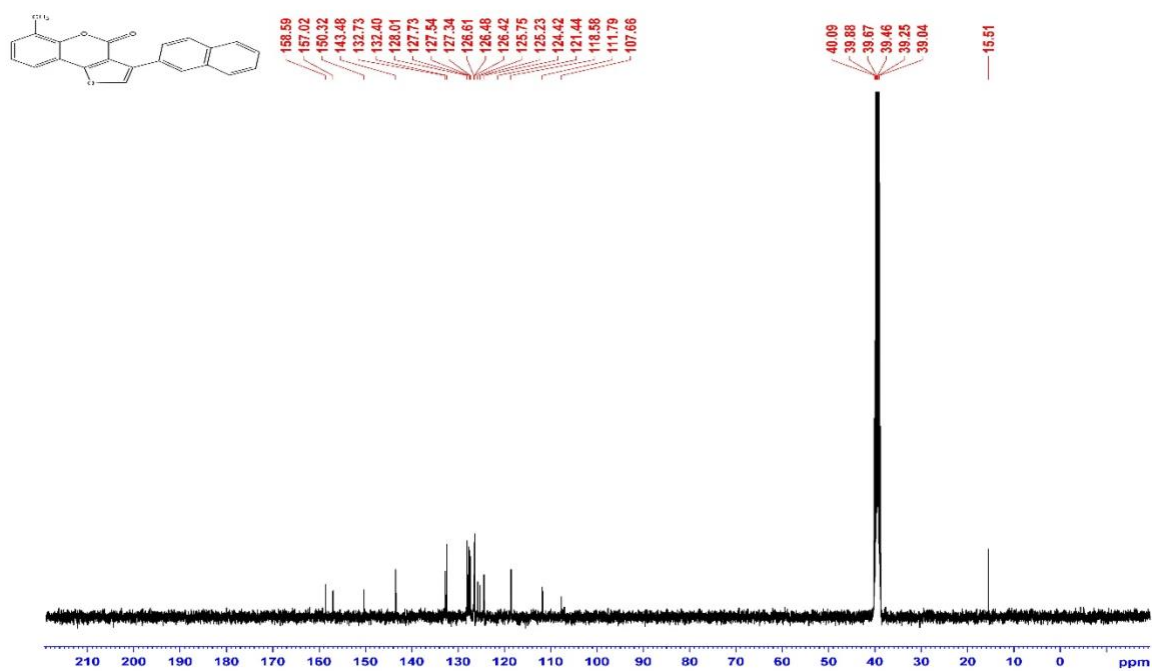


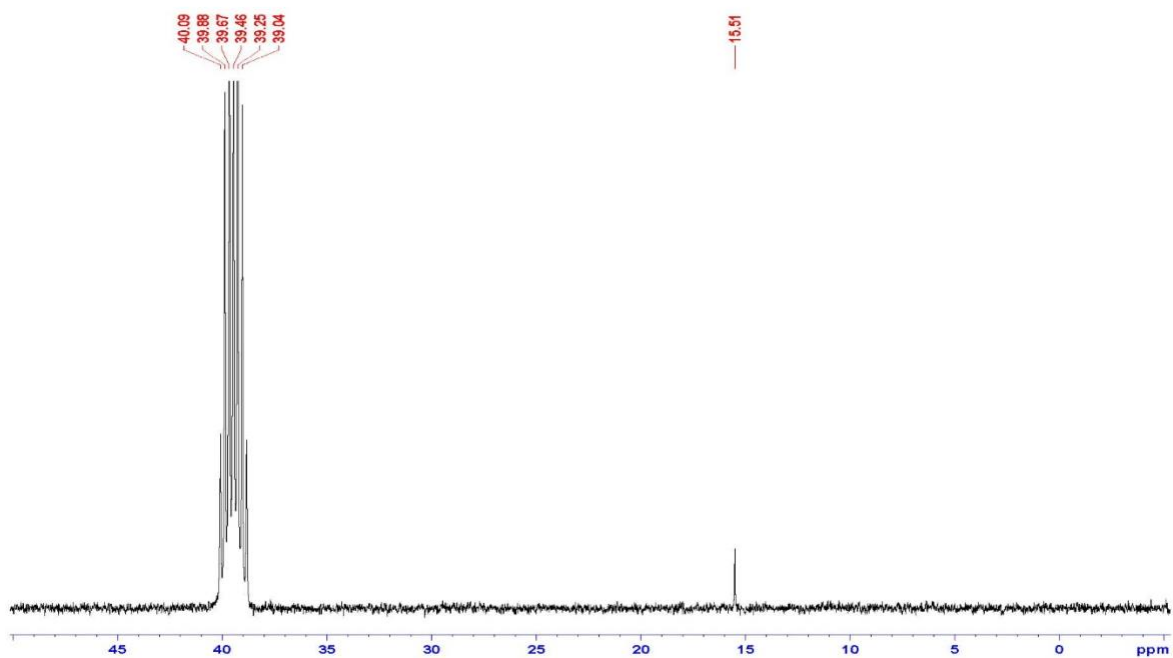
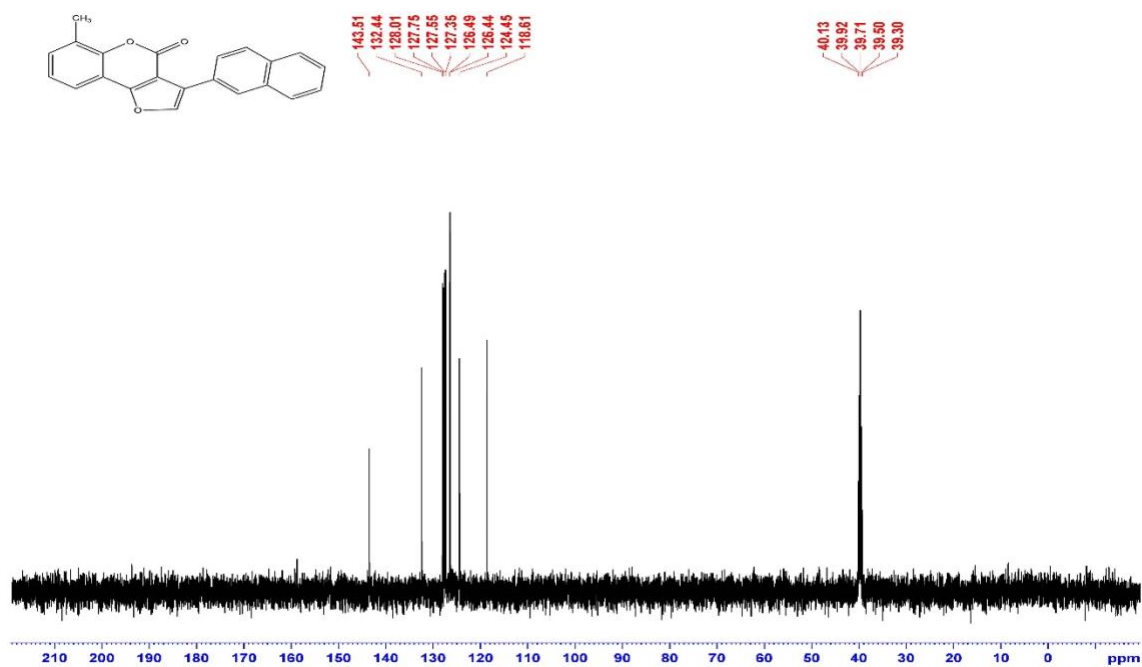
Line#: 1 R.Time: 2.7 (Scan#: 446)
MassPeaks: 86
RawMode: Averaged 1.5-3.8 (201-662) BasePeak: 311.800 (25882)
BG Mode: None Group 1 - Event 1

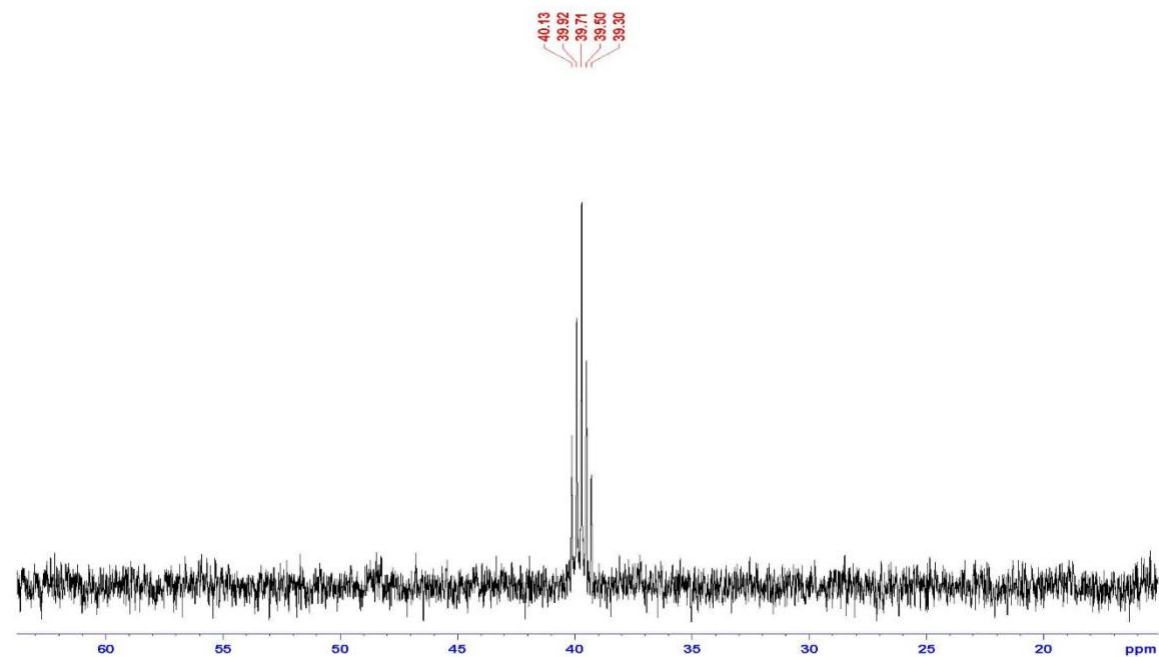
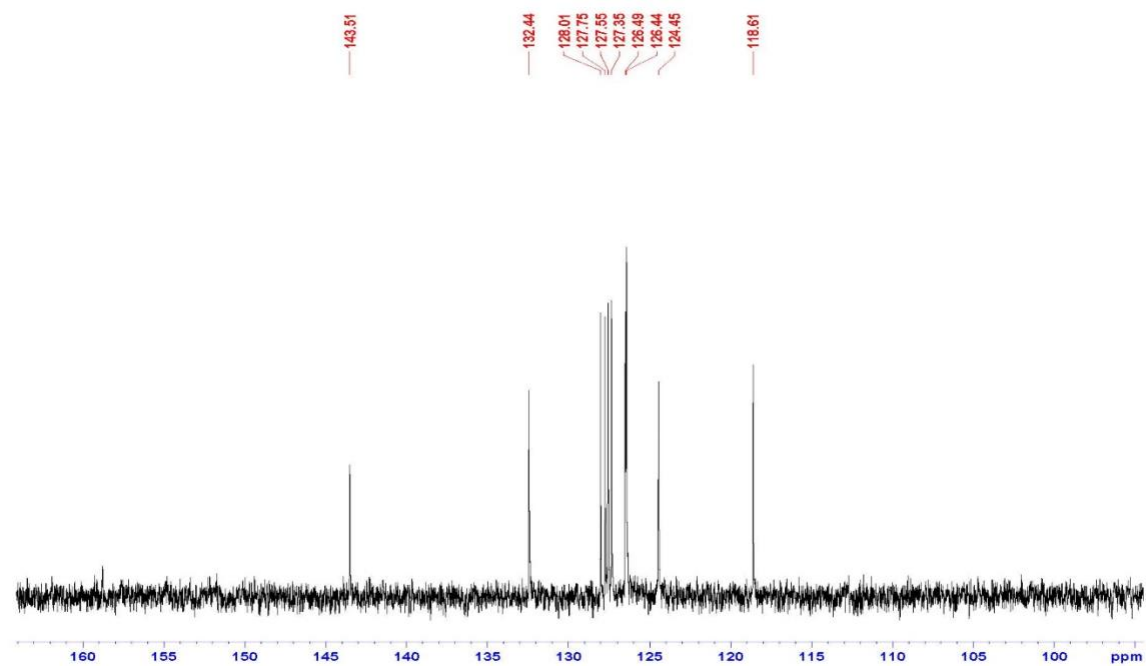




Compound 2b

 ^{13}C NMR spectra

**Compound 2b****DEPT-90 spectra**



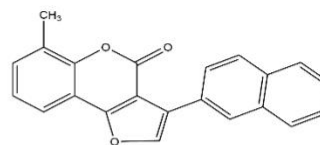
Compound 2b

Mass spectra

DEPARTMENT OF CHEMISTRY
(DST-FIST Funded & UGC-SAP Sponsored)
SAURASHTRA UNIVERSITY
RAJKOT-360005

Sample Information

Analyzed by : BHOLA GAURAV
Analyzed : 23/2015 1:11:55 PM
Sample Name : M10
Sample ID : M10
Data File : D:\OUT OF DEPQAUSHA\ALPATELM10.qgd
Tuning File : C:\GCMSolution\System1\Tune1020215_F1.MS.qgd

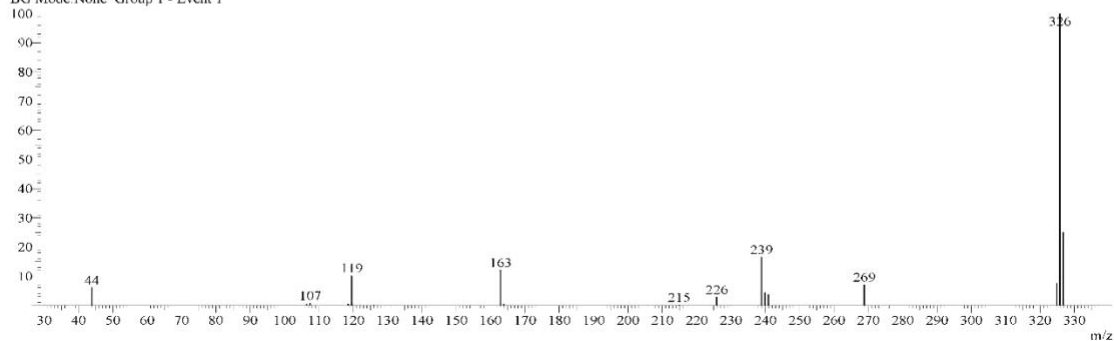


Line#: 1 R Time: 4.0 (Scan#: 426)

MassPeaks: 18

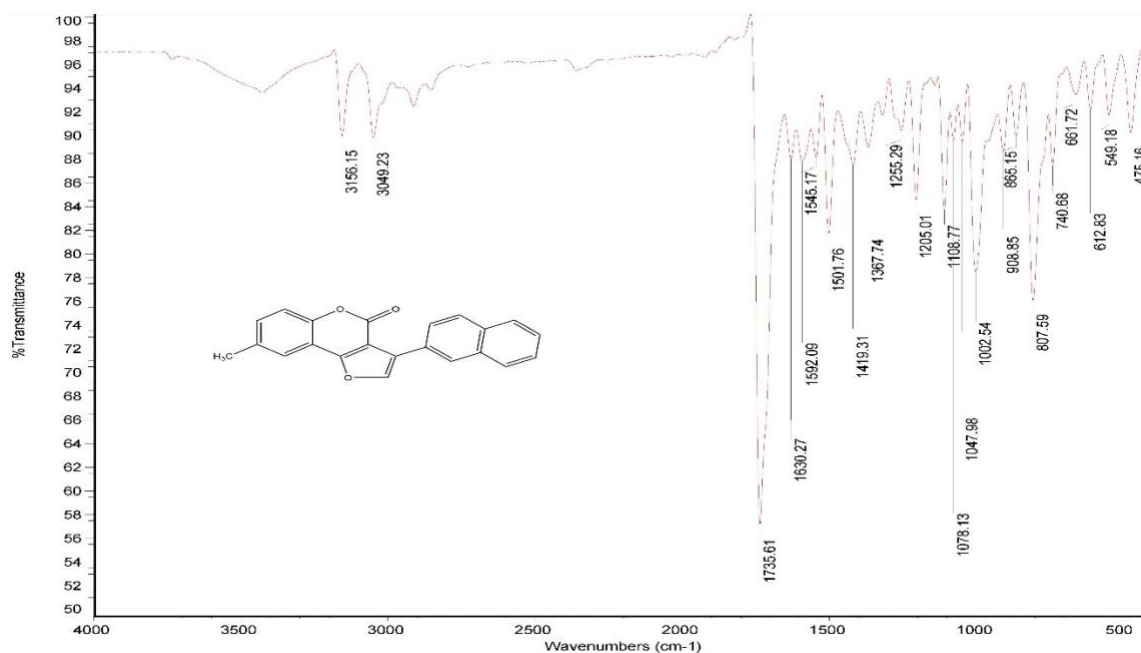
RawMode: Averaged 2.1-5.4 (189-588) BasePeak: 325.800(9383)

BG Mode: None Group 1 - Event 1

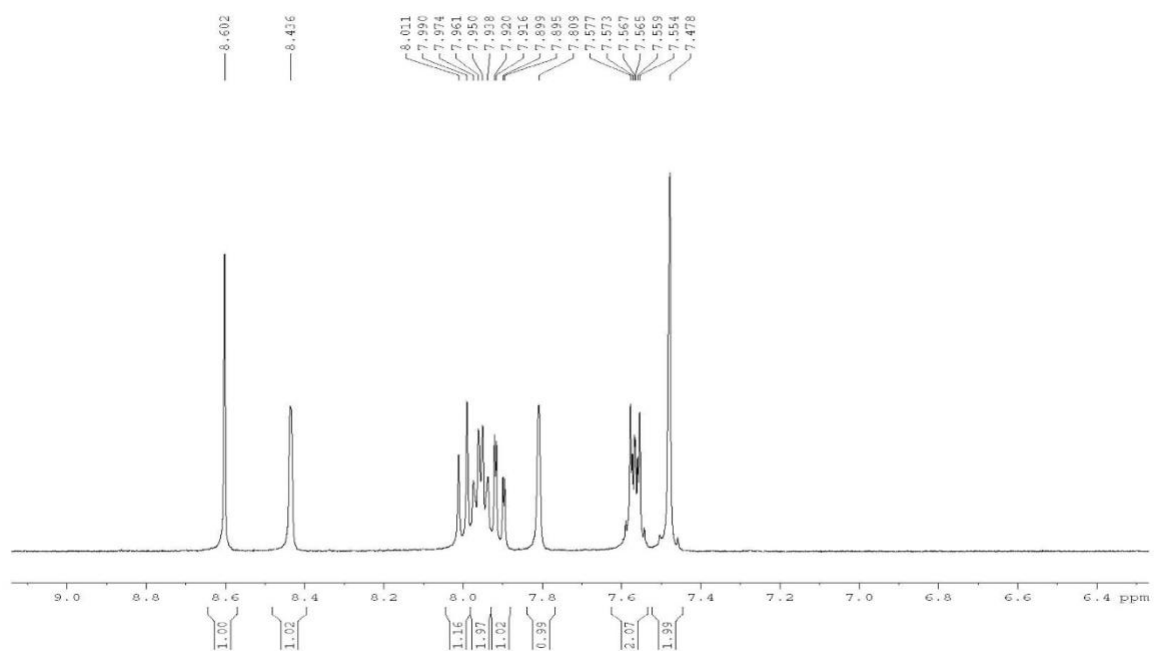
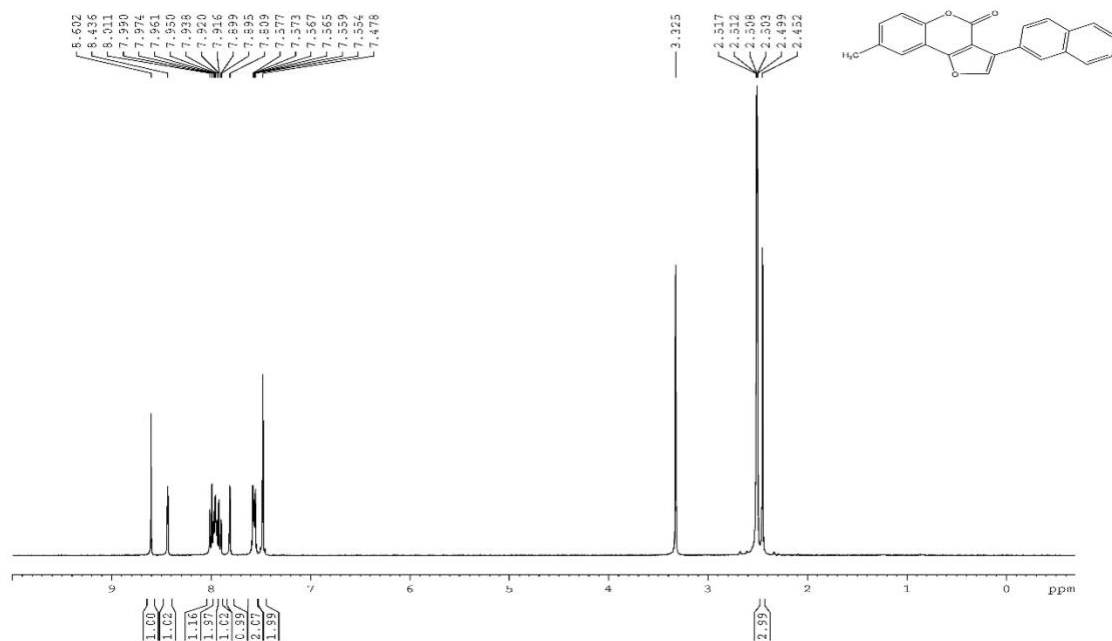


Compound 2c

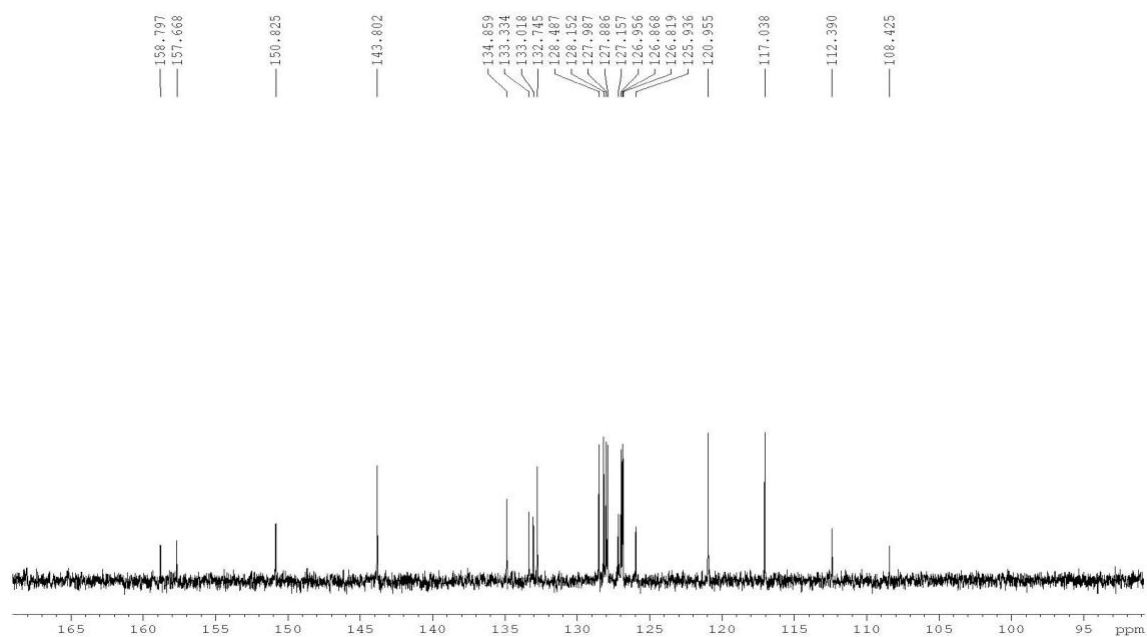
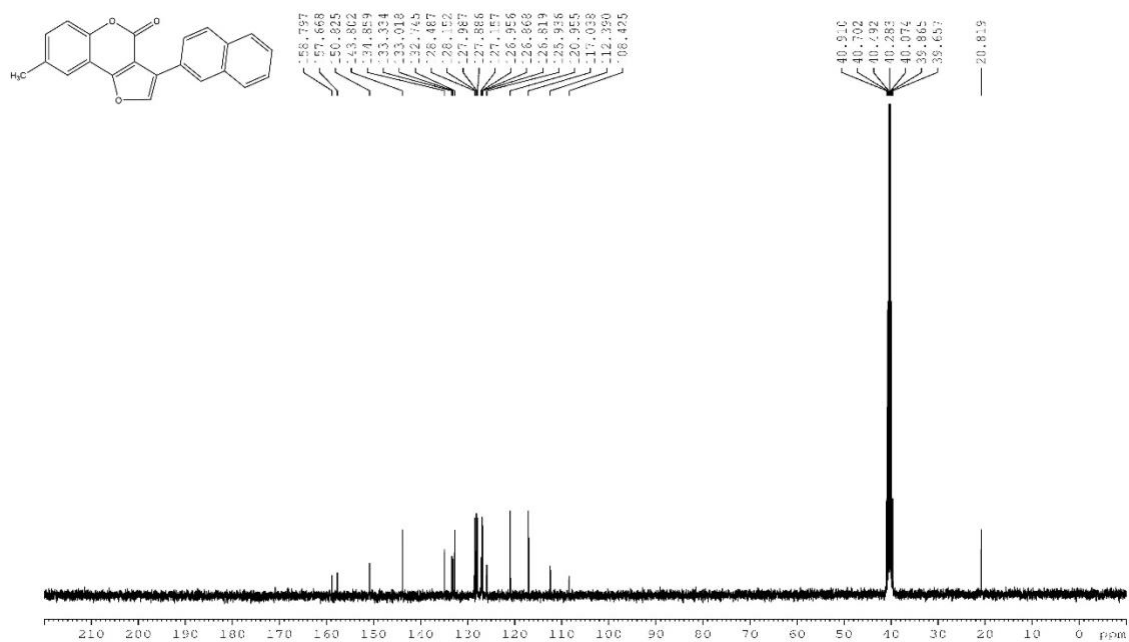
Infrared Spectra

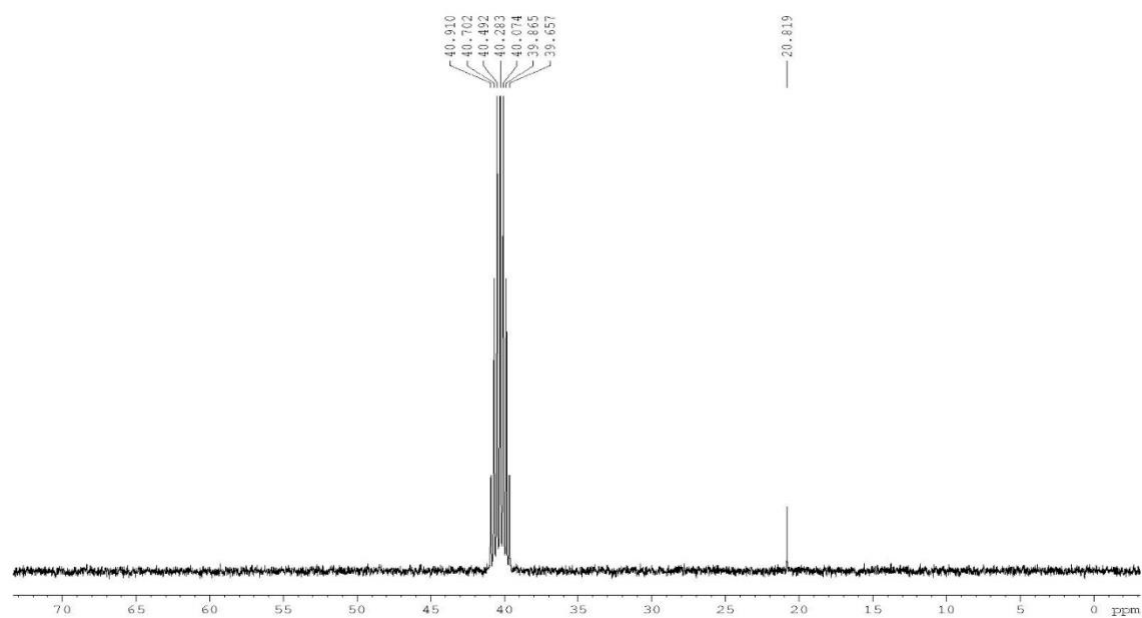
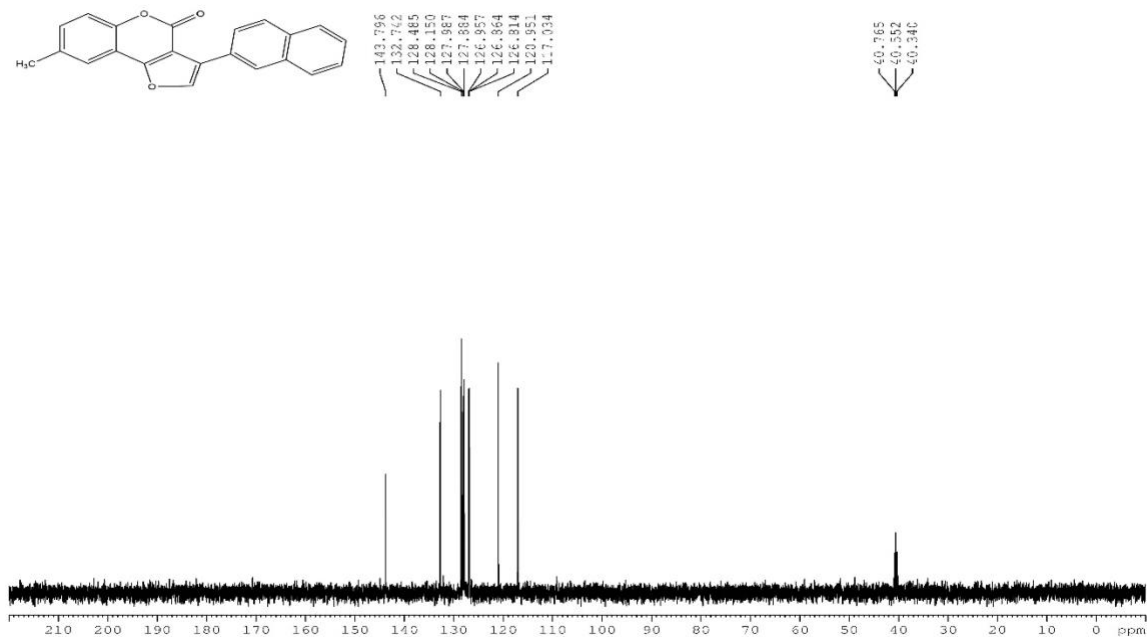


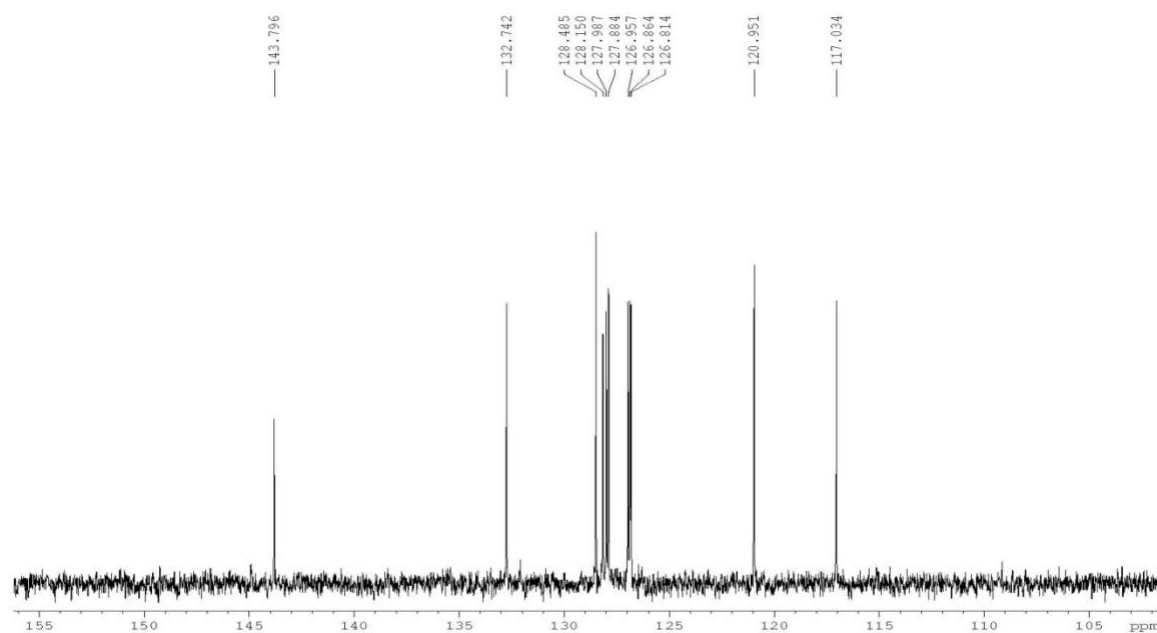
Compound 2c

 ^1H NMR spectra

Compound 2c

¹³C NMR spectra

**Compound 2c****DEPT-90 spectra**



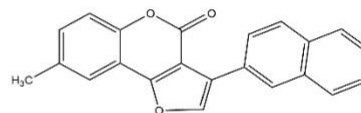
Compound 2c

Mass spectra

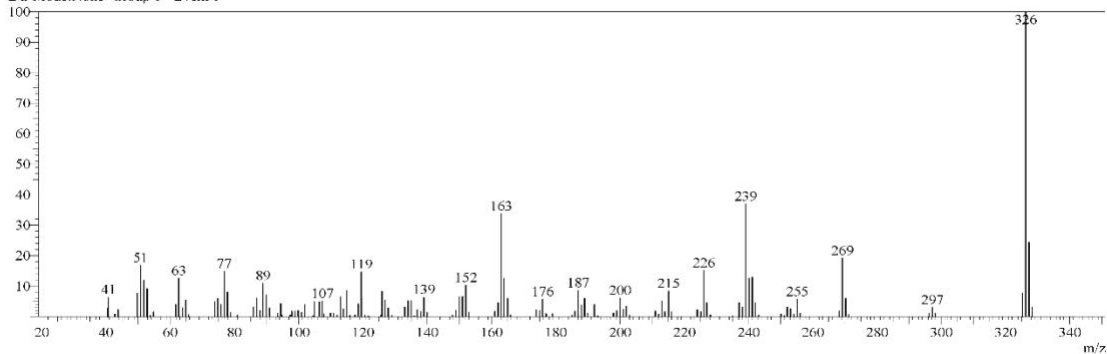
DEPARTMENT OF CHEMISTRY
(DST-FIST Funded & UGC-SAP Sponsored)
SAURASHTRA UNIVERSITY
RAJKOT-360005

Sample Information

Analyzed by : BHOLA GAURAV
Analyzed : 1/28/2015 4:21:57 PM
Sample Name : M-9
Sample ID : M-9
Data File : D:\PROJECT-1\DI.ms.qgd
Tuning File : C:\GCMSolution\System1\Tune1\240115_F1_MS.qgt

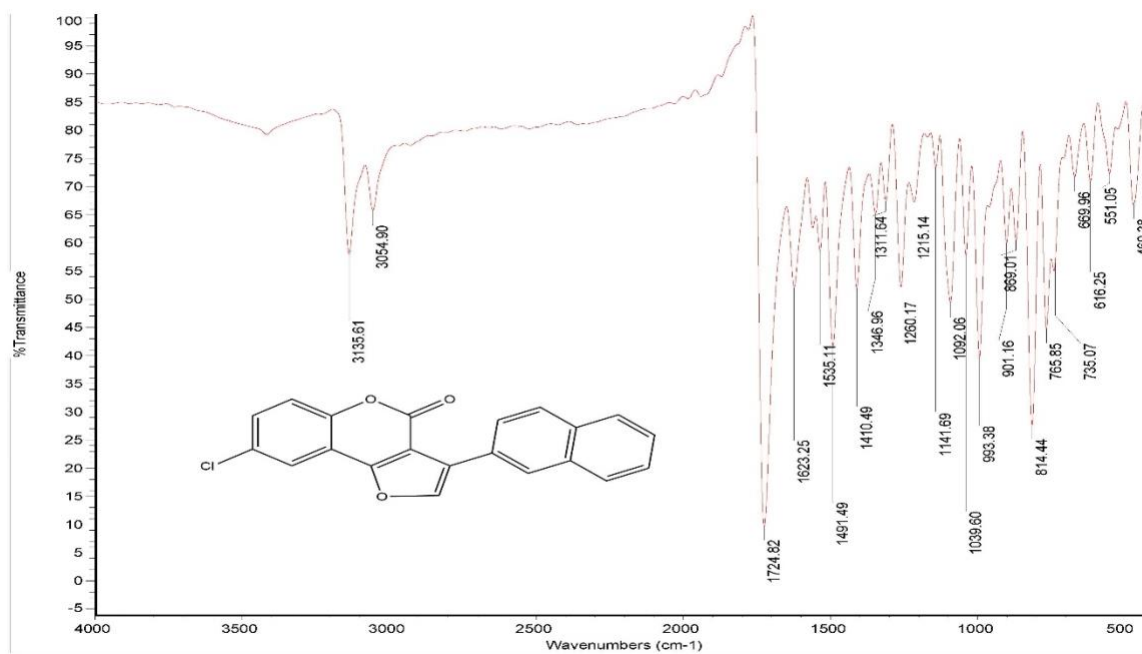


Line#: 1 RTime: 3.2 (Scan#: 319)
MassPeaks: 136
RawMode: Averaged 2.4-3.9 (224-410) BasePeak: 326.300 (3341)
BG Mode: None Group 1 - Event 1

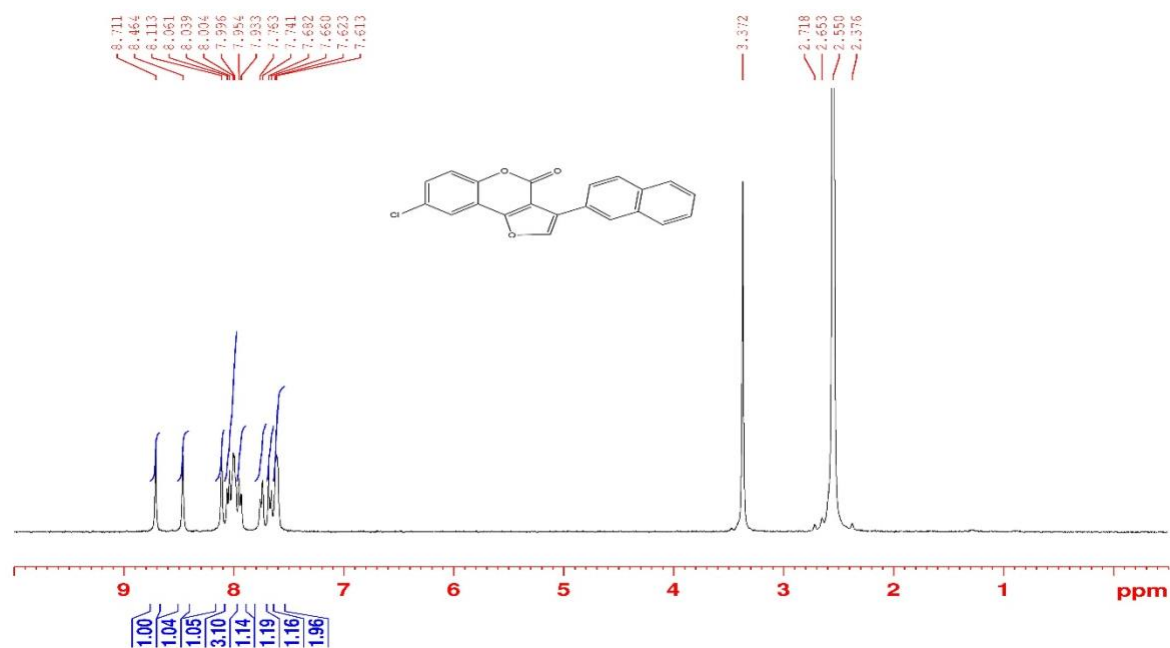


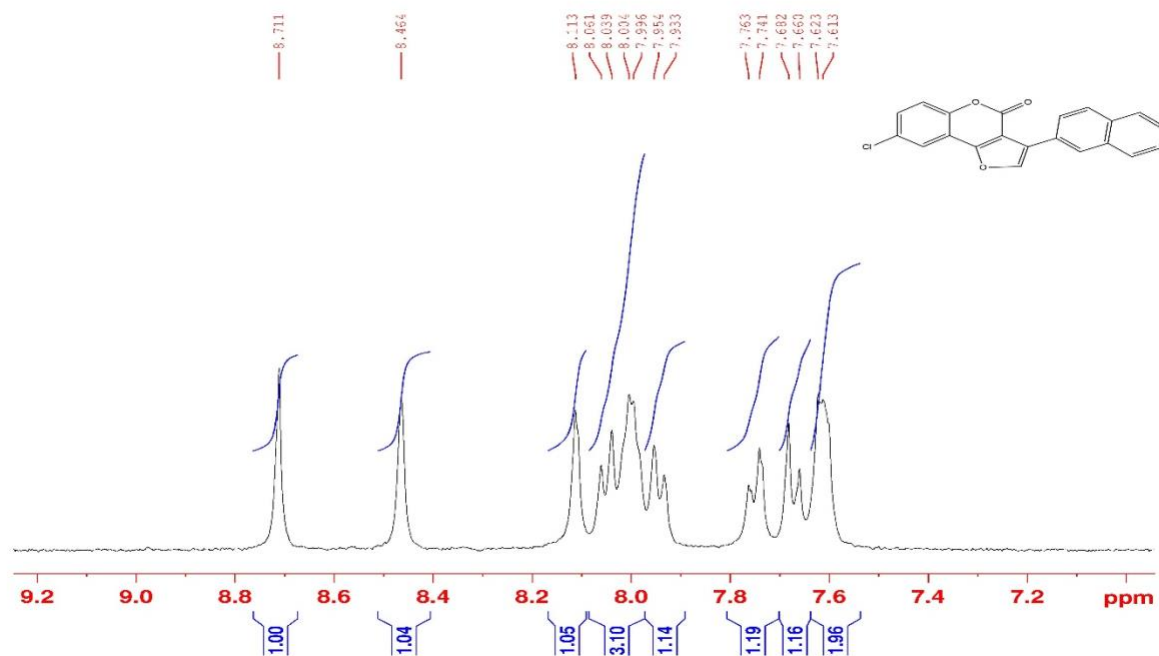
Compound 2d

Infrared Spectra

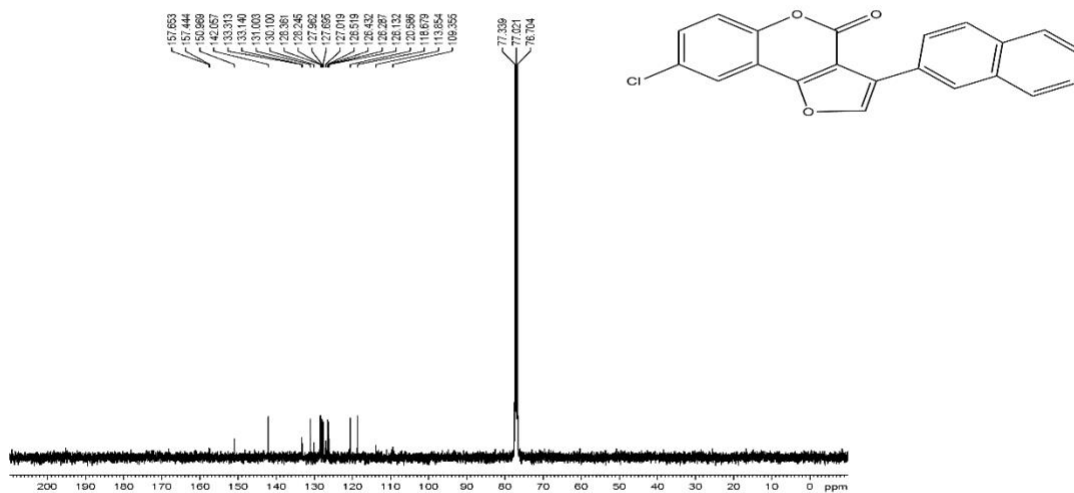


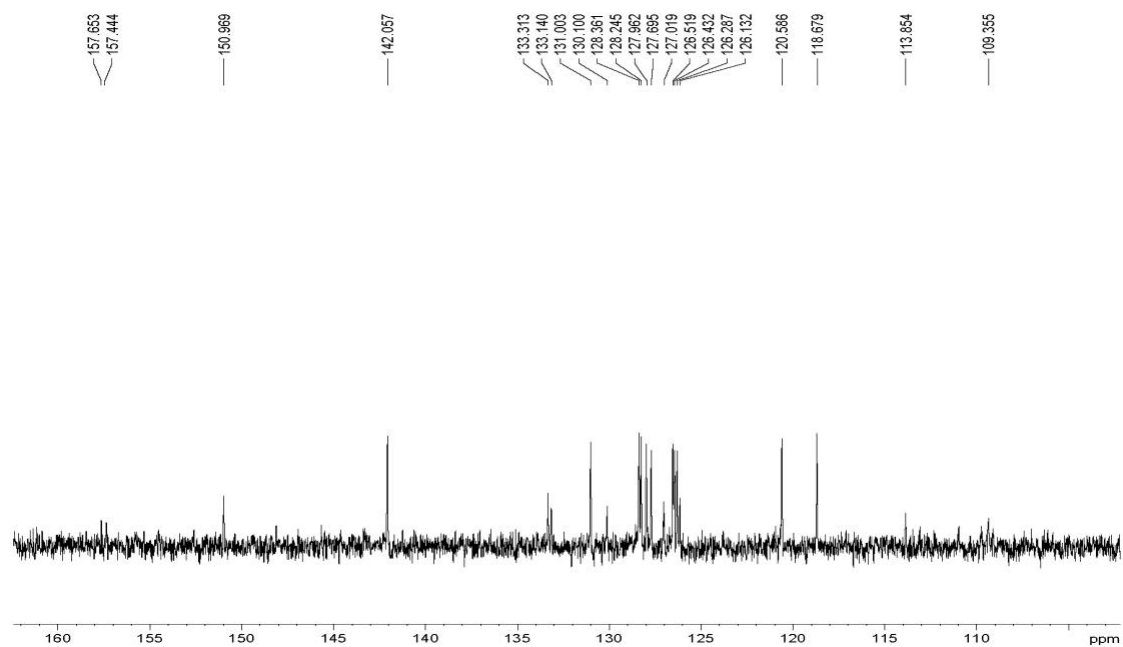
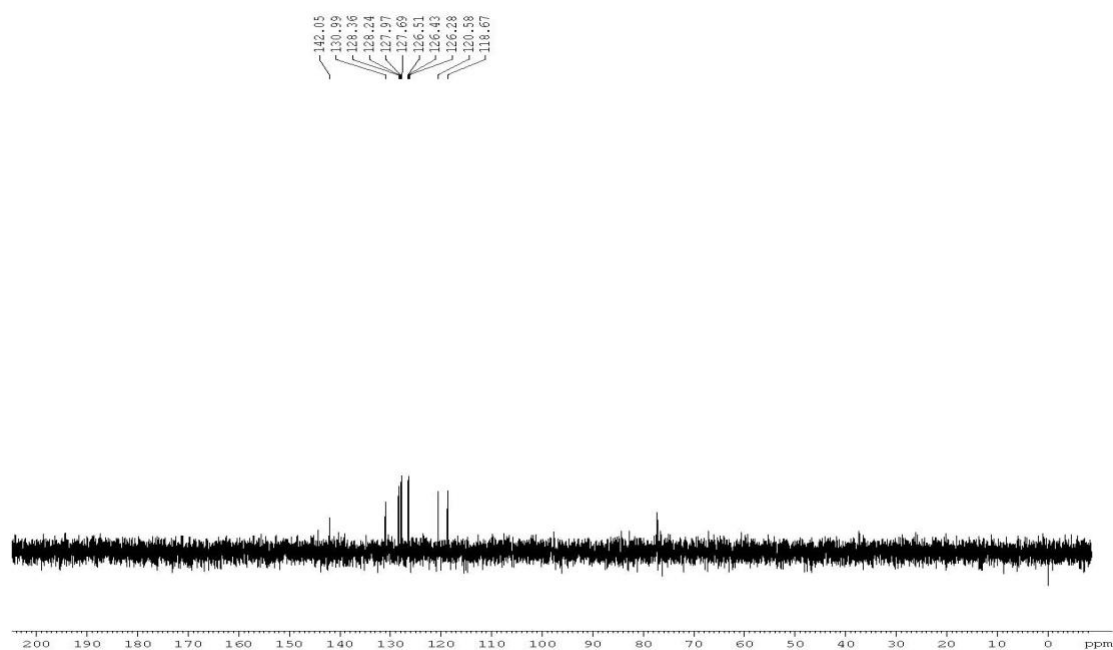
Compound 2d

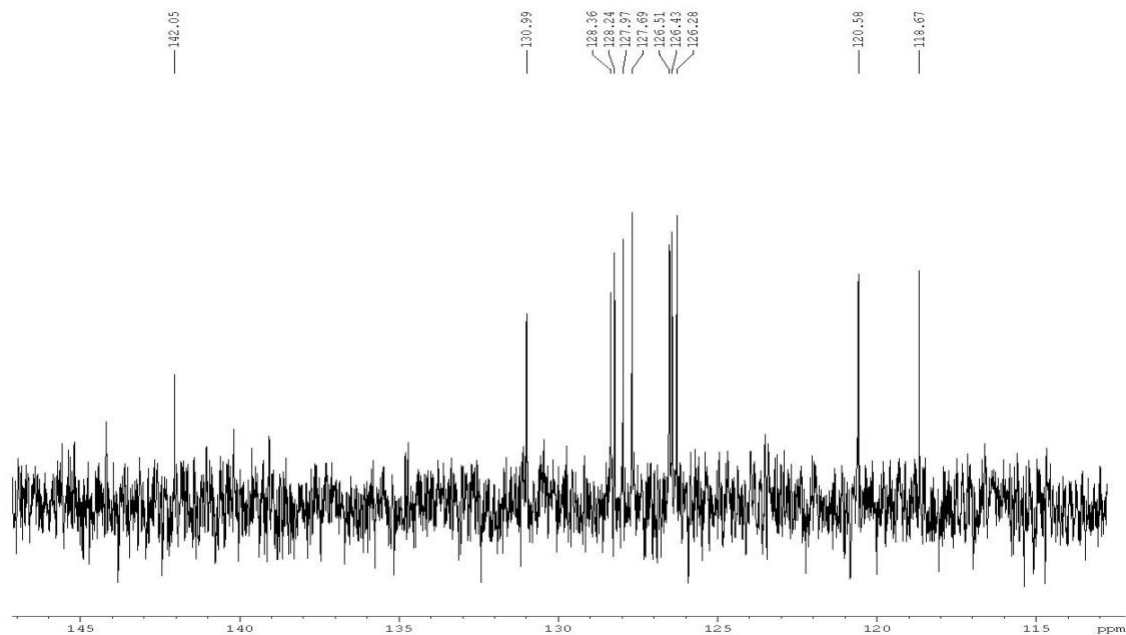
¹H NMR spectra



Compound 2d

¹³C NMR spectra

**Compound 2d****DEPT-90 spectra**



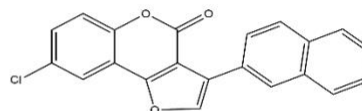
Compound 2d

Mass spectra

DEPARTMENT OF CHEMISTRY (DST-FIST Funded & UGC-SAP Sponsored) SAURASHTRA UNIVERSITY RAJKOT-360005

Sample Information

Analyzed by : BHOLA G.N.
Analyzed : 2/4/2015 2:22:16 PM
Sample Name : M 11
Sample ID : M 11
Data File : D:\OUT OF DEP\KAUSHAL PATEL\M 11_1.qgd
C:\GCM\Software\Data\Project\101.ms SPED\0.qgm
Tuning File : C:\GCM\Software\System\Tune\F020215_F1_MS.qgt

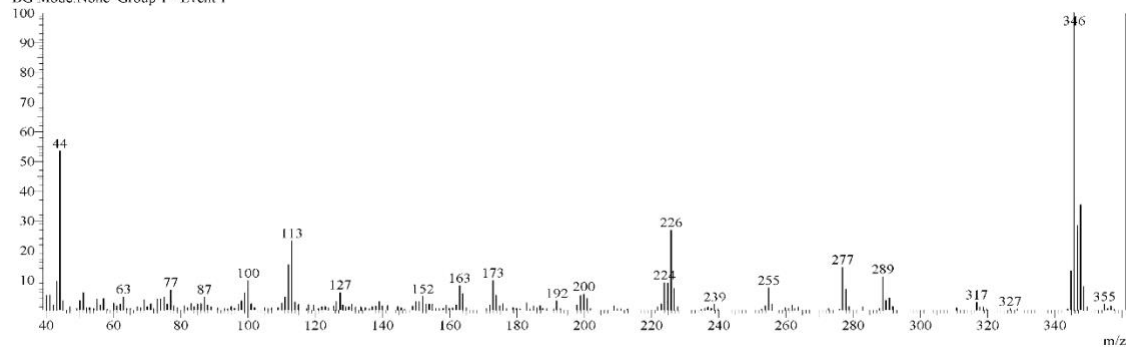


Line# 1 R Time: 4.1 (Scan#: 714)

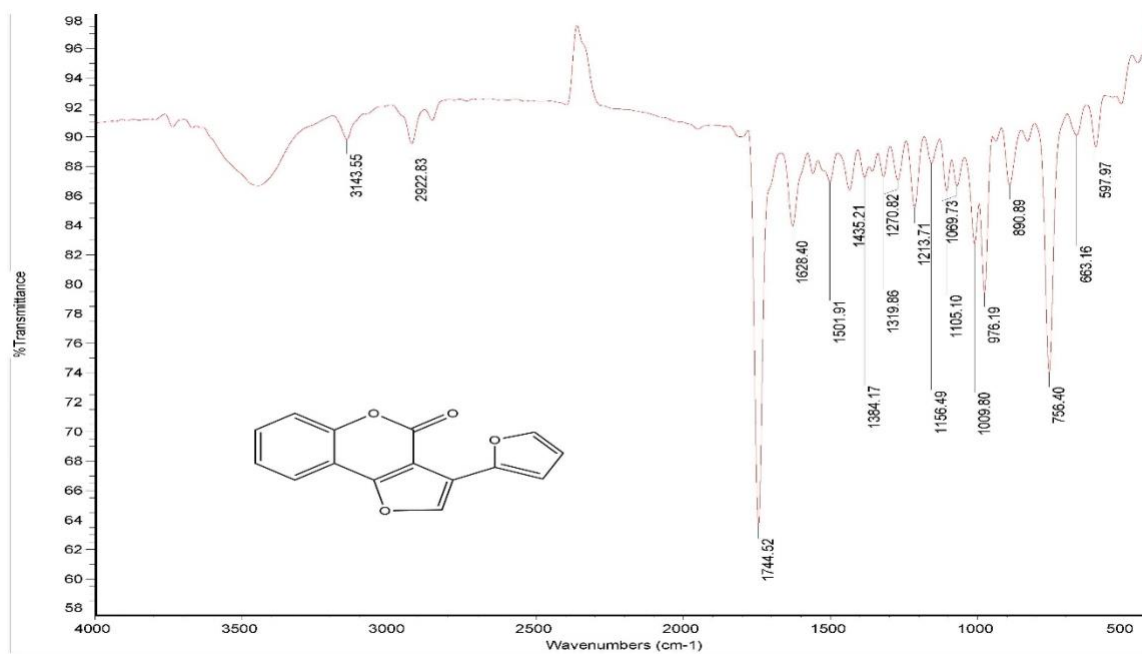
MassPeaks: 192

RawMode: Averaged 0.8-5.4 (64-971) BasePeak: 345.750 (16373)

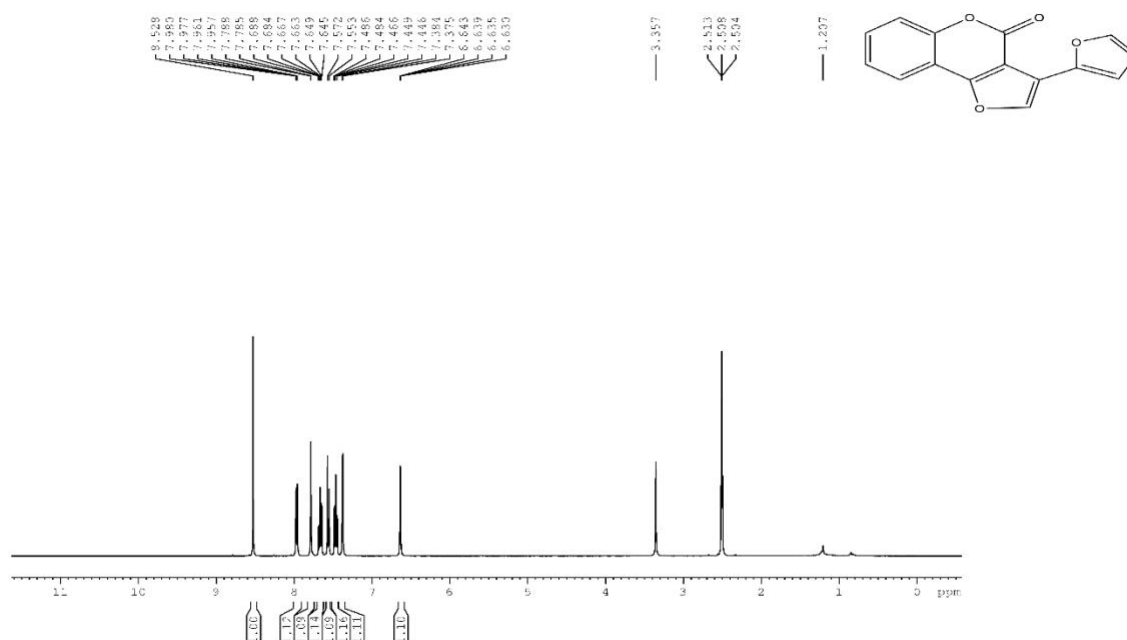
BG Mode: None Group 1 - Event 1

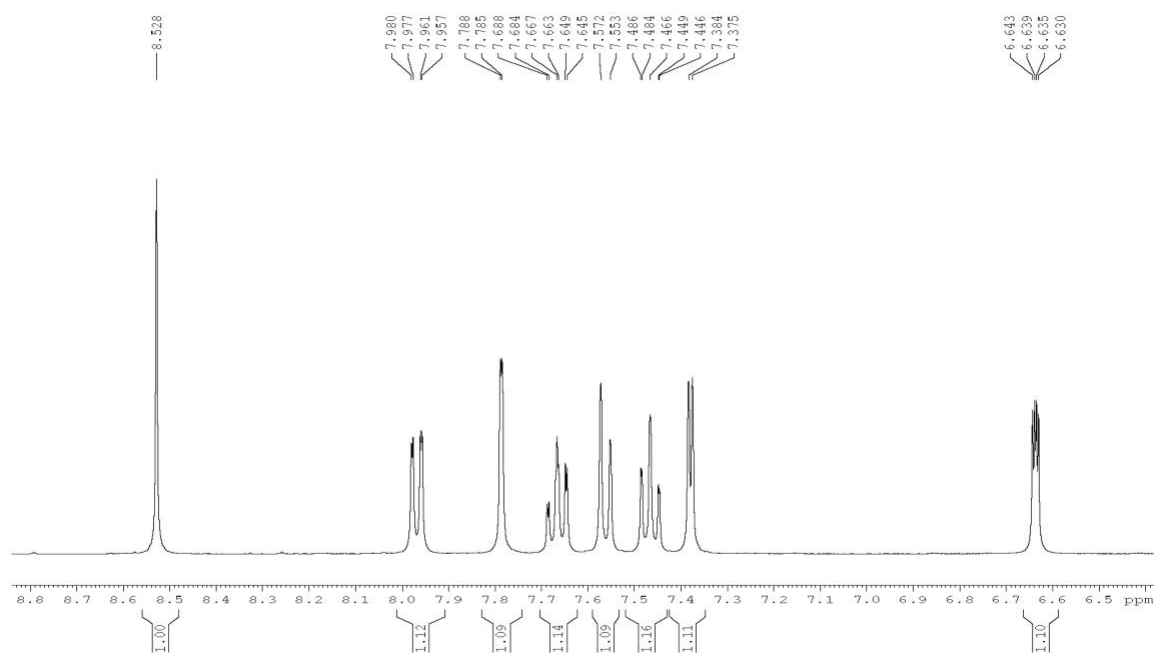


Infrared Spectra

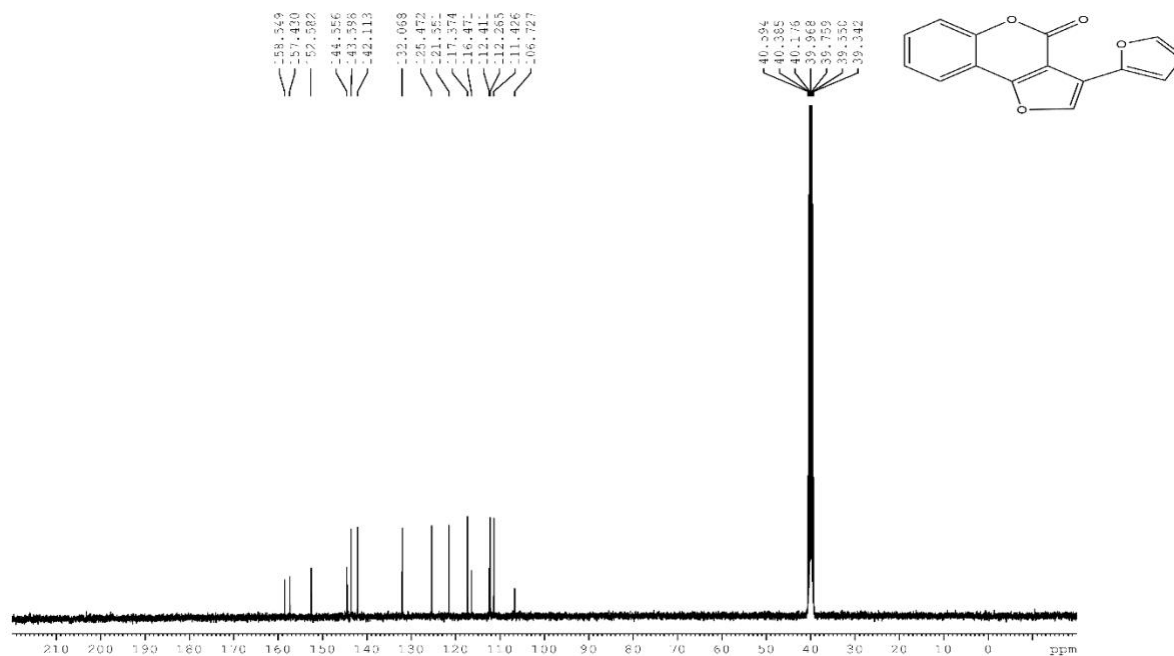


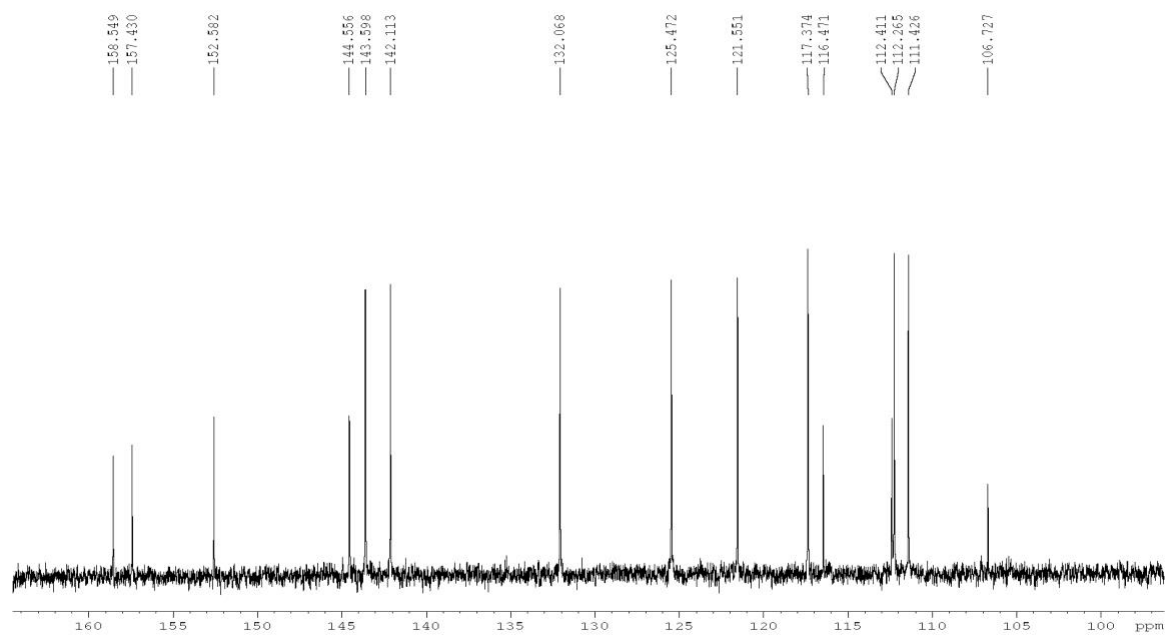
¹H NMR spectra





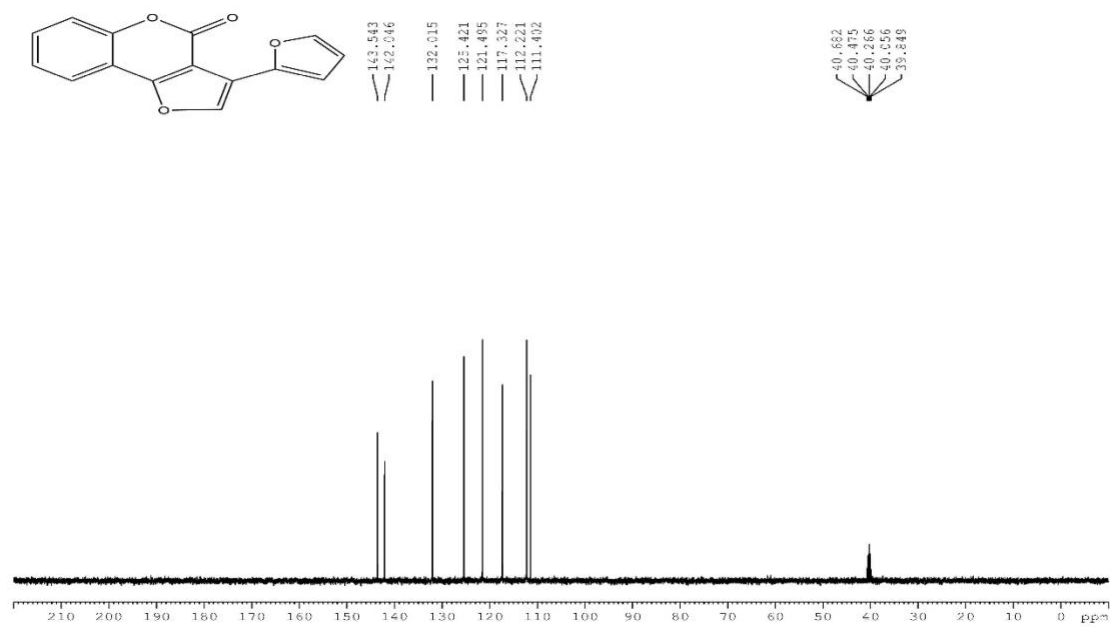
Compound 3a

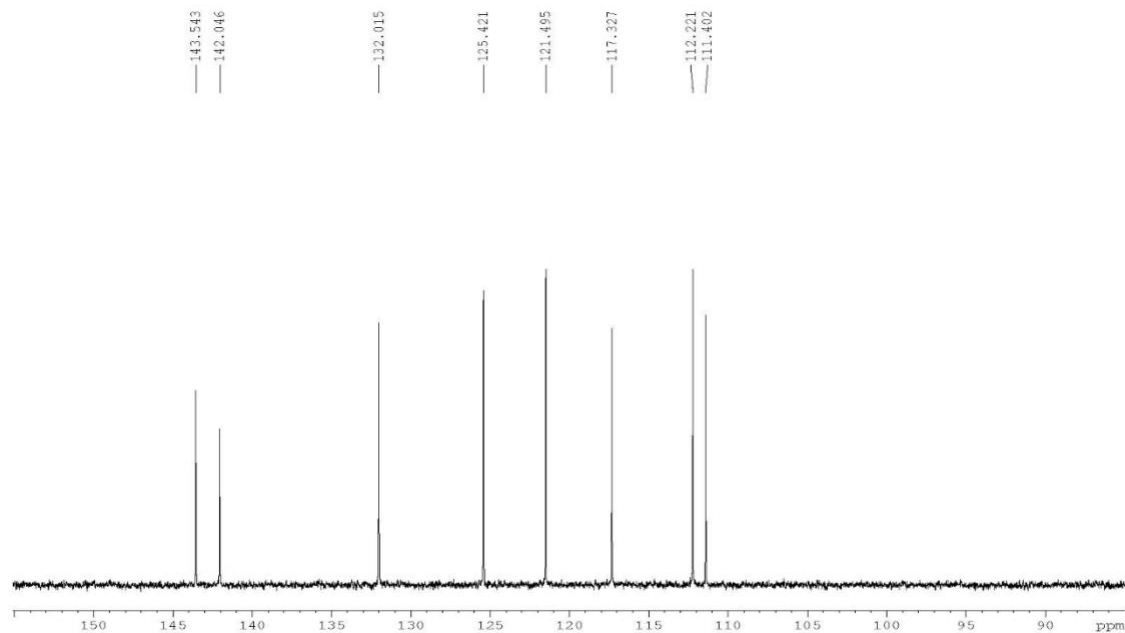
 ^{13}C NMR spectra



Compound 3a

DEPT-90 spectra





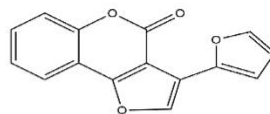
Compound 3a

Mass spectra

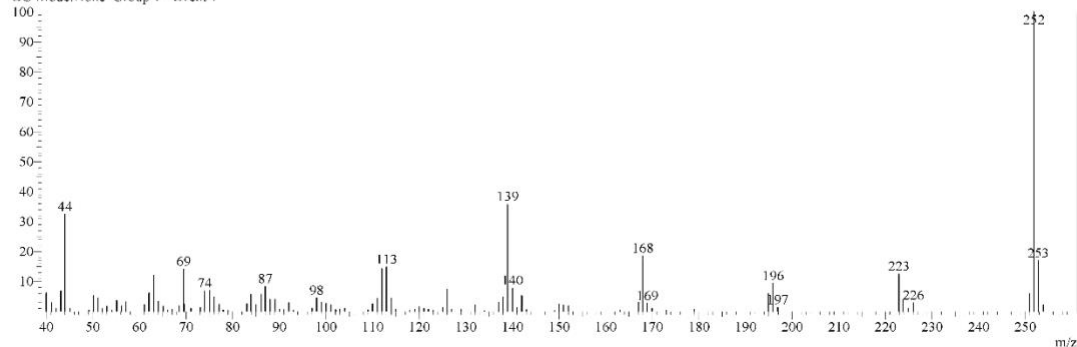
DEPARTMENT OF CHEMISTRY
(DST-FIST Funded & UGC-SAP Sponsored)
SAURASHTRA UNIVERSITY
RAJKOT-360005

Sample Information

Analyzed by : BIJOLA G.N.
Analyzed : 2/4/2015 2:44:08 PM
Sample Name : D 16
Sample ID : D 16
Data File : D:\OUT OF DEPIKA\ASHAL PATEL\16.ggd
Tuning File : C:\GCMSolution\System1\Tune1\020215_F1.MS.ggt

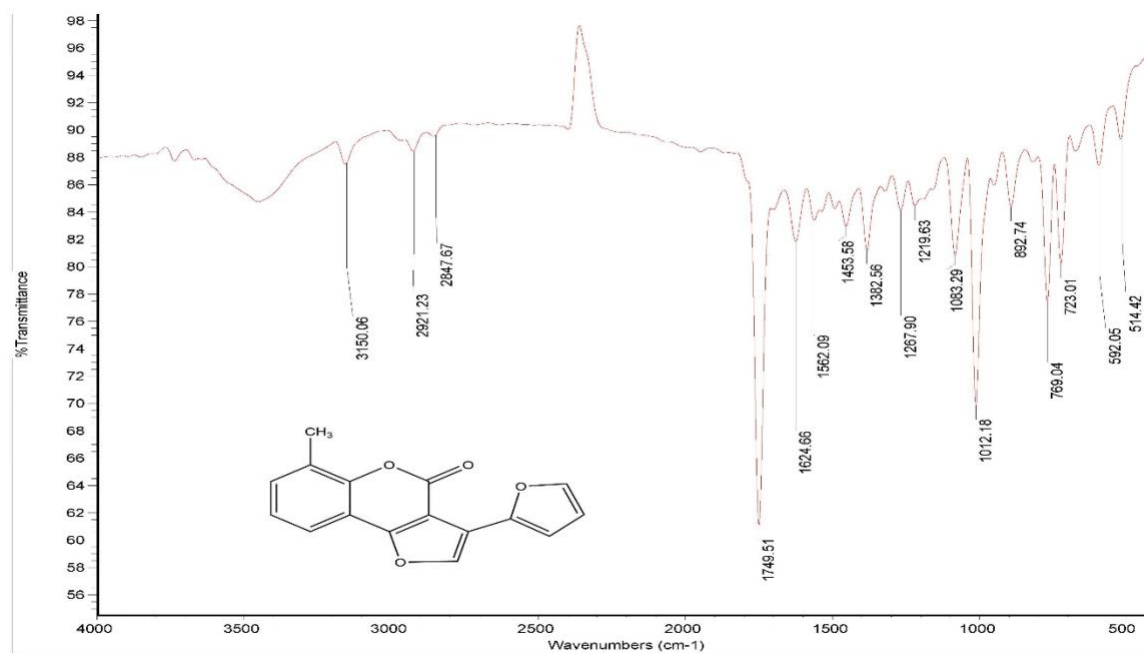


Line#:1 R.Time:1.7(Scan#:242)
MassPeaks:100
RawMode:Averaged 0.6-6.8(29-1270) BasePeak:251.850(7846)
HG Mode:None Group 1 - Event 1

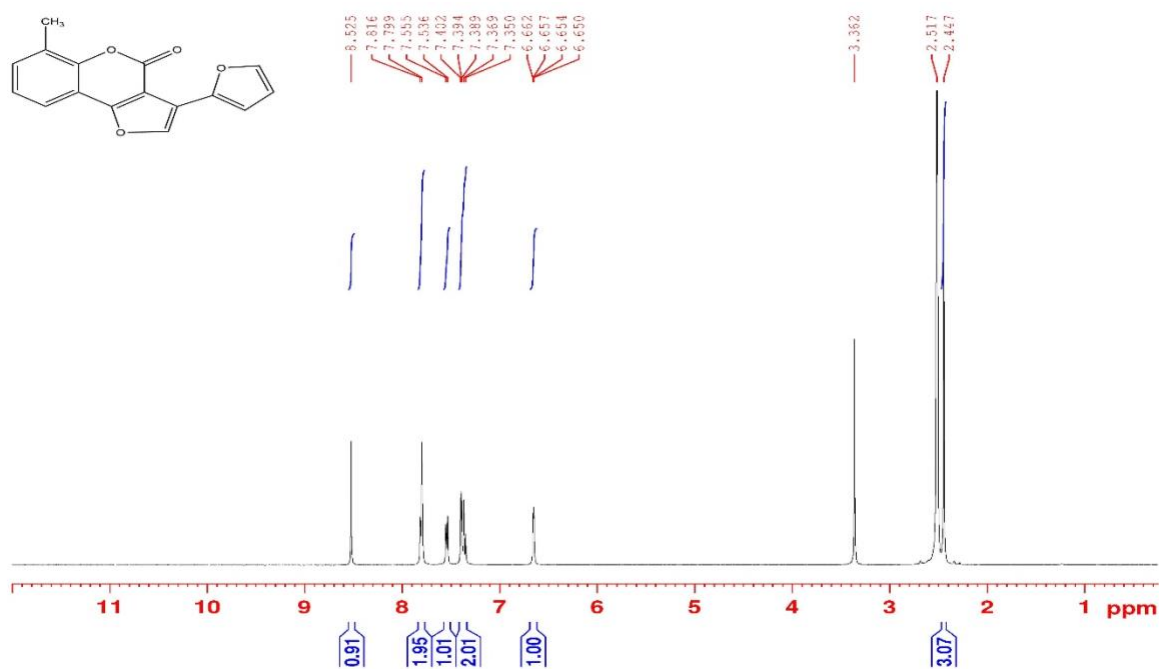


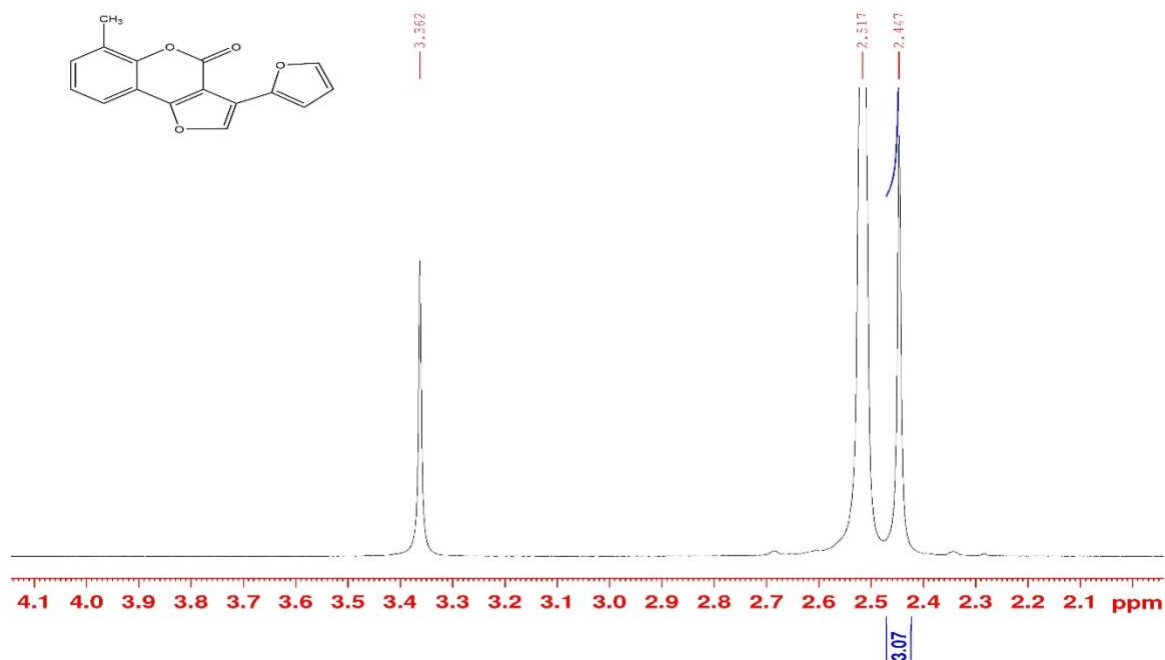
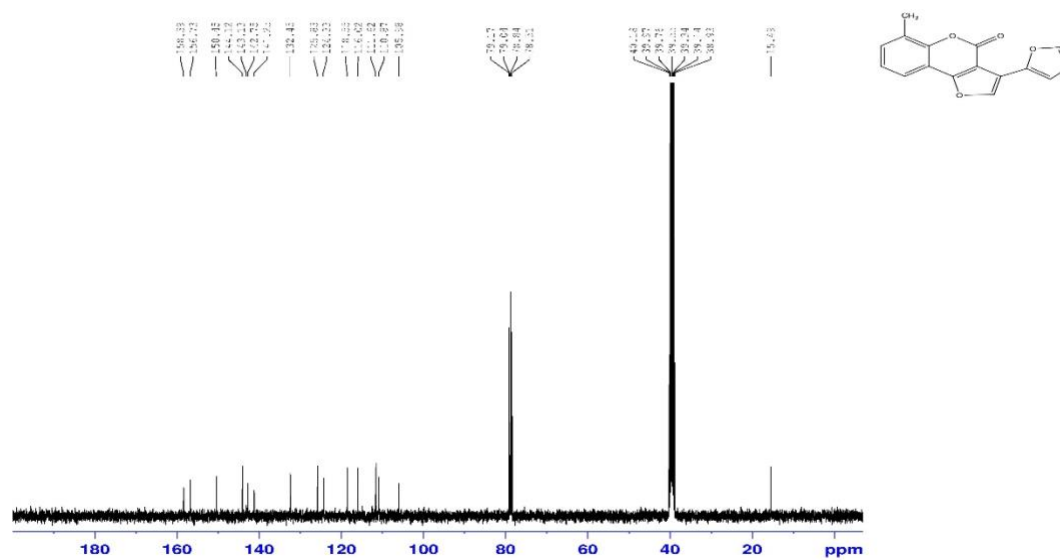
Compound 3b

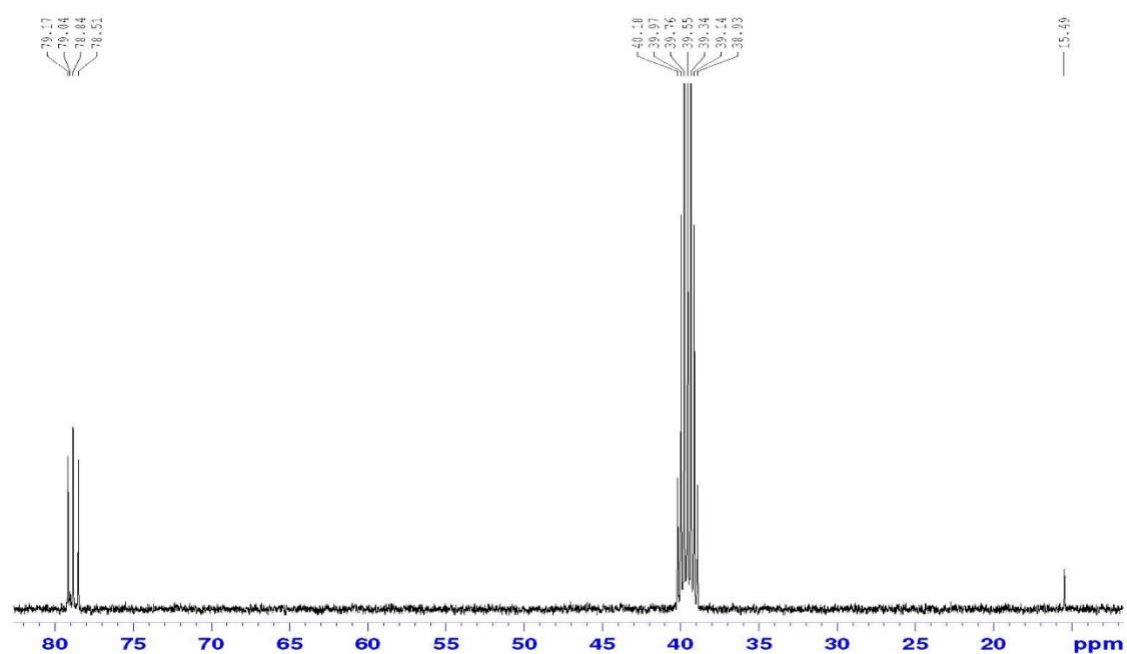
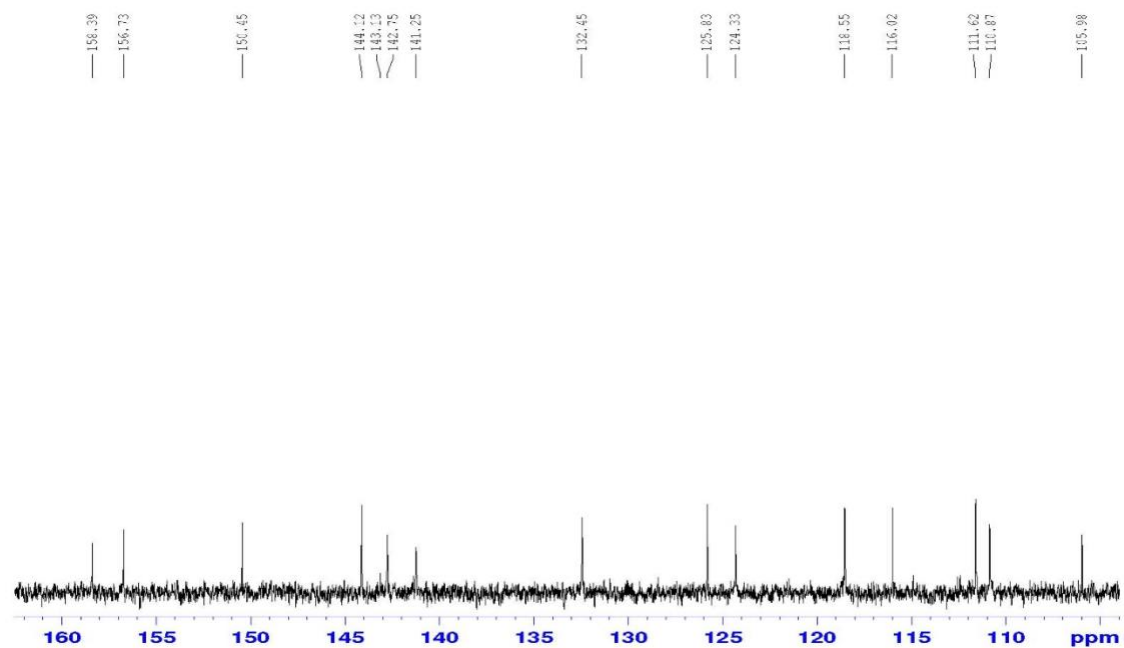
Infrared Spectra



Compound 3b

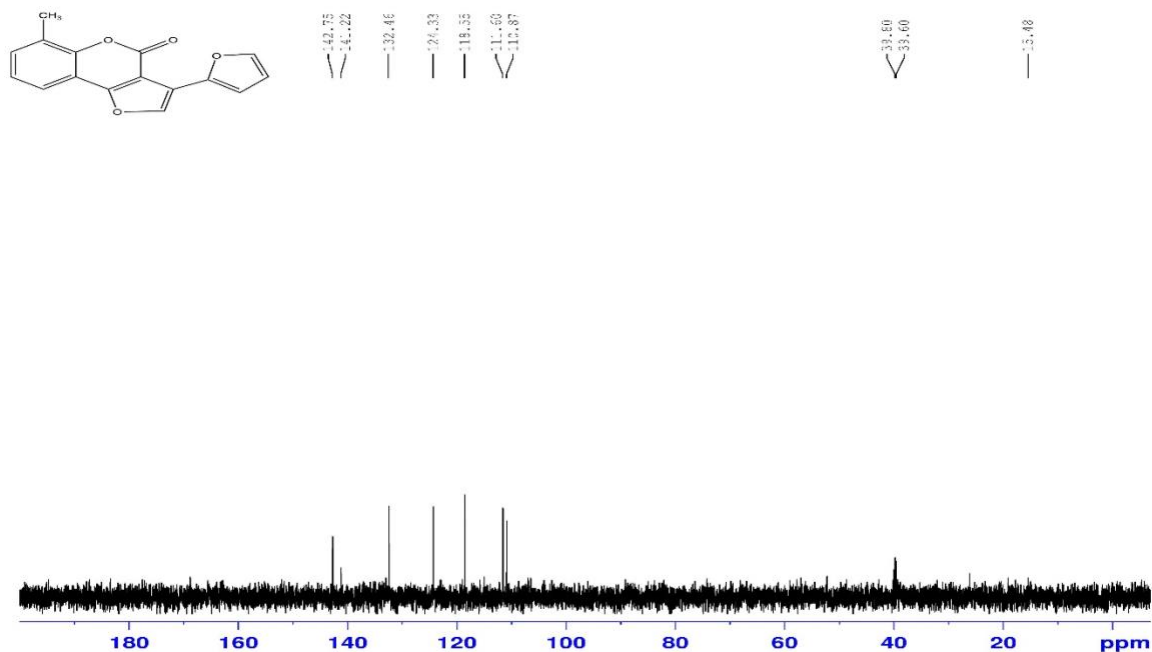
¹H NMR spectra

**Compound 3b****¹³C NMR spectra**



Compound 3b

DEPT-90 spectra



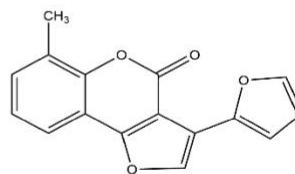
Compound 3b

Mass spectra

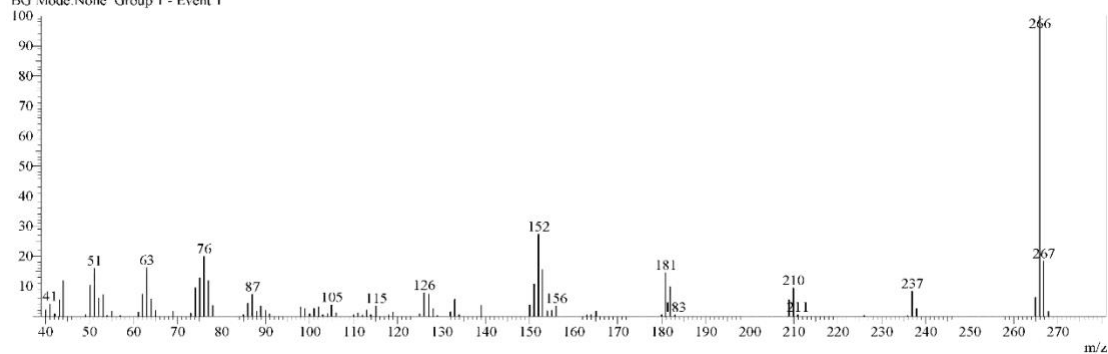
DEPARTMENT OF CHEMISTRY
(DST-FIST Funded & UGC-SAP Sponsored)
SAURASHTRA UNIVERSITY
RAJKOT-360005

Sample Information

Analyzed by: BHOLA GAURAV
Analyzed: 2/4/2015 3:24:17 PM
Sample Name: D 18
Sample ID: D 18
Data File: D:\OUT OF DEP\KAUSHAL PATEL\D 18.qsd
Tuning File: C:\GCMSolution\Data\Project1\DI m.s SPEED.qsm
C:\GCMSolution\System1\Tune1\020215_1_1 MS.qgt

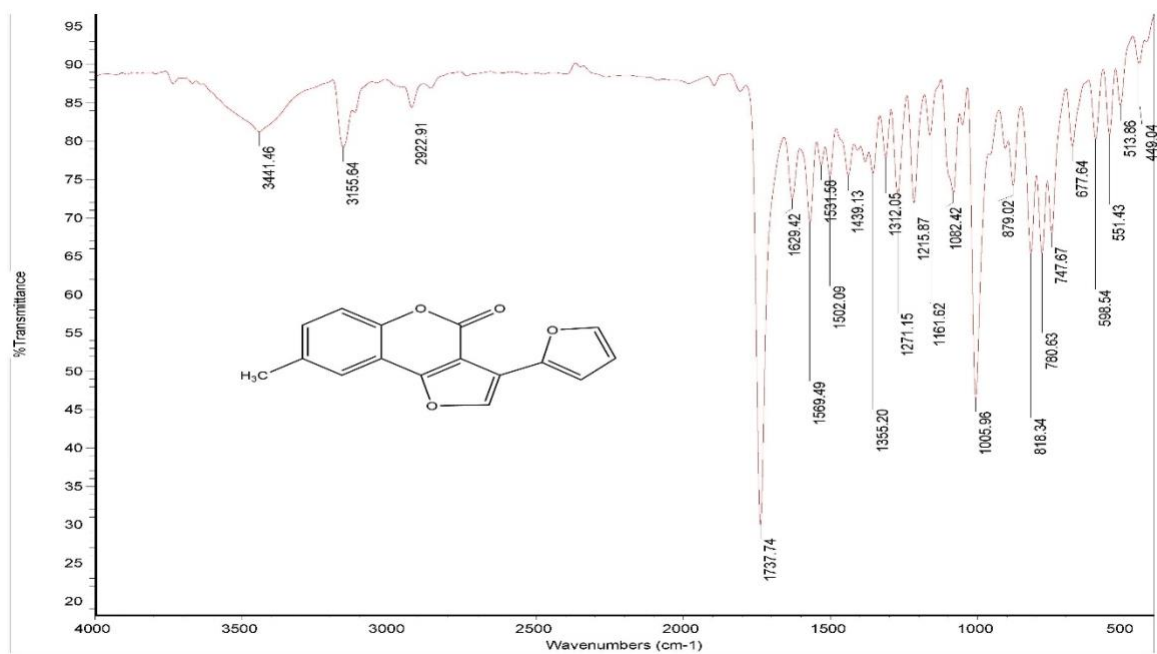


Line#: 1 R.Time: 2.0 (Scan#: 299)
MassPeaks: 83
RawMode: Averaged 0.5-3.7 (1-634) BasePeak: 265.900 (3391)
BG Mode: None Group 1 - Event 1

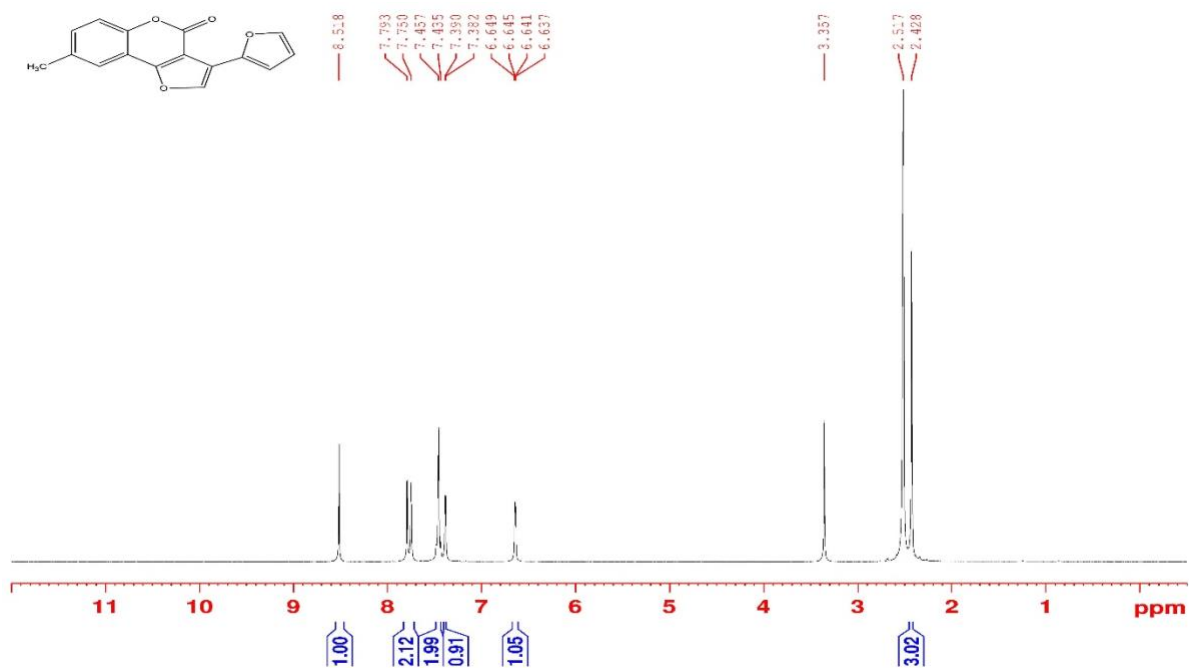


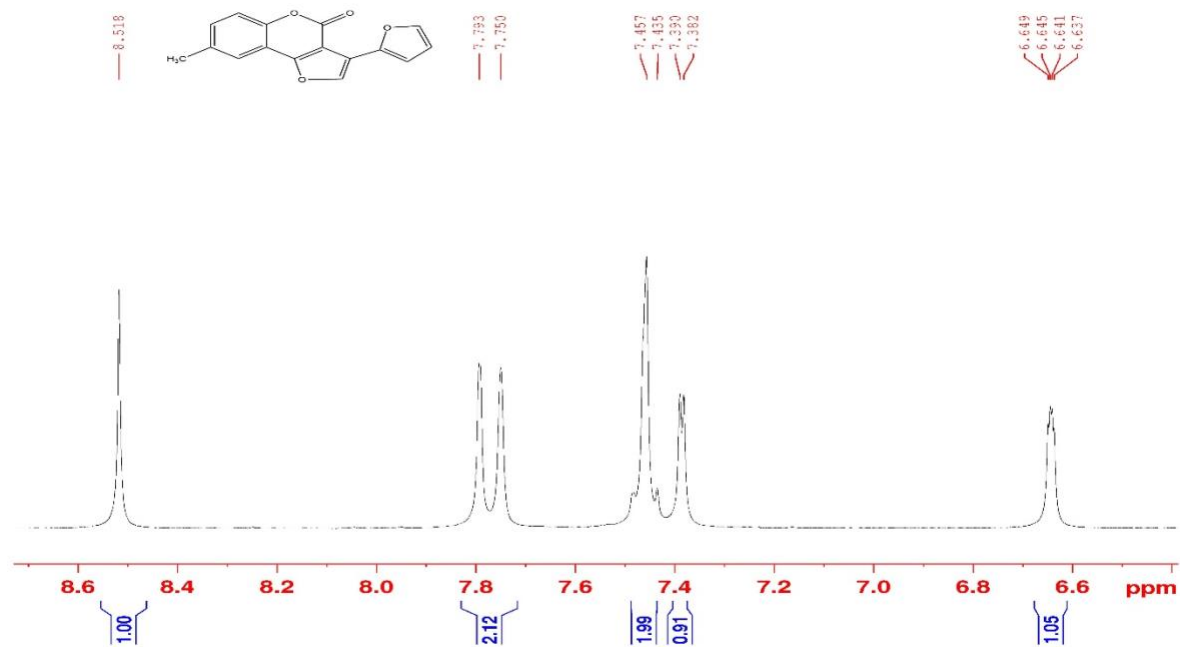
Compound 3c

Infrared Spectra

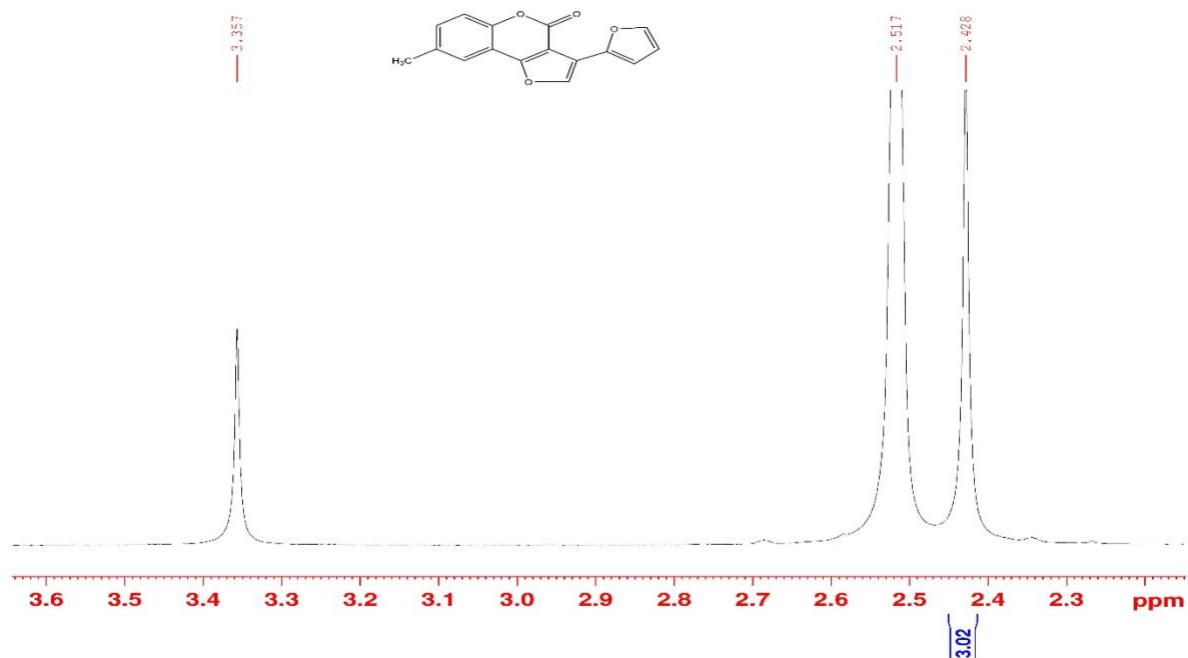


Compound 3c

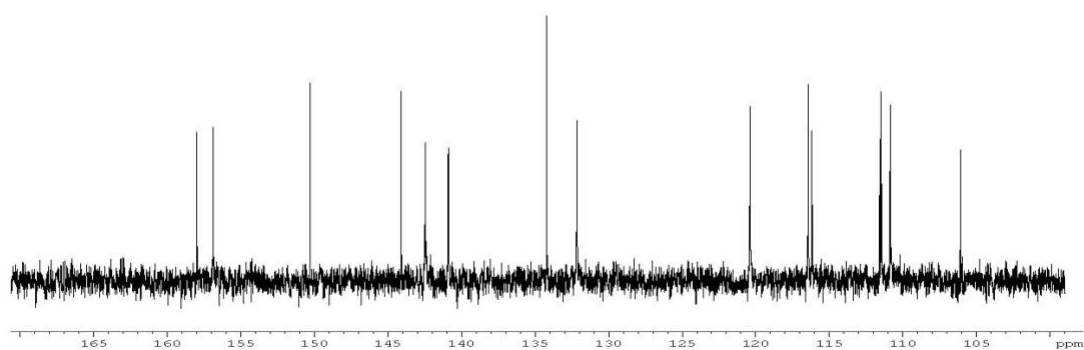
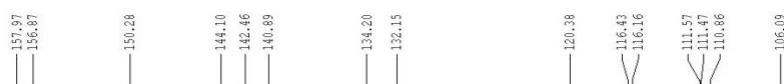
¹H NMR spectra



Compound 3c

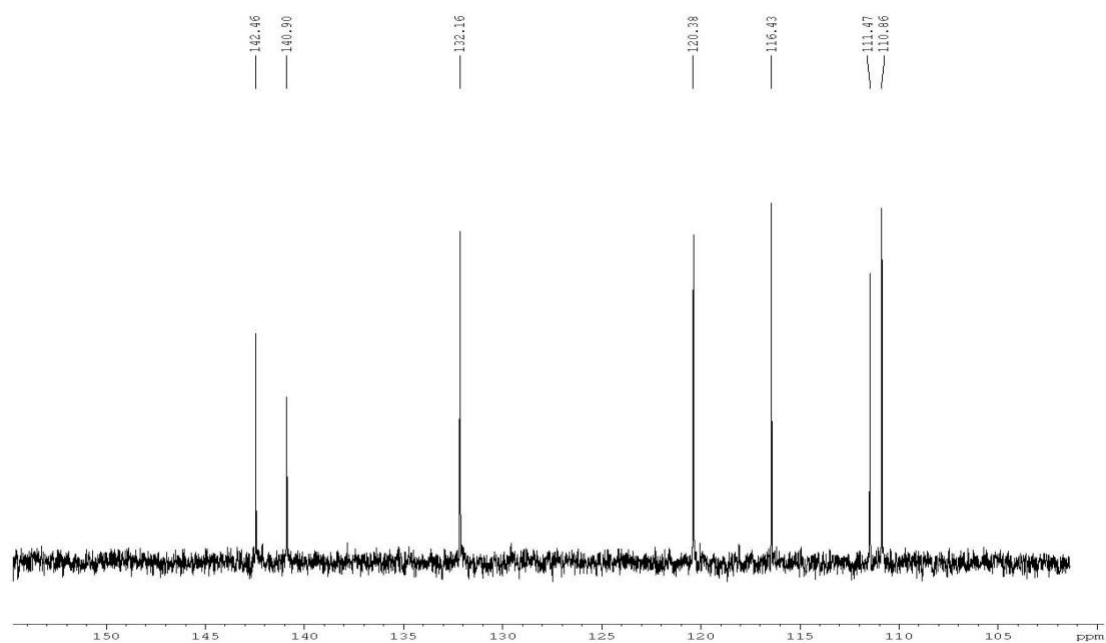
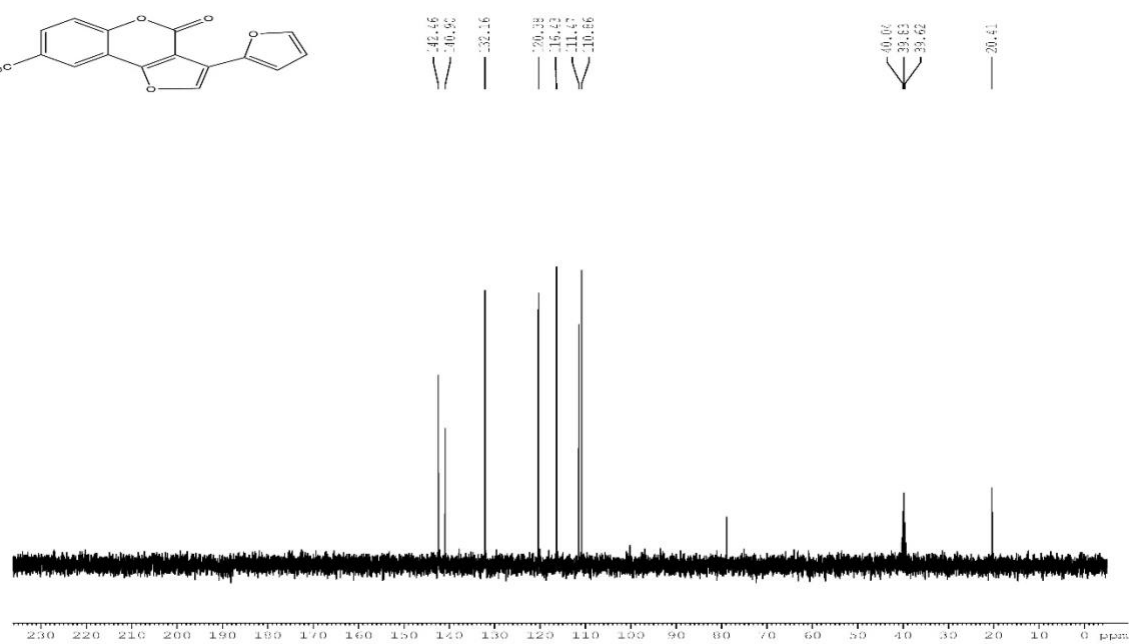
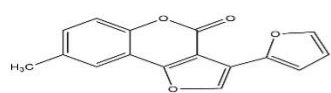
¹³C NMR spectra

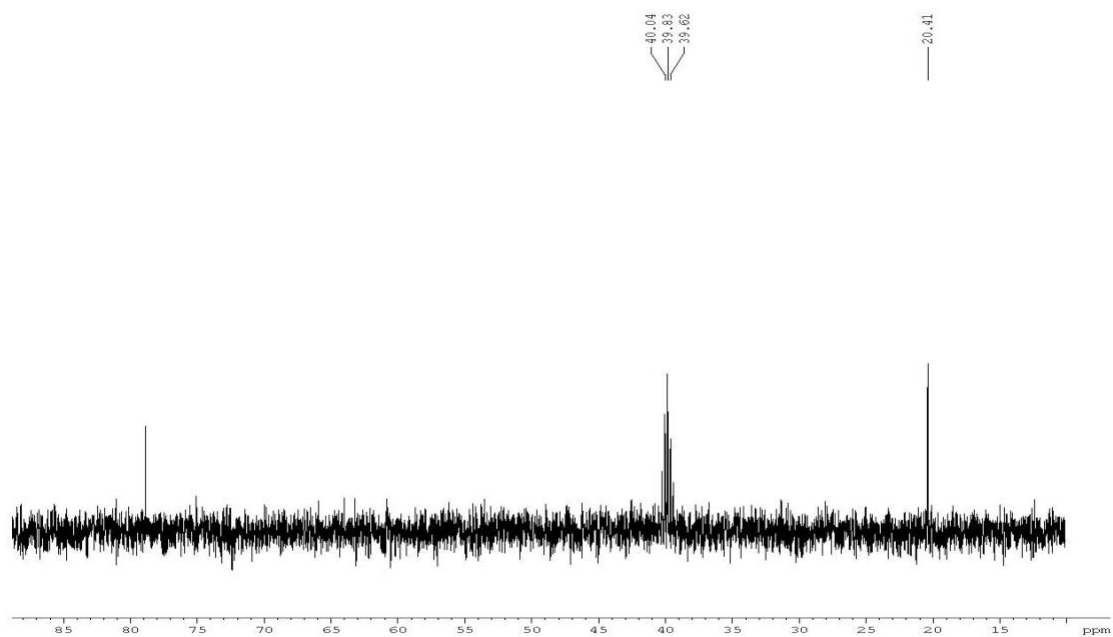
¹³C NMR Spectra



Compound 3c

DEPT-90 spectra





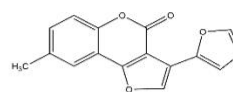
Compound 3c

Mass spectra

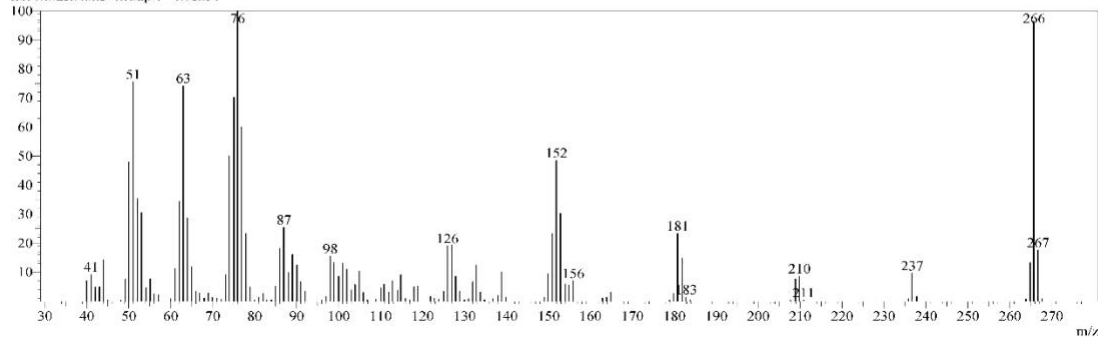
DEPARTMENT OF CHEMISTRY
(DST-FIST Funded & UGC-SAP Sponsored)
SAURASHTRA UNIVERSITY
RAJKOT-360005

Sample Information

Analyzed by: BHOLA GAURAV
Analyzed: 2/9/2015 2:36:14 PM
Sample Name: D-19
Sample ID:
Data File: D:\OUT OF DEPT\KAUSHAL PATEL\19.qcd
C:\GCMSolution\Data\Project1\DI.ms SPEED.qsm
Tuning File: C:\GCMSolution\System Tune\10020215_F1.MS.qgt

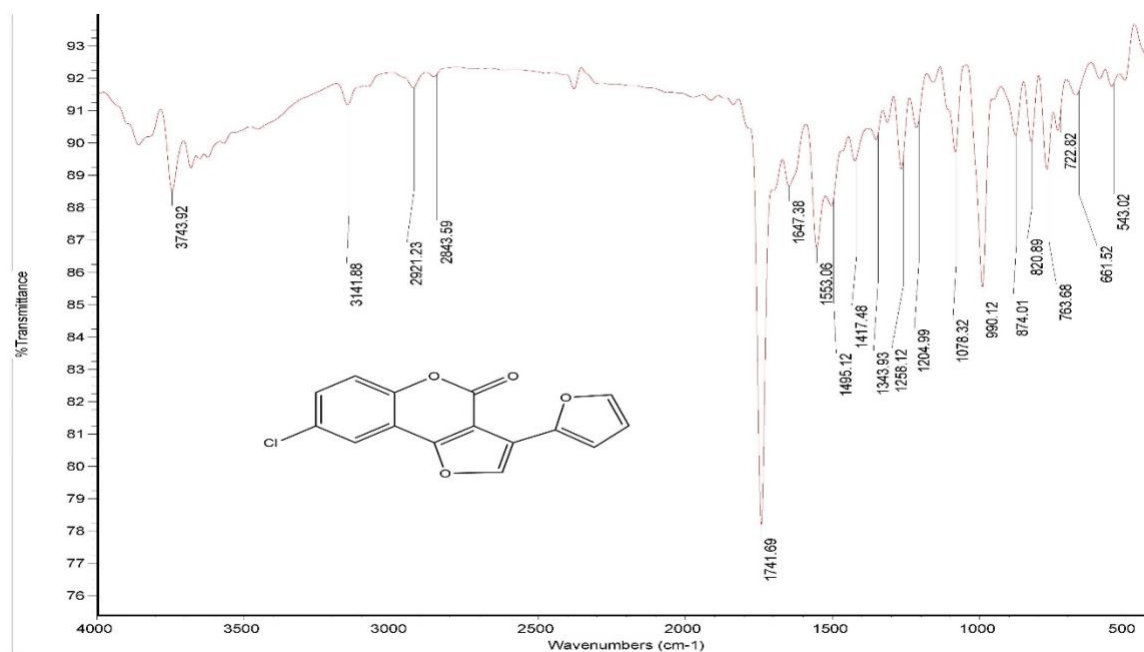


Line#:1 R.Time:1.9(Scan#:289)
MassPeaks:119
RawMode:Averaged 1.4-2.7(179-440) BasePeak:75.900(2037)
BG Mode:None Group 1 - Event 1

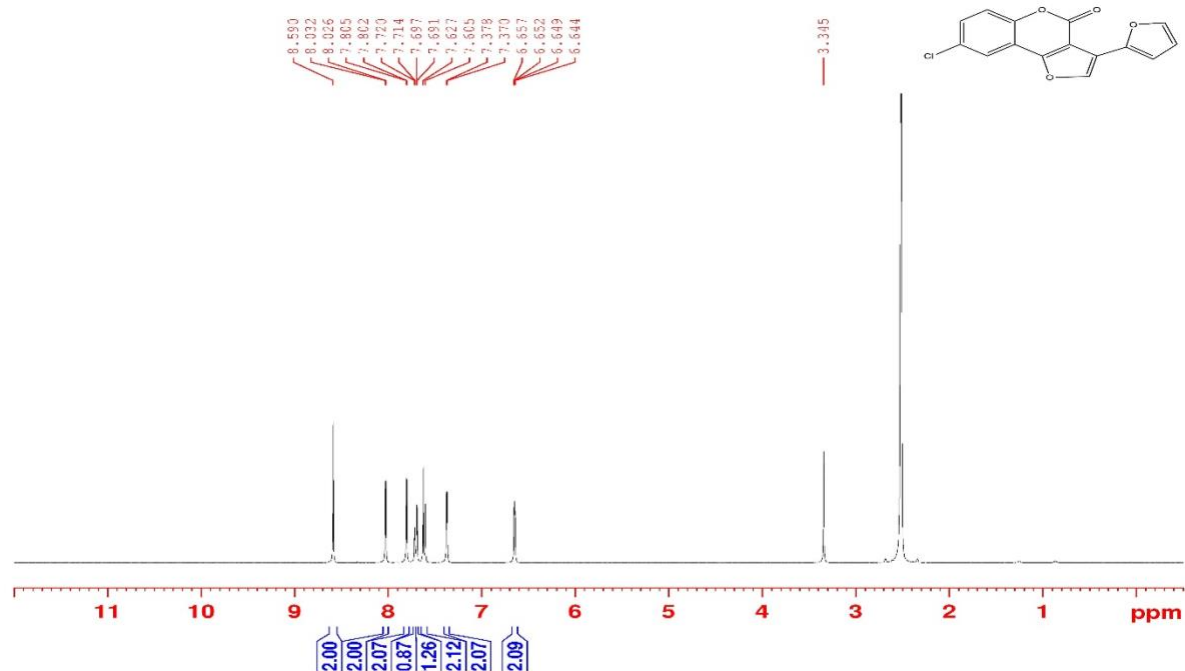


Compound 3d

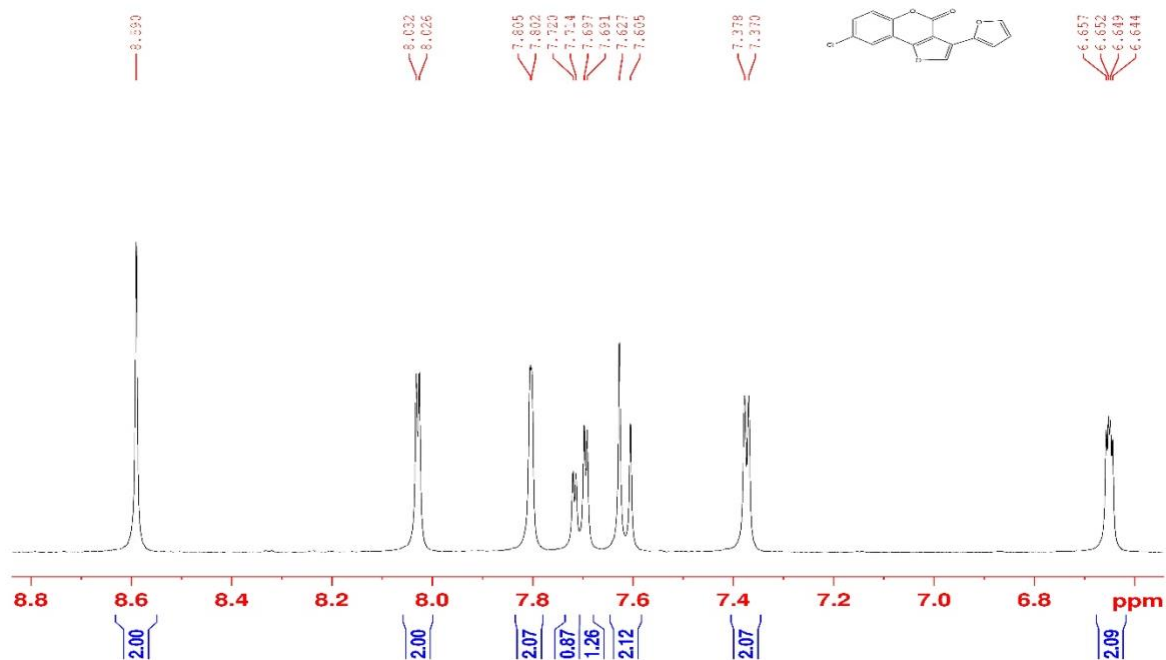
Infrared Spectra



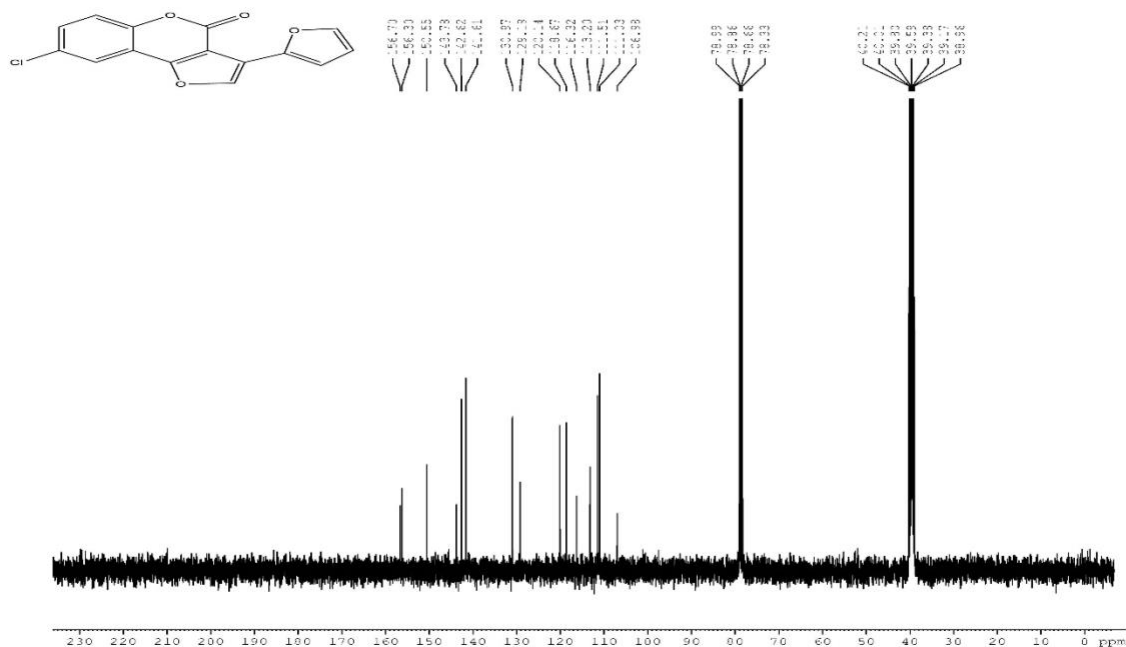
Compound 3d

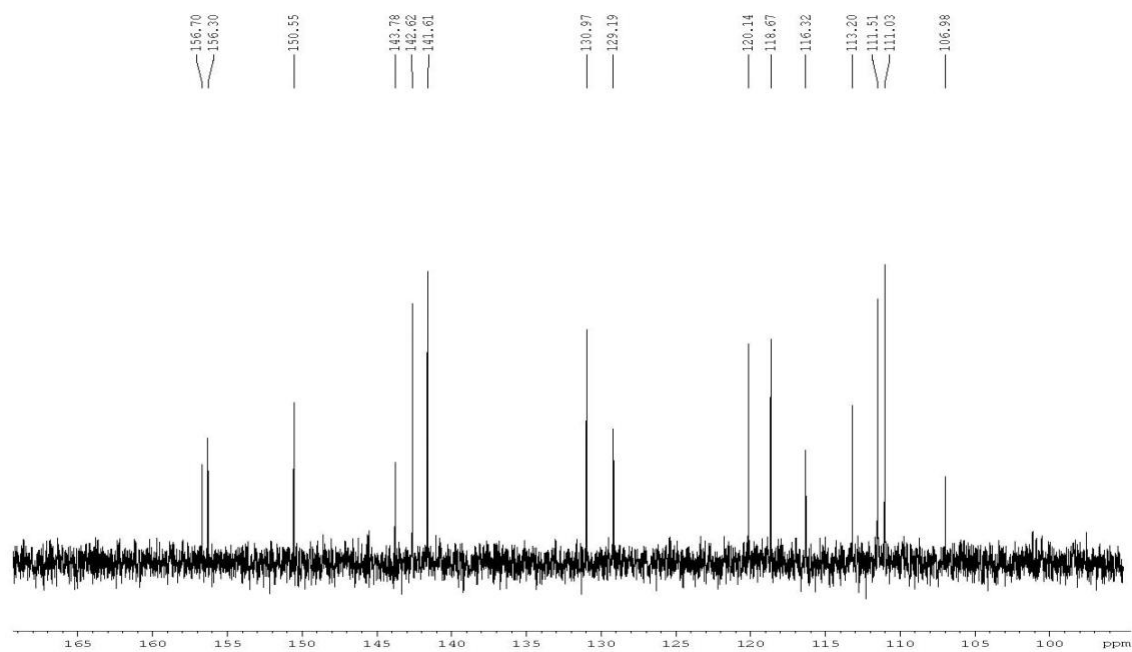
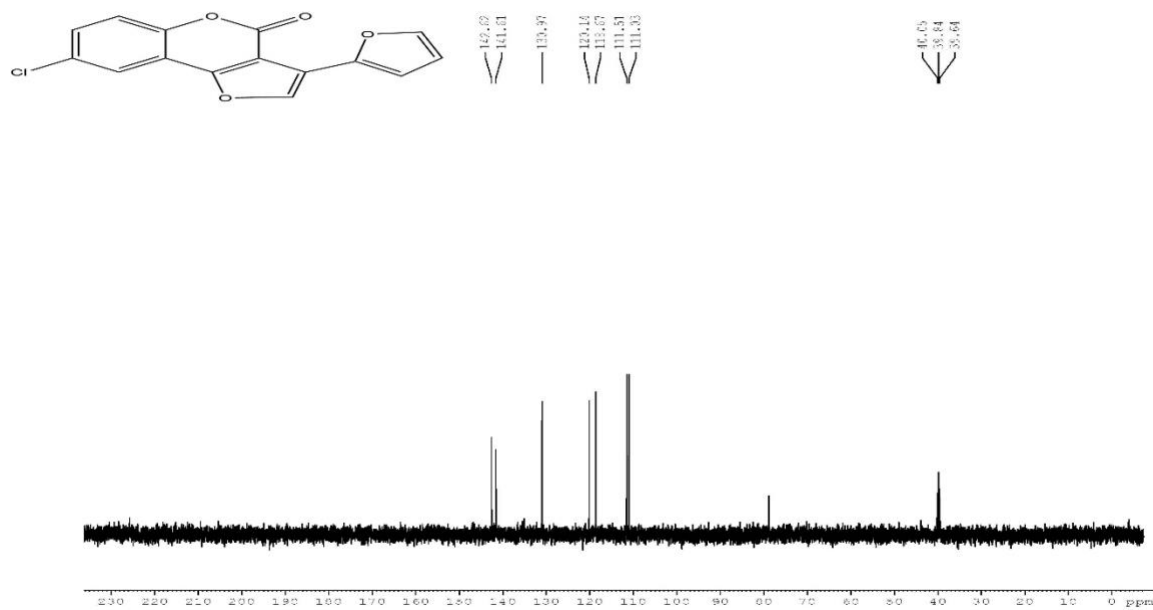
¹H NMR spectra

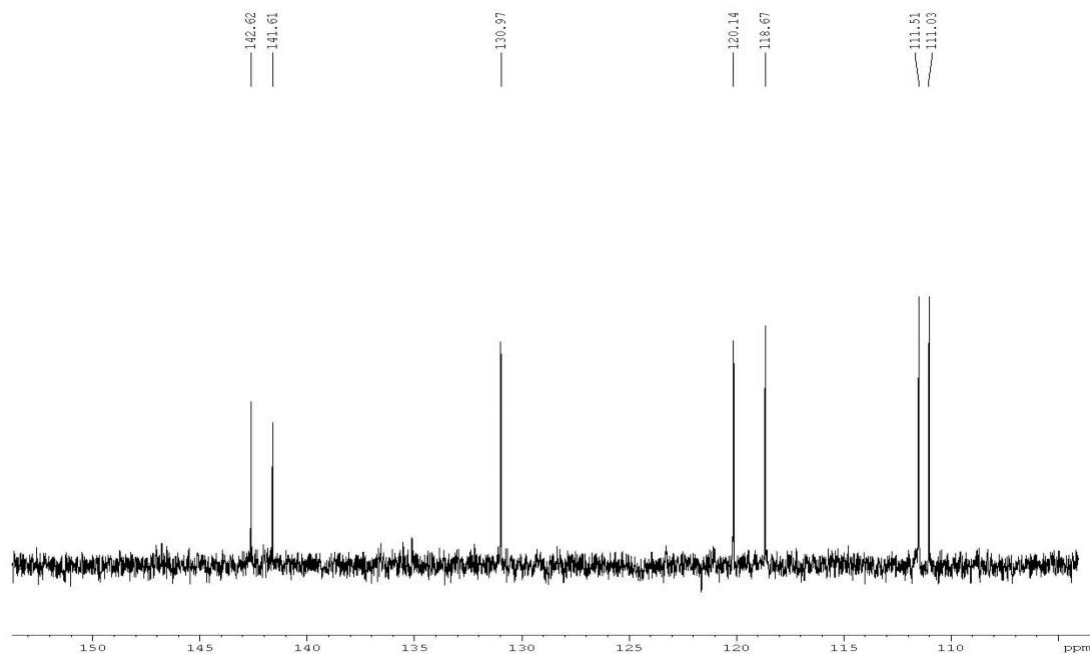
Compound 3d



Compound 3d

¹³C NMR spectra

**Compound 3d****DEPT-90 spectra**



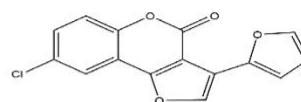
Compound 3d

Mass spectra

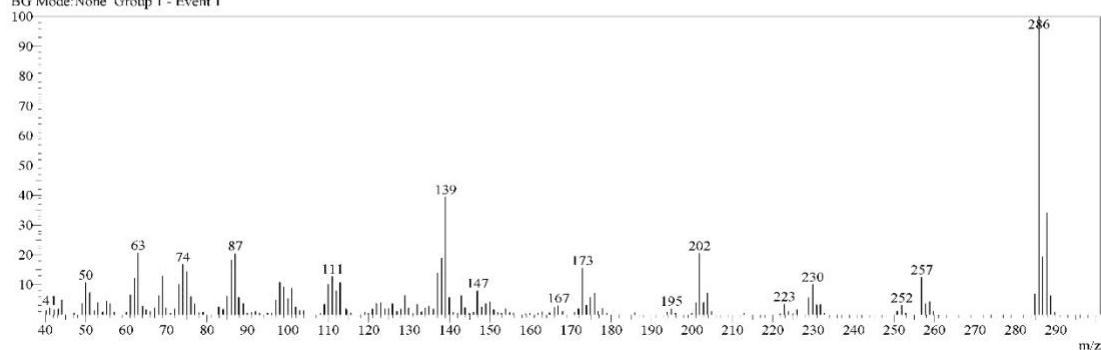
DEPARTMENT OF CHEMISTRY
(DST-FIST Funded & UGC-SAP Sponsored)
SAURASHTRA UNIVERSITY
RAJKOT-360005

Sample Information

Analyzed by : BELOLA G.N.
Analyzed : 24/2015 3:04:17 PM
Sample Name : D 17
Sample ID : D 17
Data File : D:\OUT OF DEP\KAUSHAL PATEL\D 17.qsd
C:\GCMSSolution\Data\Project\FDI ms SPEED.qgm
Tuning File : C:\GCMSSolution\System1\Tune1\020215_F1_MS.qgt

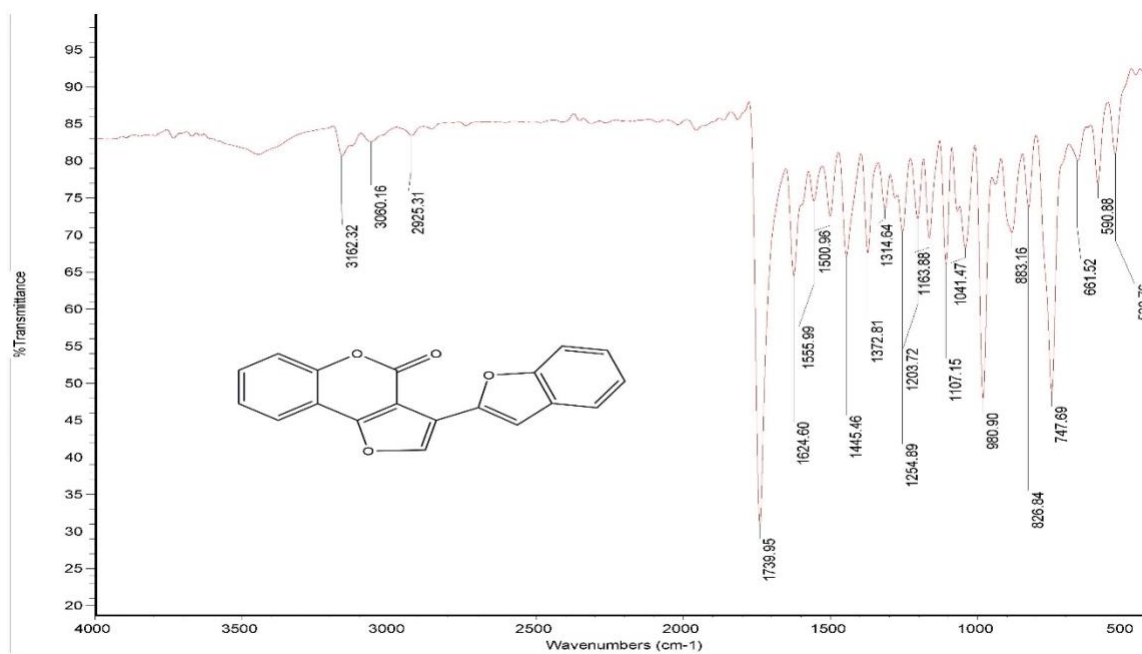


Line#: 1 R: Time: 2.5 (Scan#: 408)
Mass Peaks: 154
Raw Mode: Averaged 0.6-3.3 (17-569) Base Peak: 285.800 (16122)
BG Mode: None Group 1 - Event 1

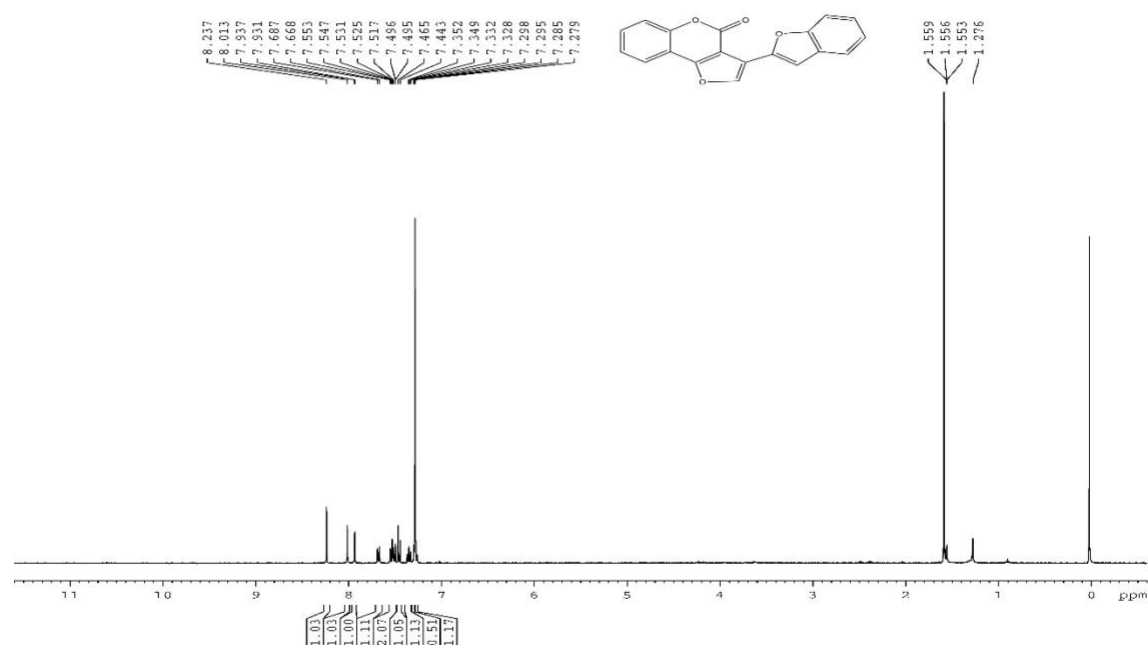


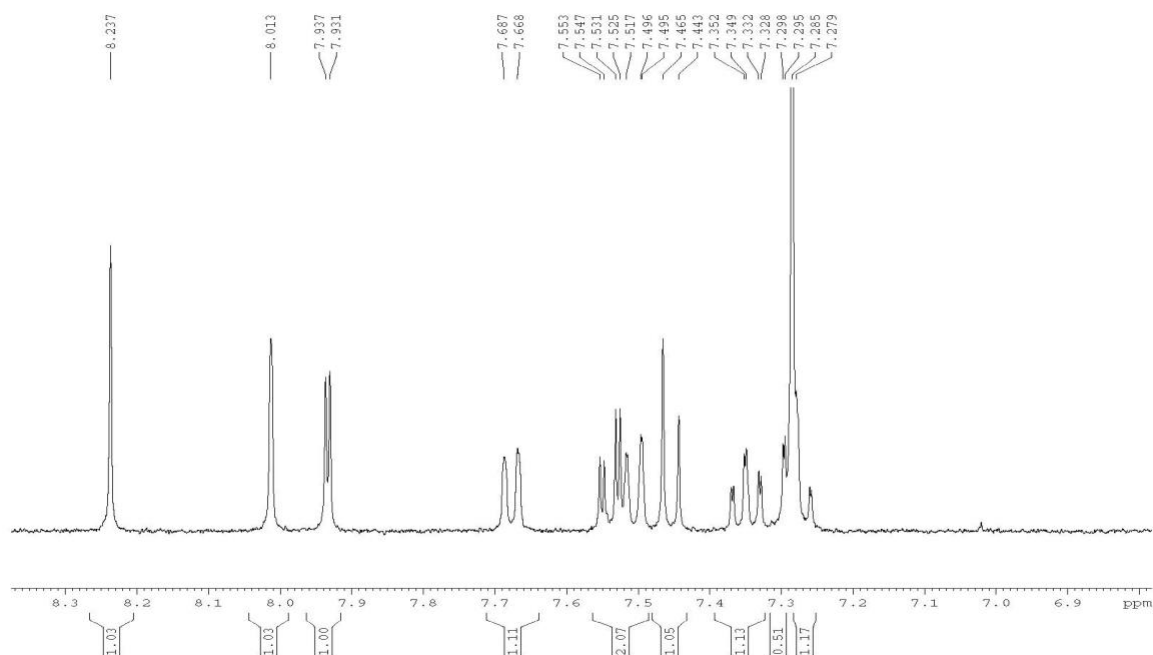
Compound 4a

Infrared Spectra

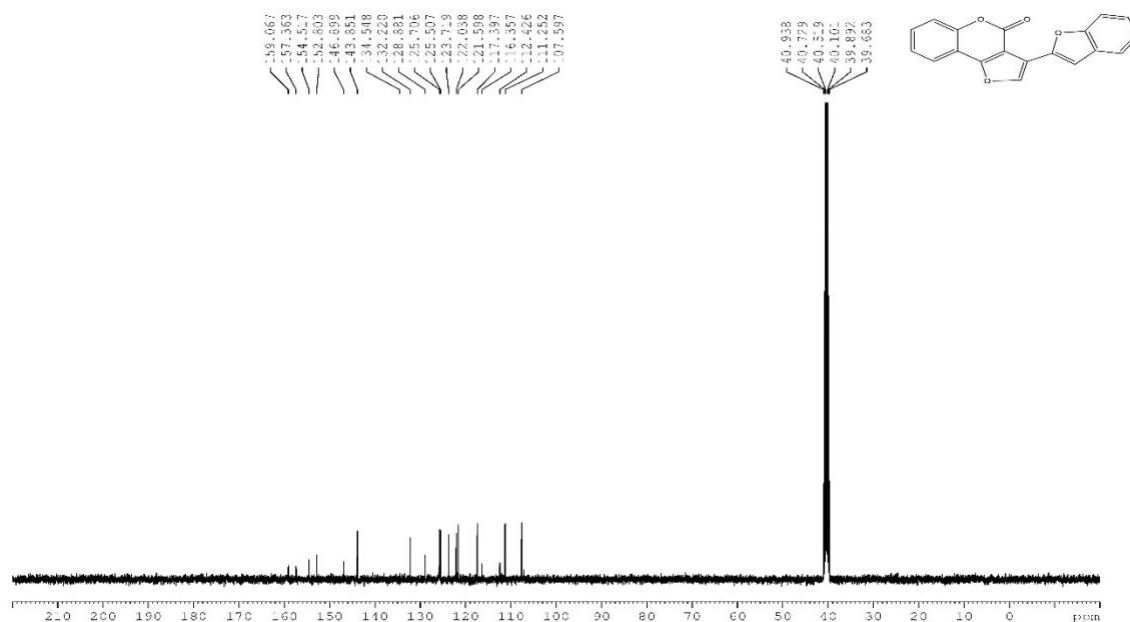


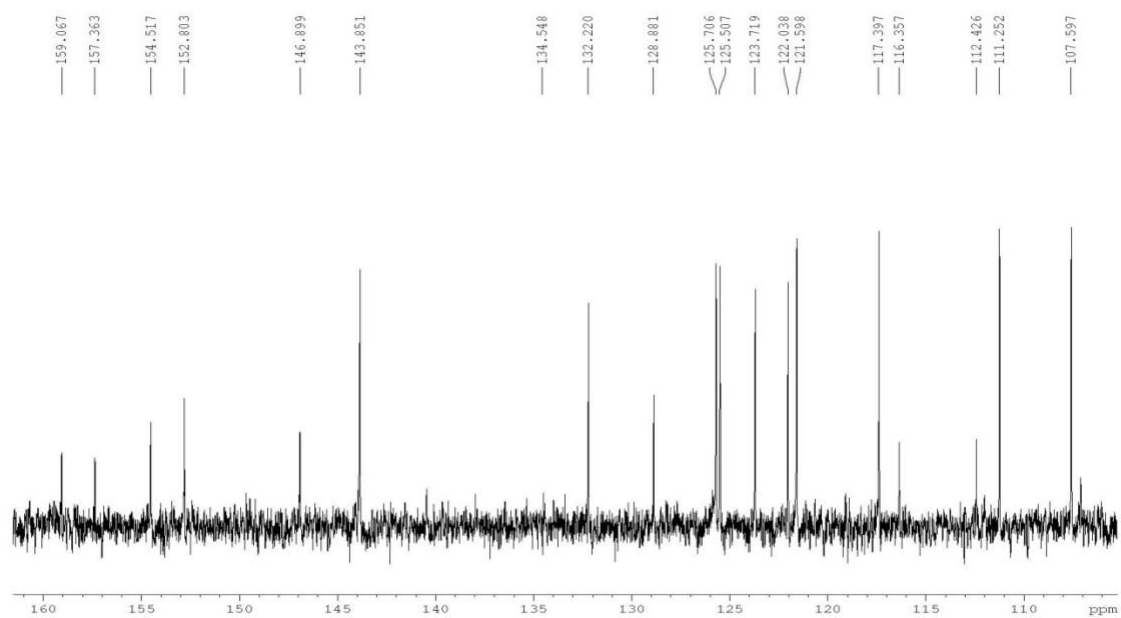
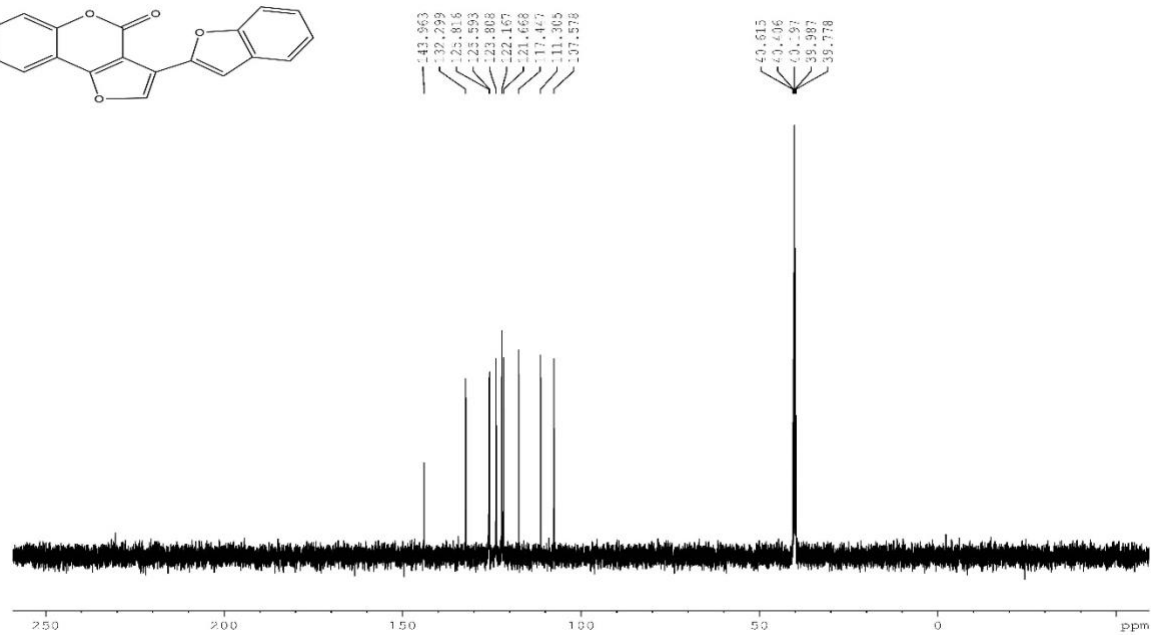
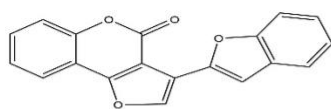
Compound 4a

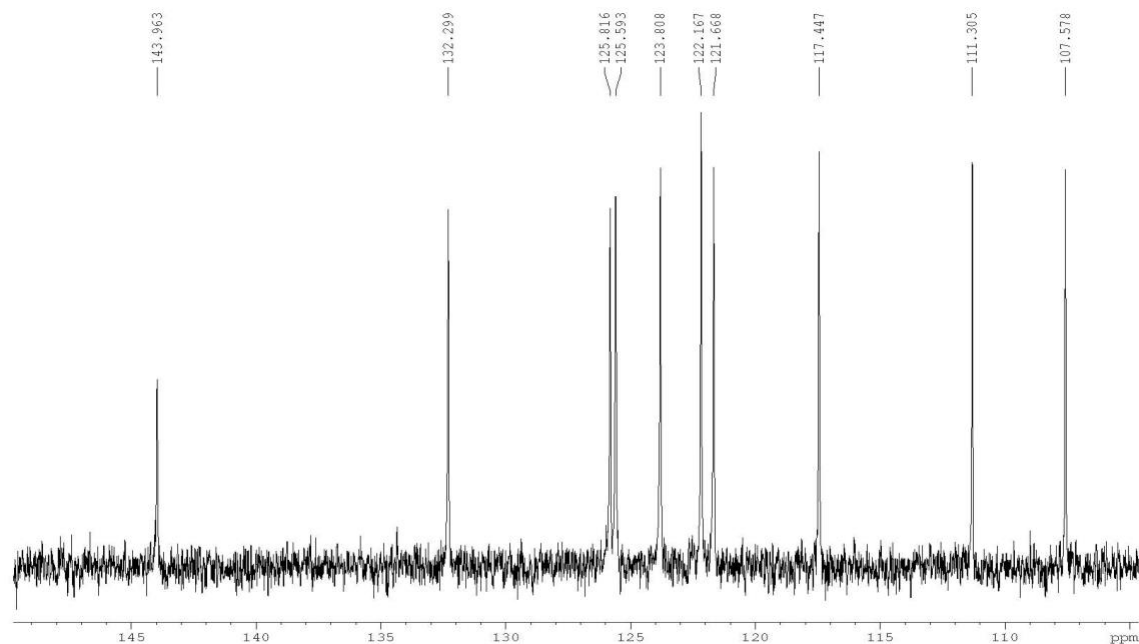
¹H NMR spectra



Compound 4a

¹³C NMR spectra

**Compound 4a****DEPT-90 spectra**



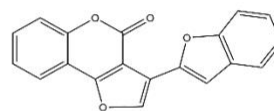
Compound 4a

Mass spectra

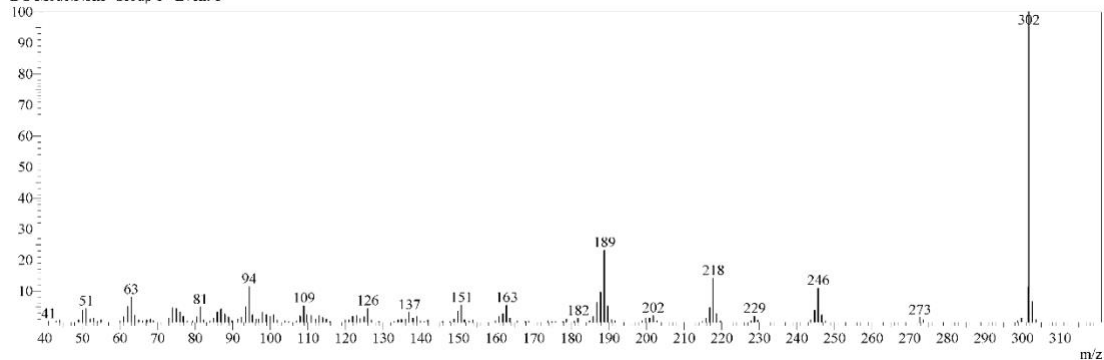
DEPARTMENT OF CHEMISTRY
(DST-FIST Funded & UGC-SAP Sponsored)
SAURASHTRA UNIVERSITY
RAJKOT-360005

Sample Information

Analyzed by : BHOLA GAURAV
Analyzed : 2/9/2015 11:41:03 AM
Sample Name : D12
Sample ID : D12
Data File : D:\OUT OF DEP\KAUSHAL PATEL\D12.qgd
C:\GCMSSolution\Data\Project\DI12.ms SPEED.qgm
Tuning File : C:\GCMSSolution\System1\Tune1\020215_F1_MS.qgf

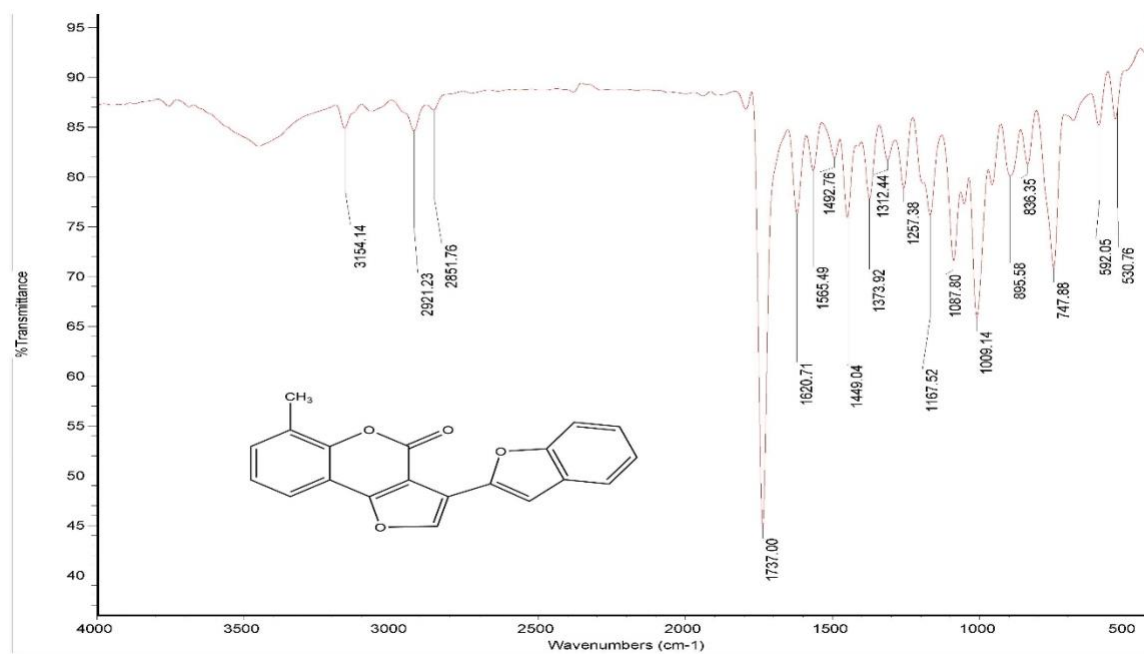


Line#:1 R Time:3.5(Scan#:595)
MassPeaks:138
RawMode:Averaged 1.8-4.8(257-857) BasePeak:301.650(113433)
BG Mode:None Group 1 - Lvent 1

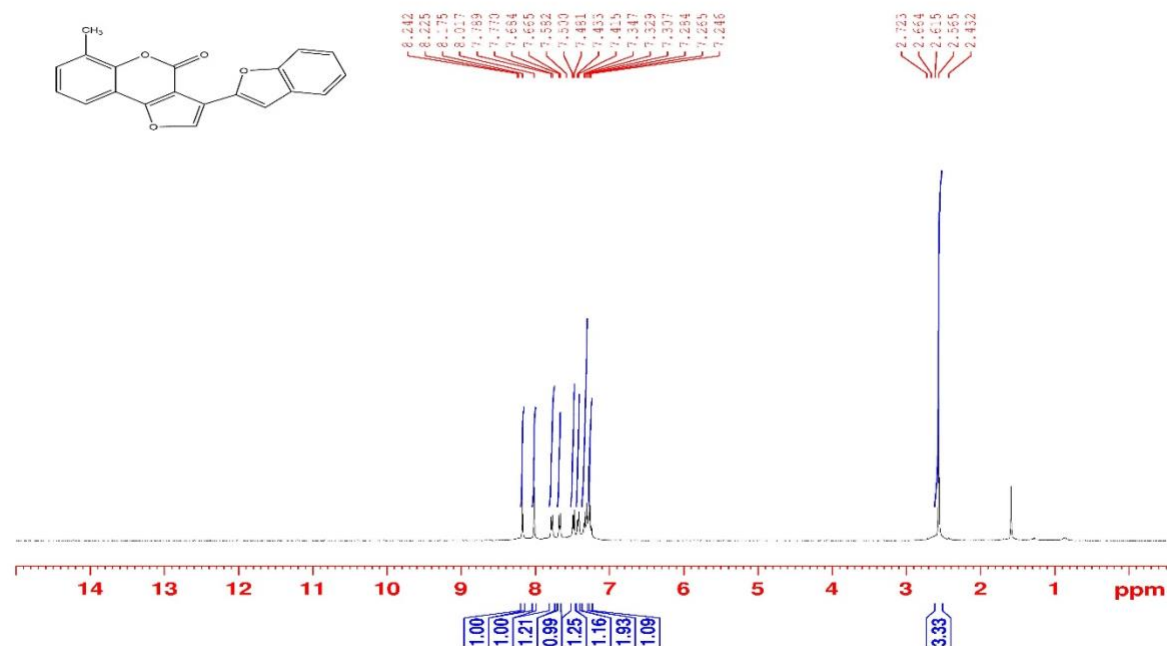


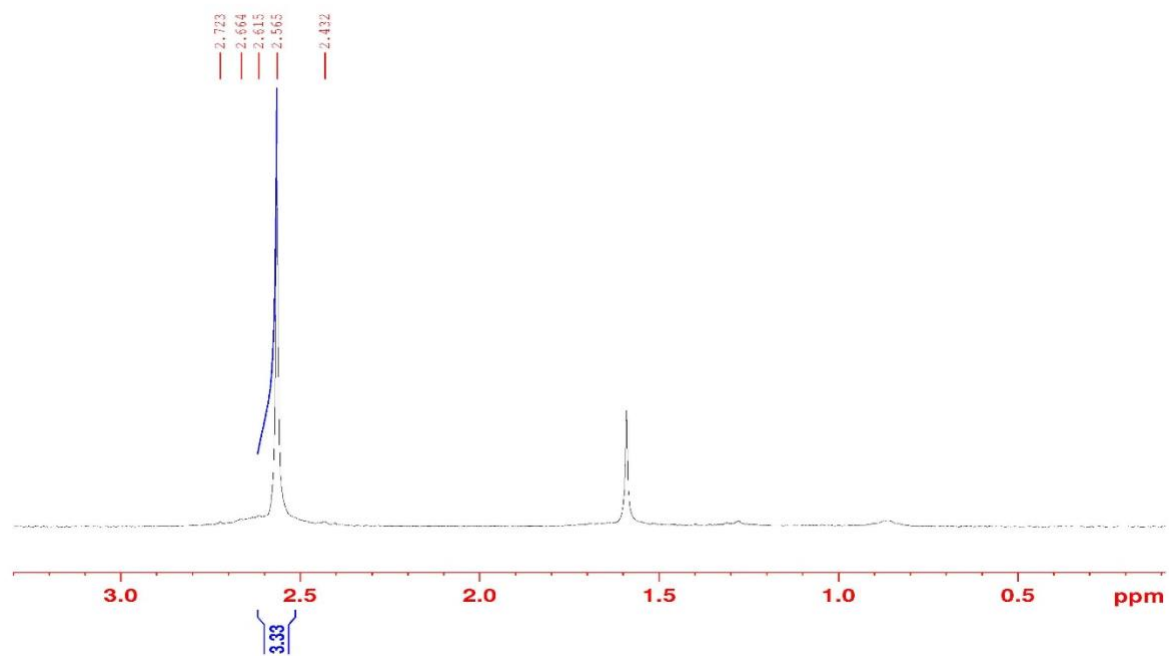
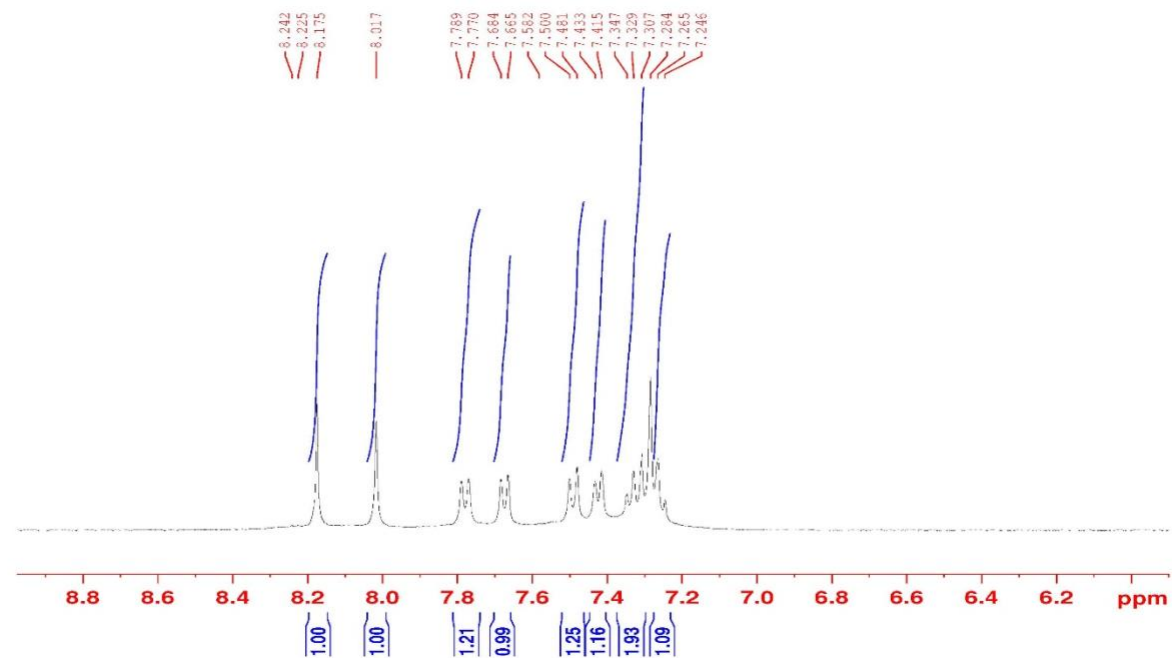
Compound 4b

Infrared Spectra

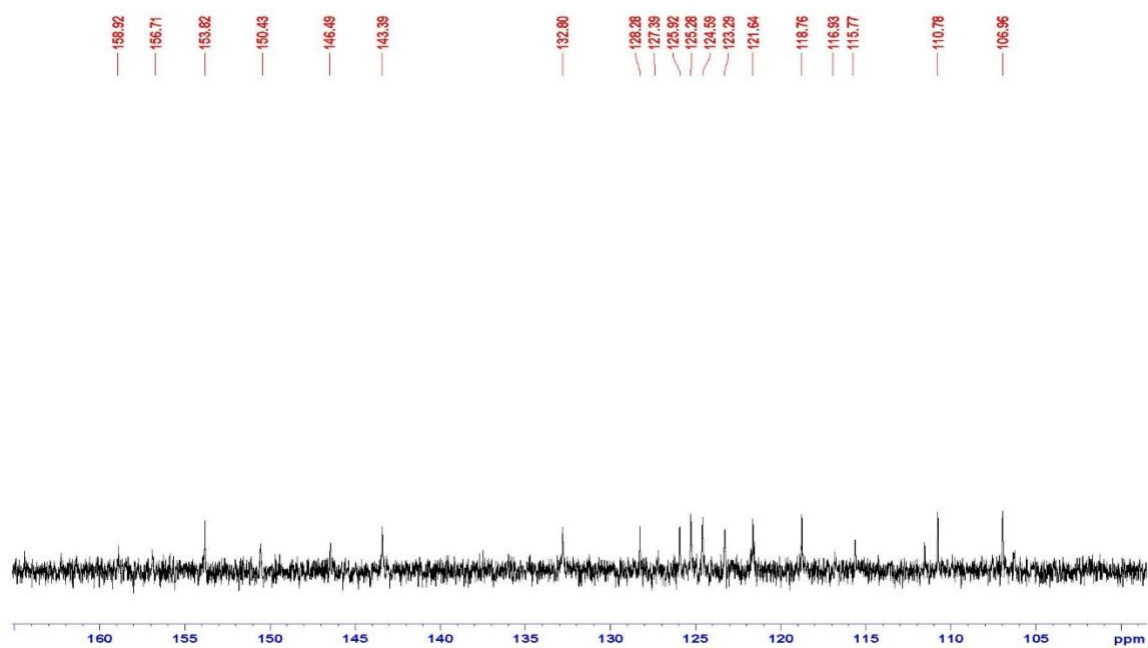
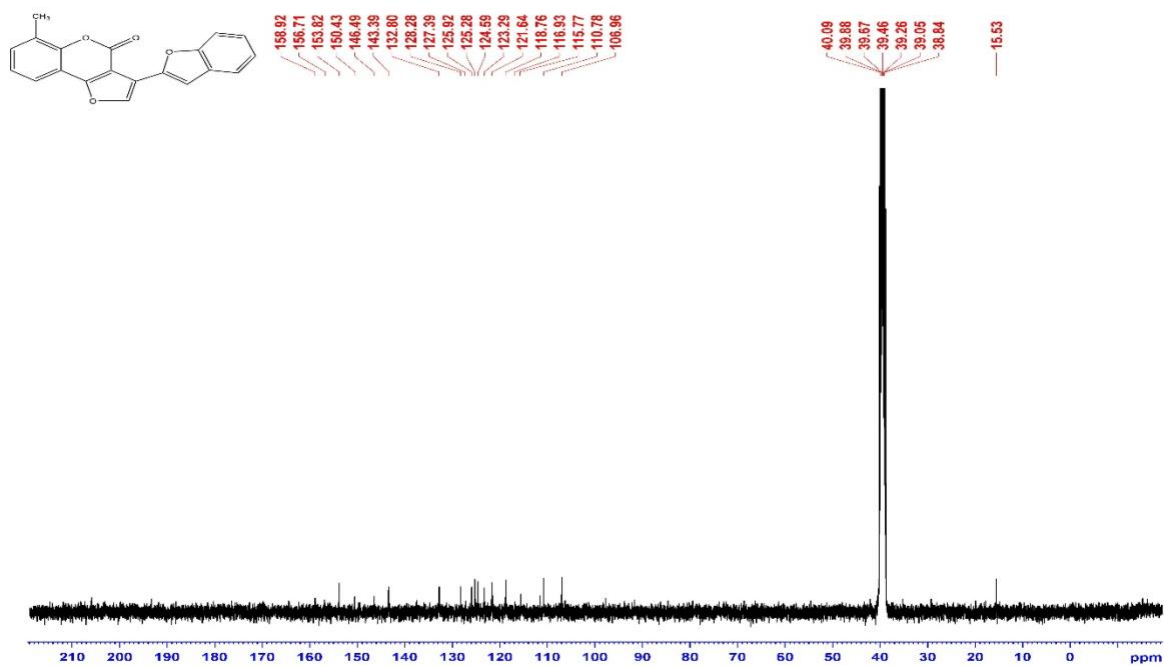


Compound 4b

¹H NMR spectra

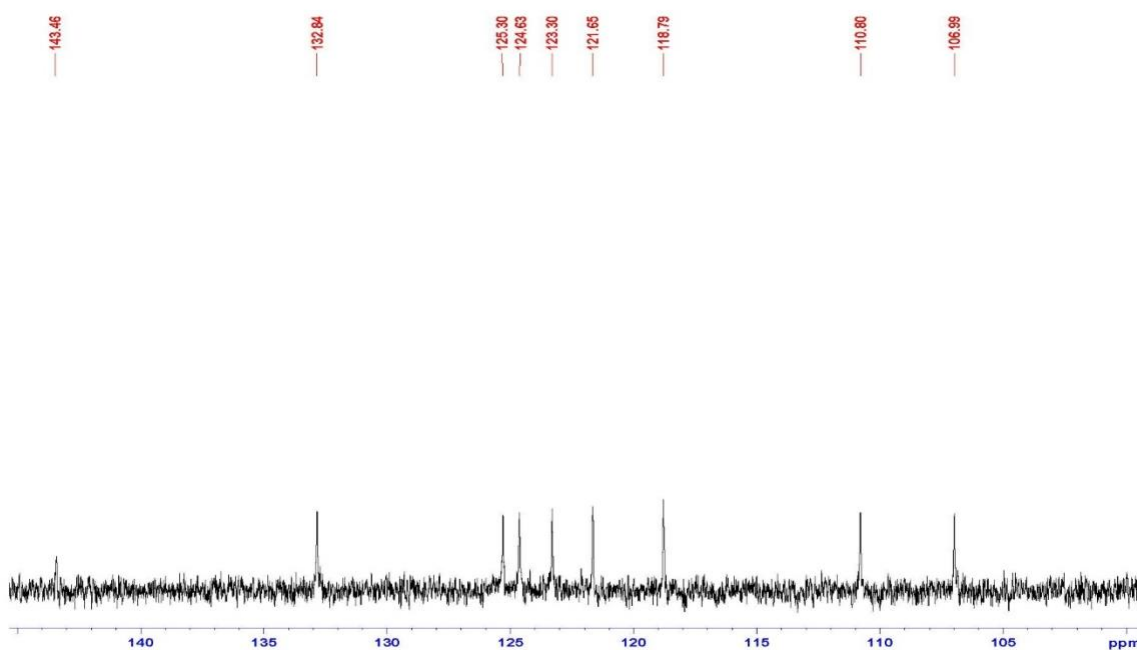
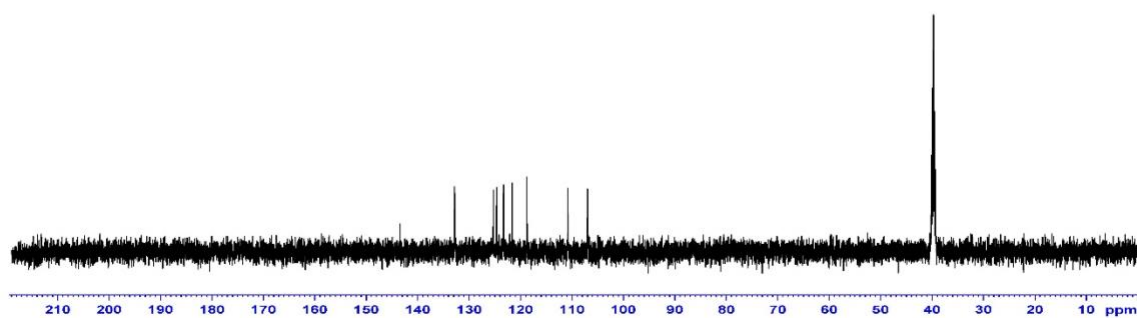
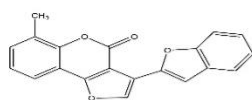


Compound 4b

 ^{13}C NMR spectra

Compound 4b

DEPT-90 spectra



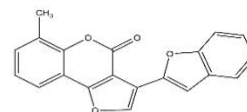
Compound 4b

Mass spectra

DEPARTMENT OF CHEMISTRY
(DST-FIST Funded & UGC-SAP Sponsored)
SAURASHTRA UNIVERSITY
RAJKOT-360005

Sample Information

Analyzed by :BHOLA GAURAV
Analyzed : 2/9/2015 2:16:23 PM
Sample Name : D 15
Sample ID : D 15
Data File : D:\OUT OF DEPKAUSTHA\PATH\MD 15.ngd
Tuning File : C:\GCMS\software\System1\msd1020215_F1.MS.gct

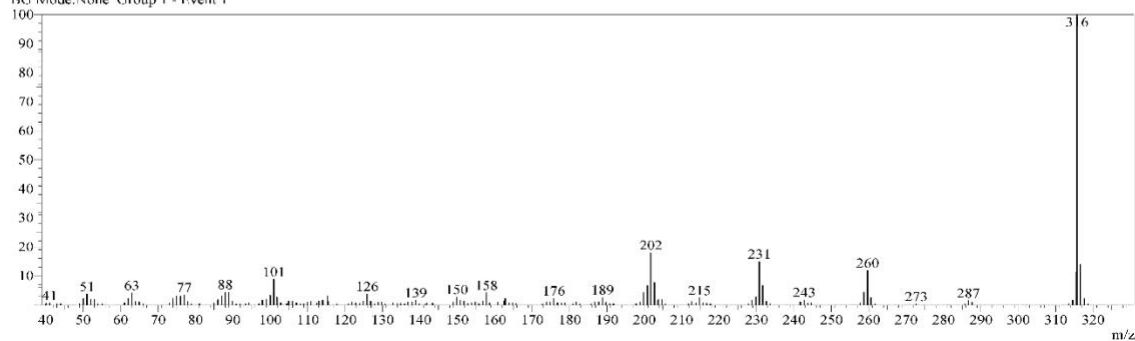


Line# : 1 R Time: 3.0 (Scan#: 507)

Mass Peaks: 156

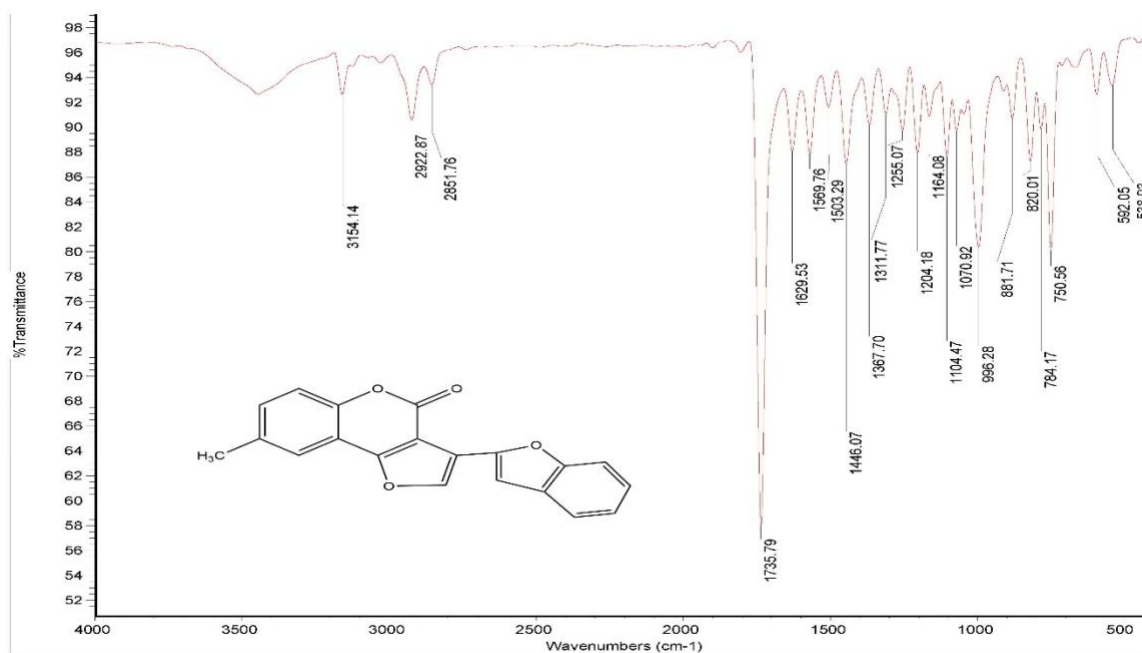
Raw Mode: Averaged 2.0-3.8 (302-656) Base Peak: 315.700 (1100008)

BG Mode: None Group 1 - Event 1

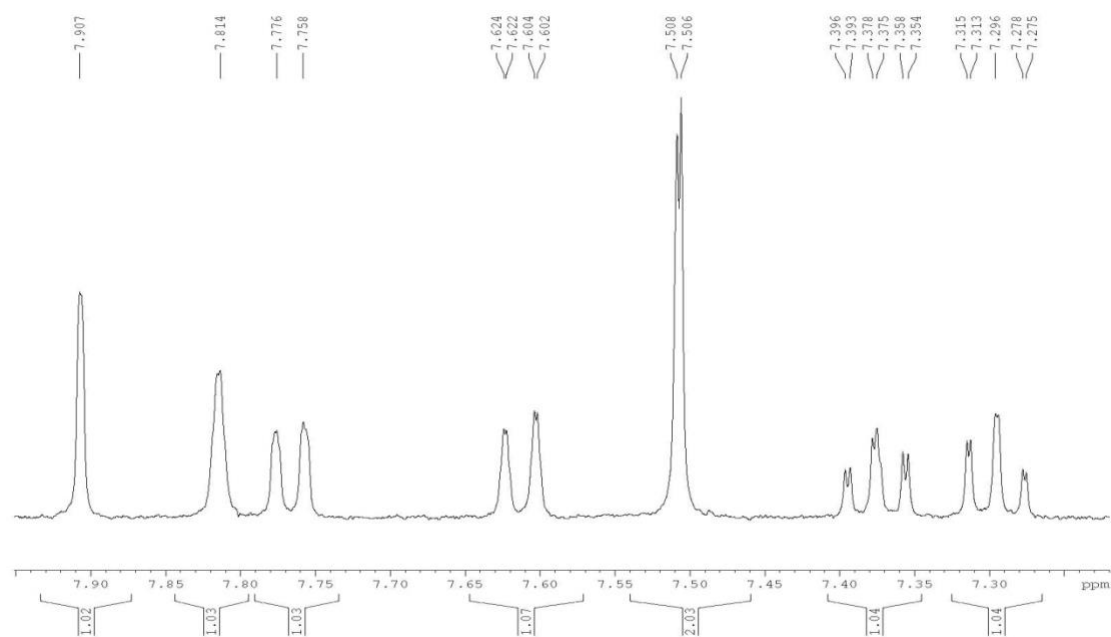
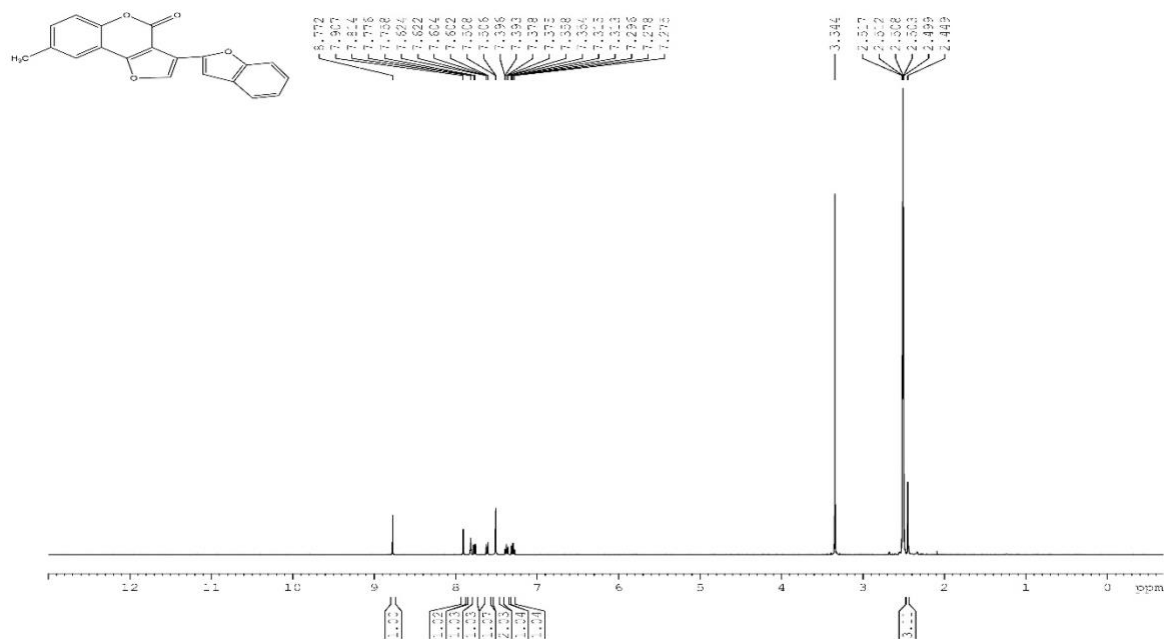


Compound 4c

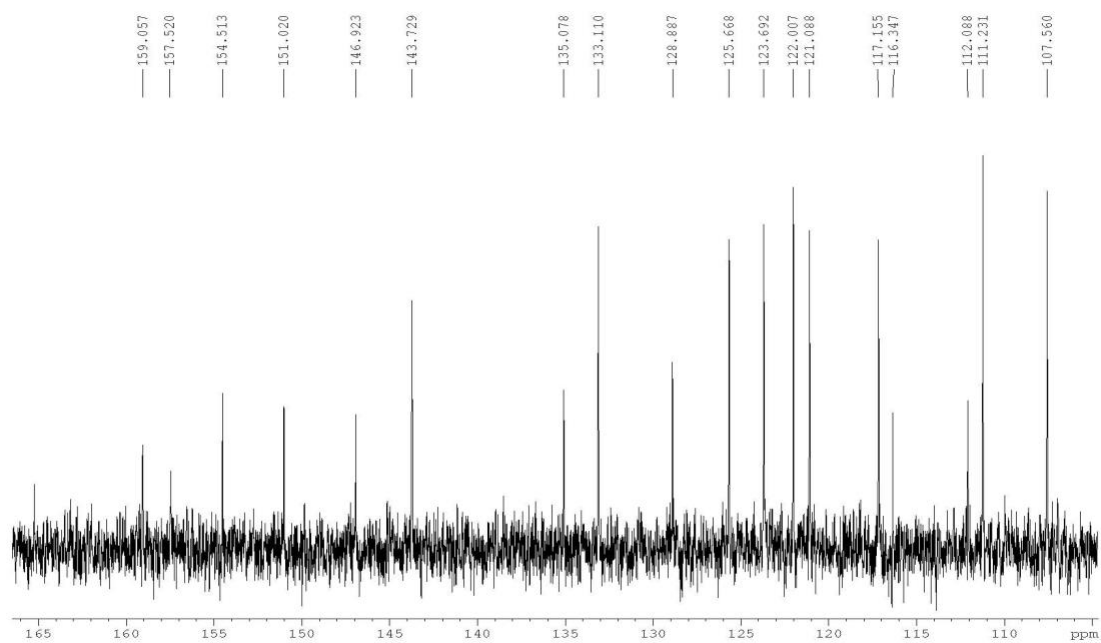
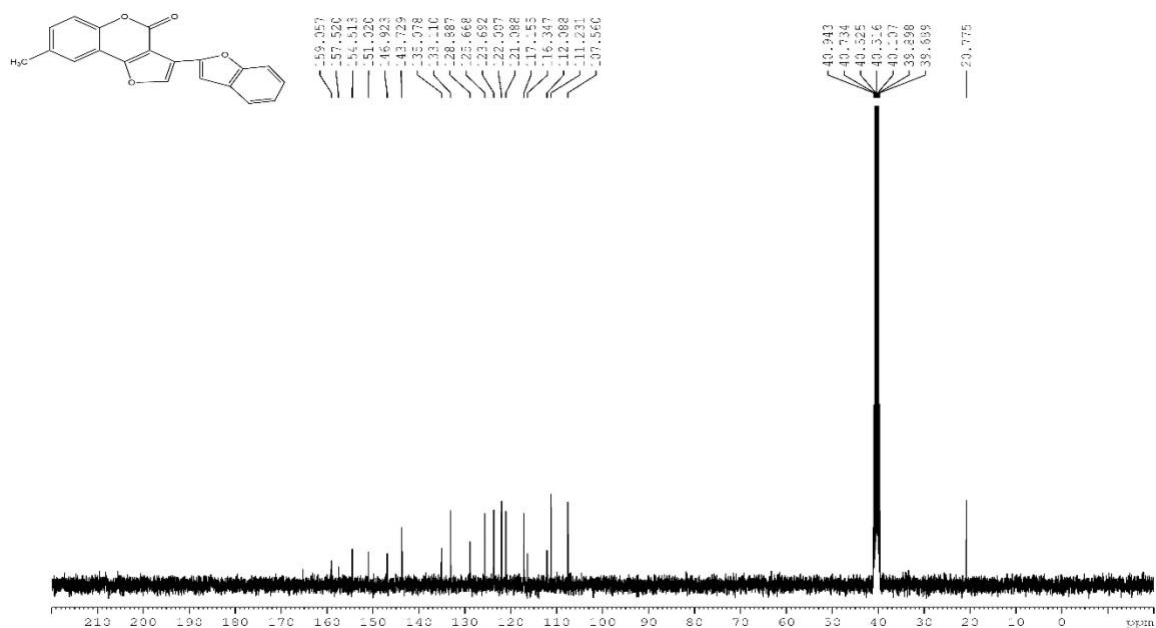
Infrared Spectra

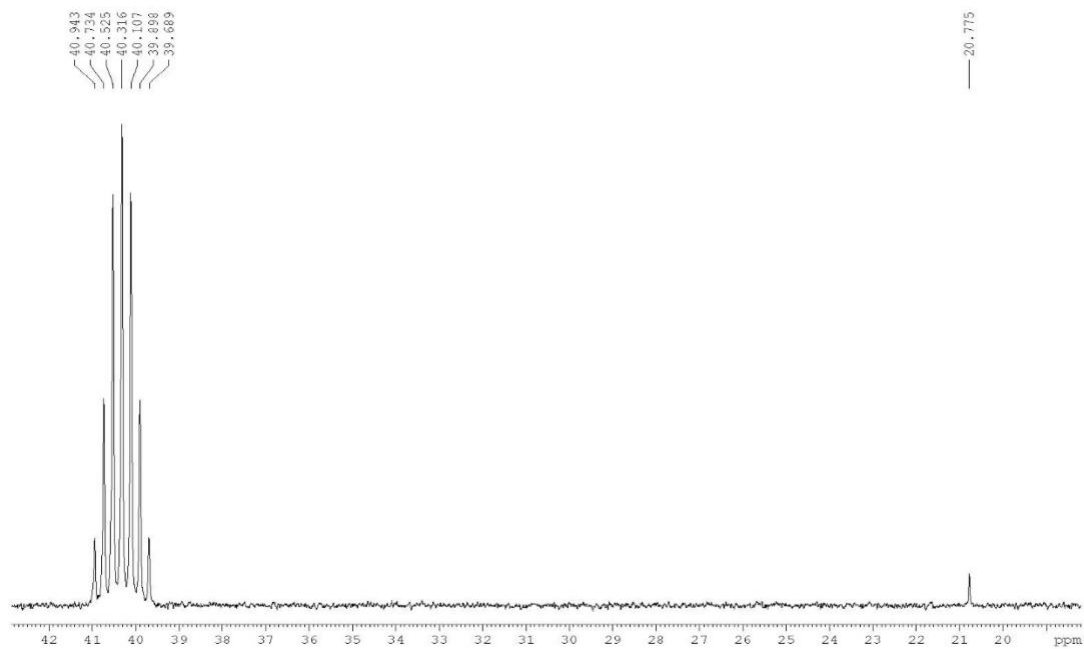
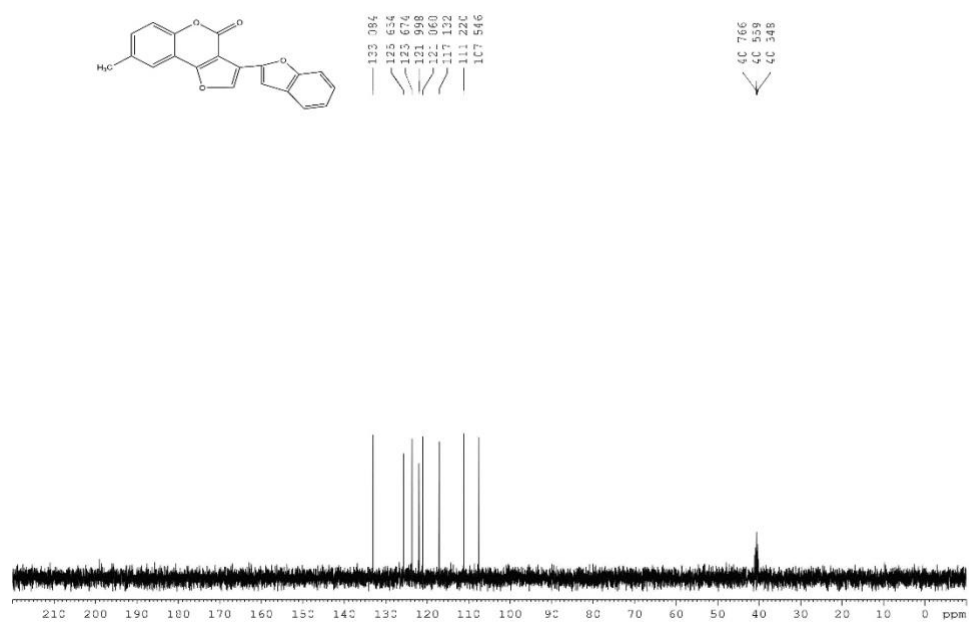


Compound 4c



Compound 4c

¹³C NMR spectra

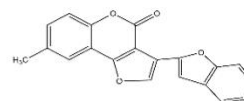
**Compound 4c****DEPT-90 spectra**

Compound 4c

Mass spectra

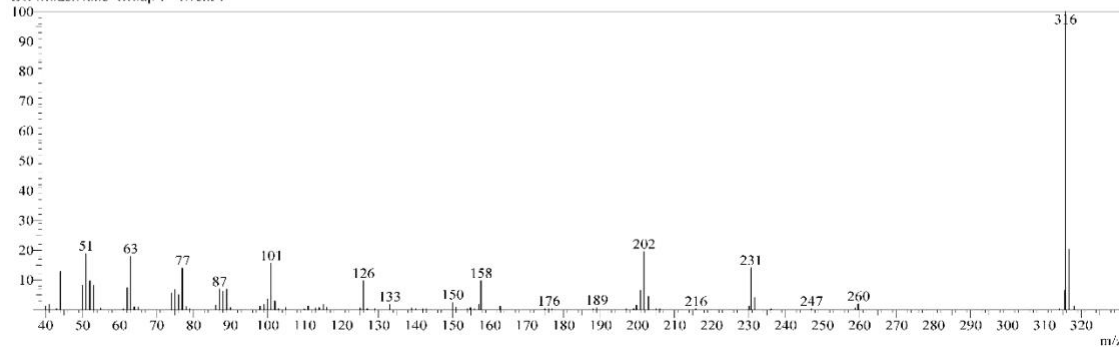
DEPARTMENT OF CHEMISTRY
(DST-FIST Funded & UGC-SAP Sponsored)
SAURASHTRA UNIVERSITY
RAJKOT-360005

Sample Information



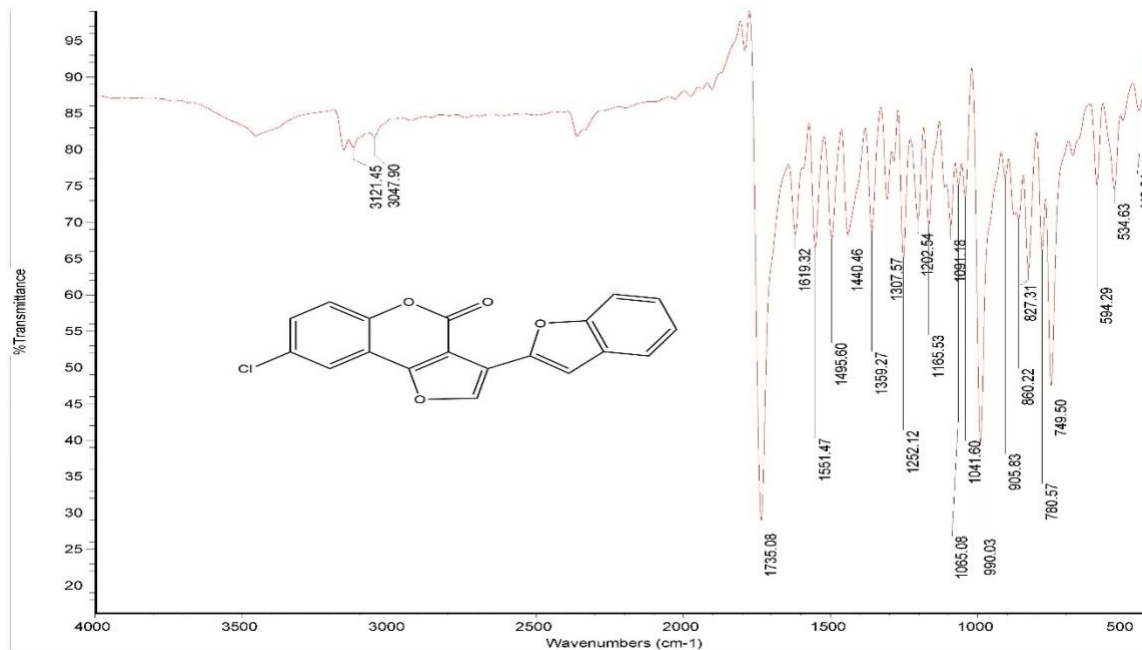
Analyzed by : BHOLA GAURAV
Analyzed : 2/9/2015 3:16:09 PM
Sample Name : D13
Sample ID :
Data File : D:\OUT OF DEP\KAUSHAL PATEL\D13.qgd
C:\GCMSolution\Data\Project1\DI.ms.SPEED.qgm
Tuning File : C:\GCMSolution\System1\Tune1\020215_F1_NSR.qgt

Line#:1 R.Time:2.3(Scan#:351)
MassPeaks:81
RawMode:Averaged 1.3-3.5(153-597) BasePeak:315.700(764)
BG Mode:None Group 1 - Event 1

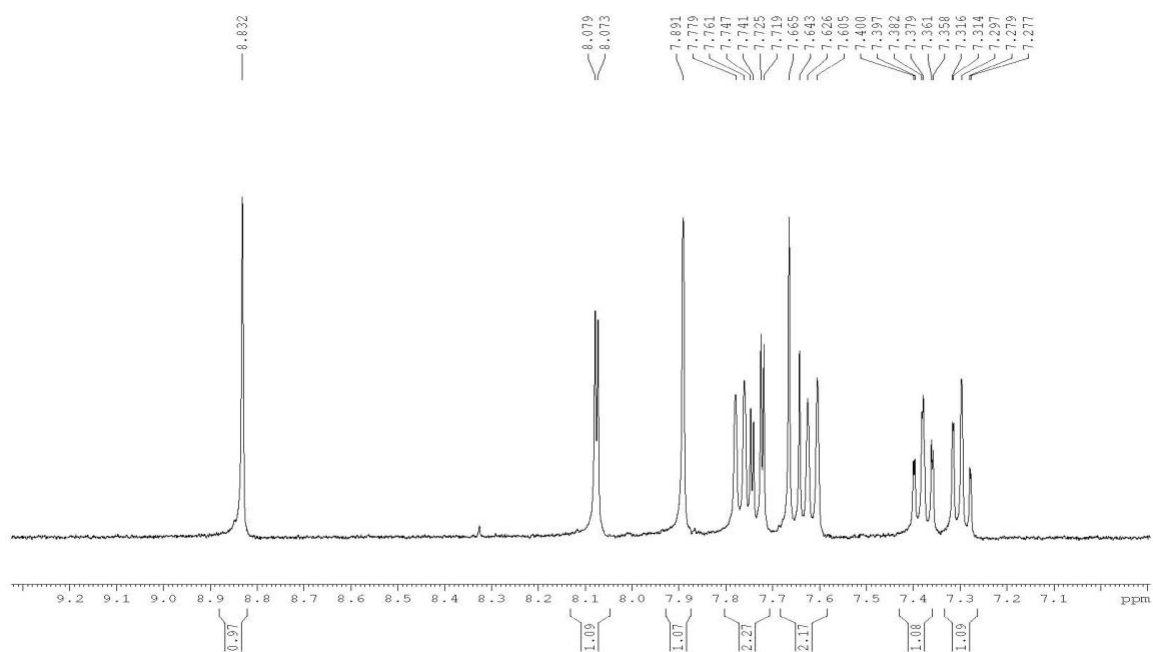
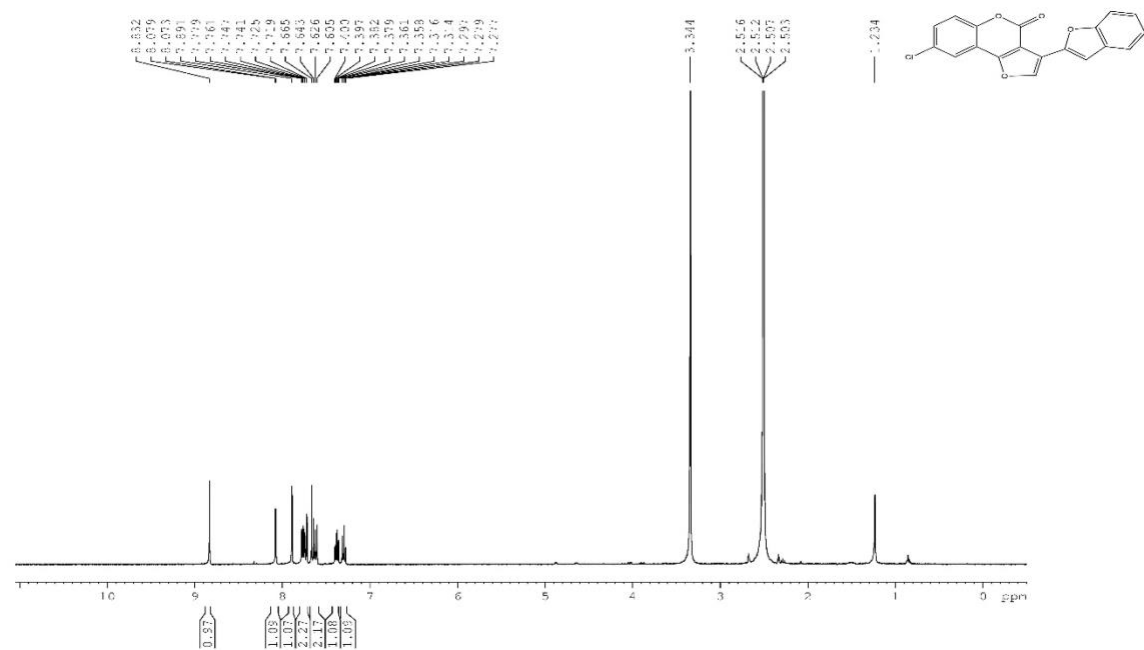


Compound 4d

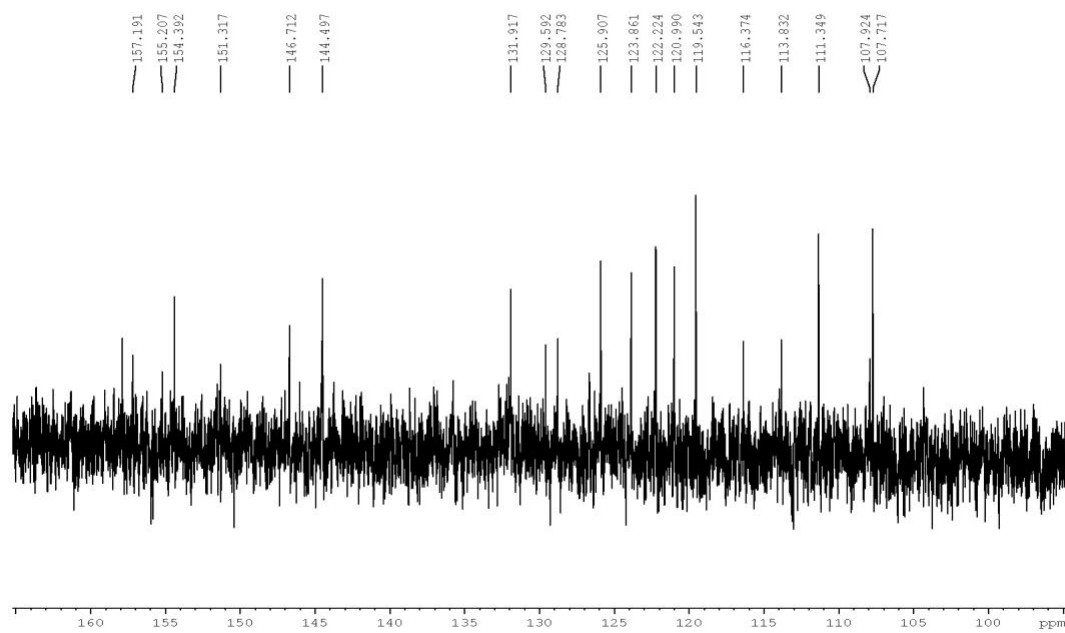
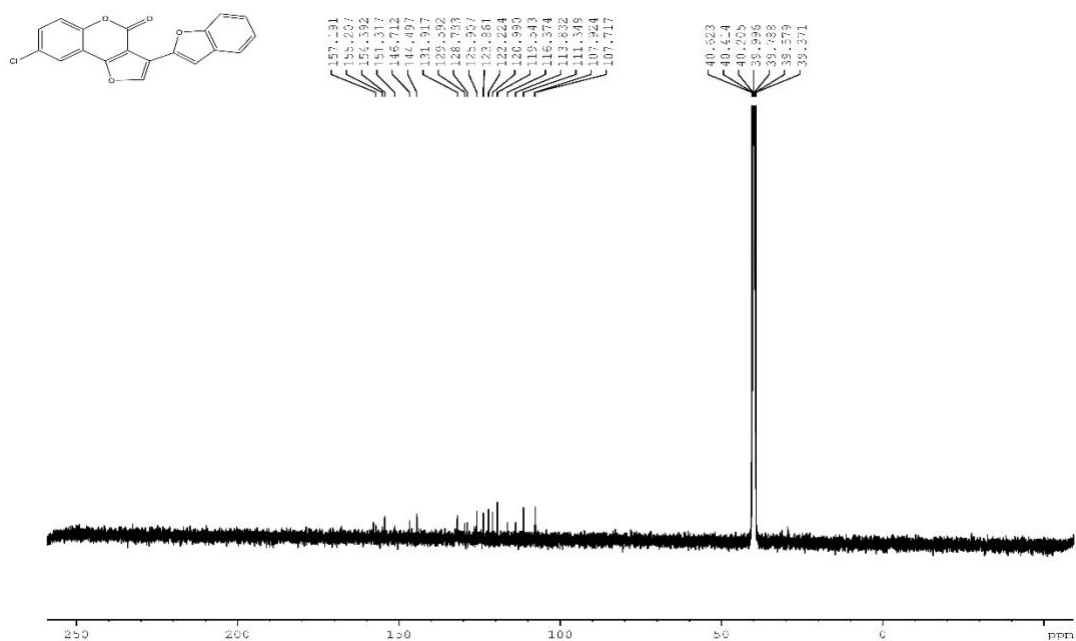
Infrared Spectra



Compound 4d

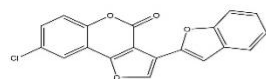
 ^1H NMR spectra

Compound 4d

 ^{13}C NMR spectra

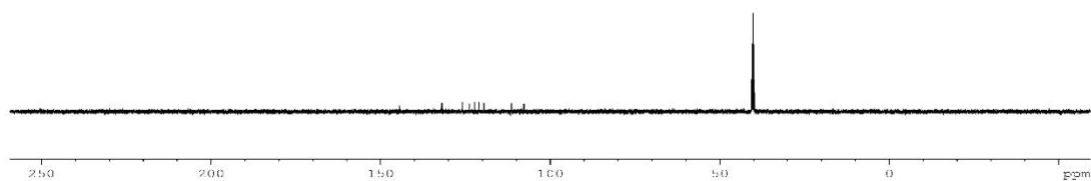
Compound 4d

DEPT-90 spectra



144.498
131.916
125.999
123.860
122.228
120.990
119.540
111.345
107.710

40.636
40.527
40.219
40.009
39.800



144.498

131.916

125.999

123.860

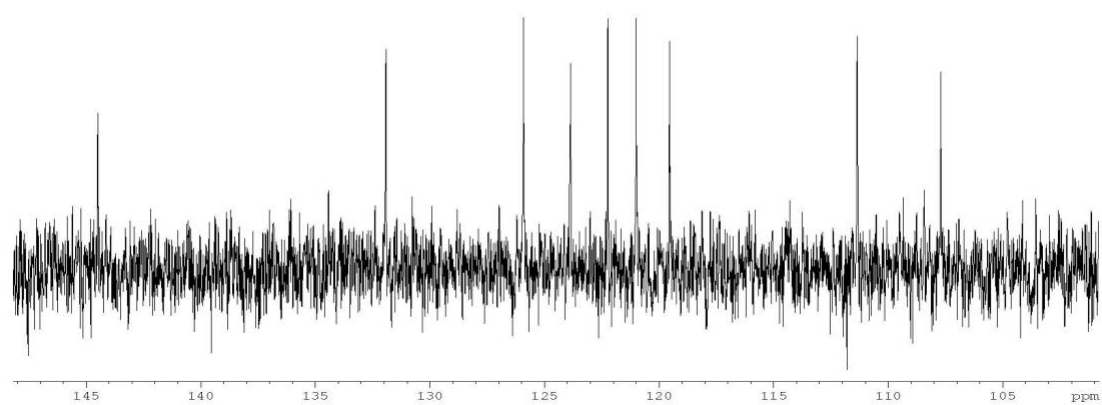
122.228

120.990

119.540

111.345

107.710



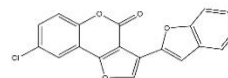
Compound 4d

Mass spectra

DEPARTMENT OF CHEMISTRY
(DST-FIST Funded & UGC-SAP Sponsored)
SAURASHTRA UNIVERSITY
RAJKOT-360005

Sample Information

Analyzed by BHOLA GAURAV
Analyzed 2/9/2015 3:36:13 PM
Sample Name D 14
Sample ID
Data File D:\OUT OF DEP\KAUSHAL PATEL\14.qgd
Tuning File C:\GCMSolution\Data\Project\14.ms.SPL1.D.qgm
C:\GCMSolution\System\Tune\1/020215_F1.MS.qgt



Line#:1 R.Time:3.3(Scan#:552)
MassPeaks:138
RawMode:Averaged 2.5-3.7(405-640) BasePeak:335.600(672168)
BG Mode:None Group 1 - Event 1

