Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplimentary Data

X-ray crystal structures and anti breast cancer property of 3-*tert*-butoxycarbonyl-2-arylthiazolidine-4-carboxylic acids

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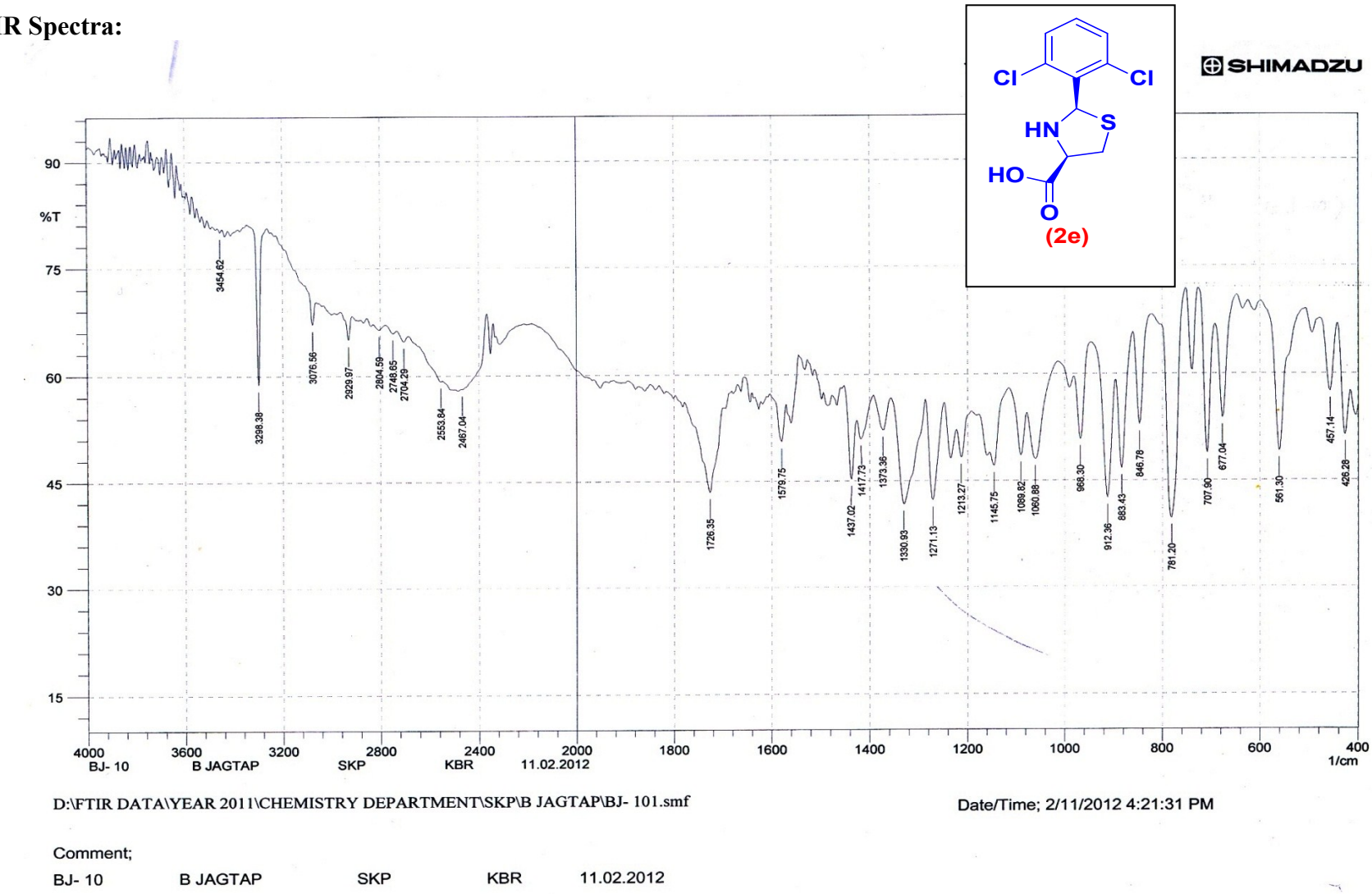
[b]Center for Materials Characterization (CMC), National Chemical Laboratory, Dr. Homi Bhabha Road, Pune-411008, India

- **Characterization of compounds (2e-3e)**
- **IR Spectrum**
- **^{1}H NMR Spectrum**
- **^{13}C NMR Spectrum**
- **LCMS Spectrum**
- **Crystal structure images**
- **Sigmoid fitted curves for IC_{50} values of compounds**

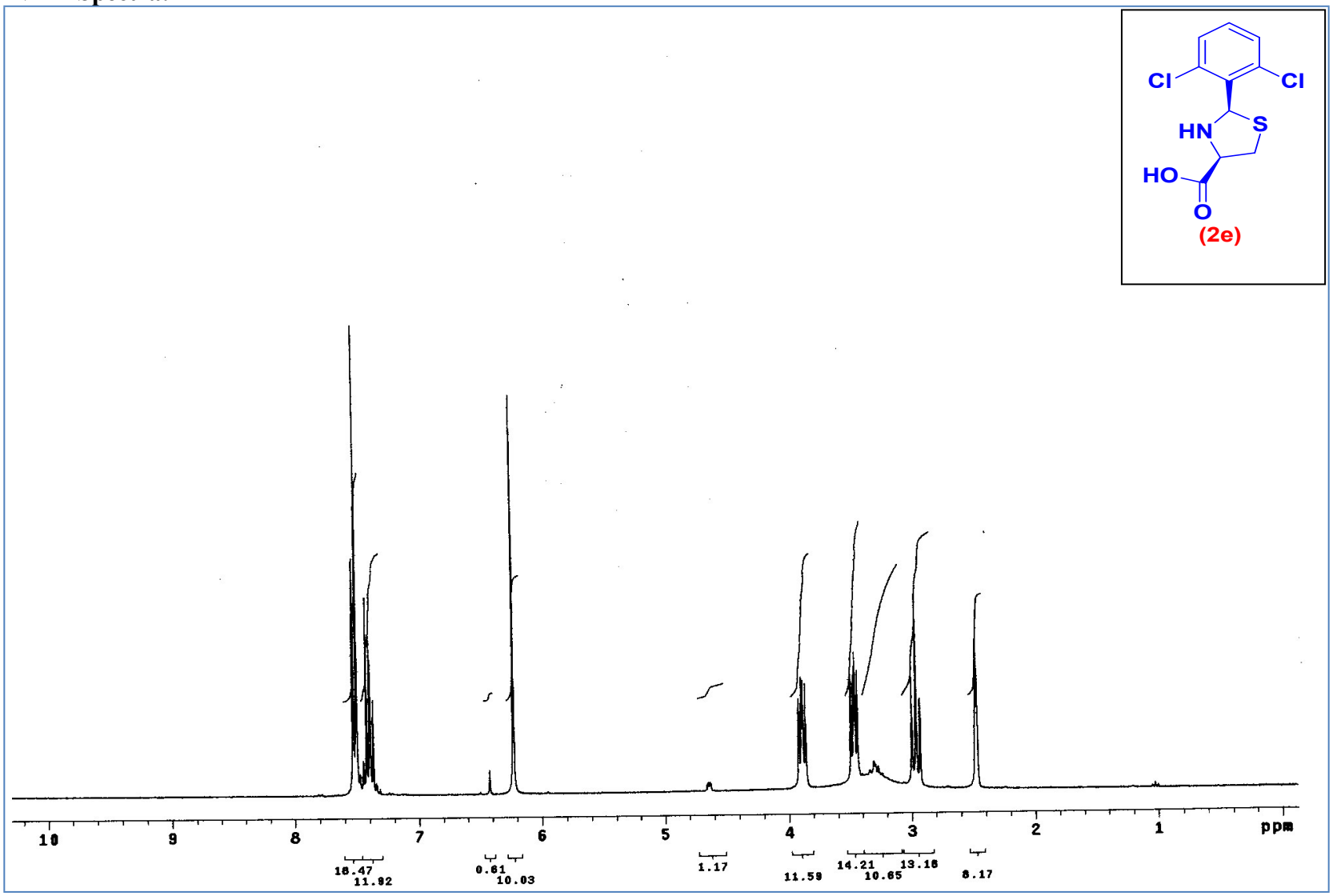
Characterization of compounds (2e-3e):

(*2S, 4R*)- 2-(2, 6-dichlorophenyl) thiazolidine-4-carboxylic acid (2e):[34]

IR Spectra:

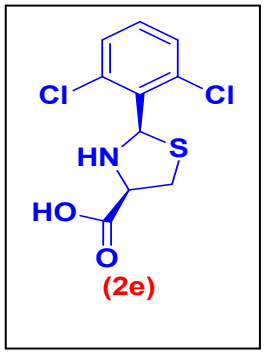


[1]H NMR Spectra:



GCMS (APCI) : 277.90 (M^++1)

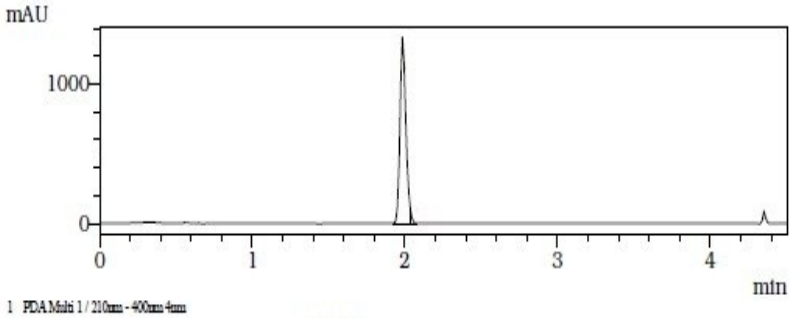
LCMS REPORT



Sample Information

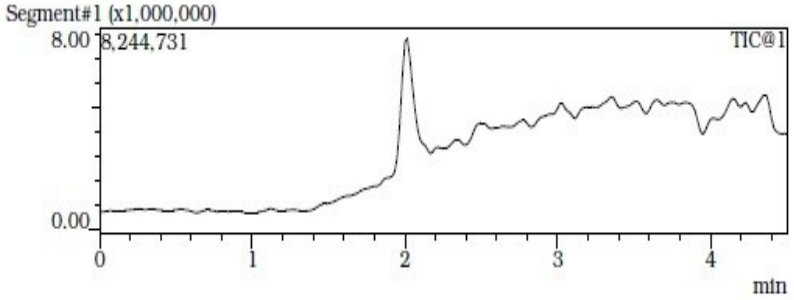
Acquired by	: Admin
Date Acquired	: 3/10/2012 12:07:43 PM
Sample Name	:
Sample ID	: BJ-10
Data File	: 108.lcd
Method File	: LCMS_ Method (4.5 min_).lcm
AR number	:

Chromatogram



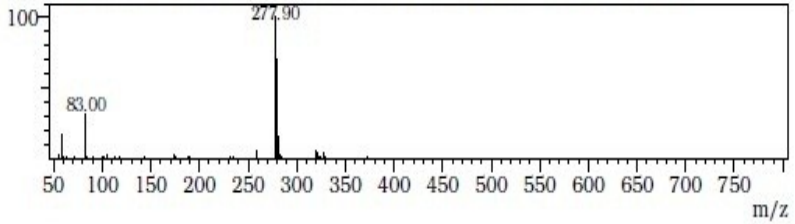
1 PDA Multi 1 / 210nm - 400nm 4nm

MS Chromatogram

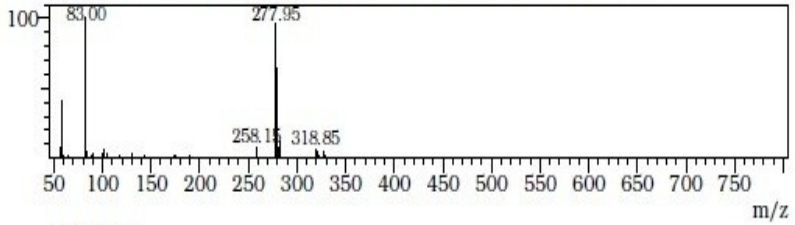


MS Spectrum Graph

Ret. Time : 2.000 min
BG Mode:Averaged 0.717-0.724(44-44)
Mass Peaks:564 Base Peak:277.90(2400488) Polarity:Pos Segment1 - Event1



Ret. Time : 2.067 min
BG Mode:Averaged 0.117-0.117(8-8)
Mass Peaks:576 Base Peak:83.00(890050) Polarity:Pos Segment1 - Event1

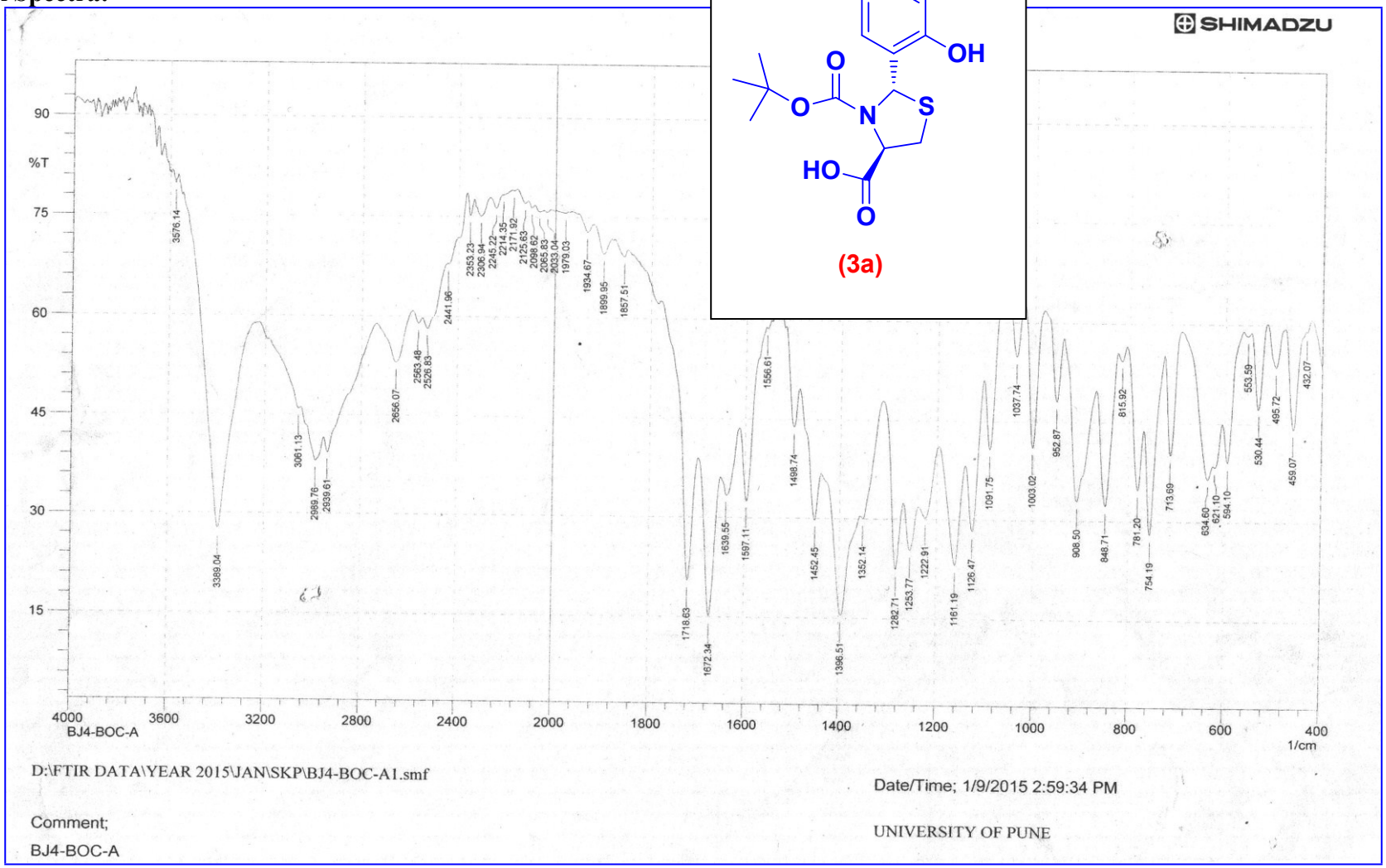


PeakTable
PDA Ch1 210nm - 400nm 4nm

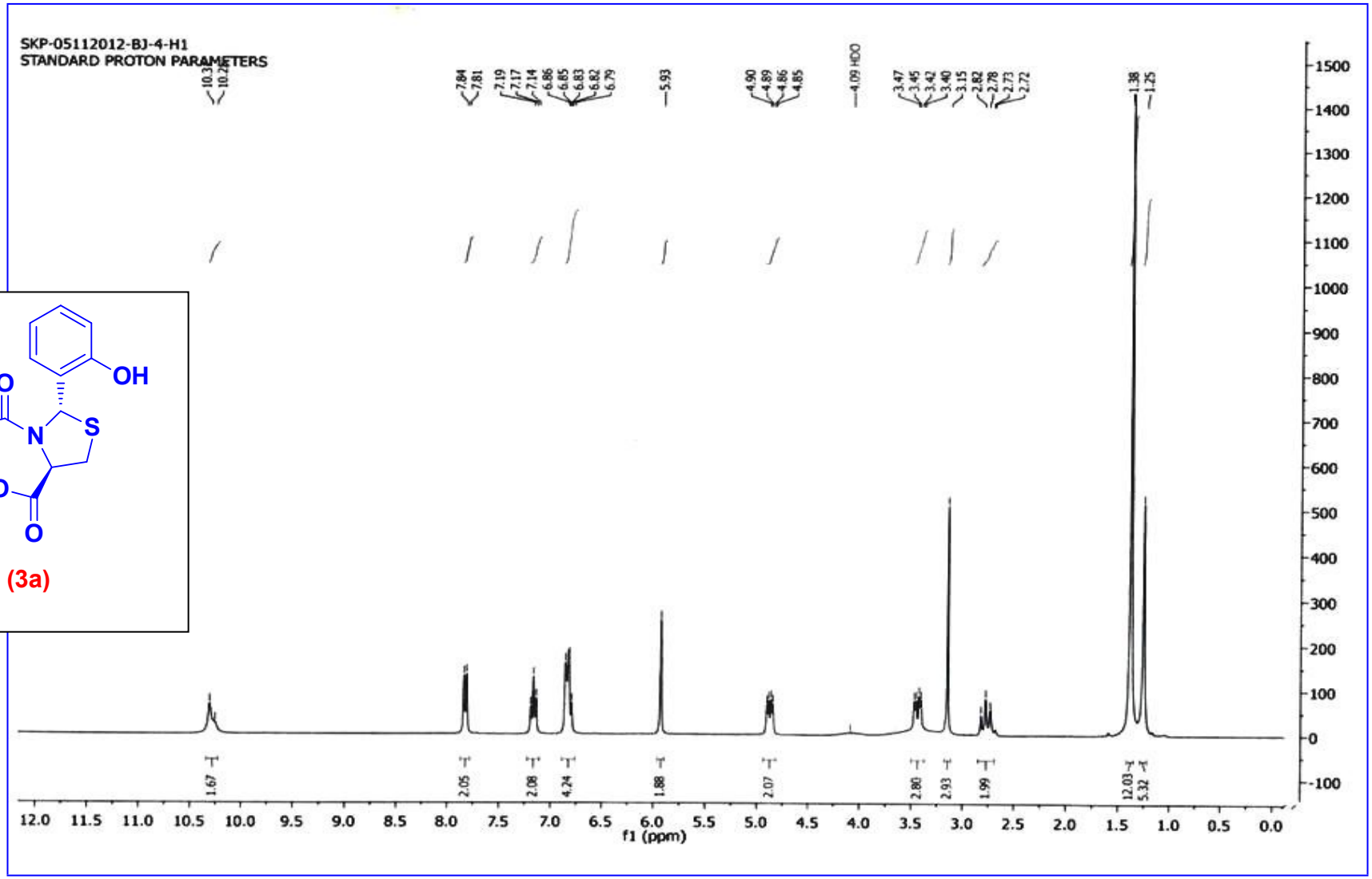
Peak#	Ret. Time	Area	Area %
1	1.980	3615970	99.163
2	2.048	30538	0.837
Total		3646508	100.000

(*2S,4R*)-3-(tert-butoxycarbonyl)-2-(2-hydroxyphenyl) thiazolidine-4-carboxylic acid (3a):[34]

IR Spectra:

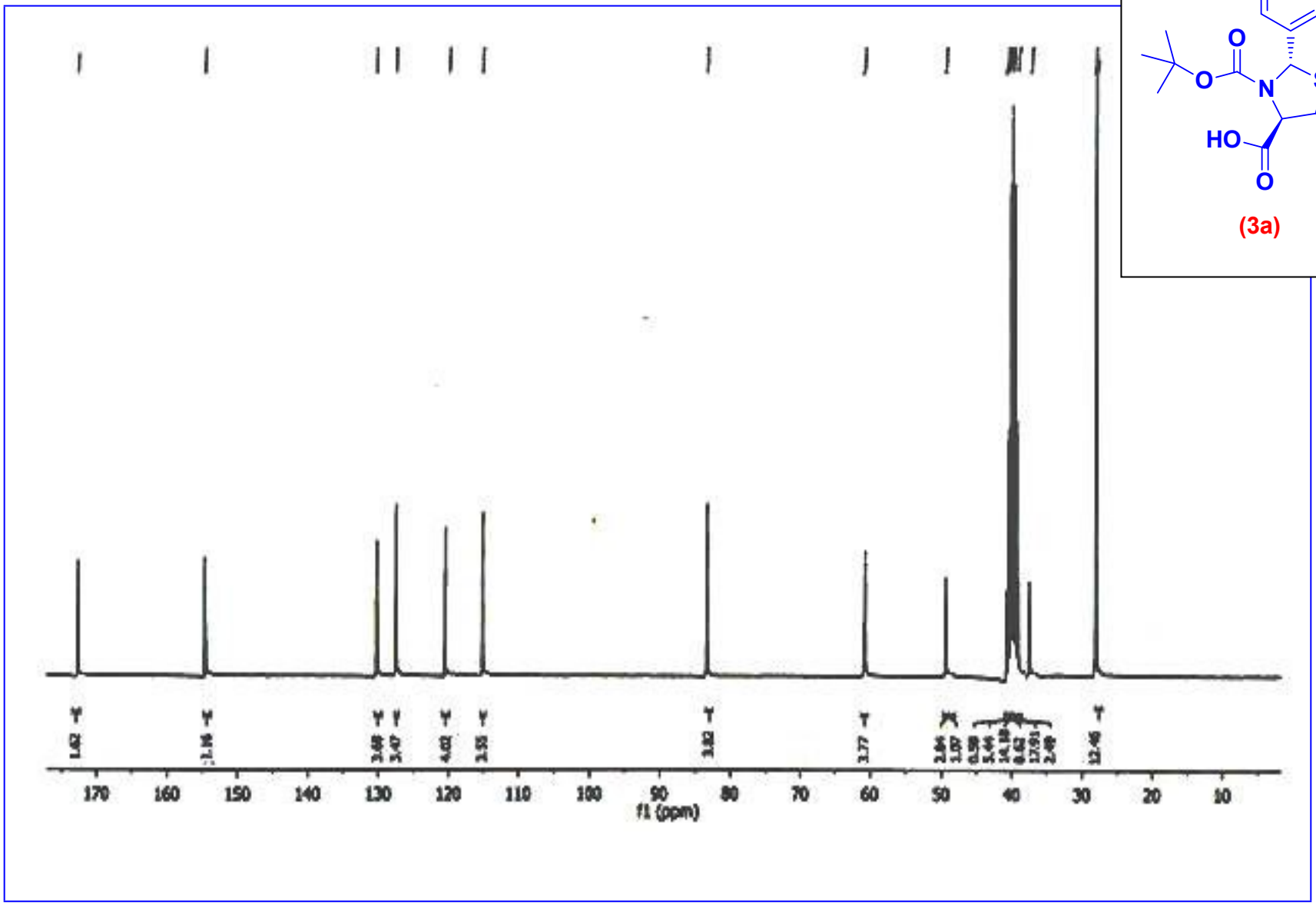


^{1}H NMR Spectra:



(3a)

^{13}C NMR Spectra:



GCMS (APCI) : 326.00 (M+1)

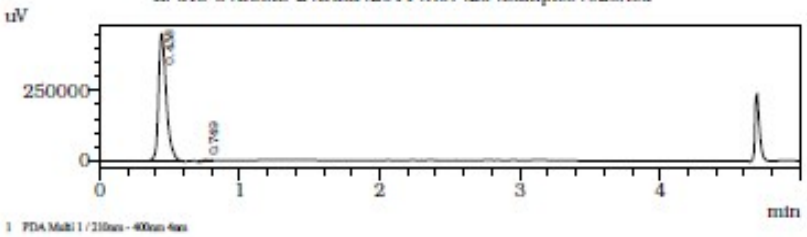
LCMS REPORT

Sample Information

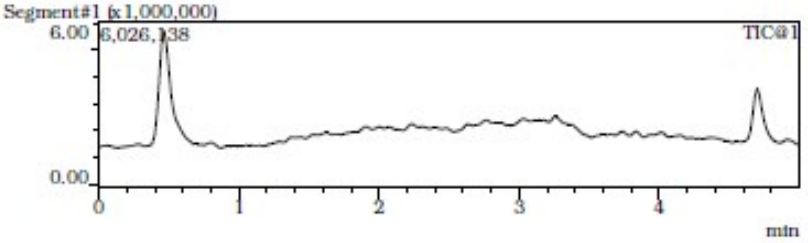
Acquired by : Admin
Date Acquired : 11/25/2013 11:23:06 AM
Sample Name :
Sample ID : ETA

Chromatogram

E:\AC-3\LCMS-2\Data\2011\Nov\25\Samples\028.lcd

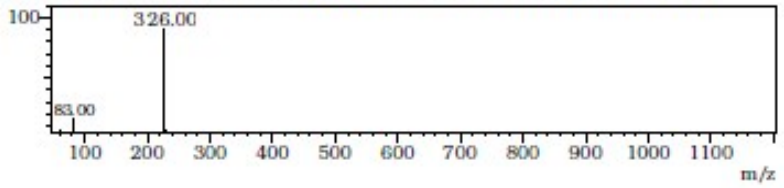


MS Chromatogram

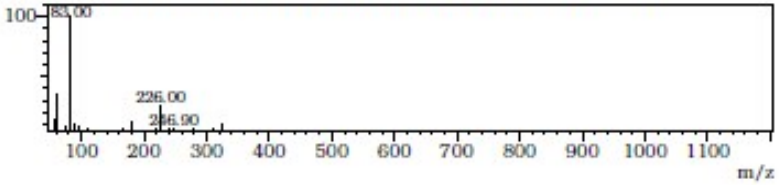


MS Spectrum Graph

Ret. Time : min
BG Mode:None
Mass Peaks:1065 Base Peak:326.00(2074780) Polarity:Pos Segment1 - Event1



Ret. Time : 0.800 min
BG Mode:Averaged 0.033-0.035(3-3)
Mass Peaks:595 Base Peak:83.00(60500) Polarity:Pos Segment1 - Event1



PeakTable

PDA Ch1 210nm - 400nm 4nm

Peak#	Ret. Time	Area	Area %
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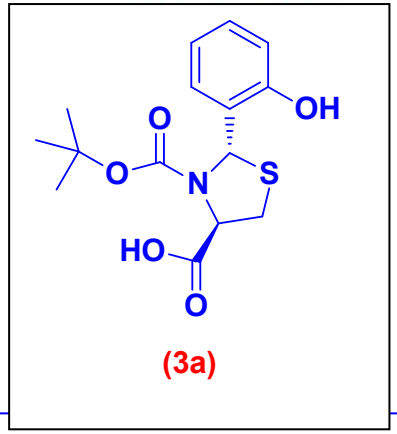
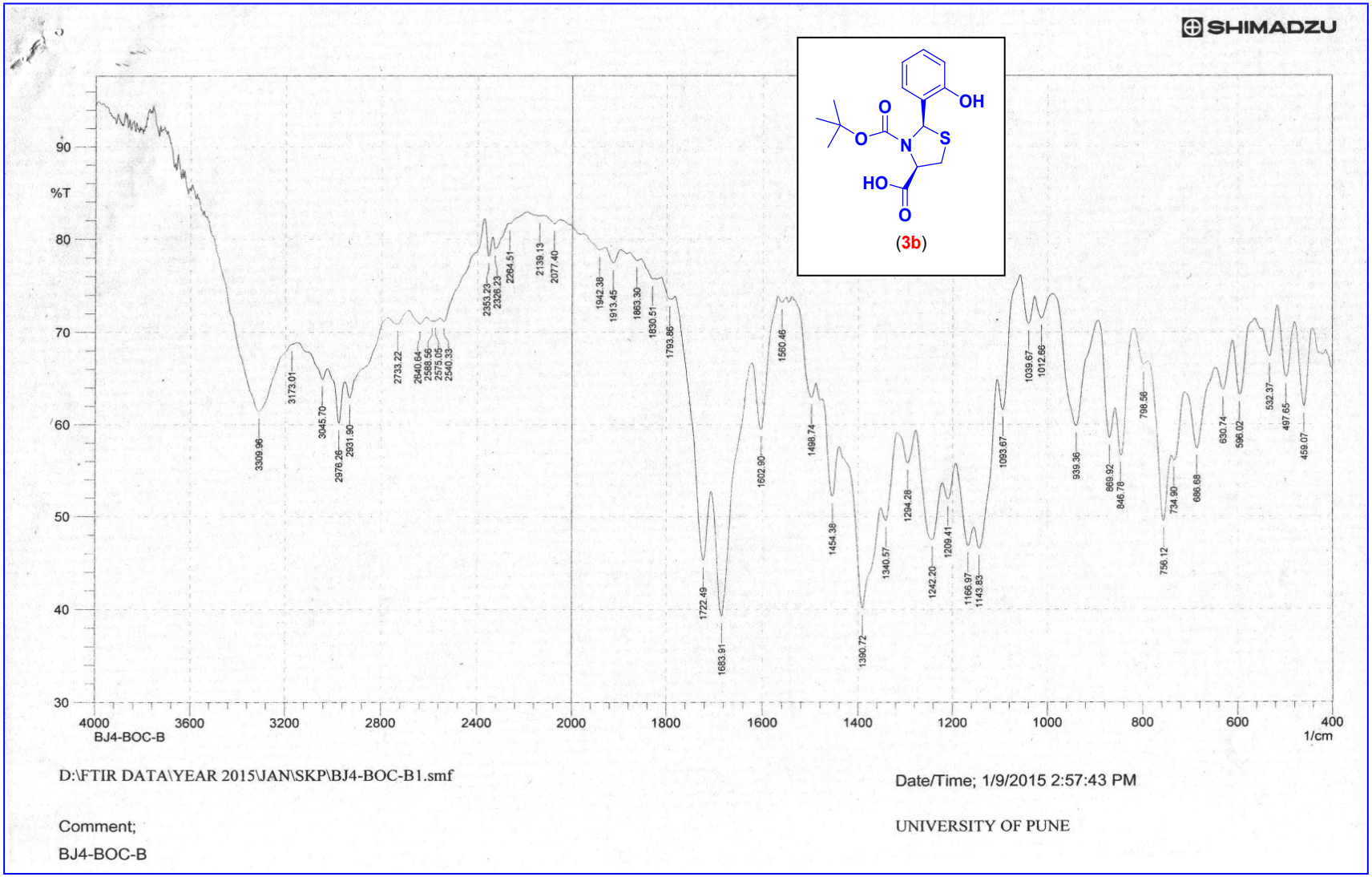
2	0.749	12144	0.691
Total		1757054	100.000



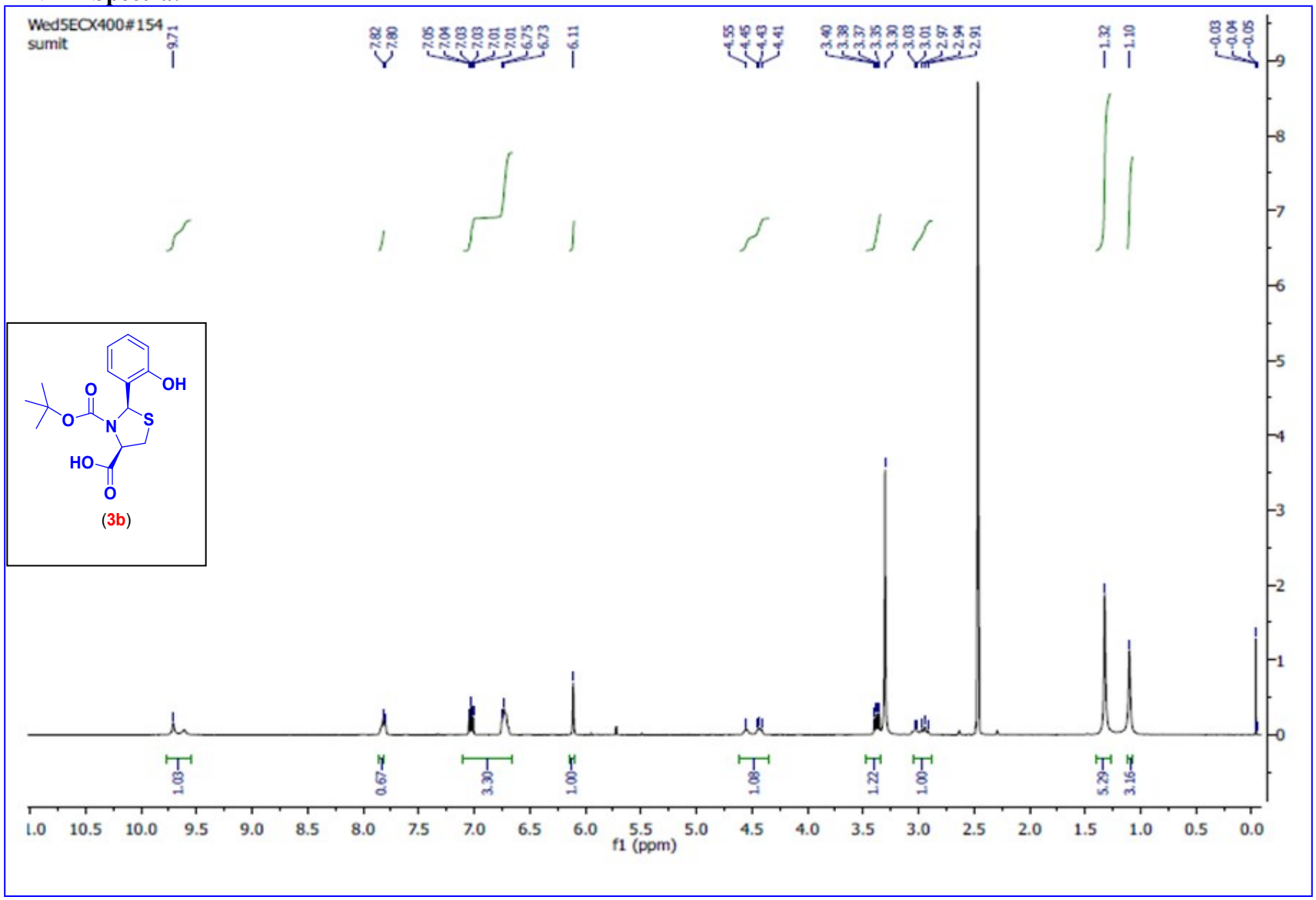
(3a)

(*2R,4R*)-3-(tert-butoxycarbonyl)-2-(2-hydroxyphenyl) thiazolidine-4-carboxylic acid (3b):[34]

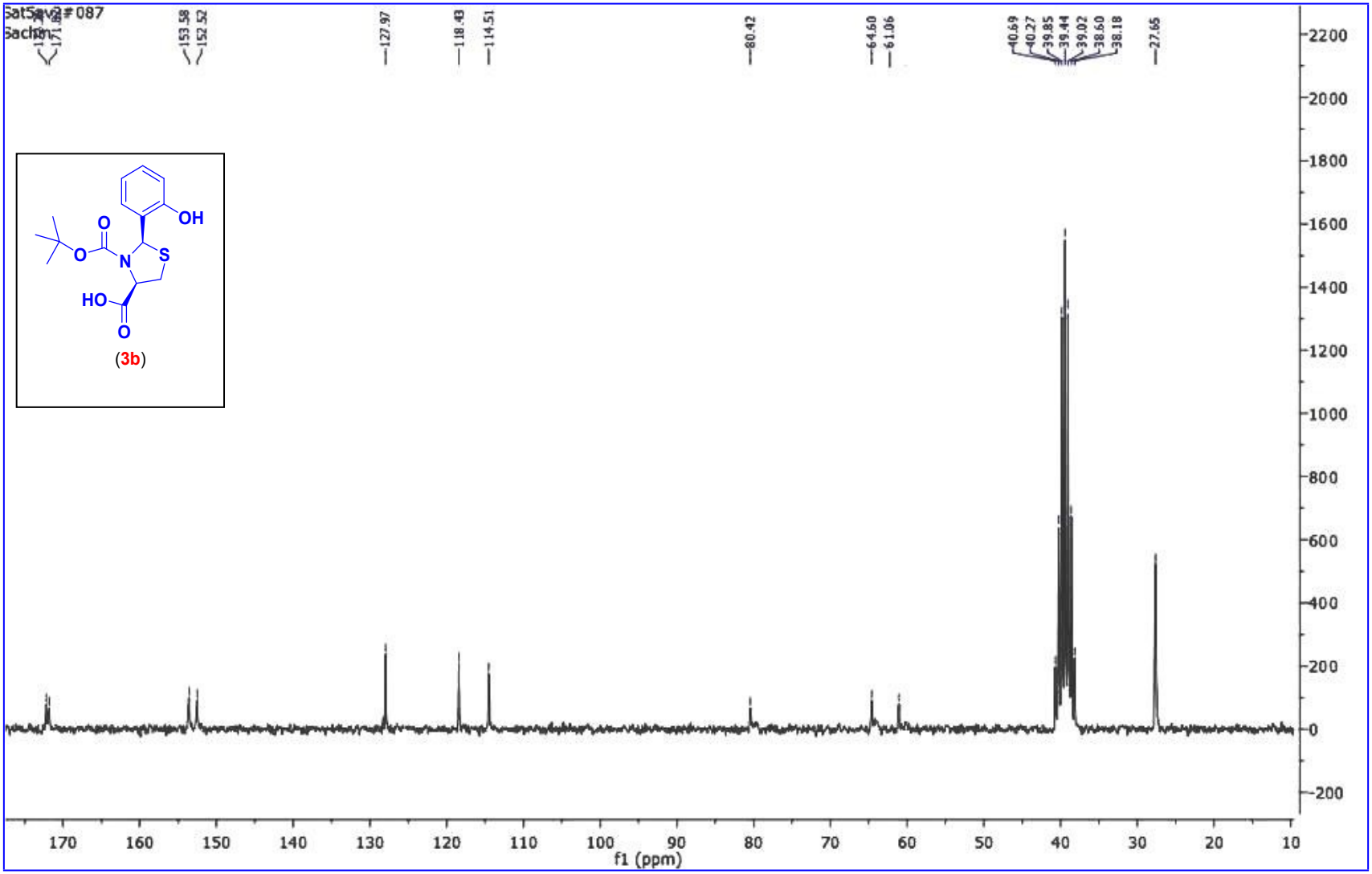
IR Spectra:



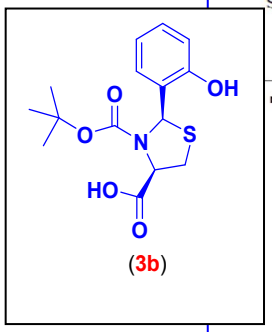
^{1}H NMR Spectra:



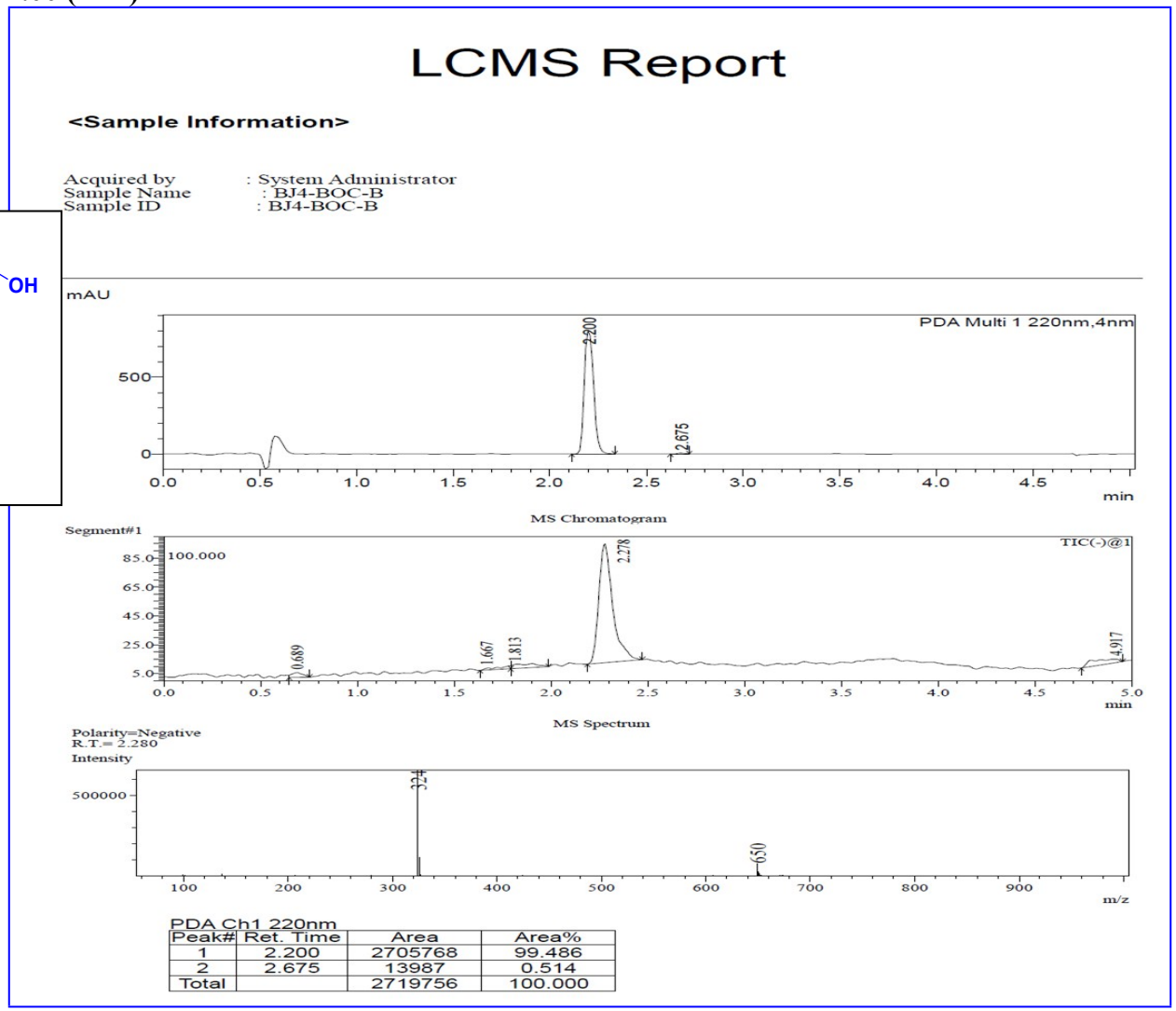
^{13}C NMR Spectra:



GCMS (APCI) : 324.00 (M-1)



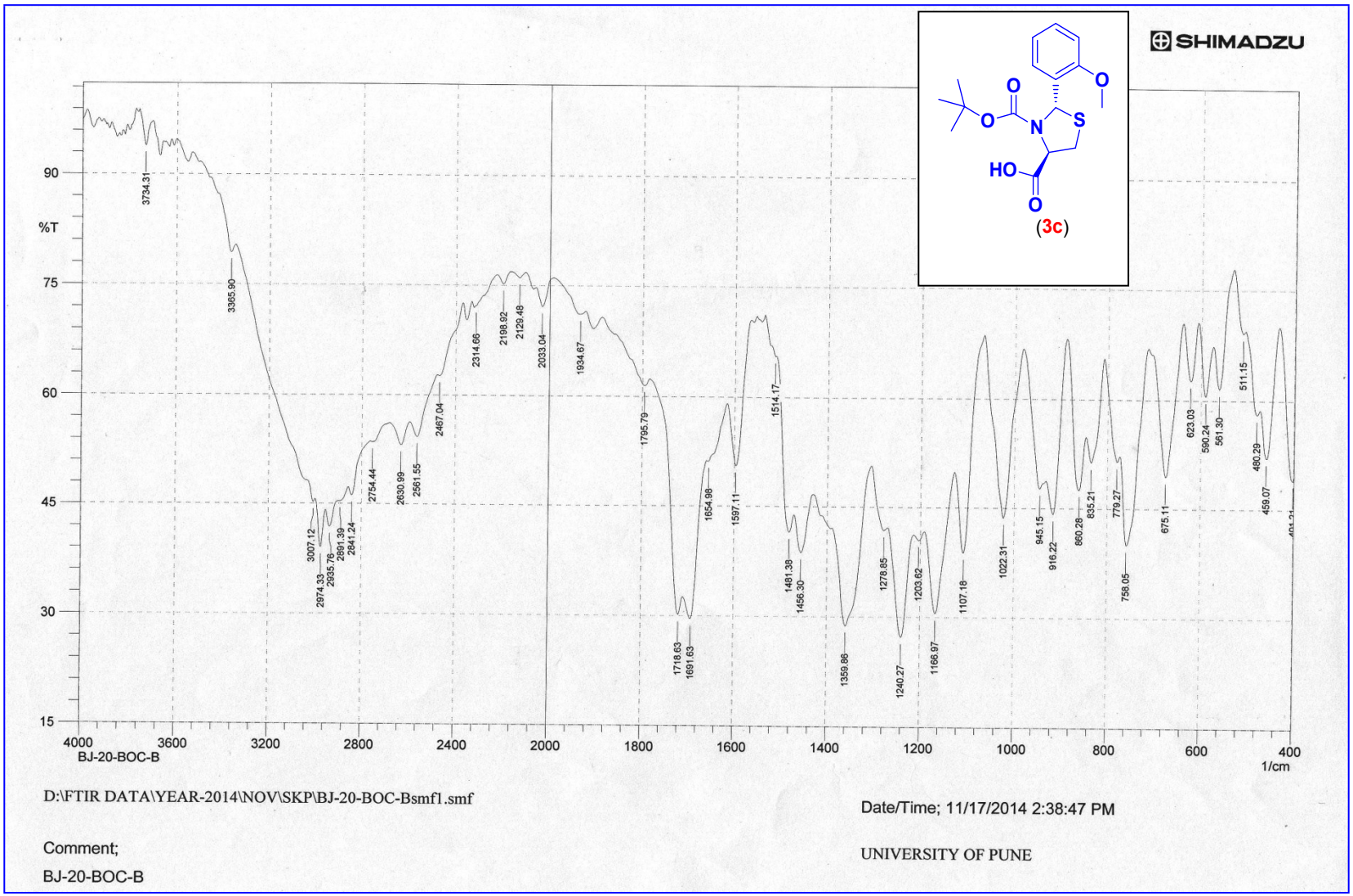
(3b)



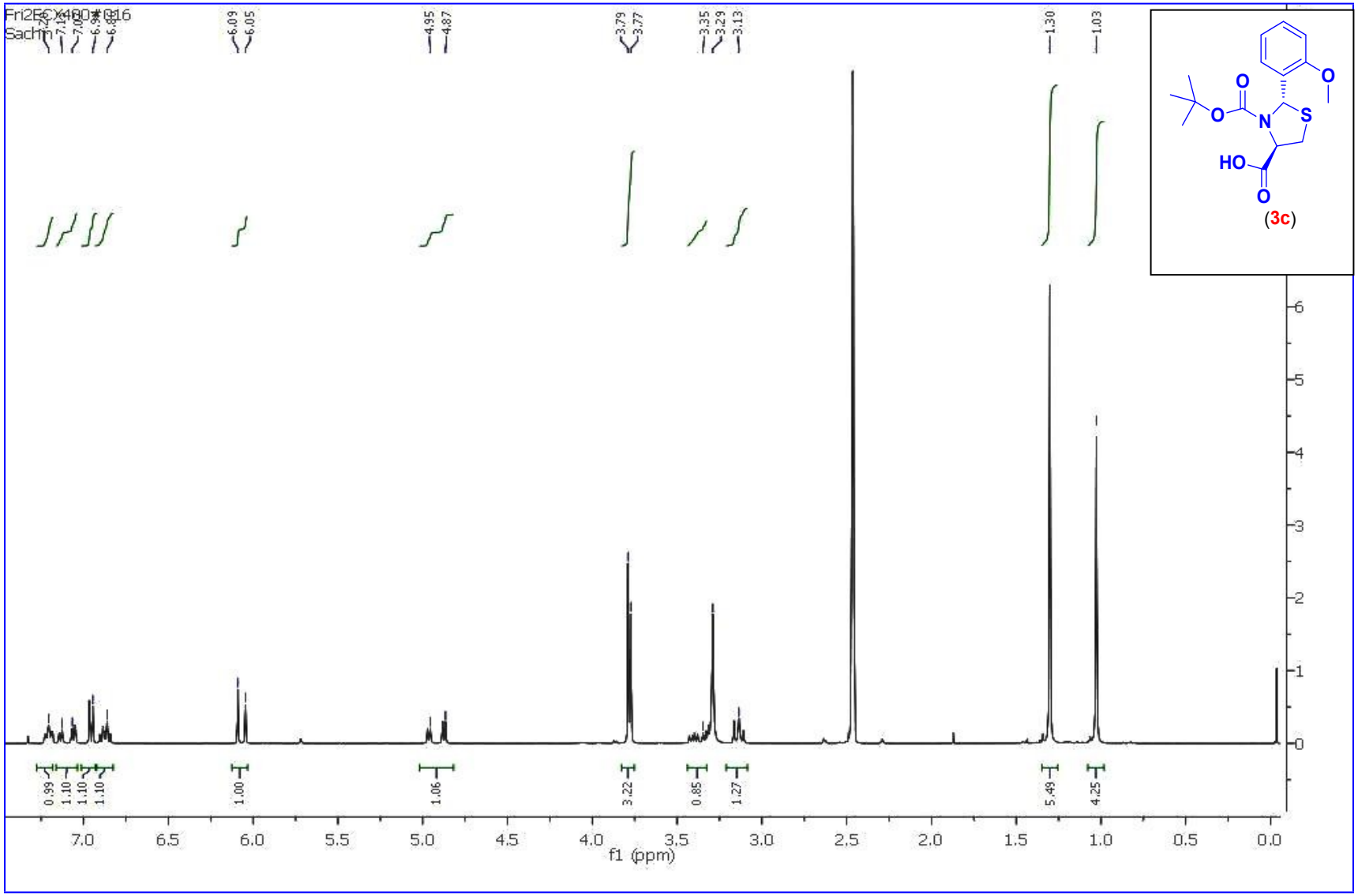
[34] R. M. Jagtap, M. A. Rizvi, Y. B. Dangat and S. K. Pardeshi, Crystal Structure, Computational studies, and stereoselectivity in the synthesis of 2-aryl-thiazolidine-4-carboxylic acids via *in situ* imine intermediate, *J. Sulfur Chem.,* 2016, 37, 401-425.

(*2S,4R*)-3-(tert-butoxycarbonyl)-2-(2-methoxyphenyl) thiazolidine-4-carboxylic acid (3c):

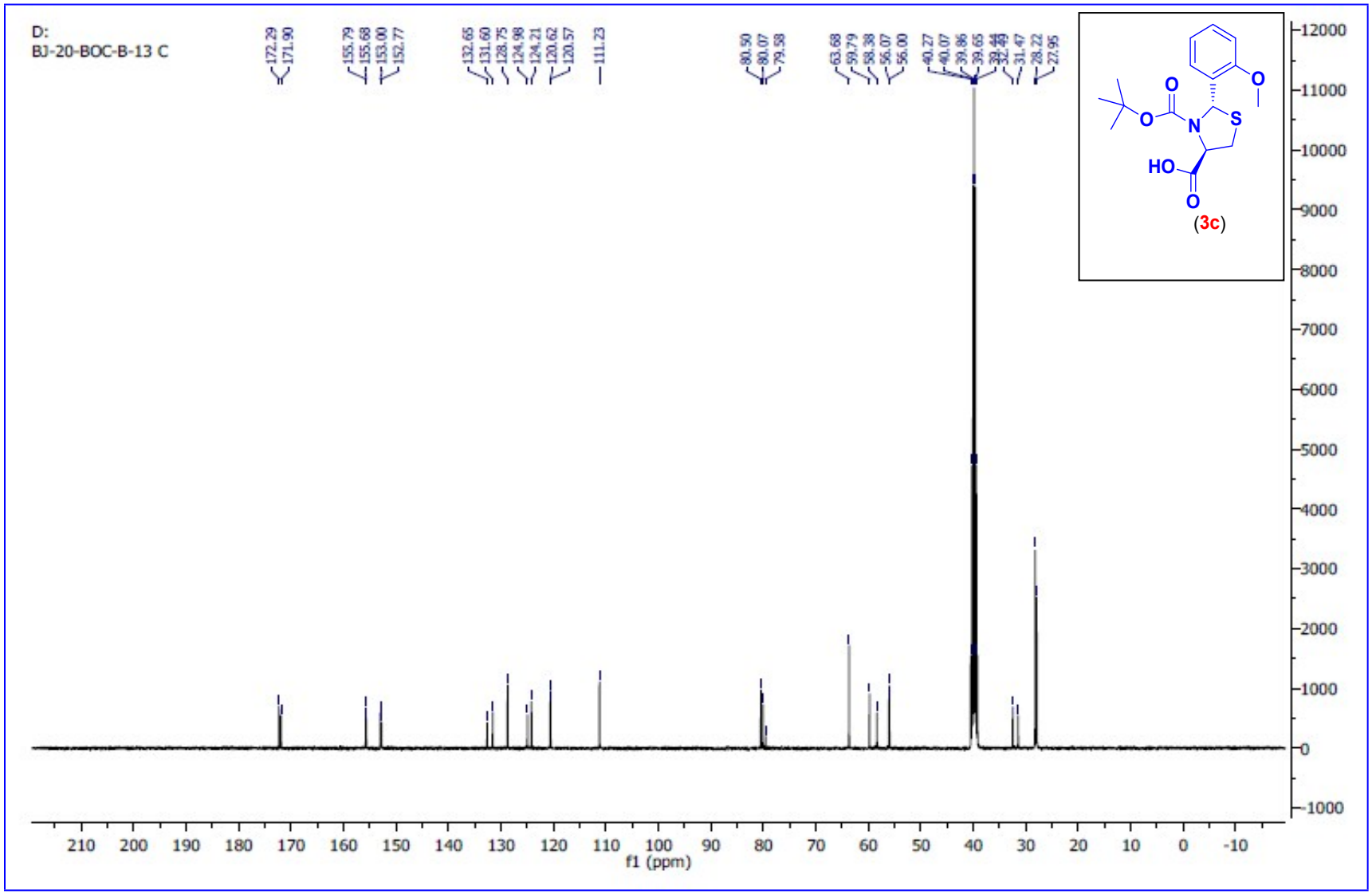
IR Spectra:



^{1}H NMR Spectra:

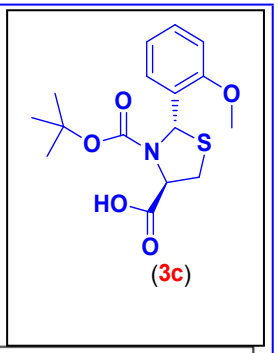


^{13}C NMR Spectra:



GCMS (APCI) : 338.00 (M-1)

LCMS Report



(3c)

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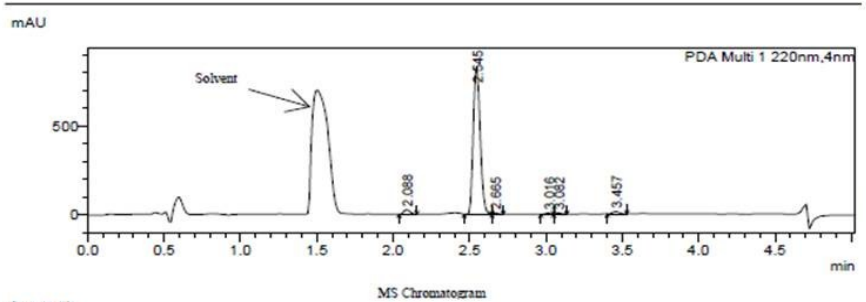
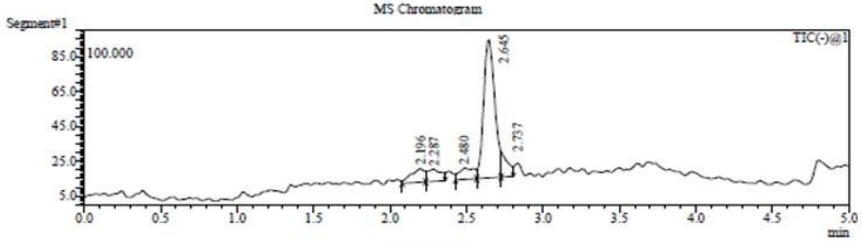
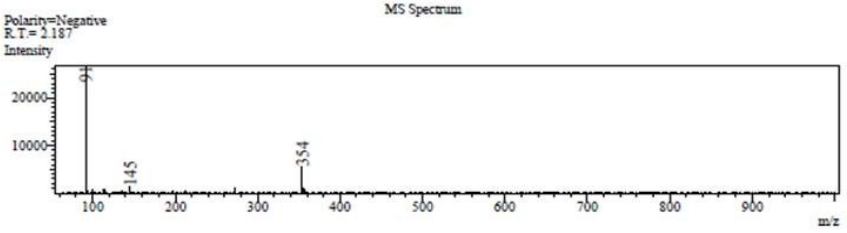
Sample Name : BJ-20-BOC-B
Sample ID : BJ-20-BOC-B

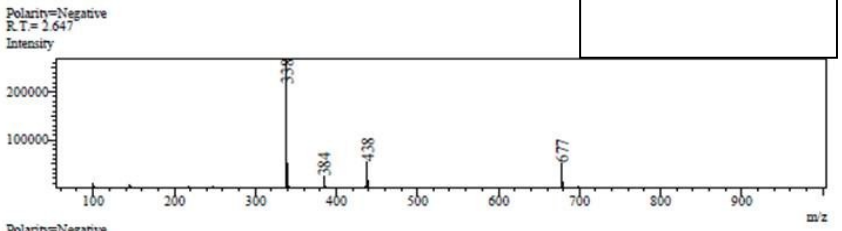


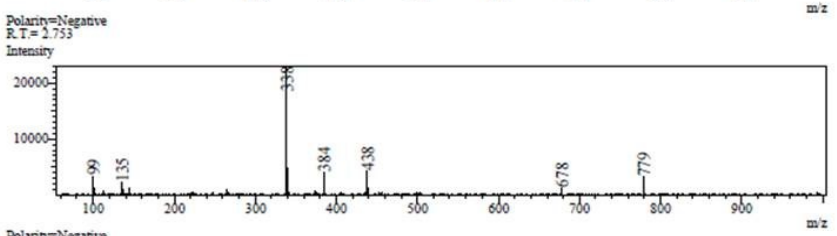
MS Chromatogram

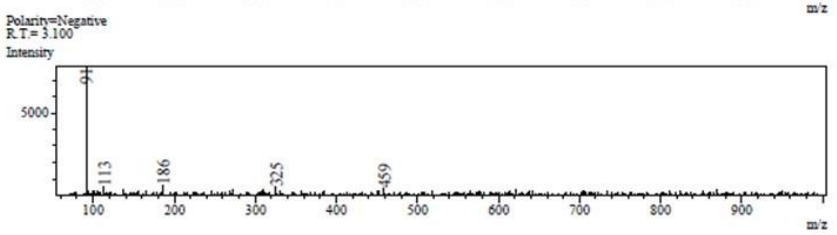


MS Spectrum







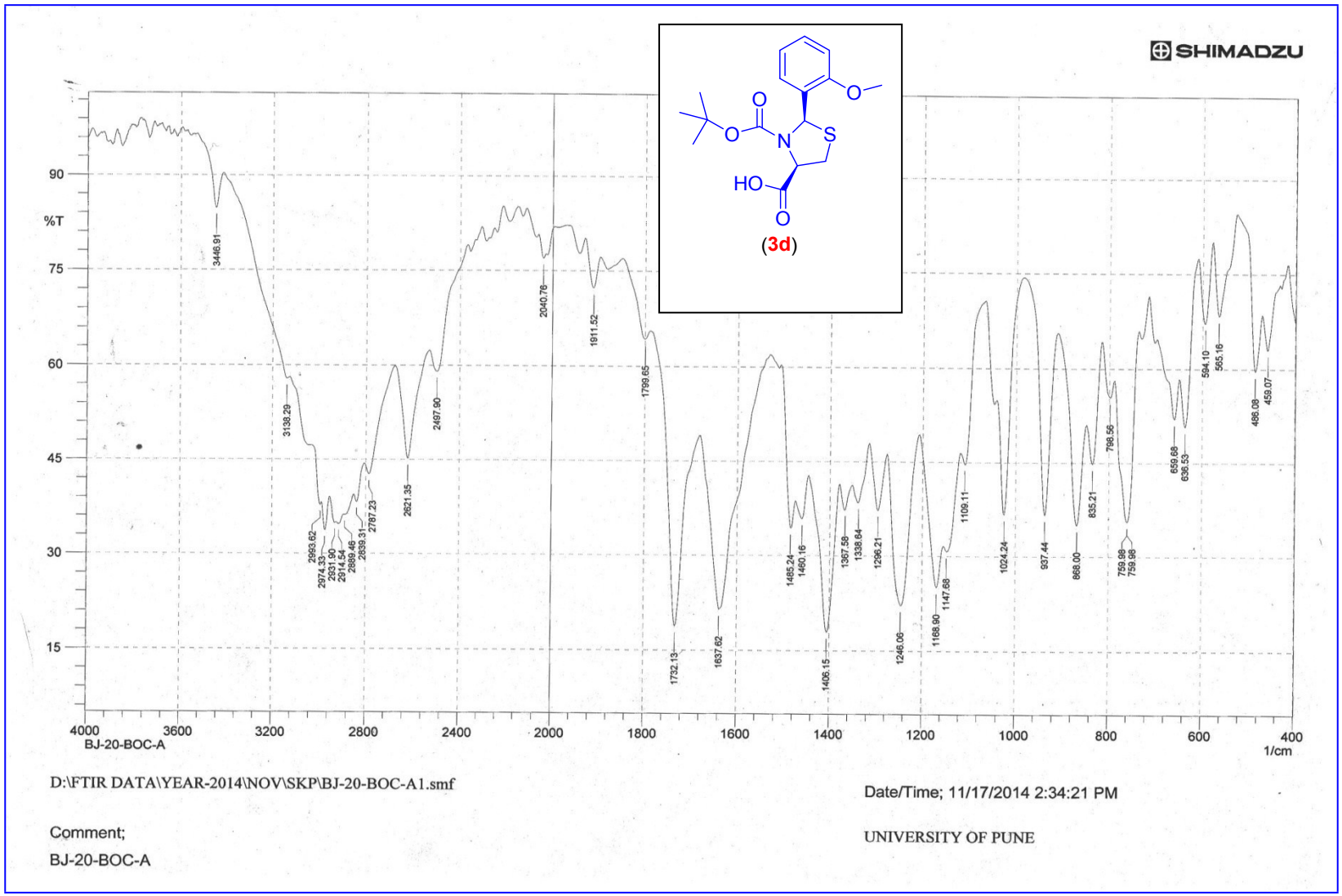


PDA Ch1 220nm

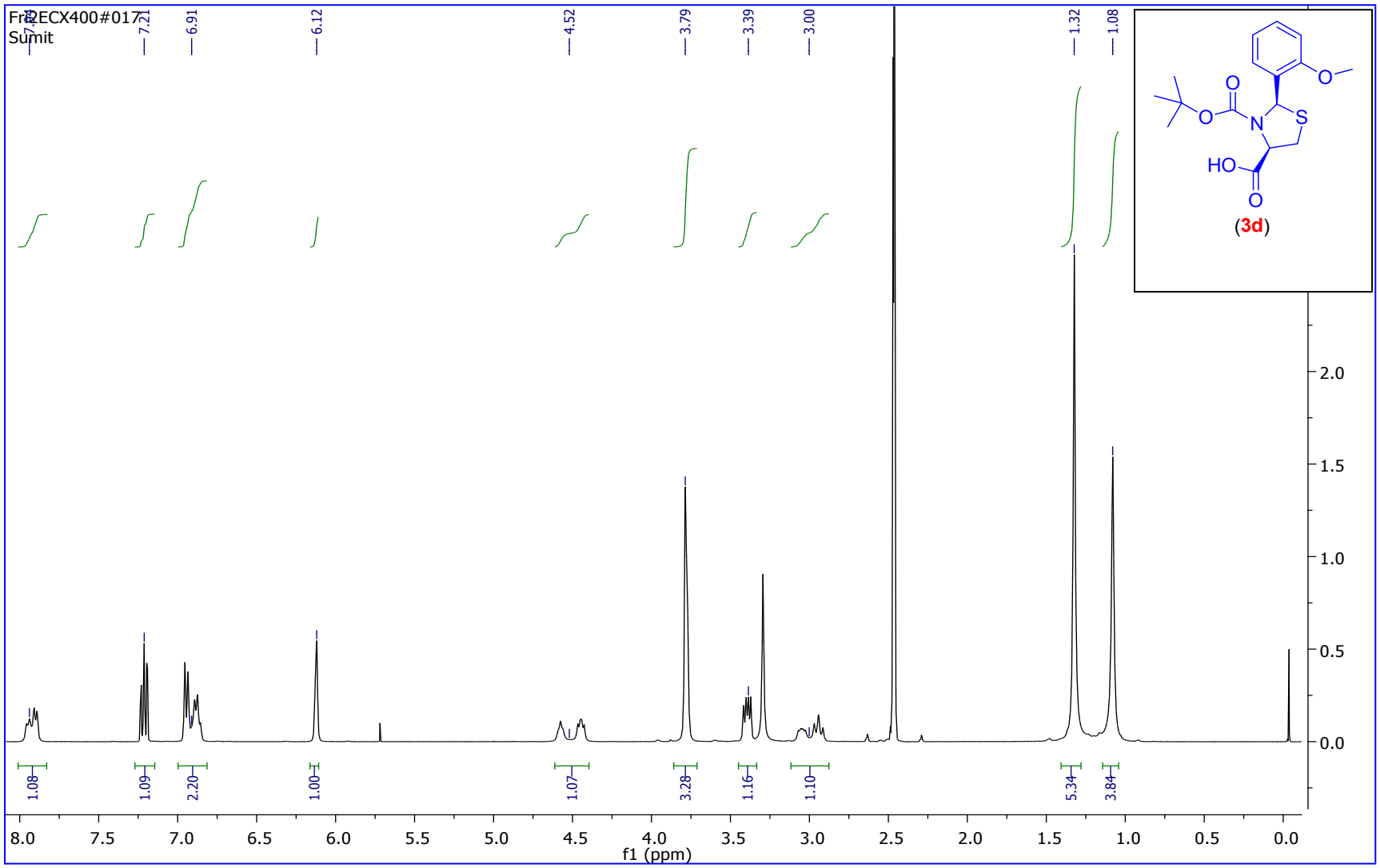
Peak#	Ret. Time	Area	Area%
1	2.088	71188	2.548
2	2.545	2629353	94.126
3	2.665	17375	0.622
4	3.016	19189	0.687
5	3.082	19076	0.683
6	3.457	37251	1.334
Total		2793432	100.000

(*2R,4R*)-3-(tert-butoxycarbonyl)-2-(2-methoxyphenyl) thiazolidine-4-carboxylic acid (3d):

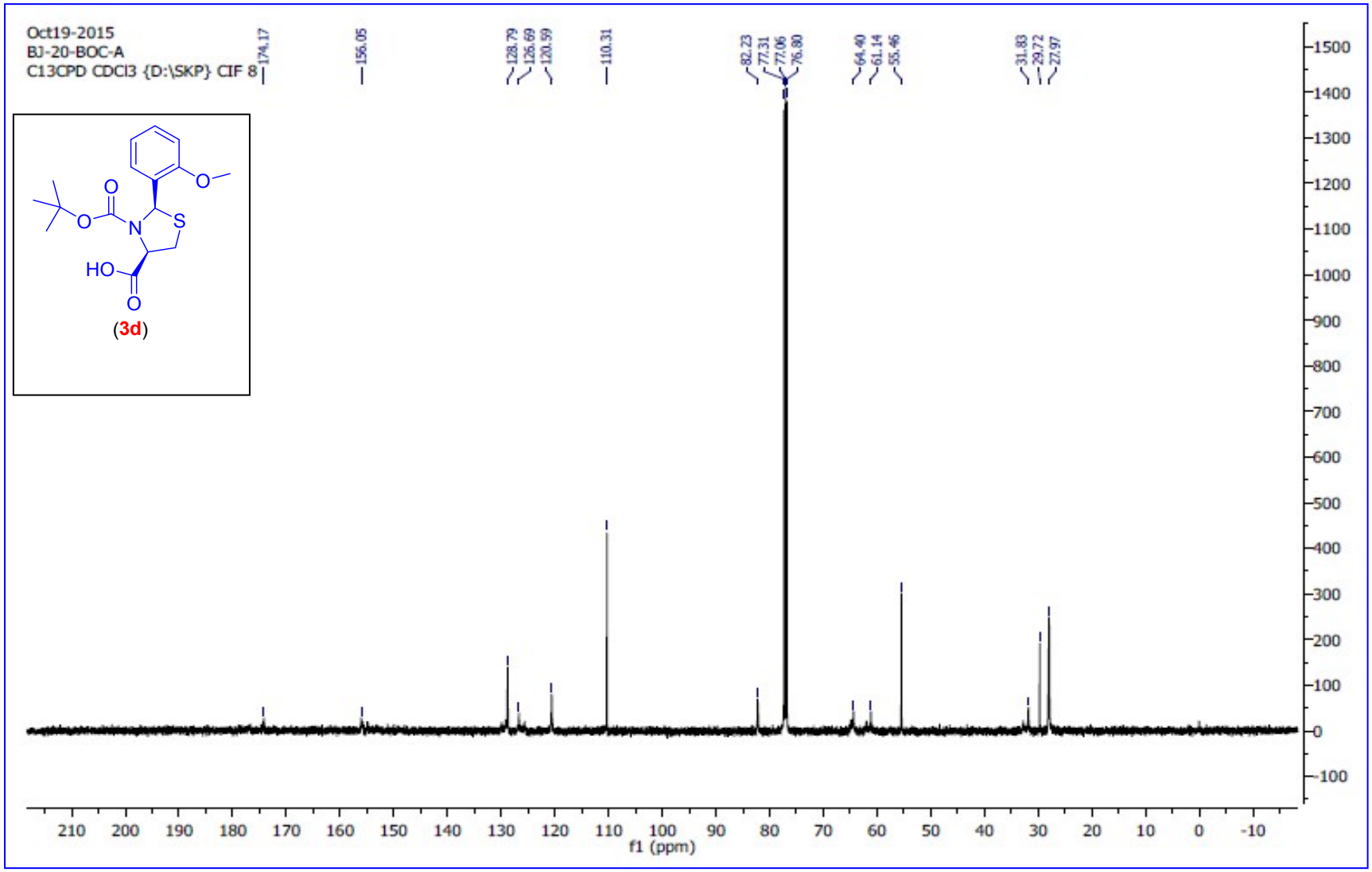
IR Spectra:



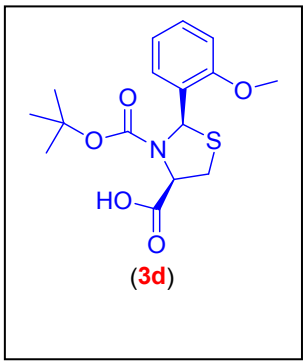
^{1}H NMR Spectra:



^{13}C NMR Spectra:



GCMS (APCI) : 338.00 (M-1)



(**3d**)

LCMS Report

<Sample Information>

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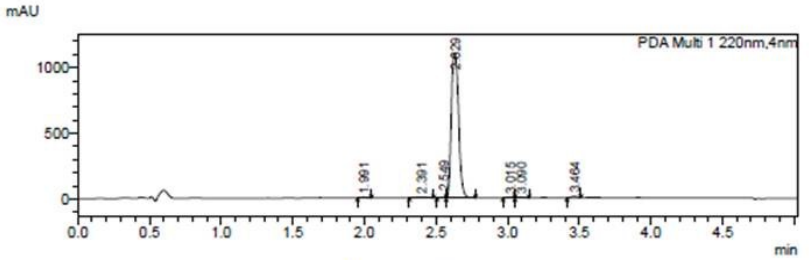
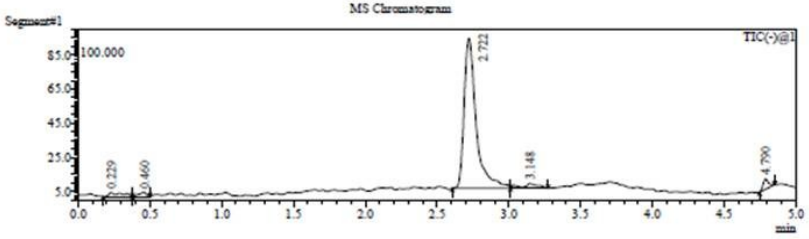
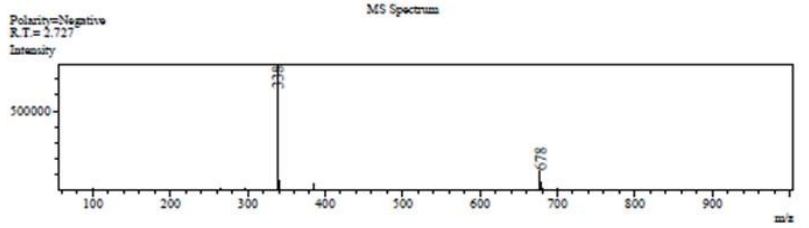
Sample ID : BJ-20-BOC-A



MS Chromatogram



MS Spectrum



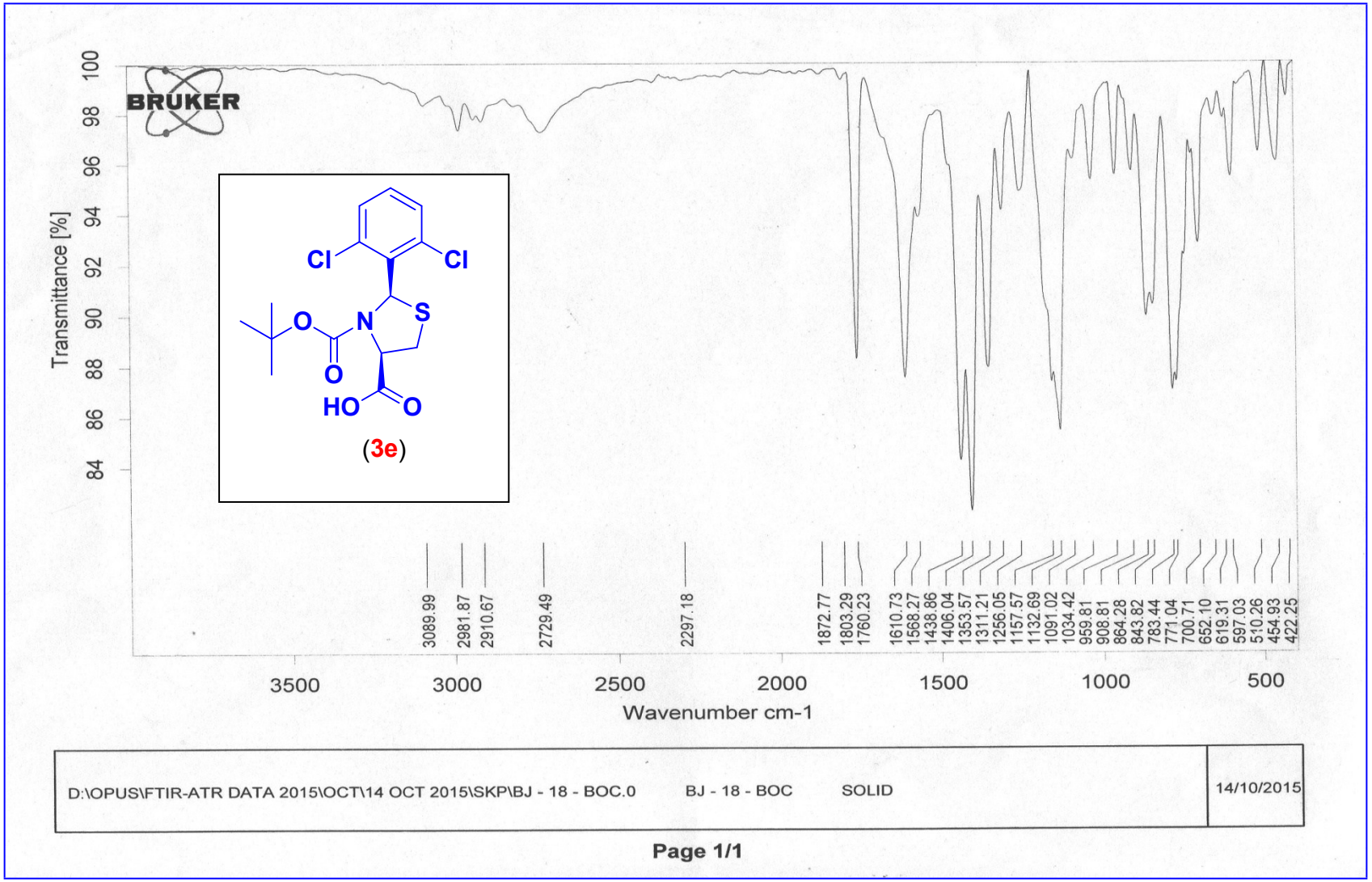
PDA Ch1 220nm

Peak#	Ret. Time	Area	Area%
1	1.991	16314	0.401
2	2.391	45643	1.123
3	2.549	13004	0.320
4	2.629	3915533	96.353

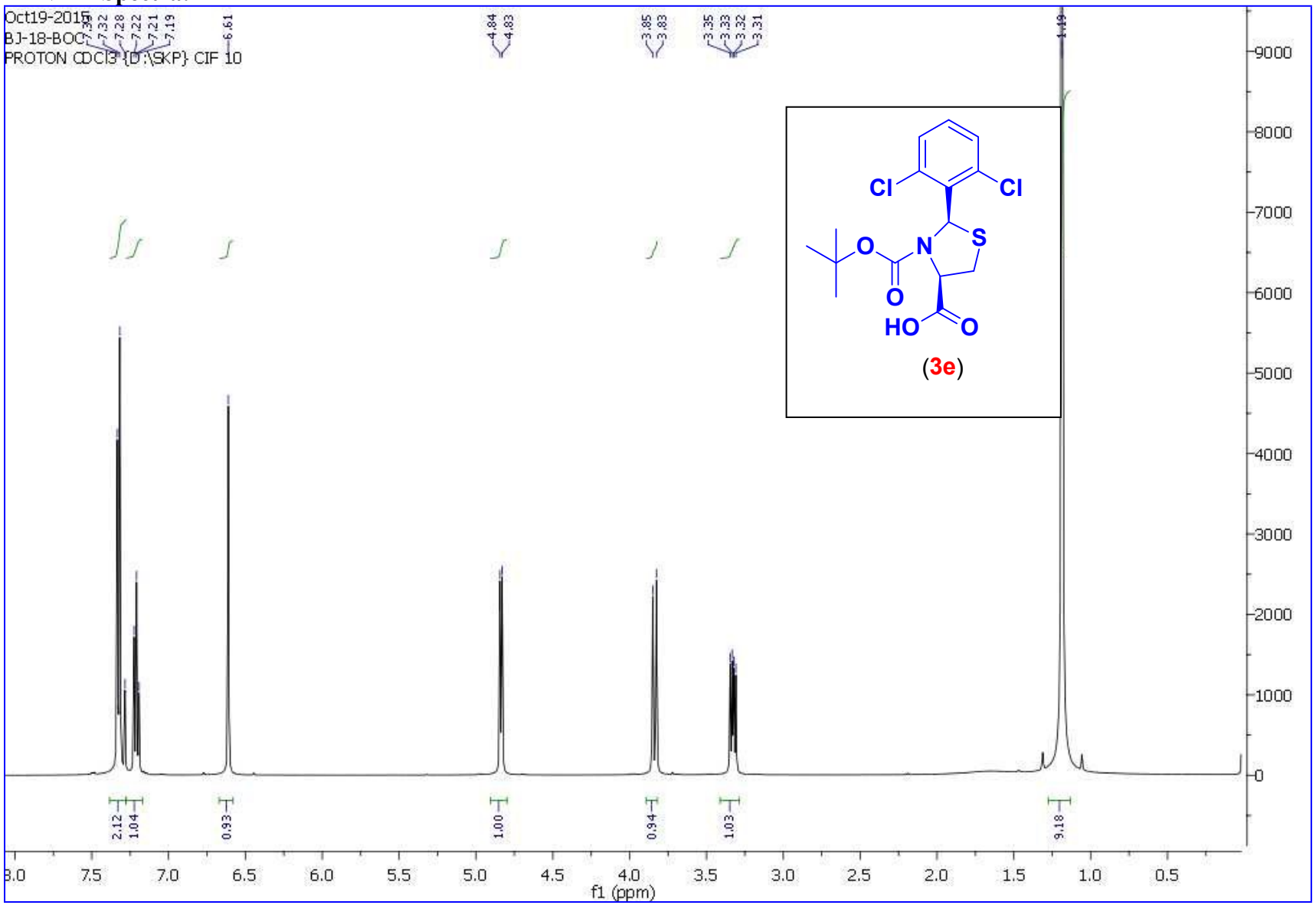
Peak#	Ret. Time	Area	Area%
5	3.015	18442	0.454
6	3.090	19353	0.476
7	3.464	35468	0.873
Total		4063756	100.000

(*2S, 4R*)-3-(tert-butoxycarbonyl)-2-(2,6-dichlorophenyl) thiazolidine-4-carboxylic acid (3e):

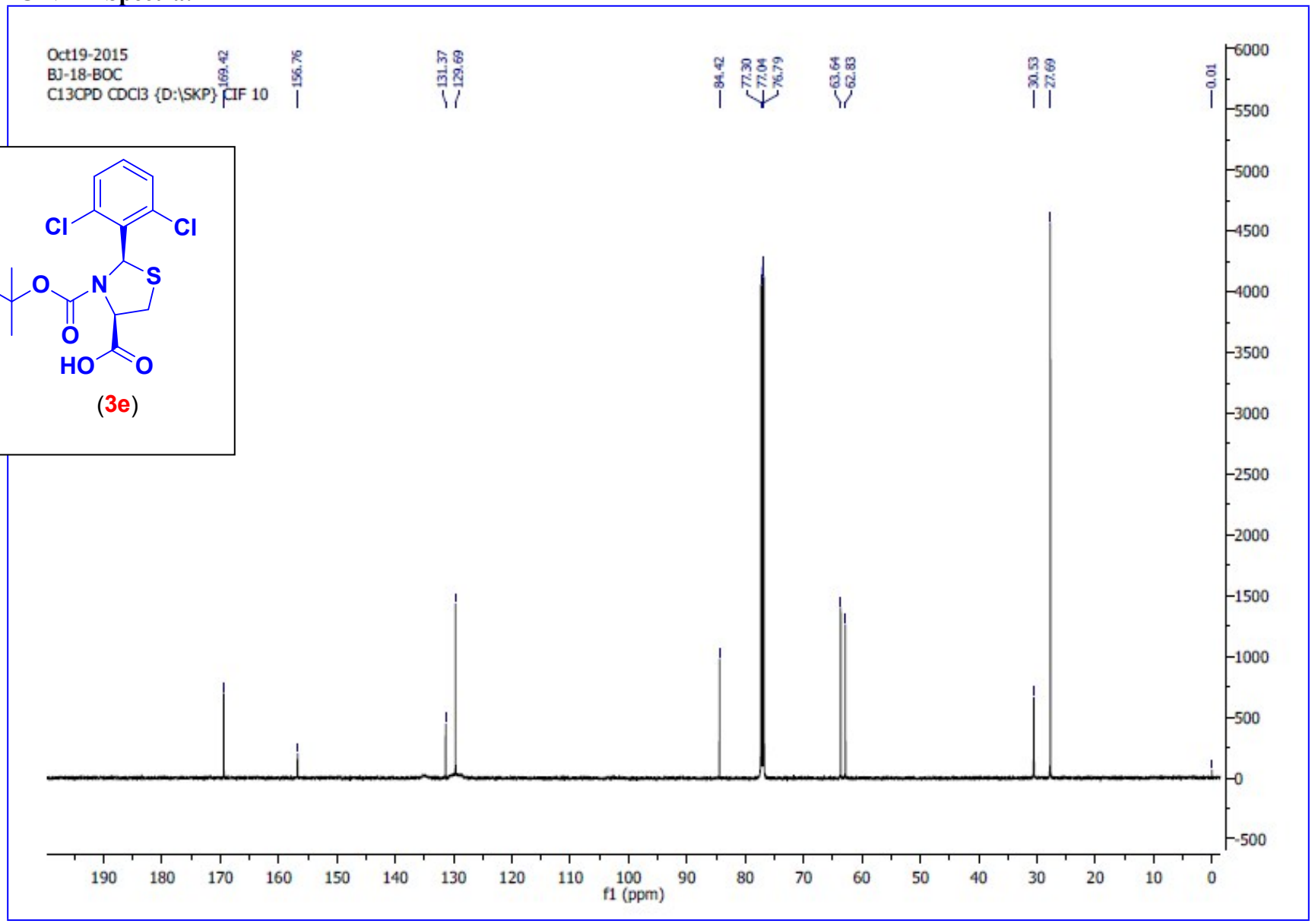
IR Spectra:



^{1}H NMR Spectra:



^{13}C NMR Spectra:



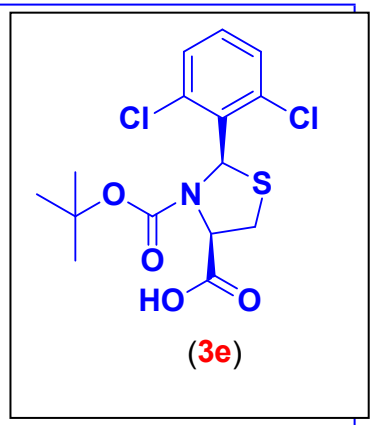
GCMS (APCI) : 376.00 (M-1)

LCMS Report

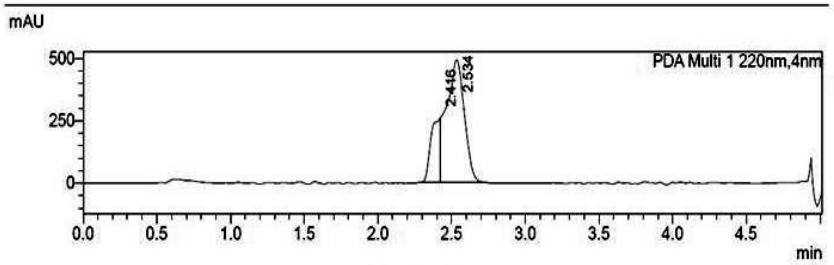
<Sample Information>

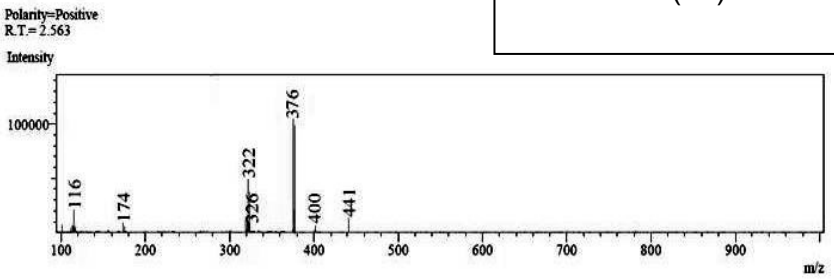
Sample Information

Sample Name : 6
Sample ID : 6

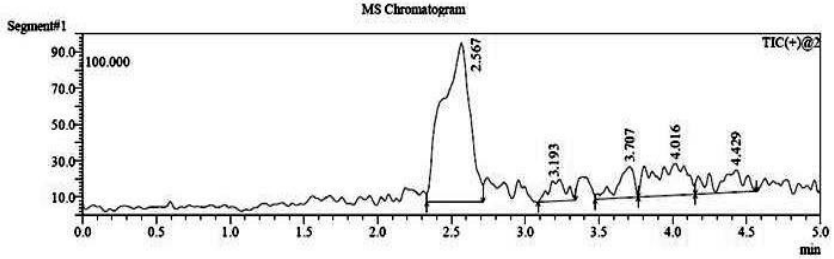


(3e)

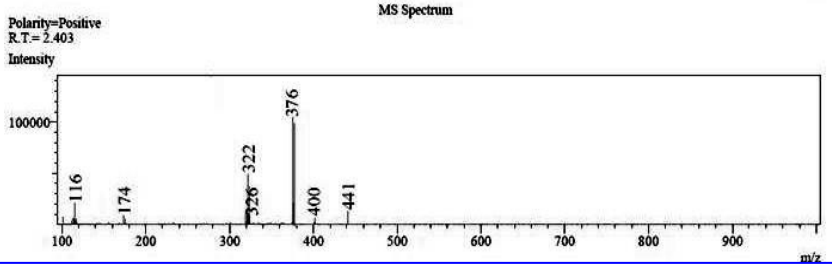




MS Chromatogram



MS Spectrum

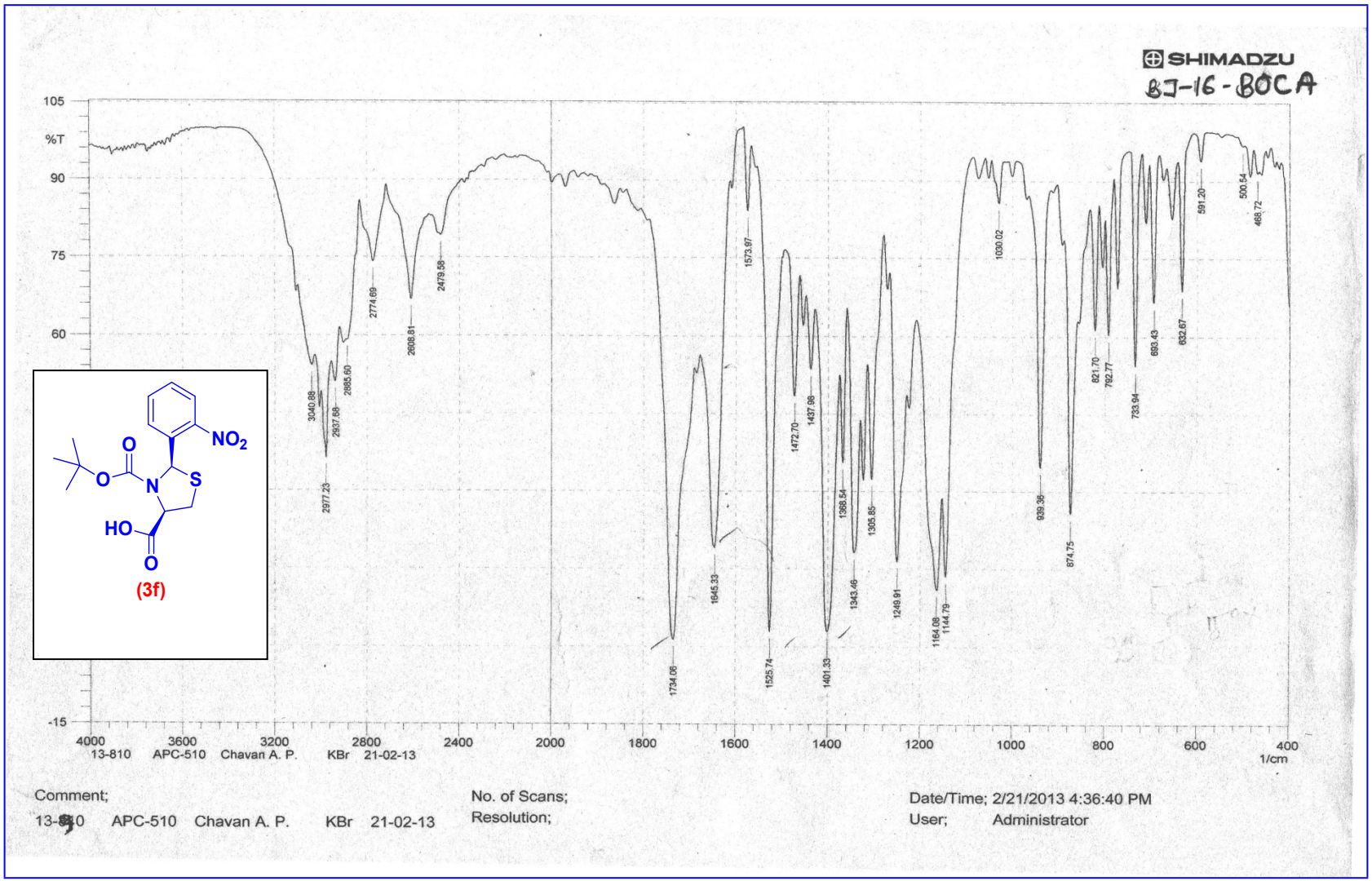


PDA Ch1 220nm

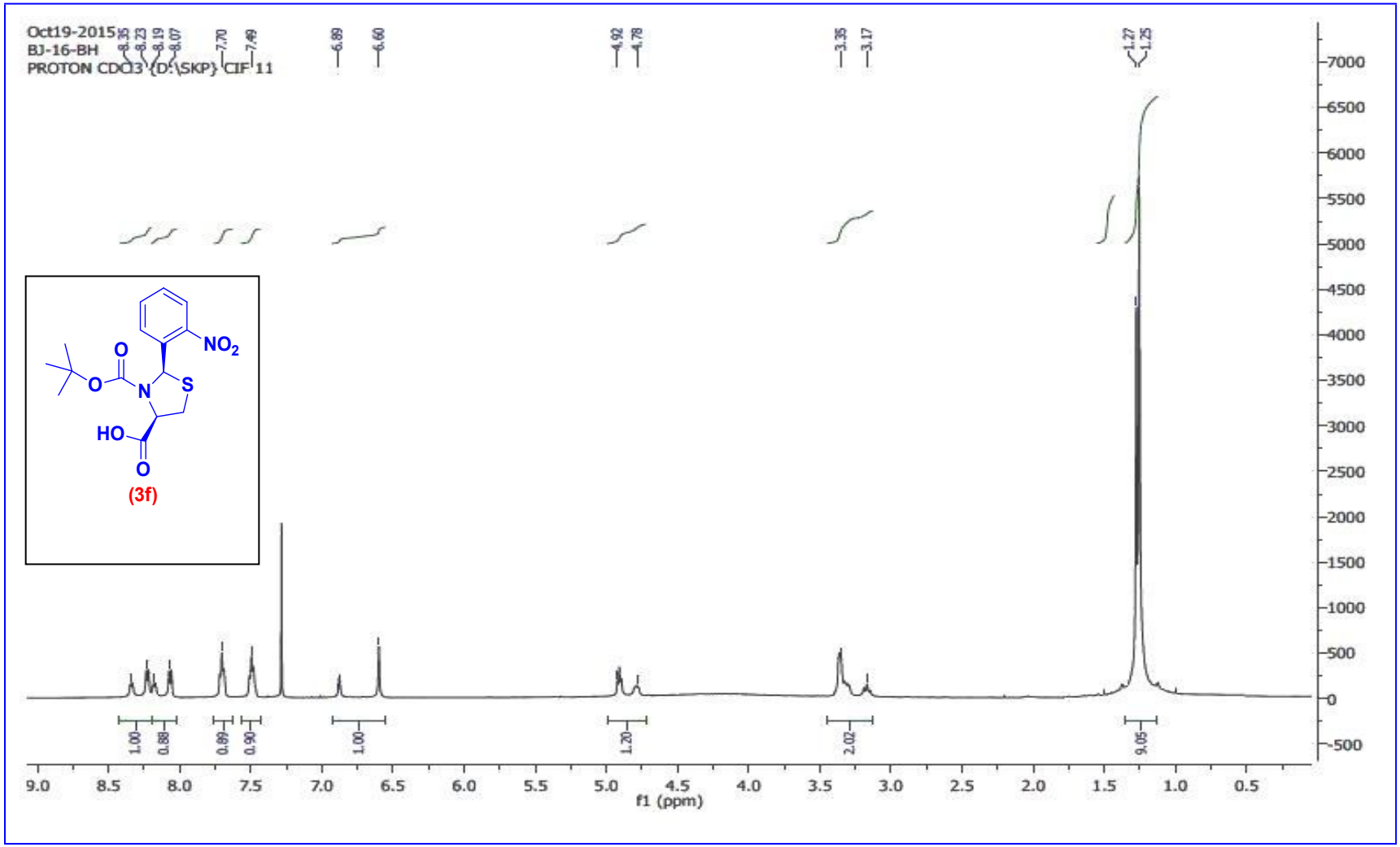
Peak#	Ret. Time	Area	Area%
1	2.416	1175929	22.038
2	2.534	4160051	77.962
Total		5335980	100.000

(*2R, 4R*)-3-(tert-butoxycarbonyl)-2-(2-nitrophenyl) thiazolidine-4-carboxylic acid (3f):

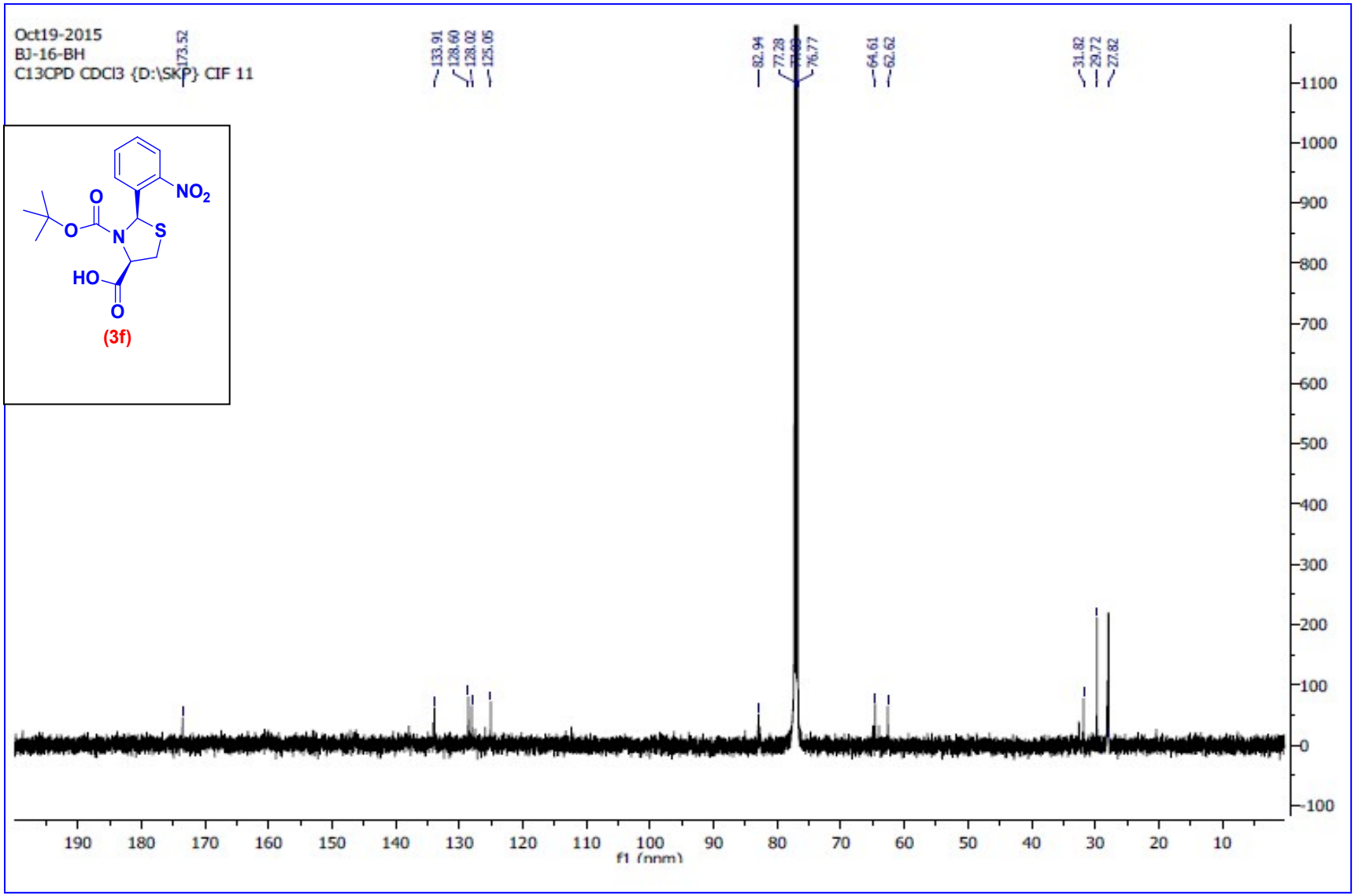
IR Spectra:



^{1}H NMR Spectra:



^{13}C NMR Spectra:



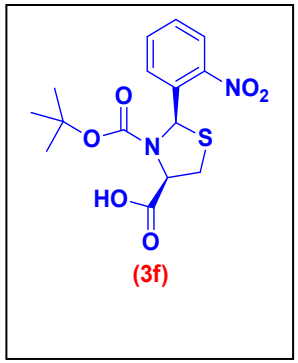
GCMS (APCI) : 354.00 (M+1)

LCMS Report

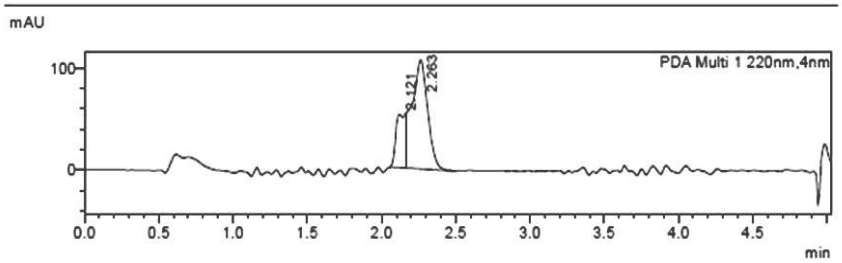
<Sample Information>

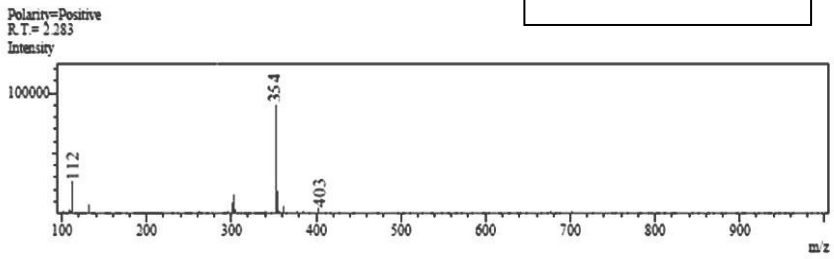
Sample Information

Sample Name : 2
Sample ID : 2

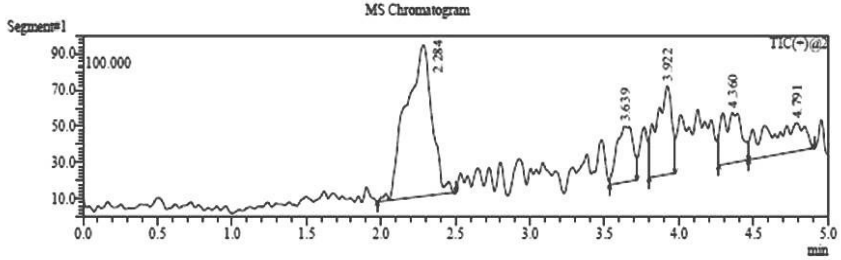


(3f)

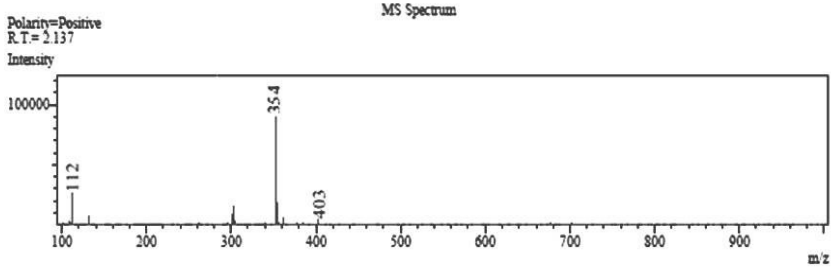




MS Chromatogram



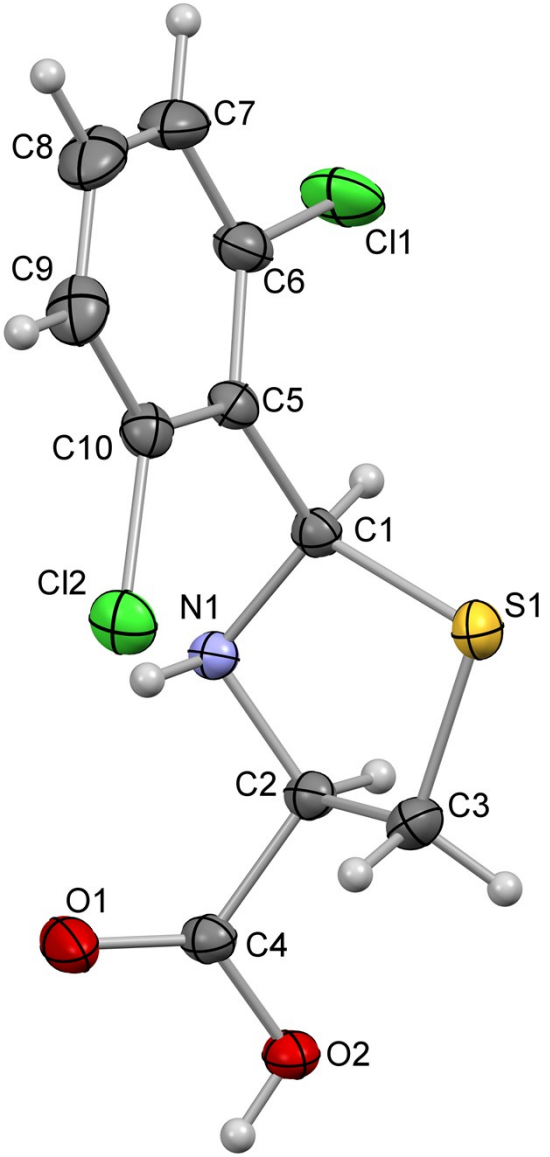
MS Spectrum



PDA Ch1 220nm

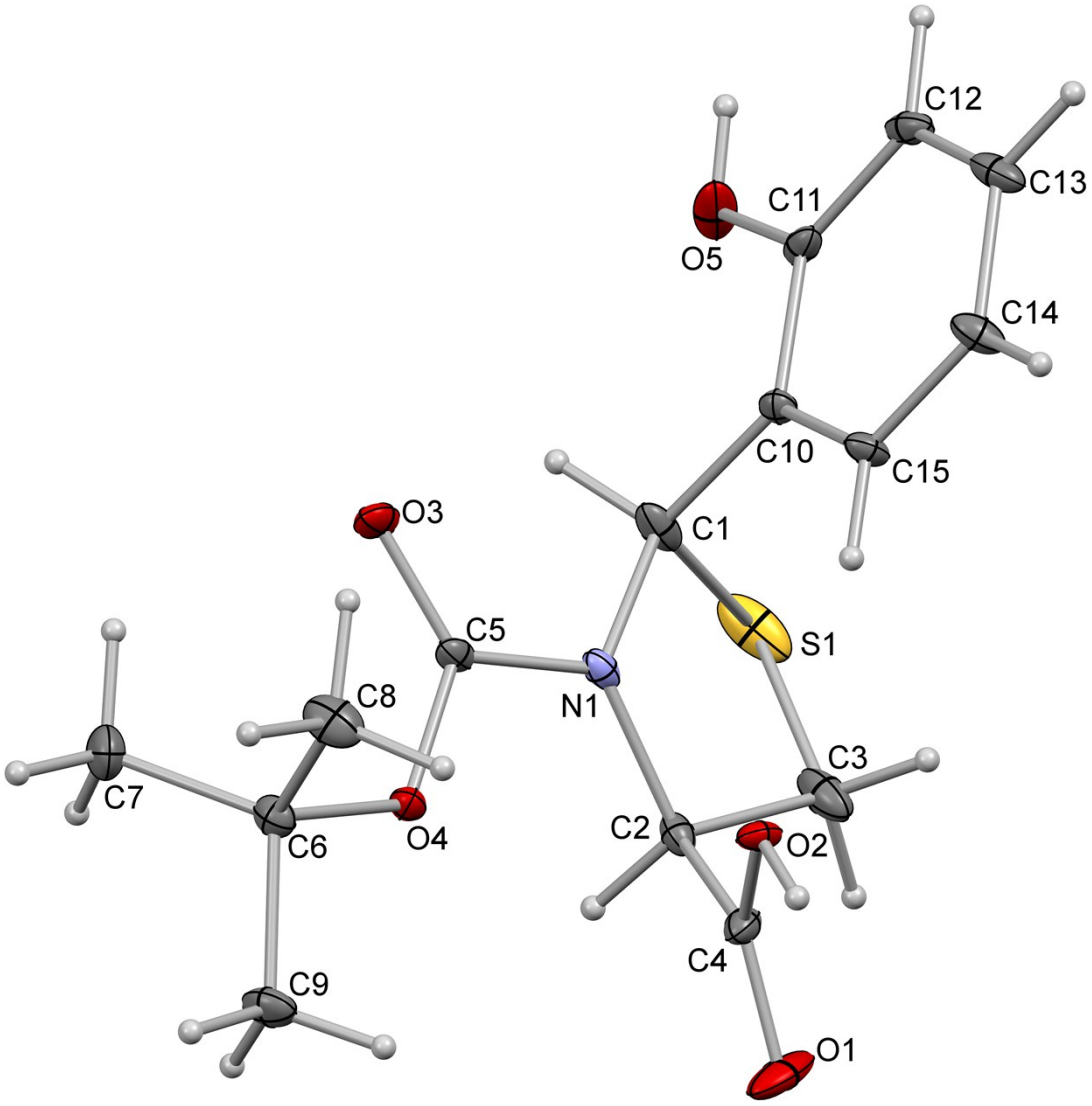
Peak#	Ret. Time	Area	Area%
1	2.121	249638	24.243
2	2.263	780083	75.757
Total		1029721	100.000

Compound 2e

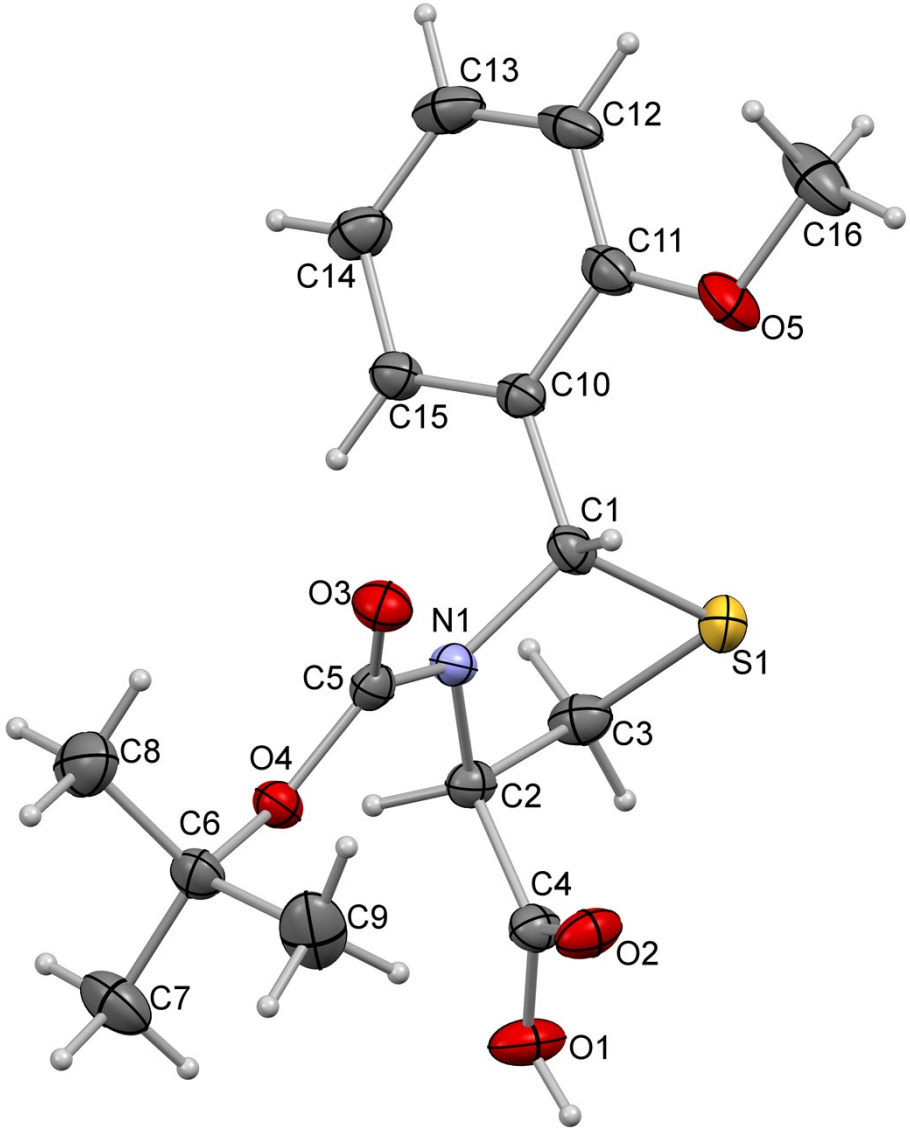


- **Crystal structure images**

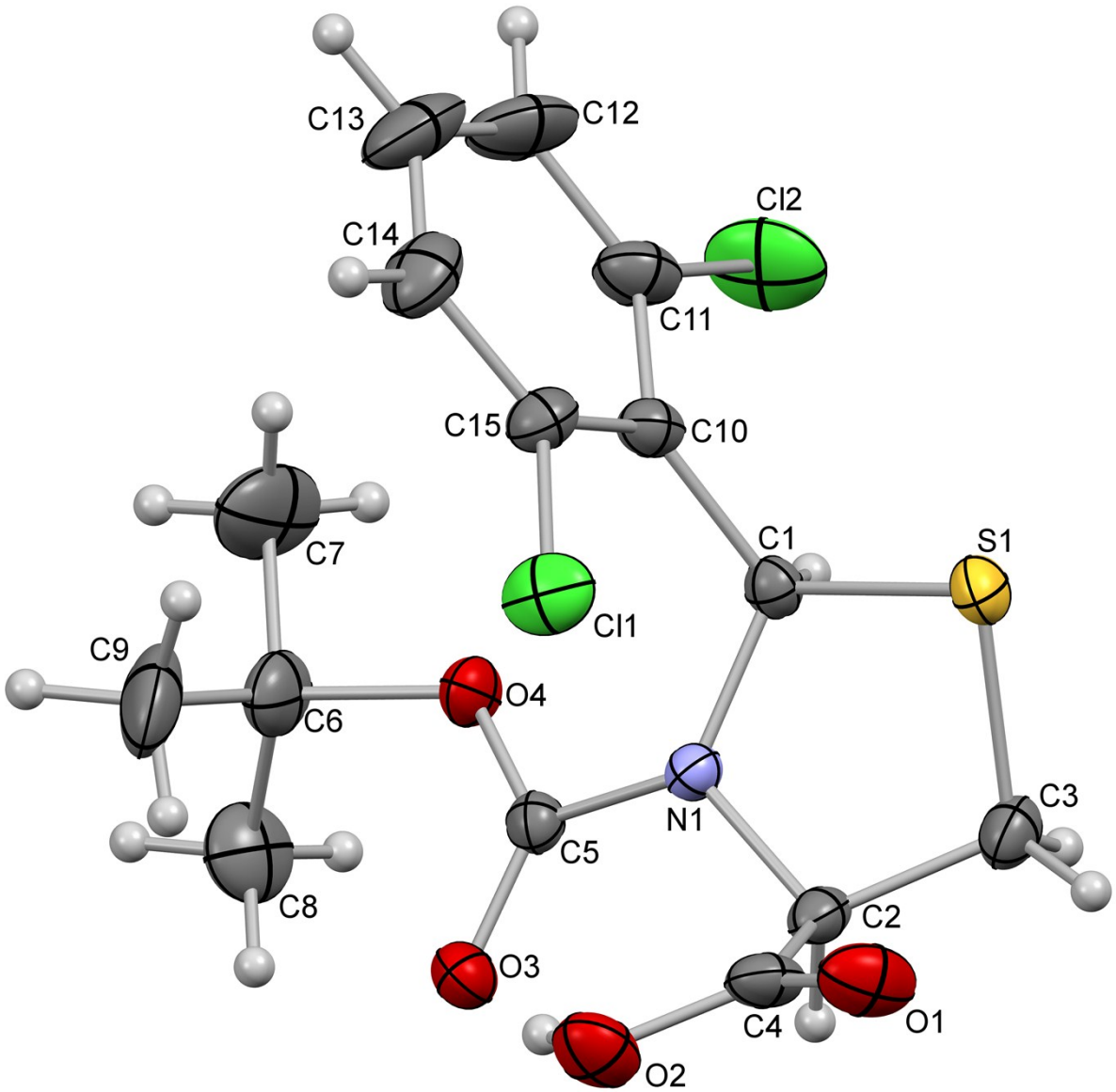
Compound 3b



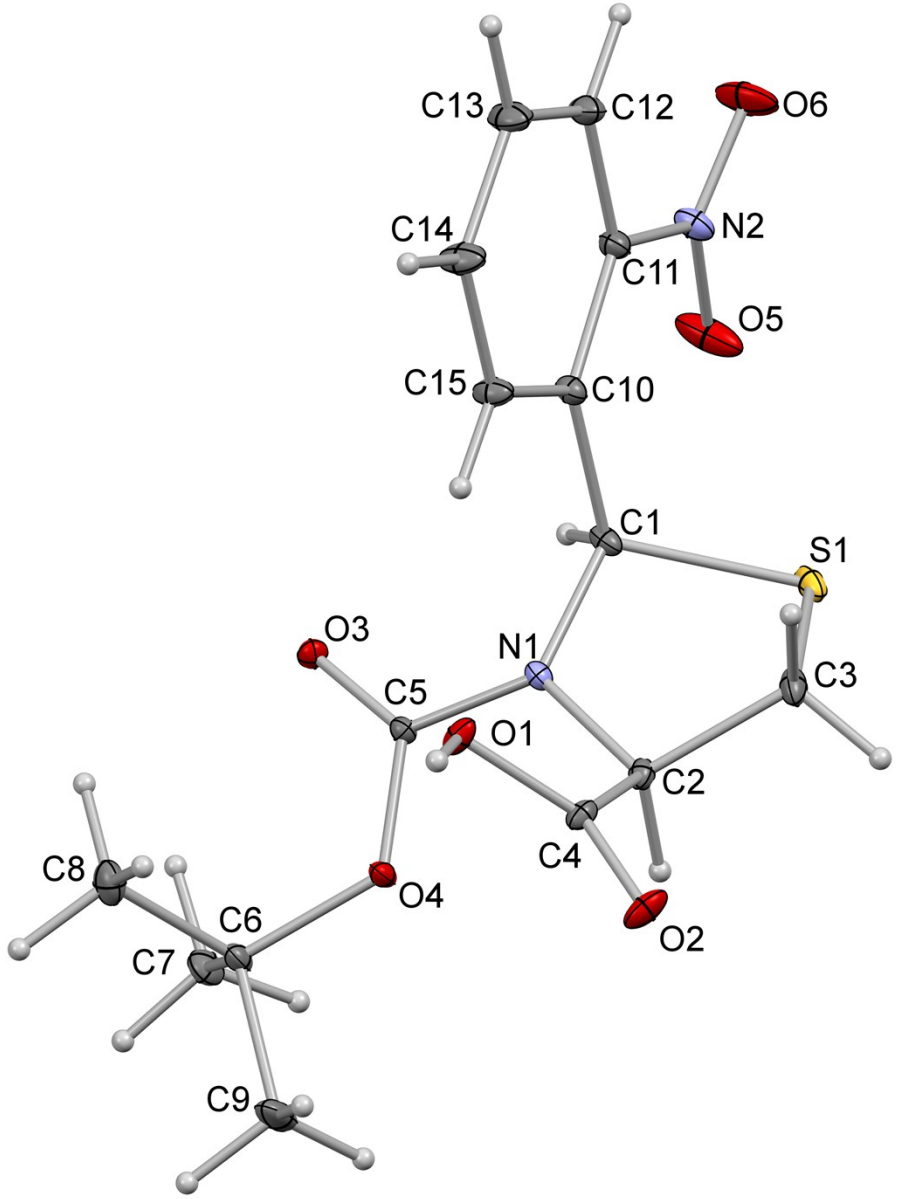
Compound 3c


C13
C12
C16
C11
C14
O5
C10
C15
C1
O3
N1
S1
C5
C3
C8
O4
C2
C6
C4
C9
O2
C7
O1

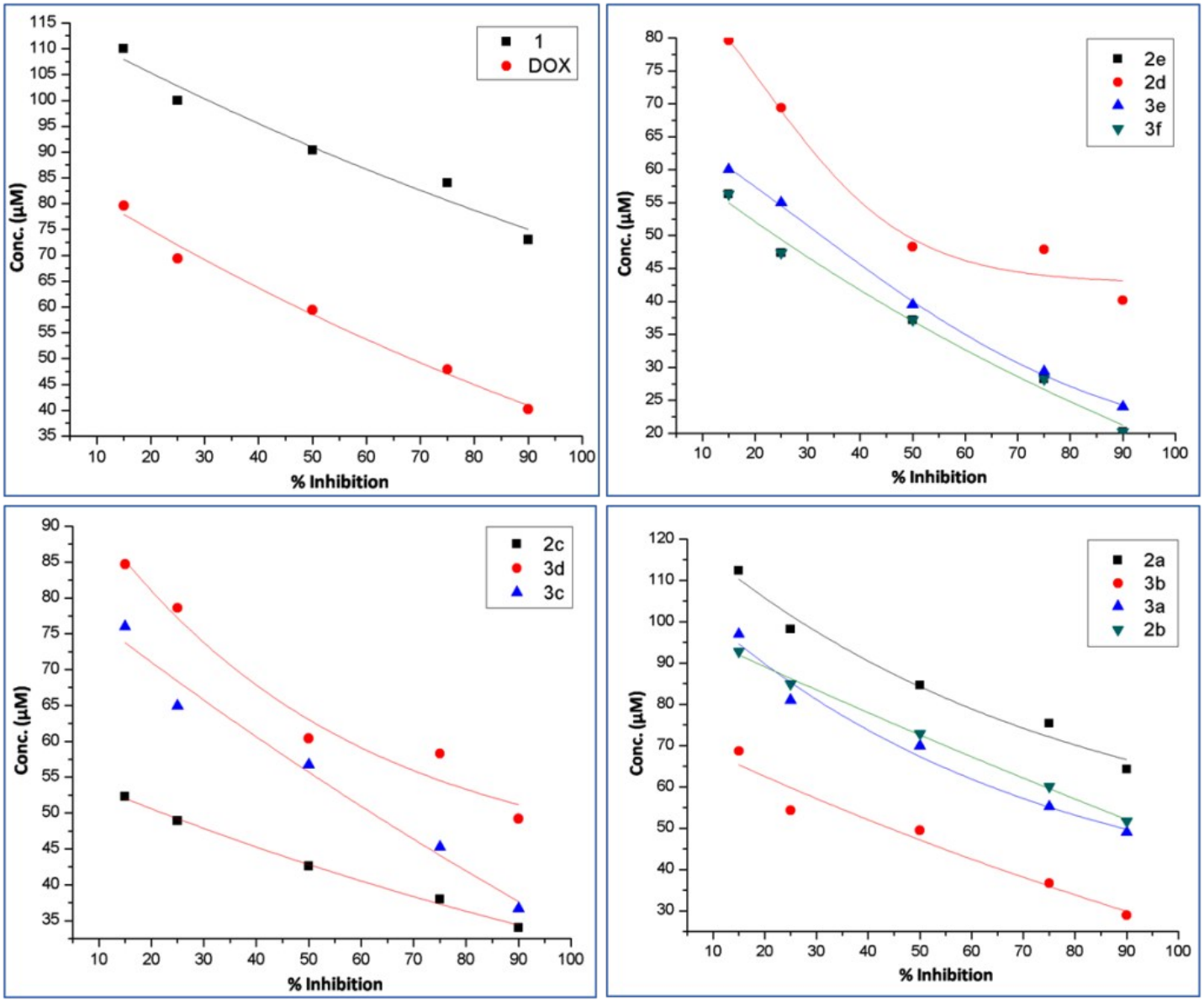
Compound 3e


C13
C12
Cl2
C14
C11
C15
C10
C1
S1
C7
Cl1
C9
O4
C6
C5
N1
C3
C8
C2
O3
C4
O1
O2

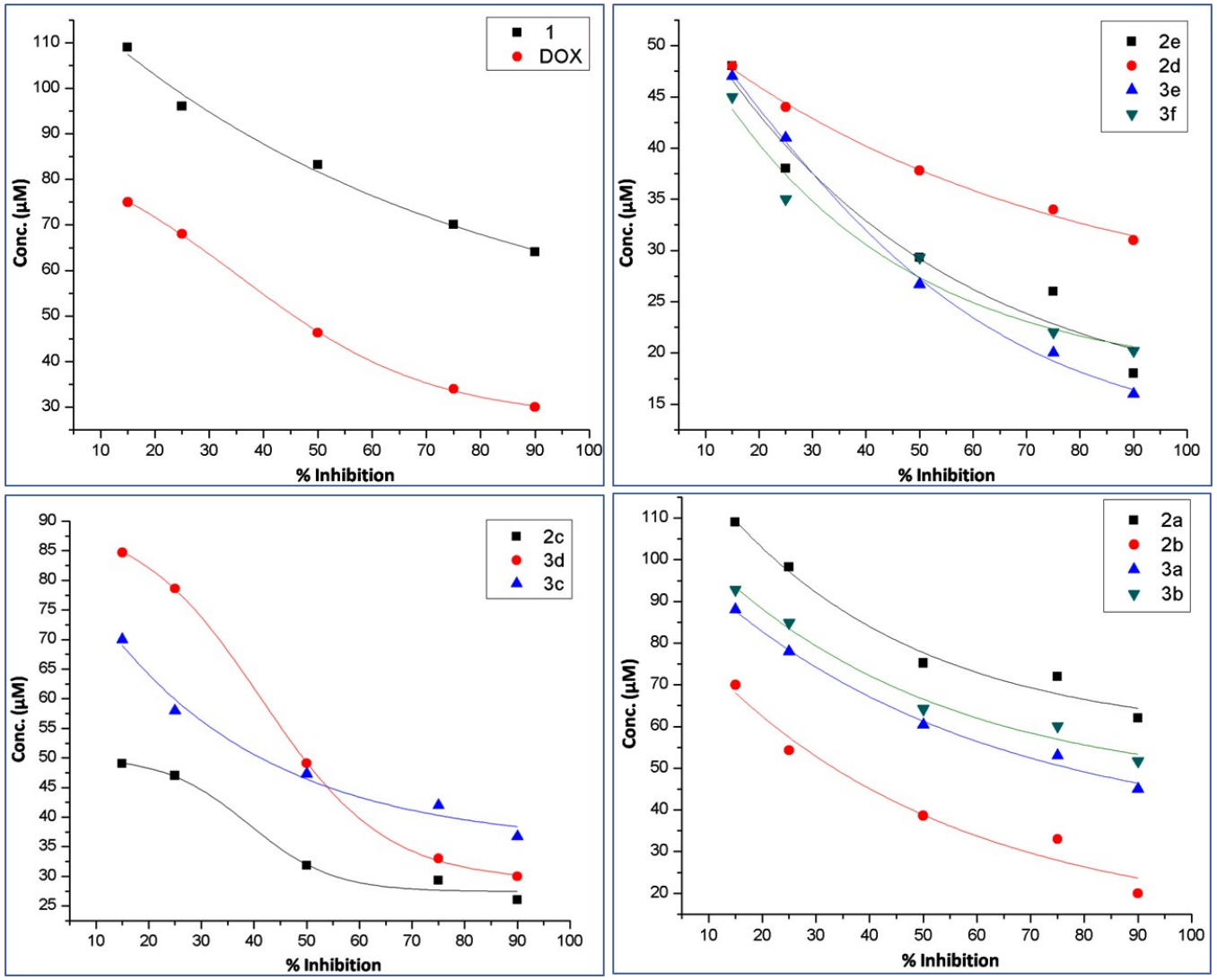
Compound 3f


C13
C12
O6
C14
N2
C11
O5
C15
C10
C1
S1
O3
N1
C3
C5
O1
C2
C4
C8
O4
C6
O2
C7
C9

Sigmoid fitted curves for IC_{50} values at 48 hrs:



Sigmoid fitted curves for IC_{50} values at 72 hrs:



Sigmoid fitted curves for IC_{50} values at 96 hrs: