Supporting Information

Stereospecific Synthesis of 3,4-Dihydro-2*H*-naphtho-1,4-oxazin-2-ones by Unification of Benzoxepine-4-carboxylates with Chiral Amino Acid Ethyl Esters

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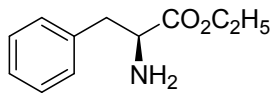
S2. The following amino acid ethyl esters **2a-v** (22 compounds) have been prepared as per the standard literature procedure from corresponding amino acids with thionyl chloride in the presence of ethyl alcohol.[10]



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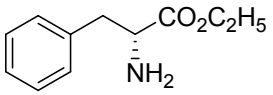

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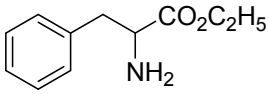

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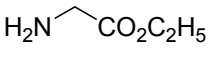

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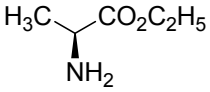

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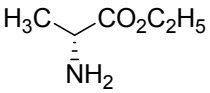

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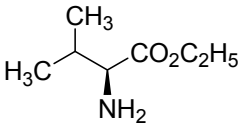

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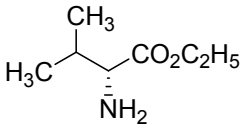

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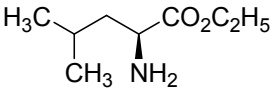

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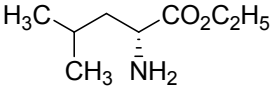

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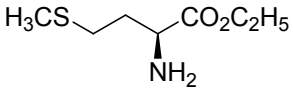

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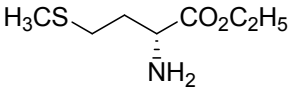

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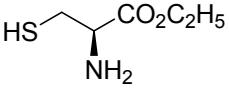

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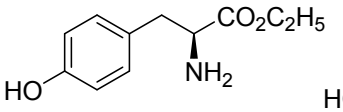

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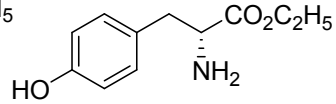

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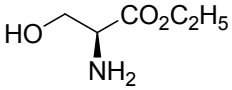

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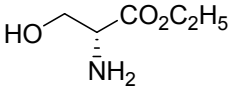

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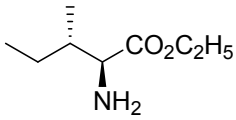

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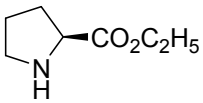

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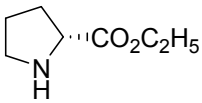

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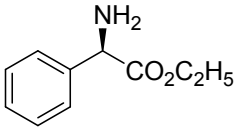

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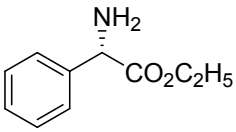

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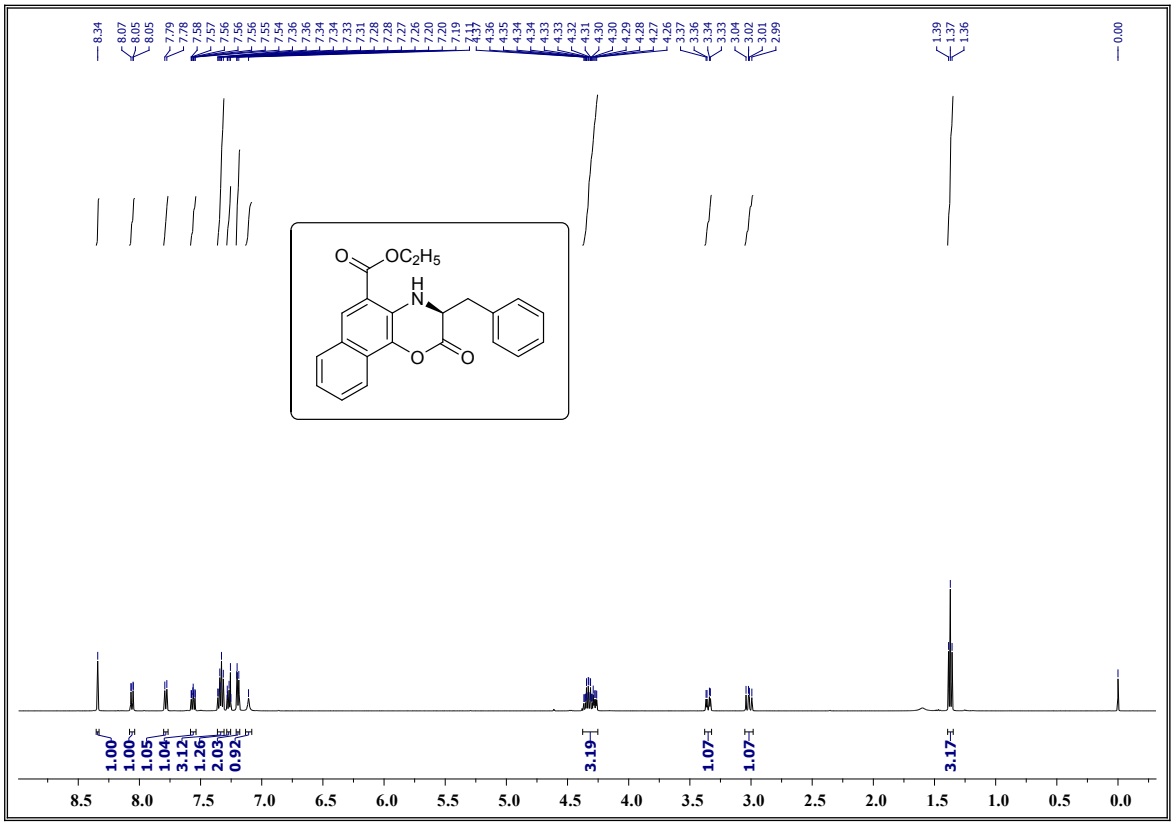
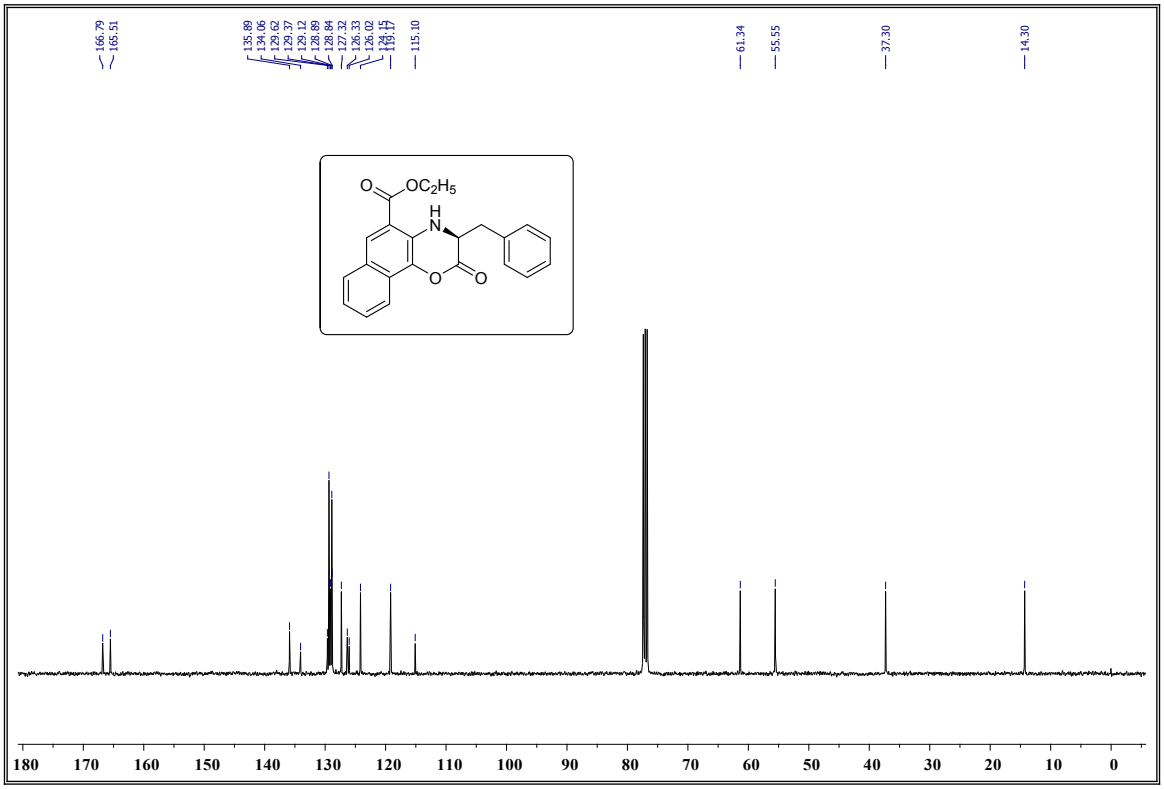
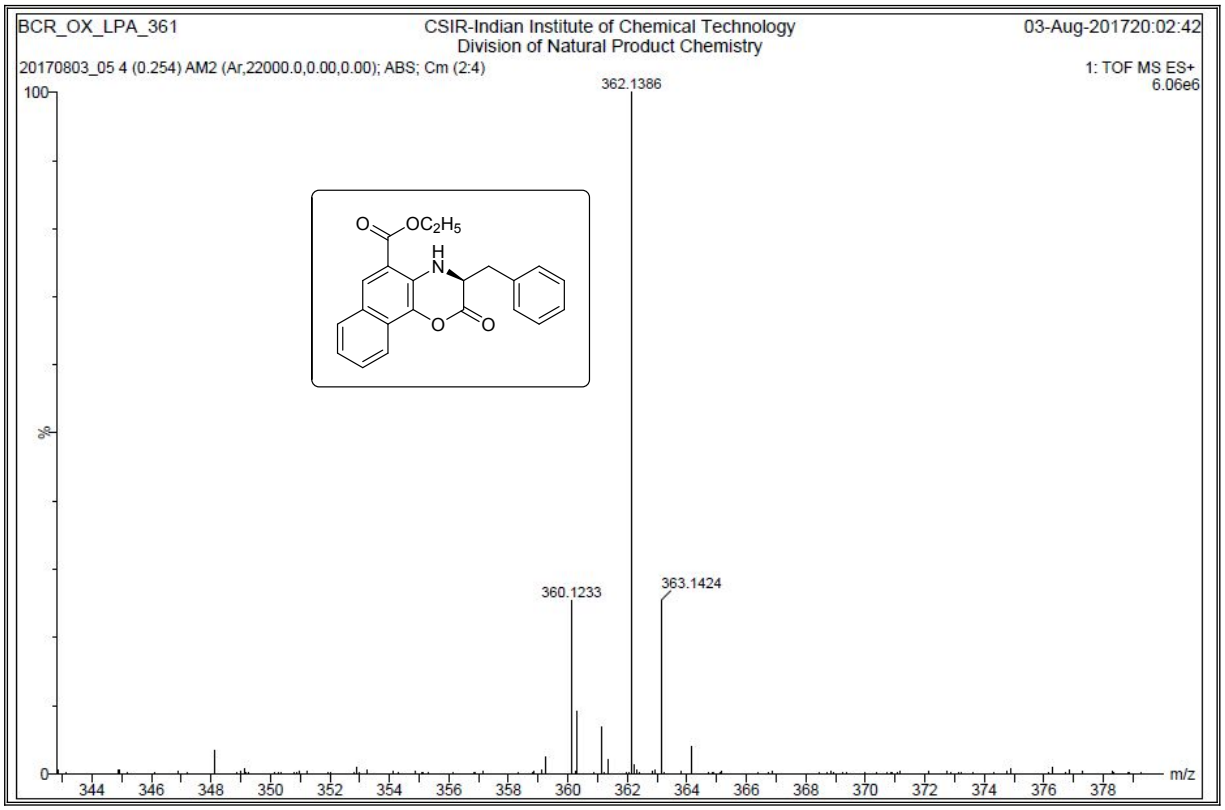
S3. Copies of ^{1}H-NMR, ^{13}C-NMR and HRMS of the compounds 3a-v, 3x-z, 3zb and 3ze-zg



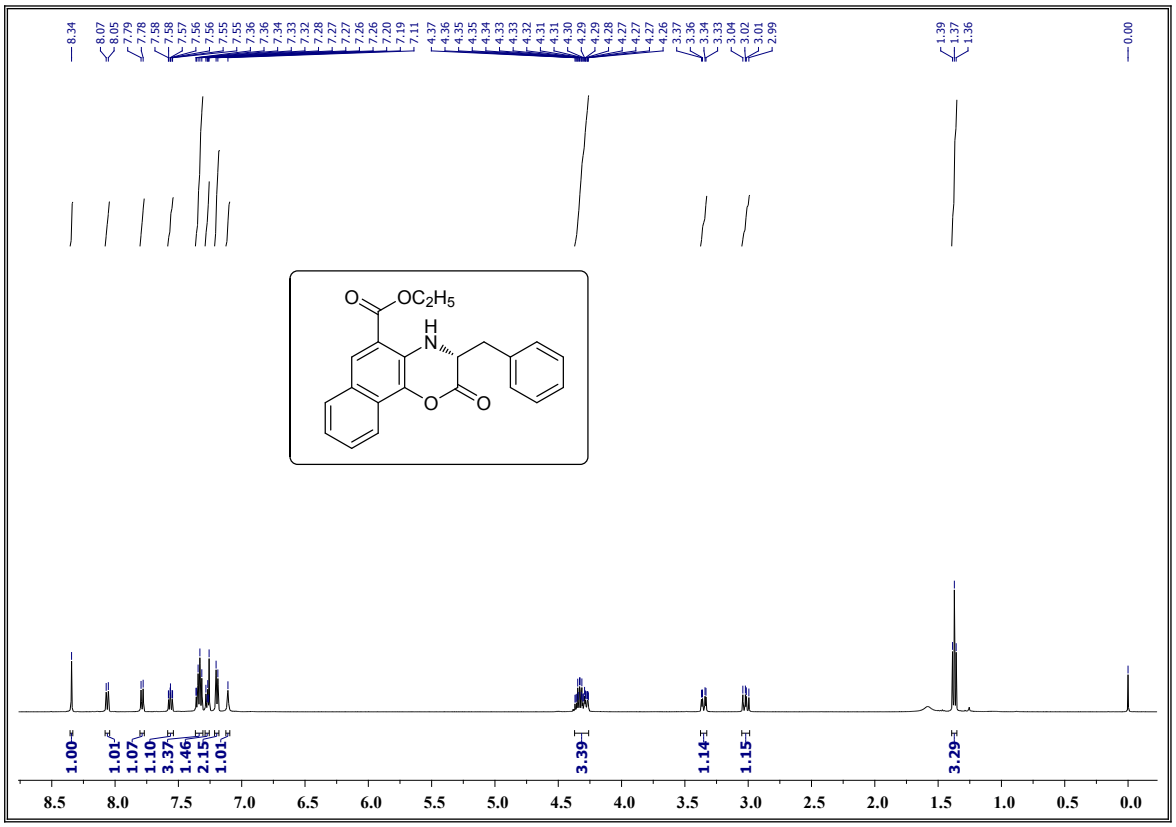
^{1}H-NMR Spectrum of compound 3a



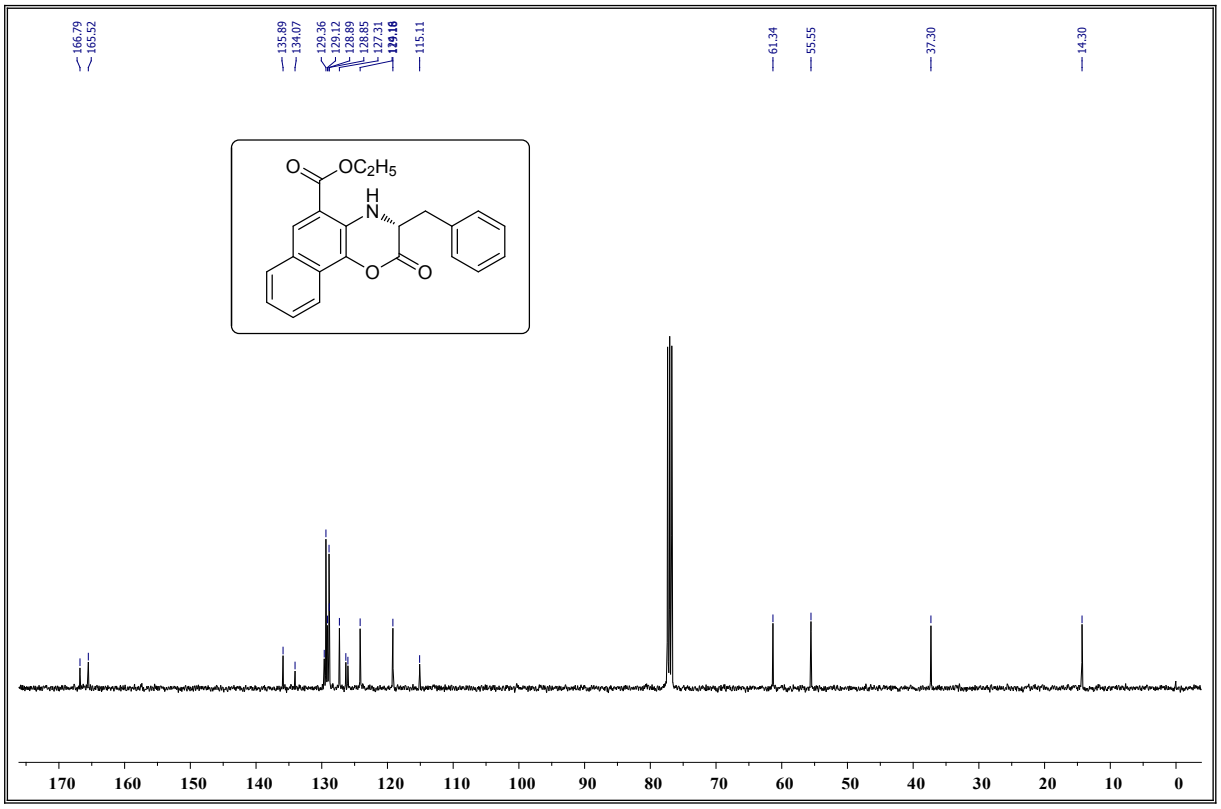
^{13}C-NMR Spectrum of compound 3a



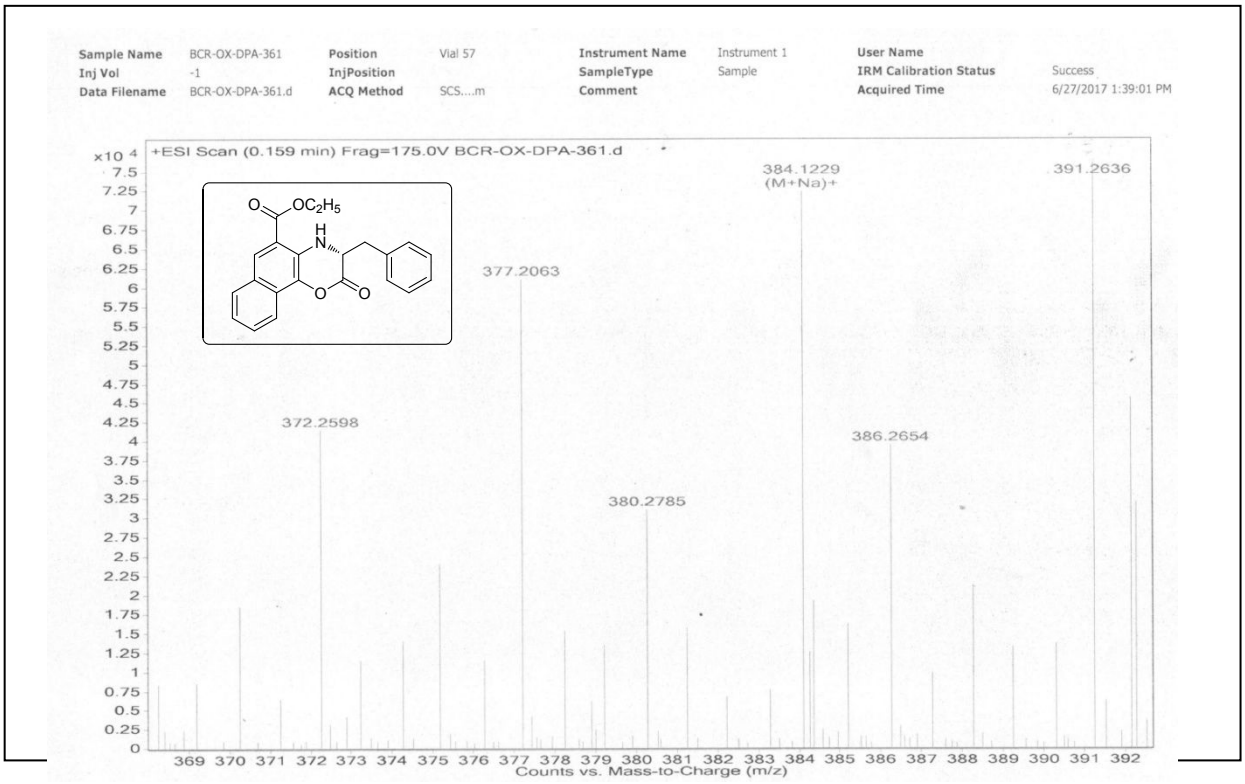
HRMS Spectrum of compound 3a



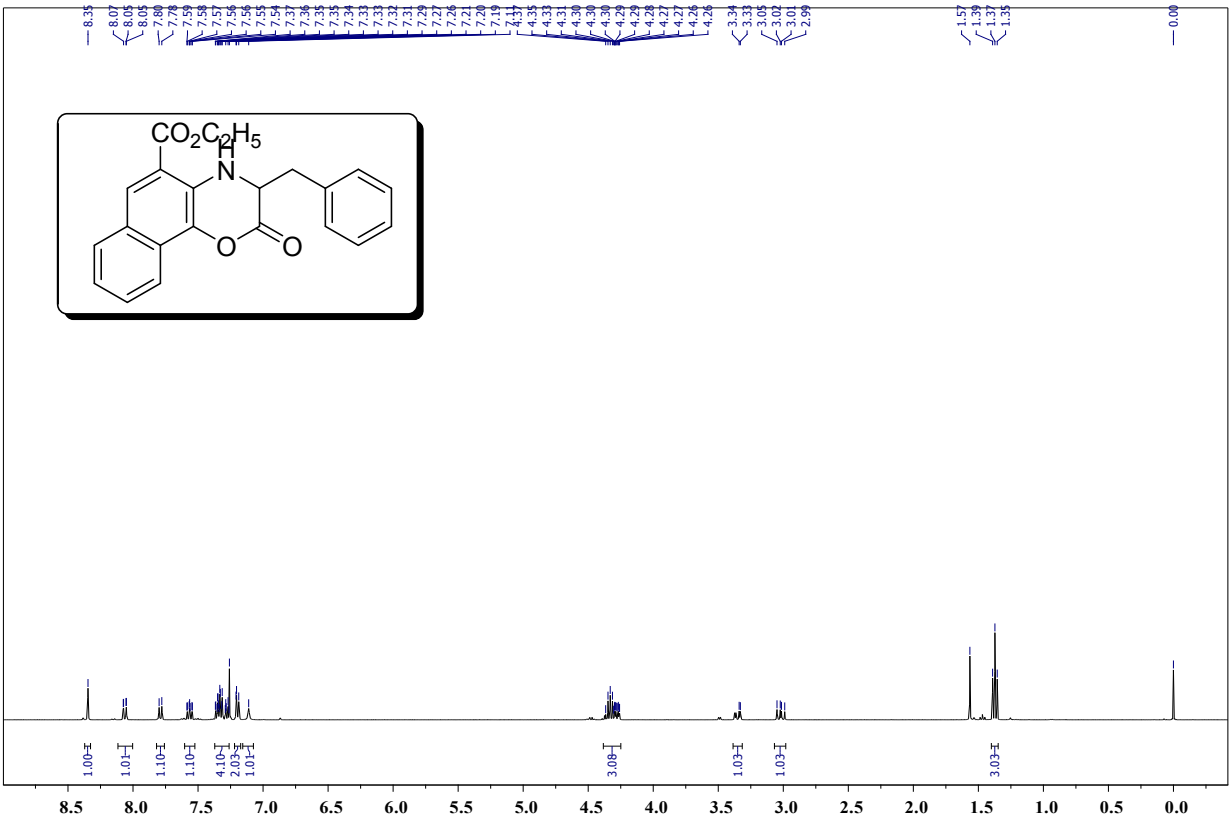
^{1}H-NMR Spectrum of compound 3b



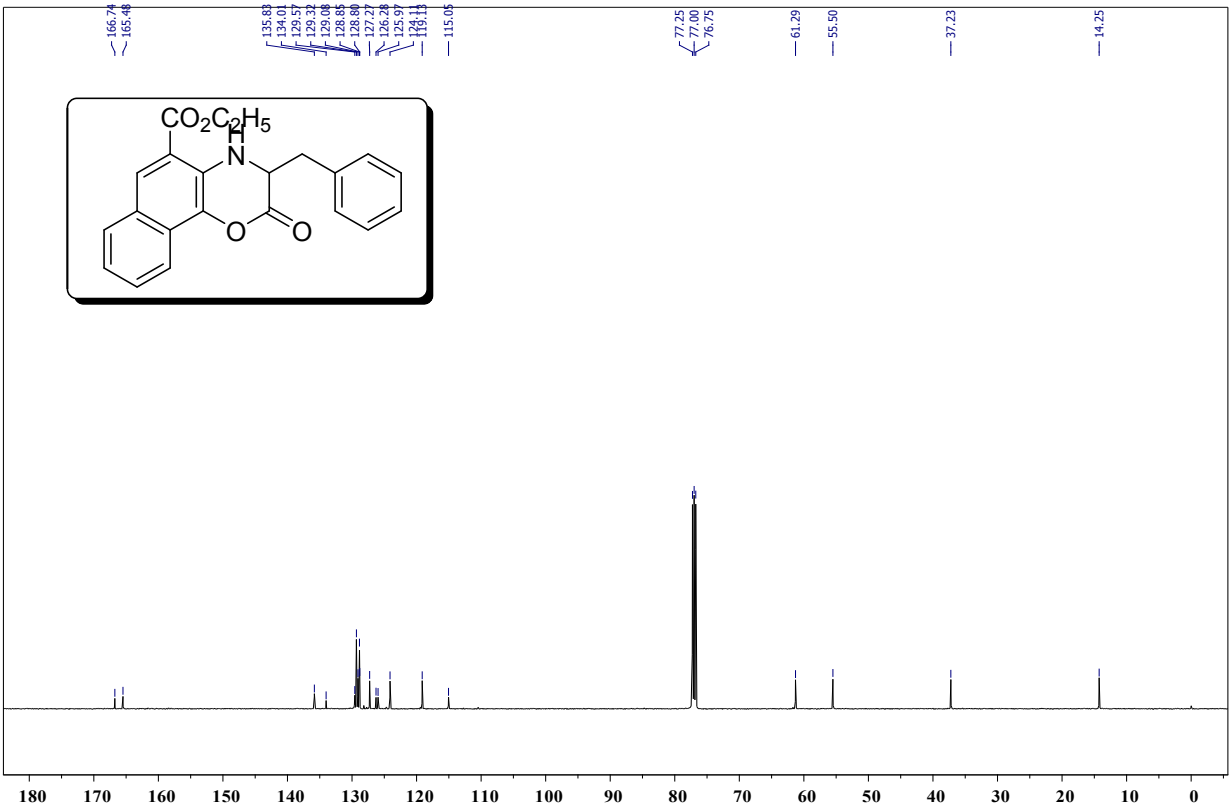
^{13}C-NMR Spectrum of compound 3b



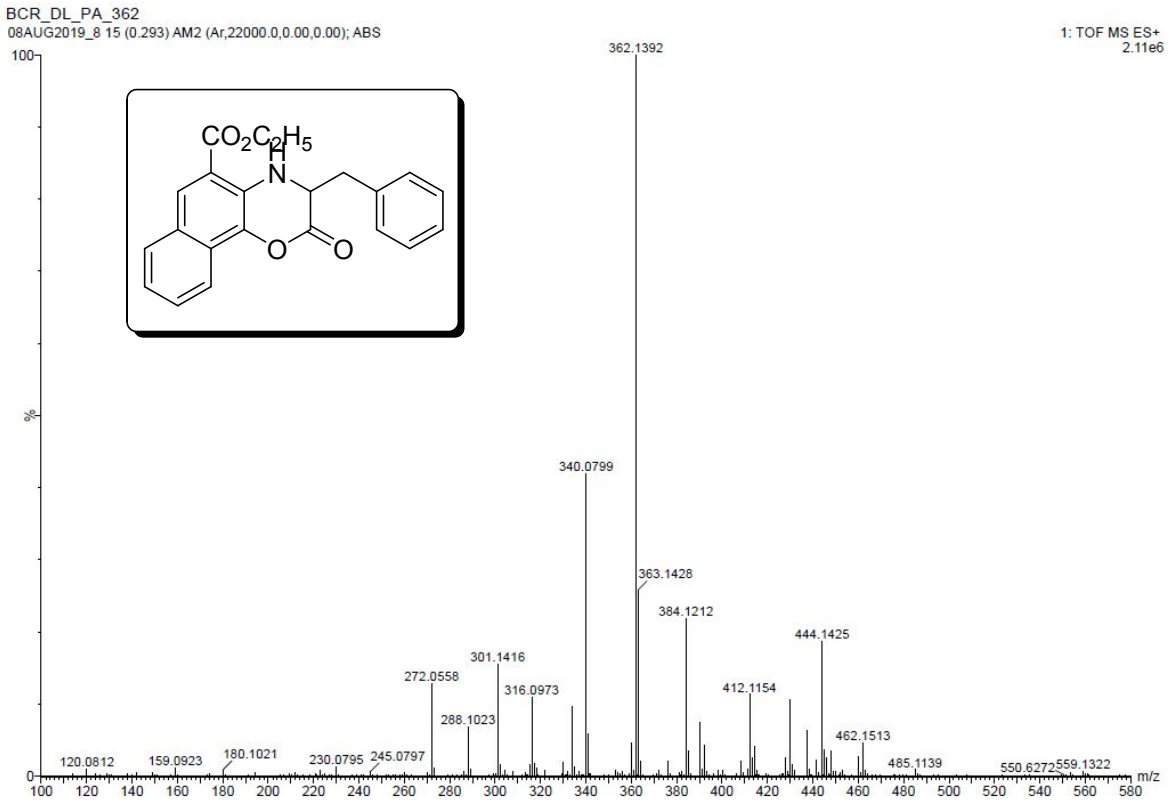
HRMS Spectrum of compound 3b



^{1}H NMR Spectrum of compound 3c



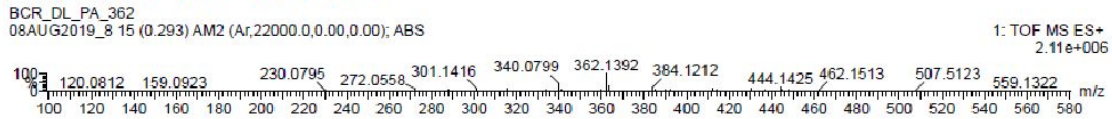
^{13}C NMR Spectrum of compound 3c



Elemental Composition Report **Page 1**

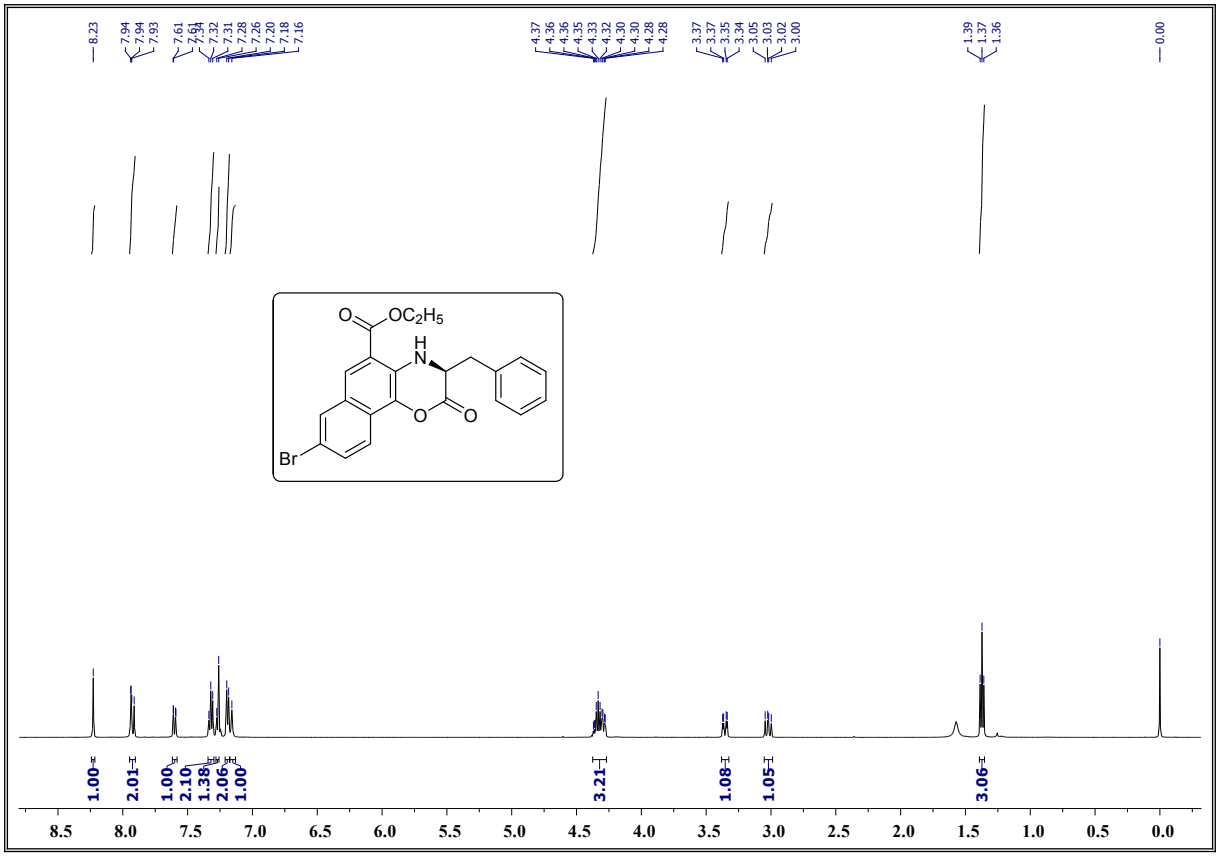
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
14 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-22 H: 0-20 N: 0-1 O: 0-4 K: 0-1

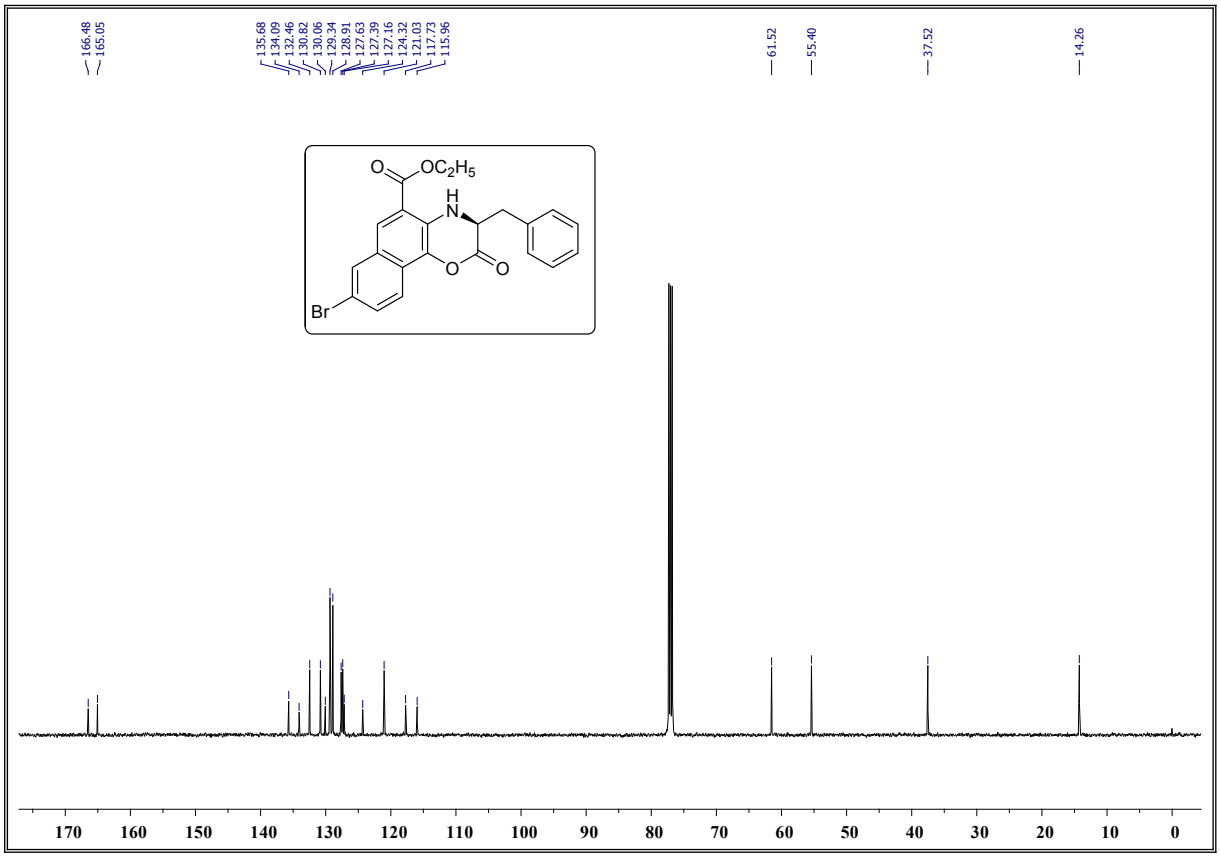


Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
362.1392	362.1392	0.0	0.0	13.5	562.4	n/a	n/a	C22 H20 N O4

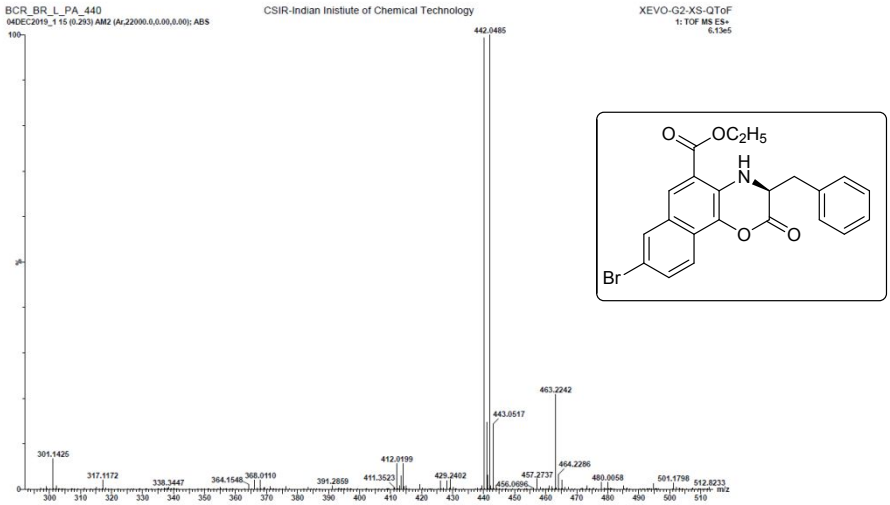
HRMS Spectrum of compound 3c



^{1}H-NMR Spectrum of compound 3d



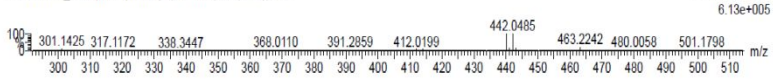
^{13}C-NMR Spectrum of compound 3d



Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
16 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-22 H: 0-19 N: 0-1 O: 0-4 Br: 0-1



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
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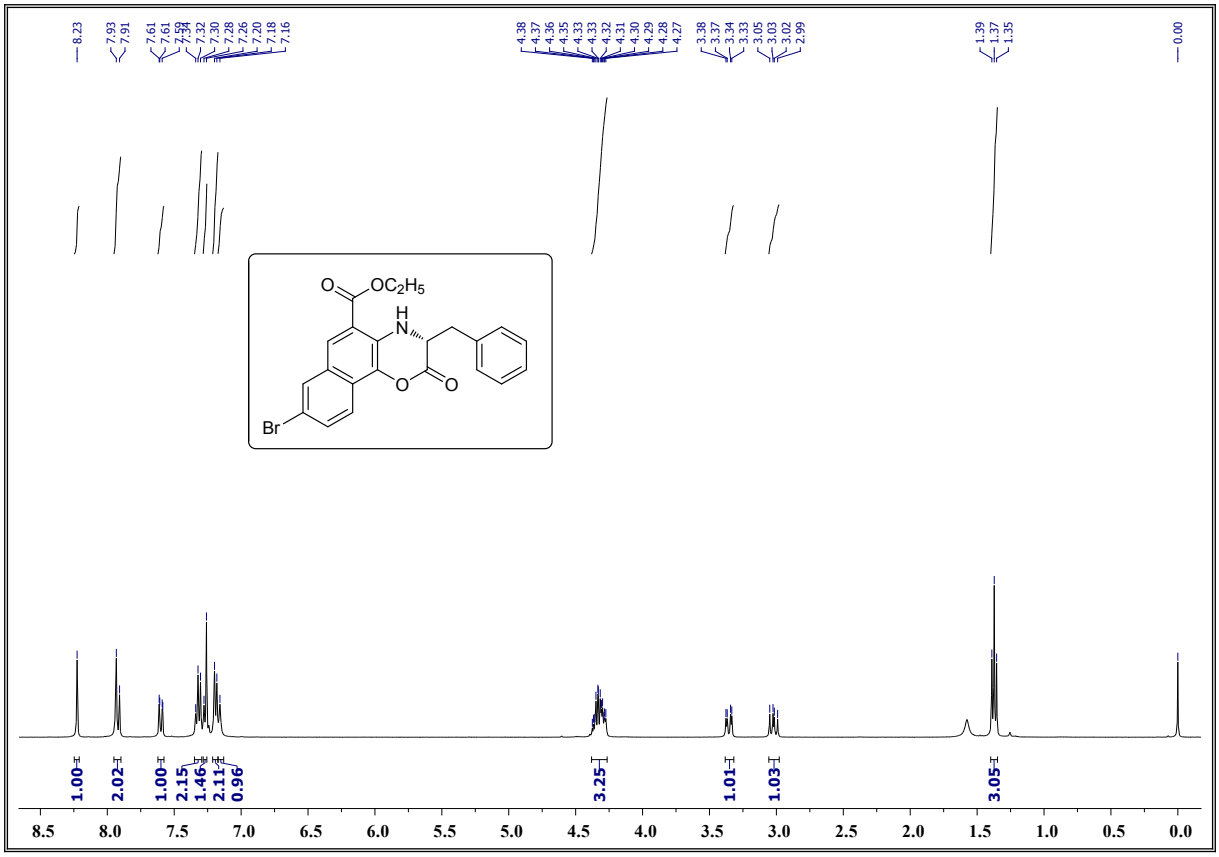
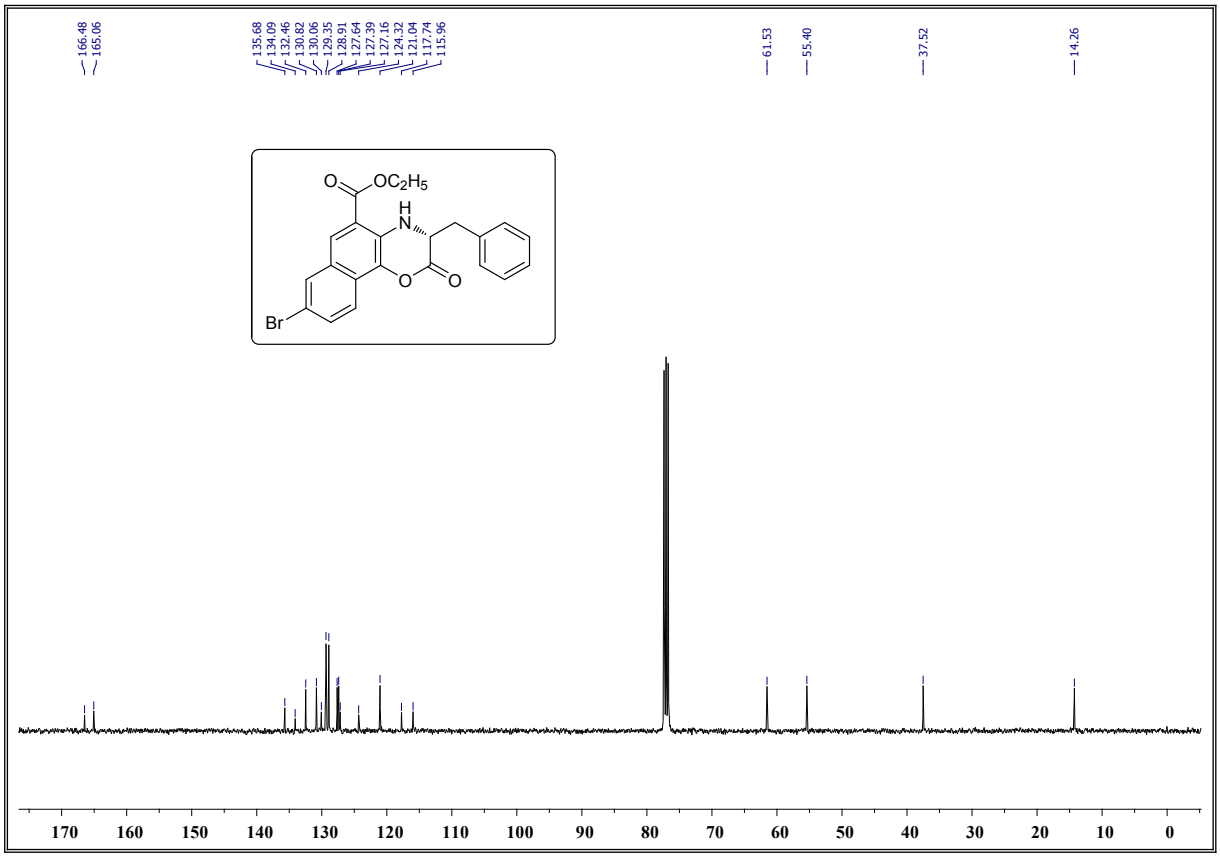
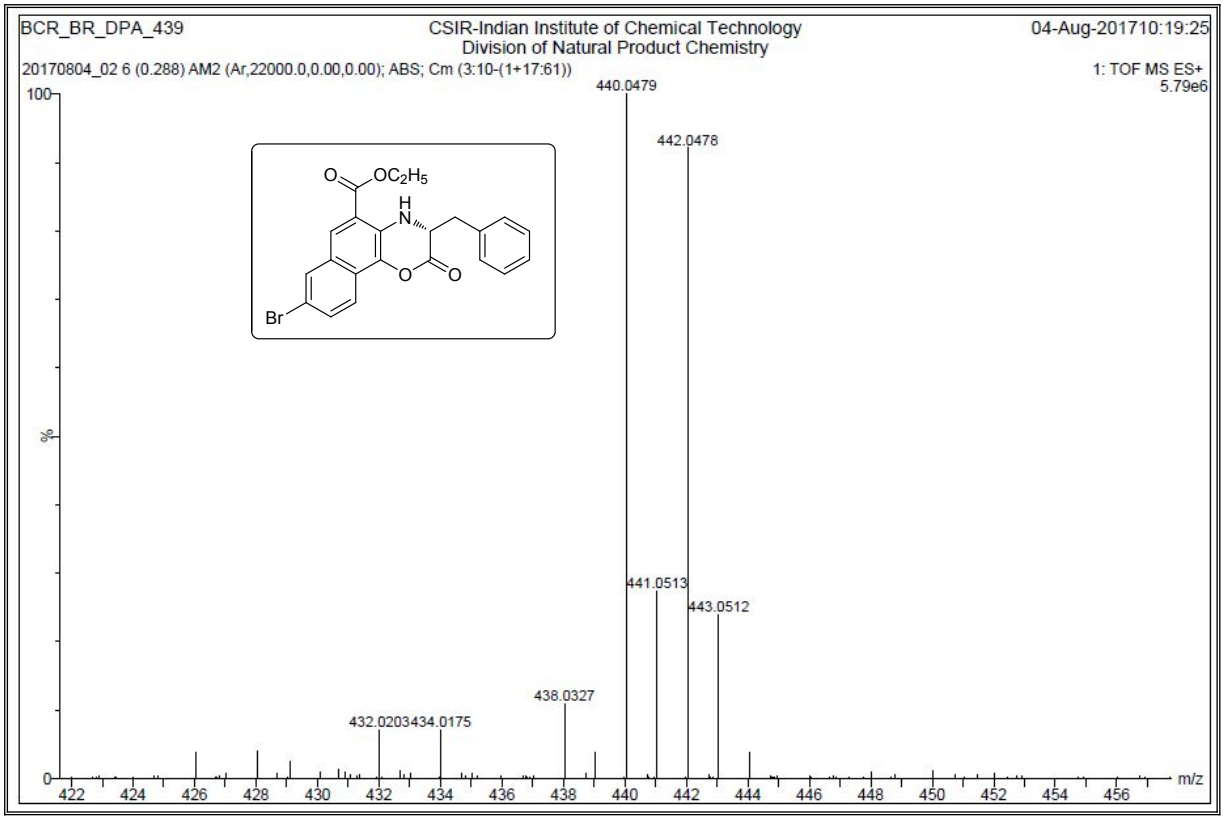
HRMS Spectrum of compound 3d



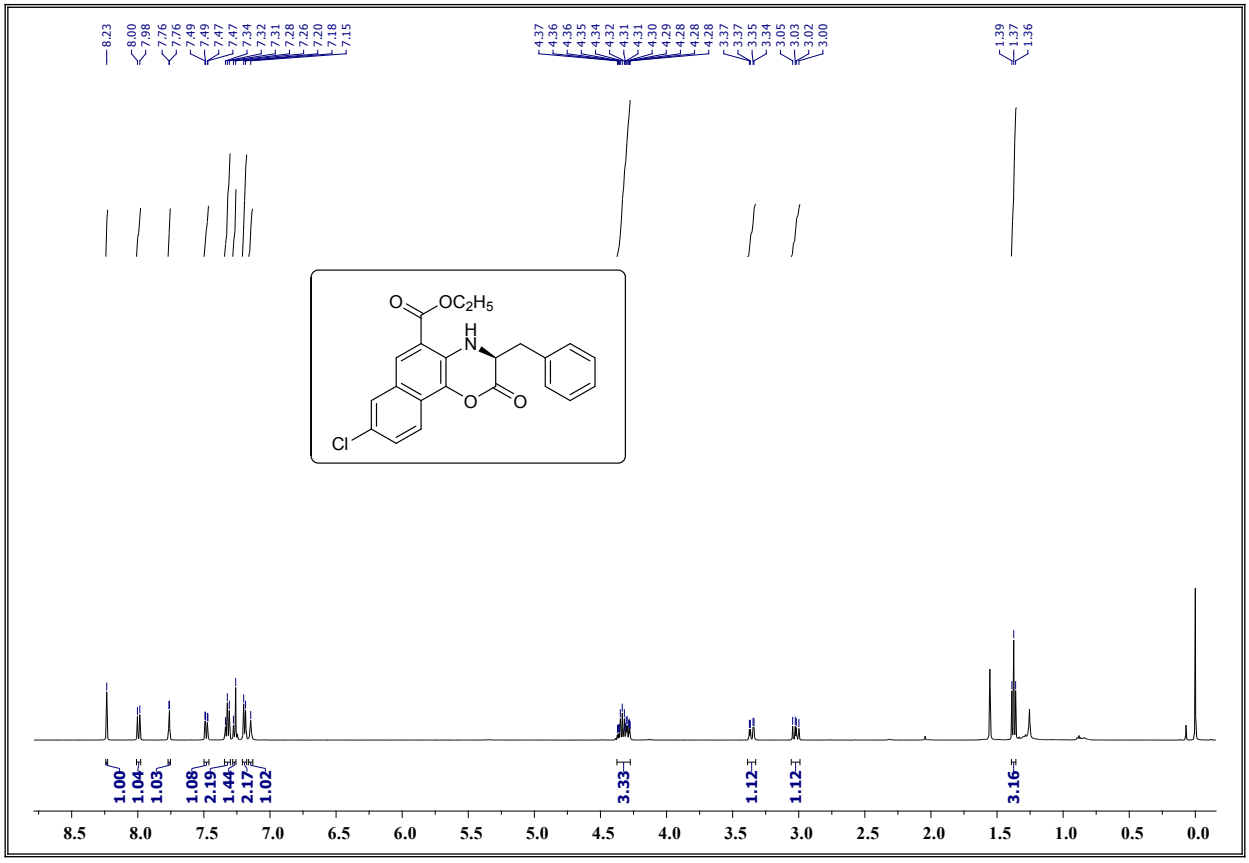
^{1}H-NMR Spectrum of compound 3e



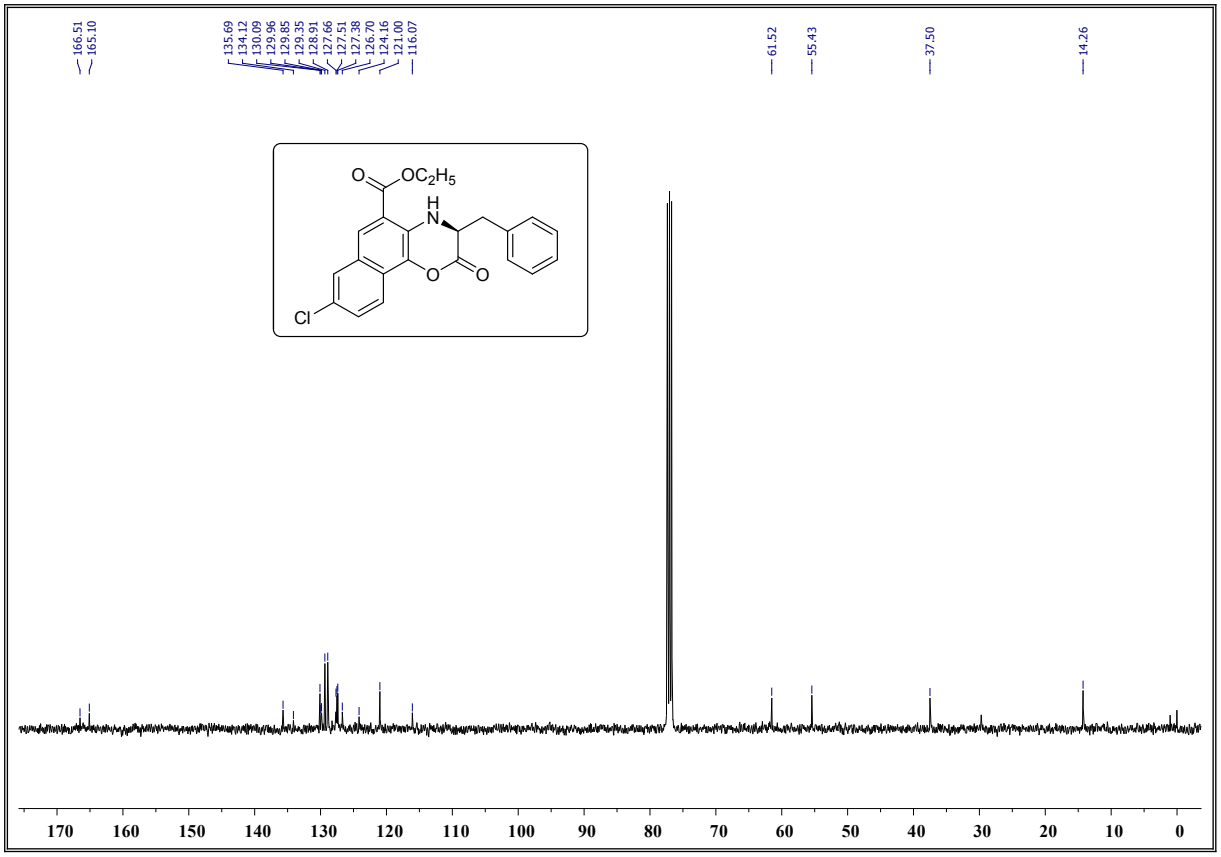
^{13}C-NMR Spectrum of compound 3e



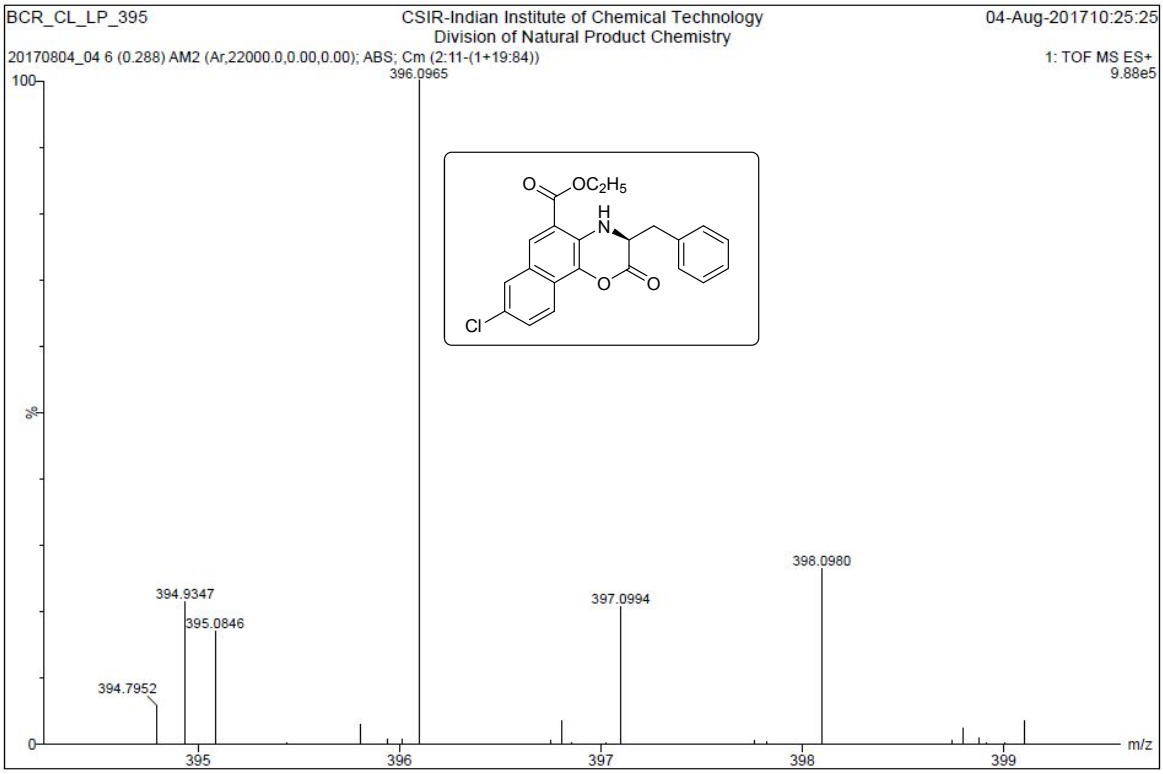
HRMS Spectrum of compound 3e



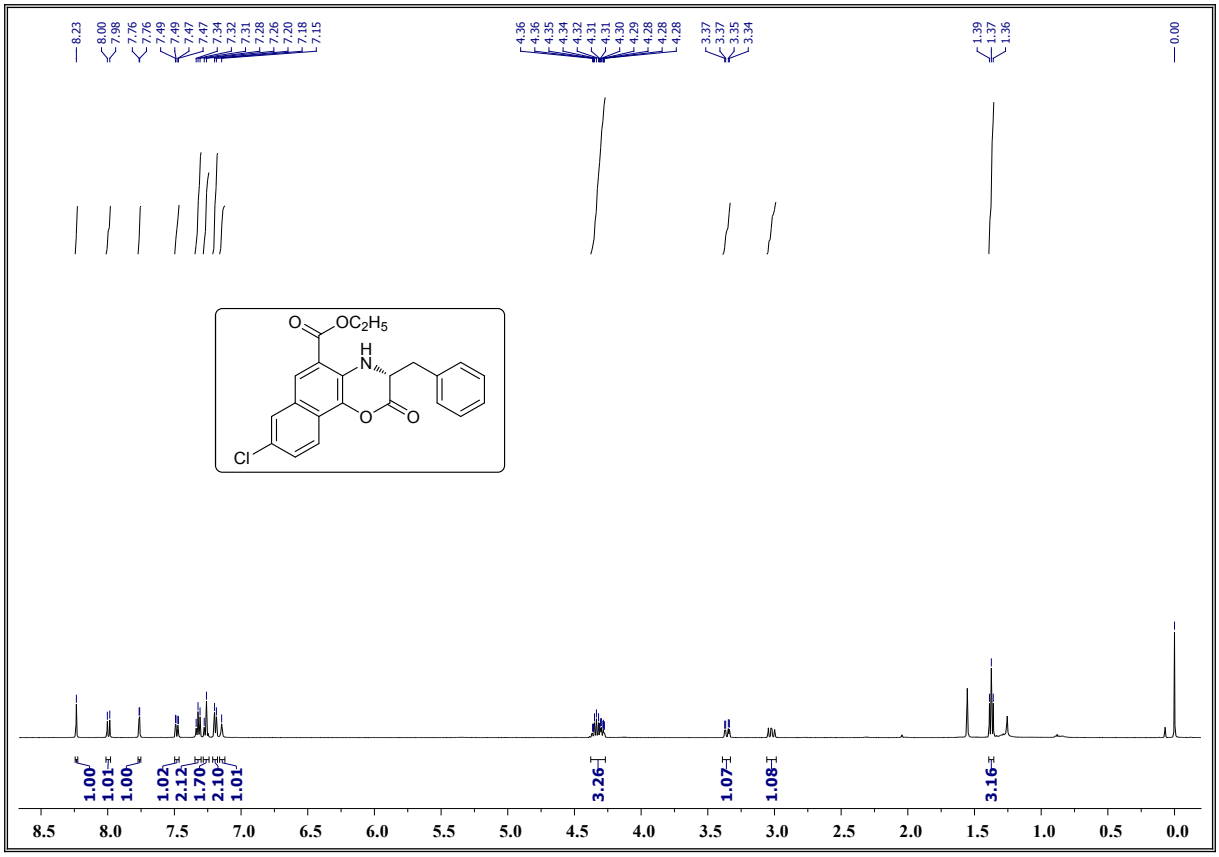
^{1}H-NMR Spectrum of compound 3f



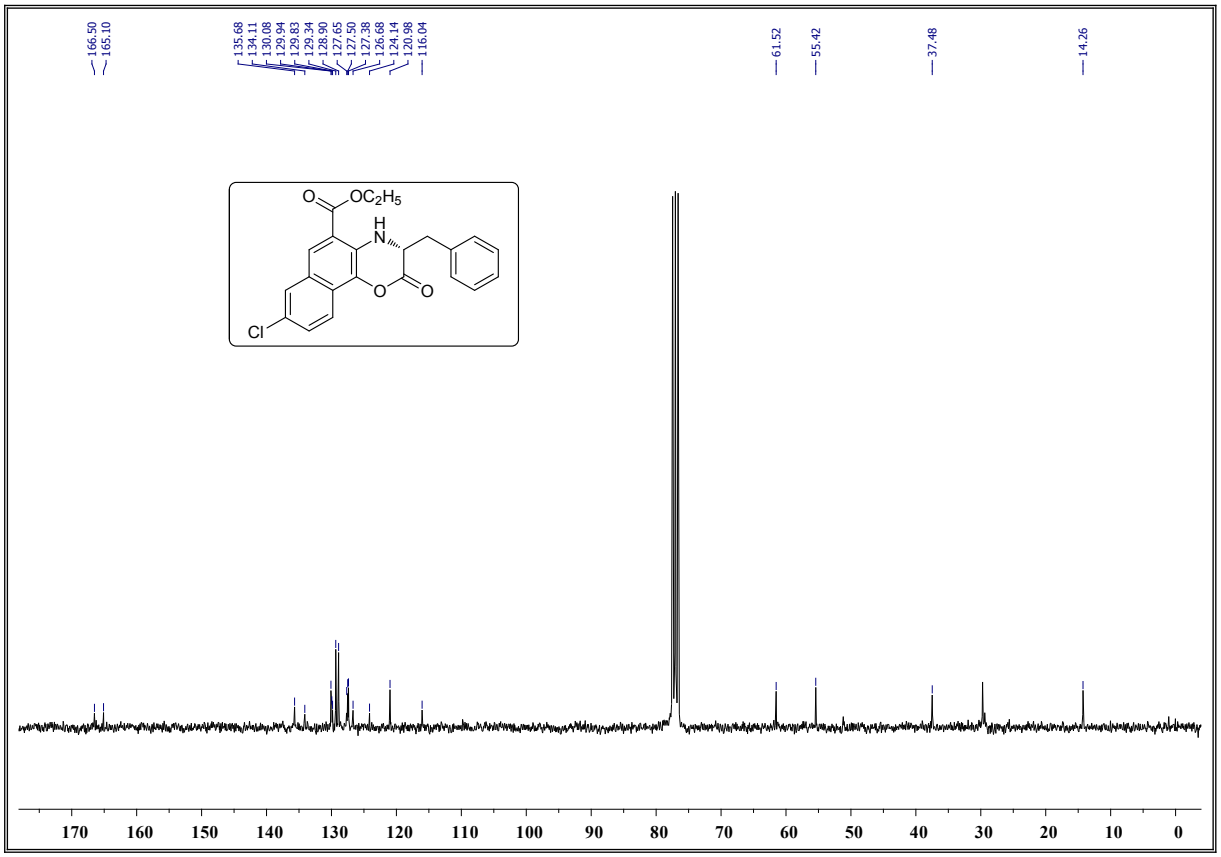
^{13}C-NMR Spectrum of compound 3f



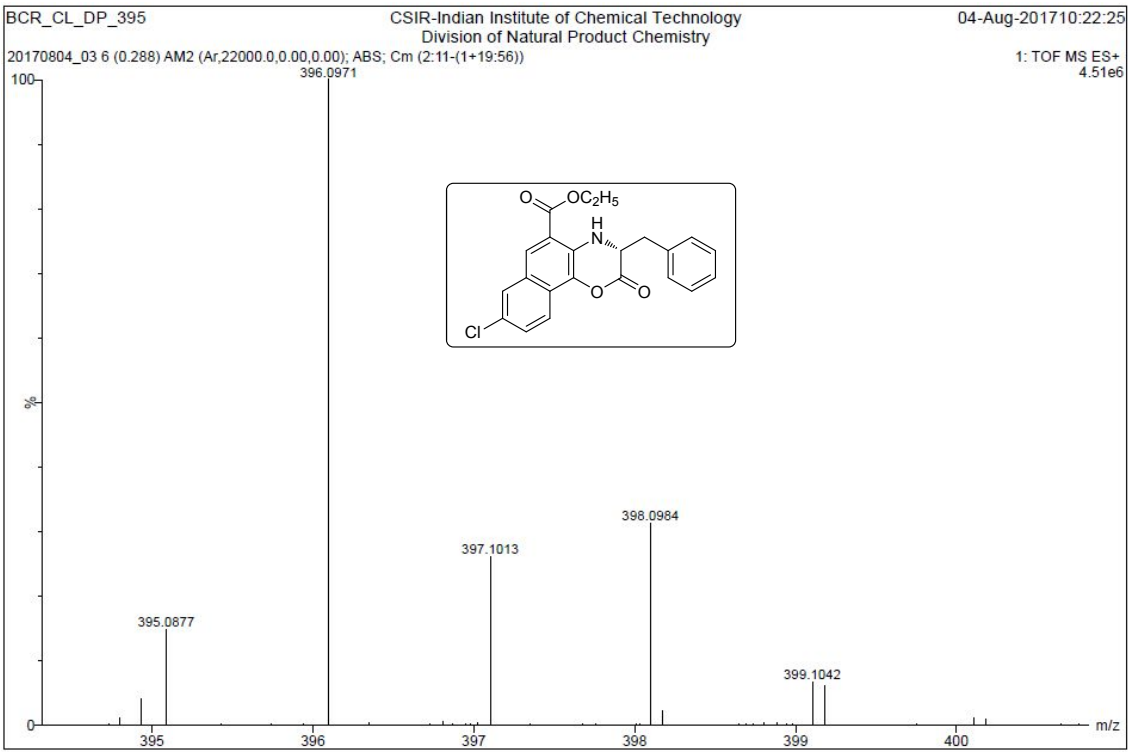
HRMS Spectrum of compound 3f



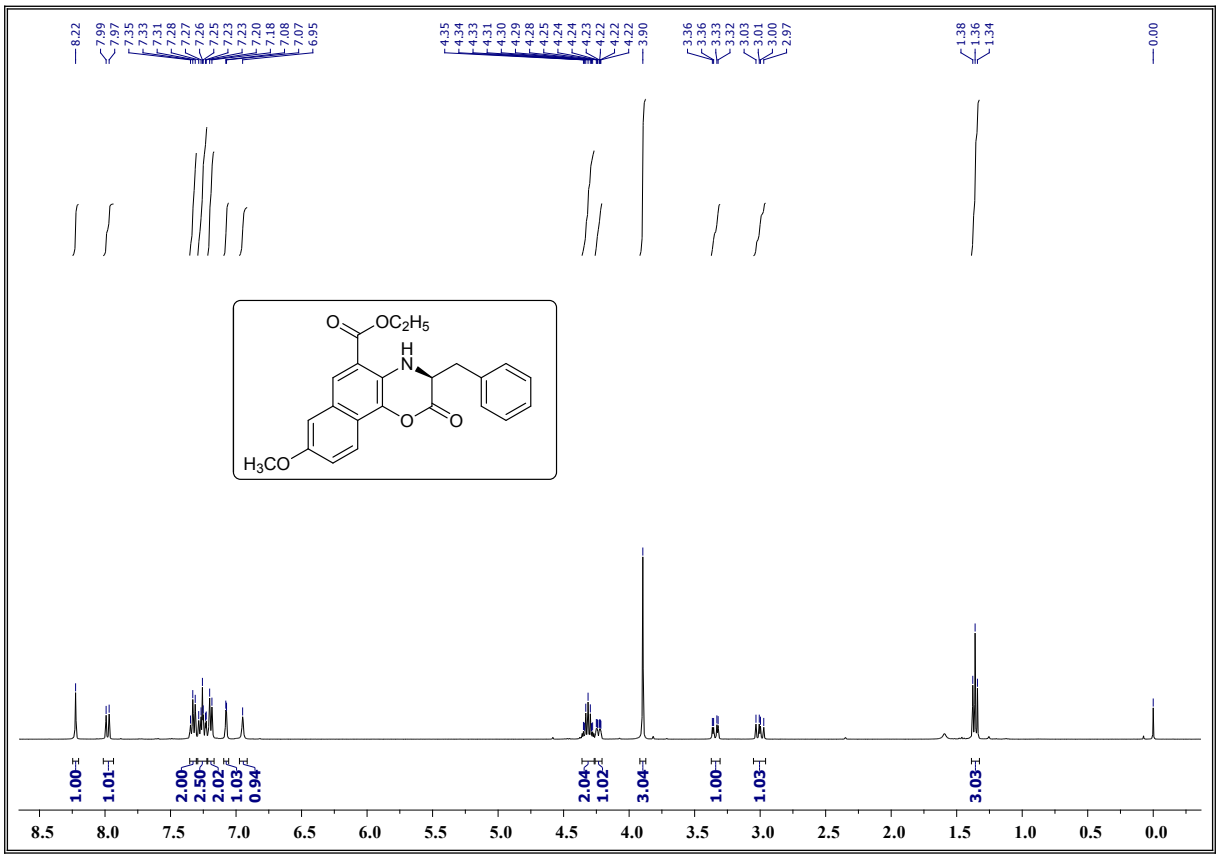
^{1}H-NMR Spectrum of compound 3g



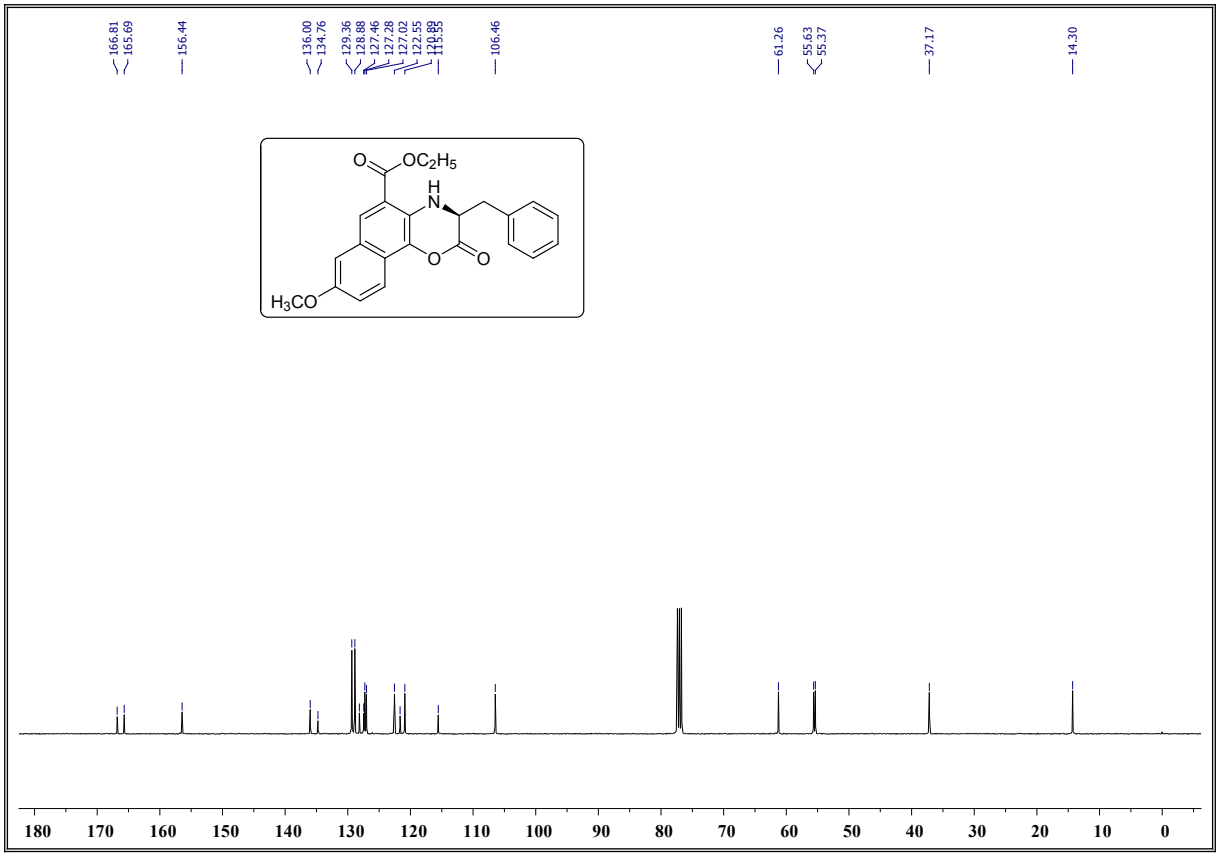
^{13}C-NMR Spectrum of compound 3g



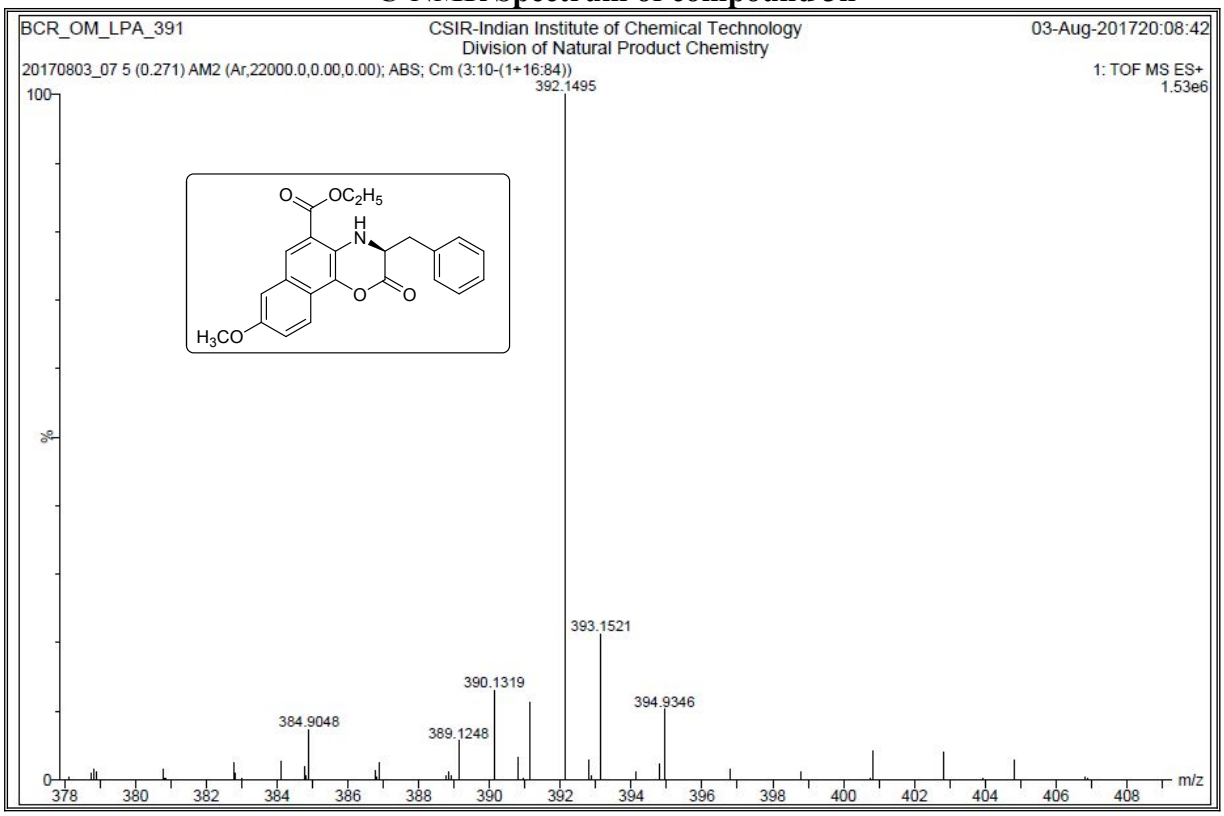
HRMS Spectrum of compound 3g



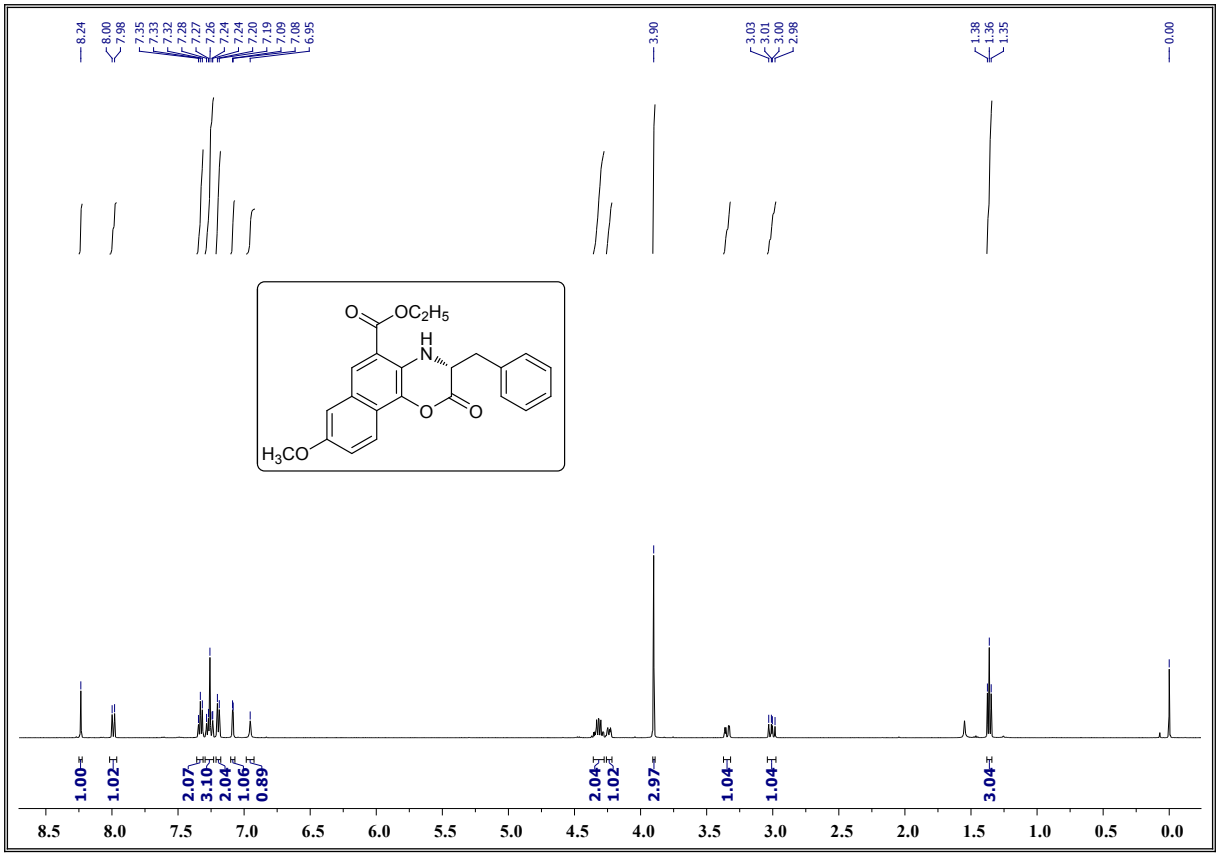
^{1}H-NMR Spectrum of compound 3h



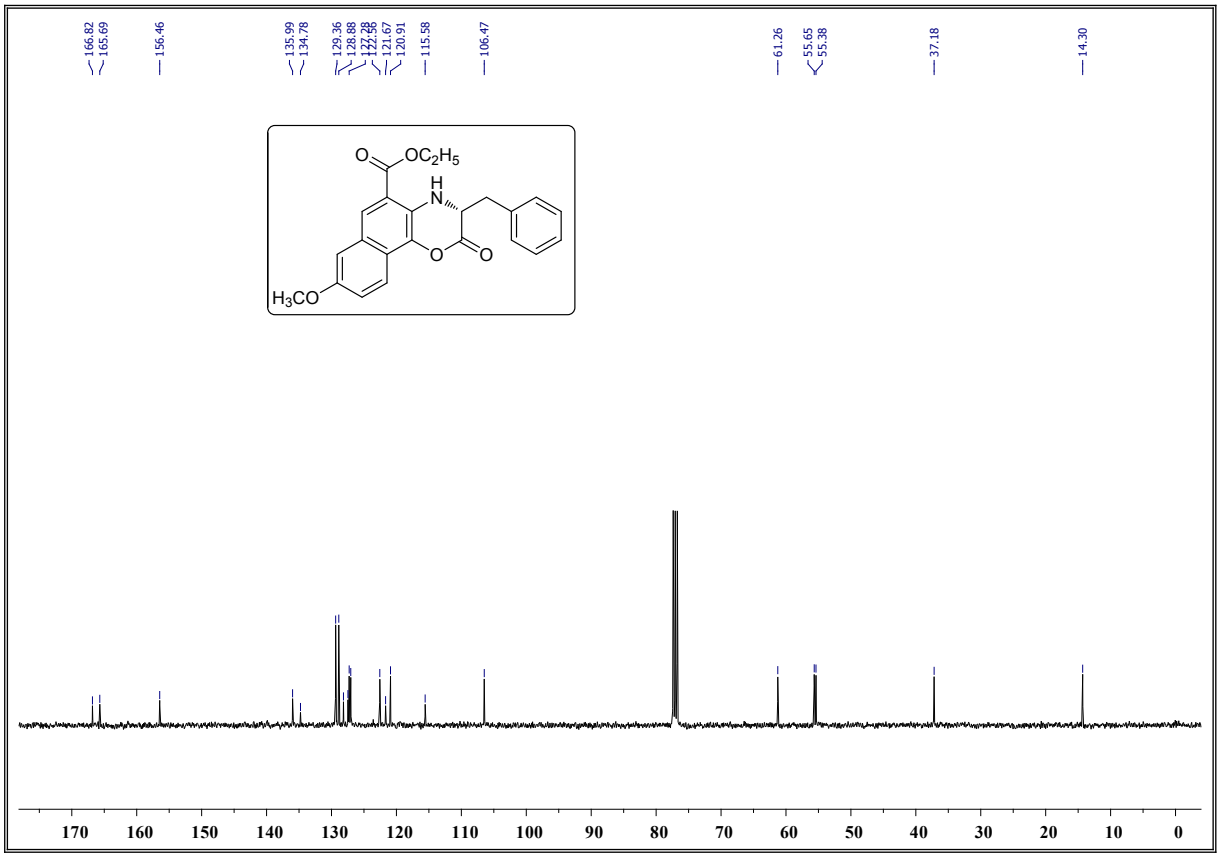
^{13}C-NMR Spectrum of compound 3h



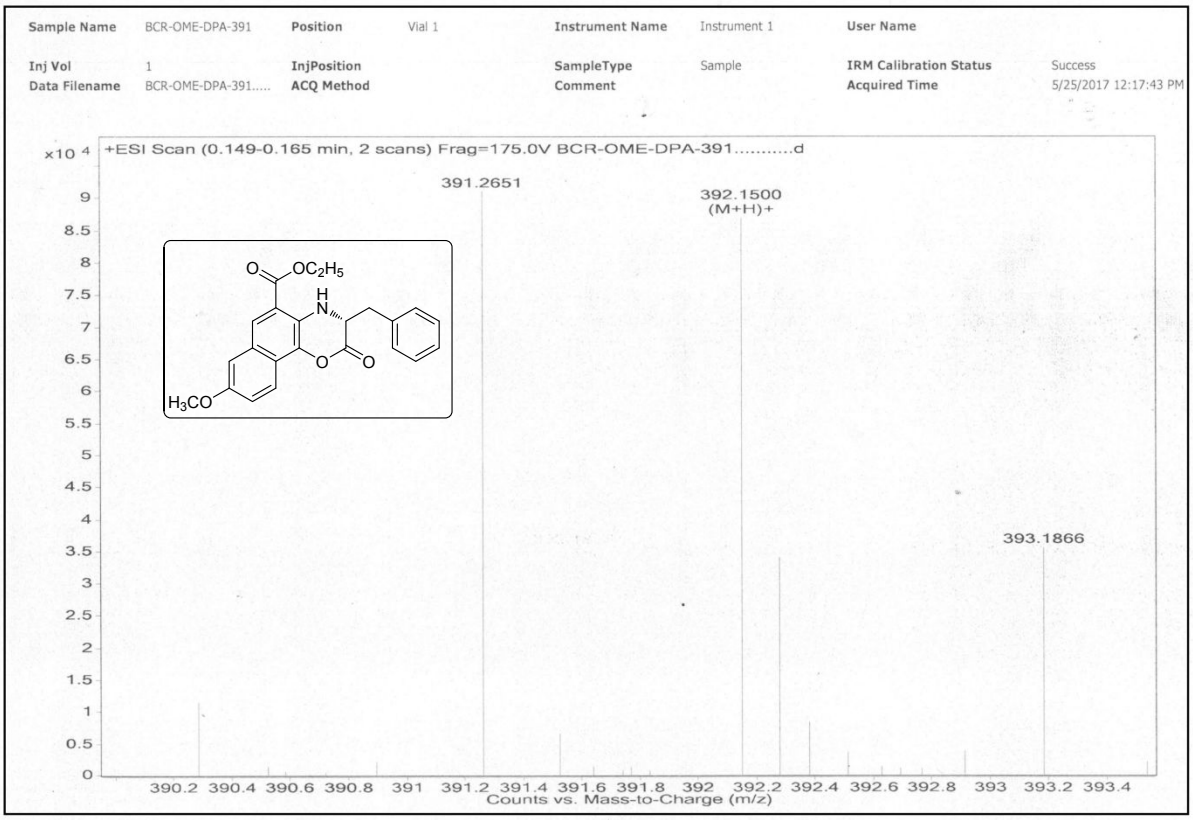
HRMS Spectrum of compound 3h



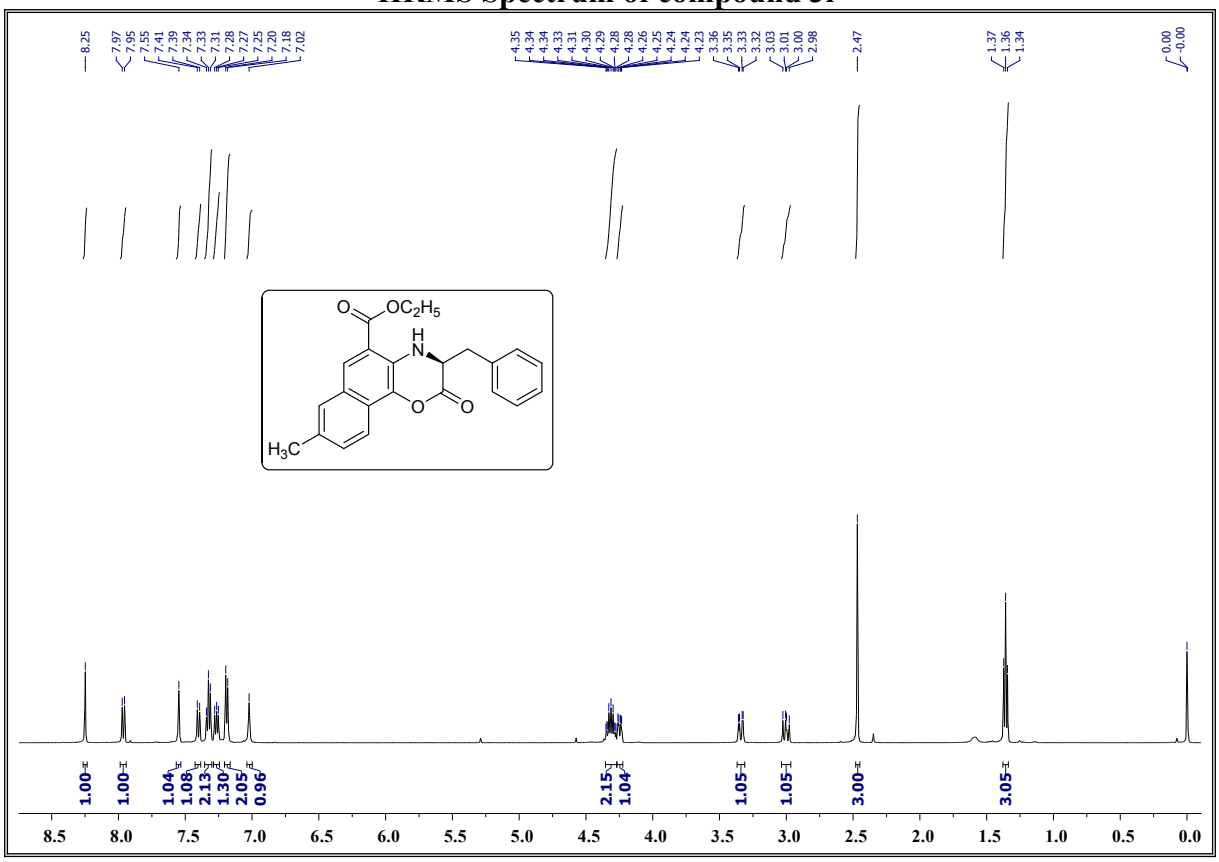
^{1}H-NMR Spectrum of compound 3i



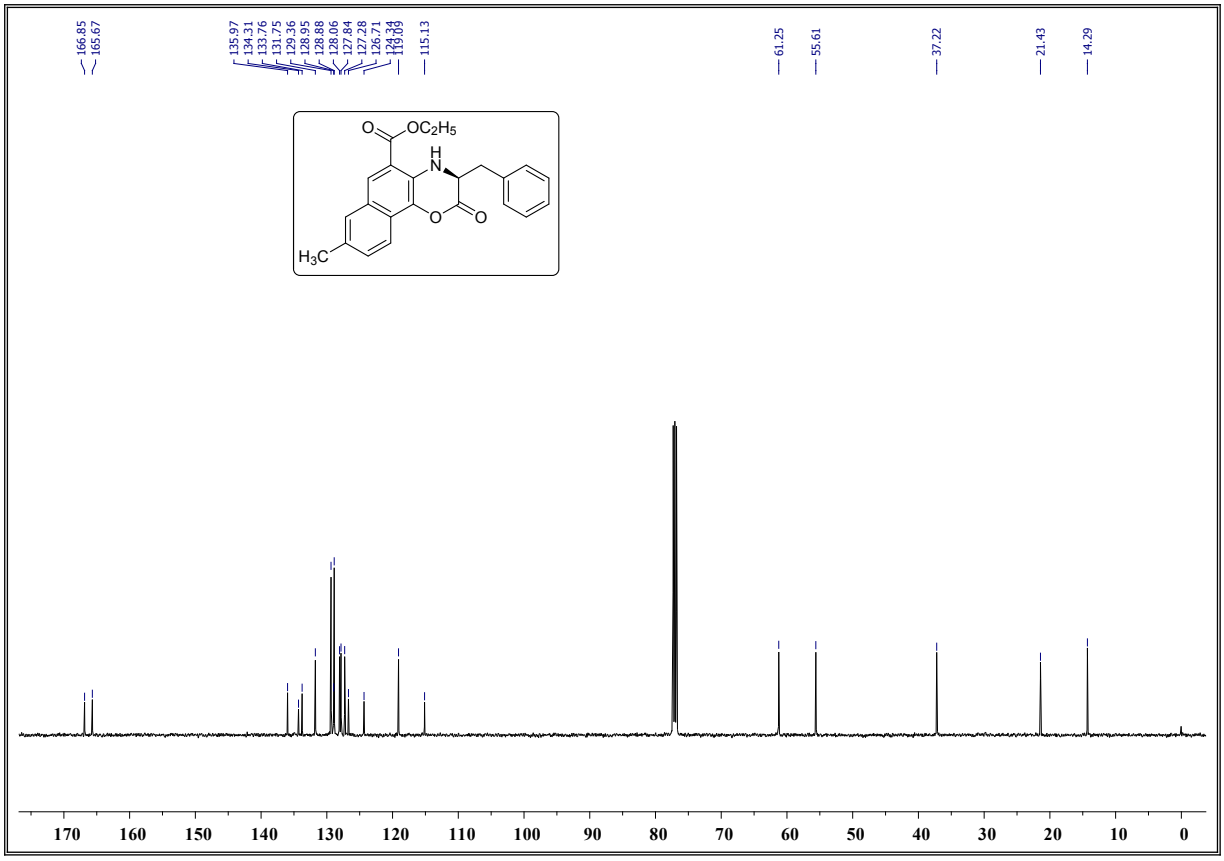
^{13}C-NMR Spectrum of compound 3i



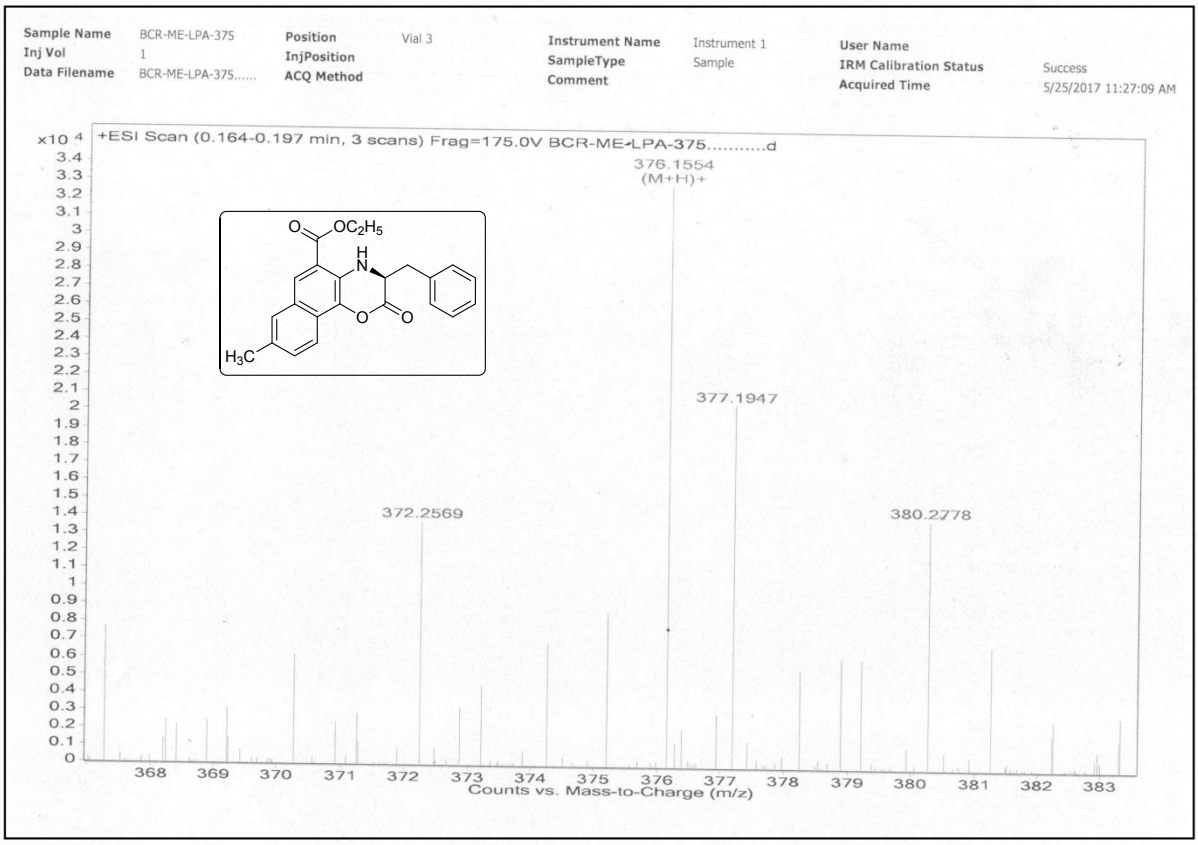
HRMS Spectrum of compound 3i



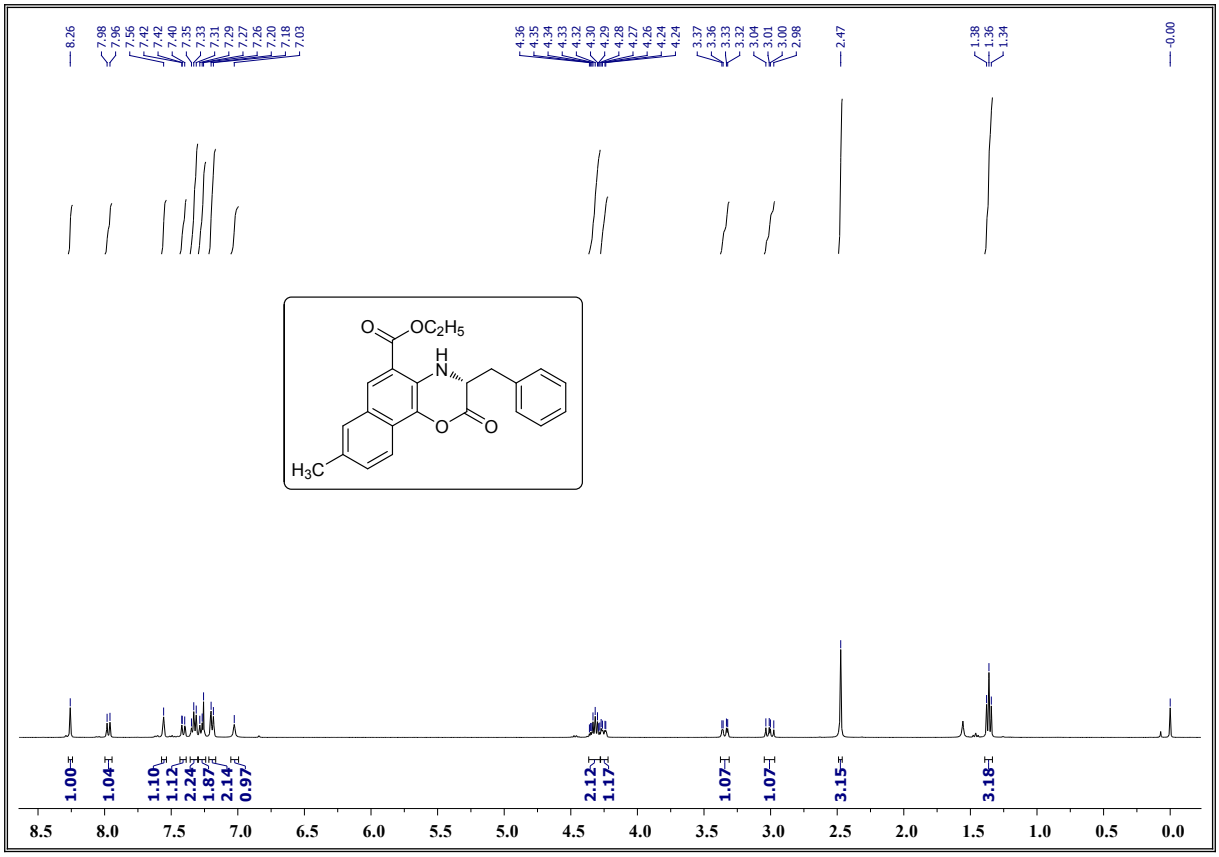
^{1}H-NMR Spectrum of compound 3j



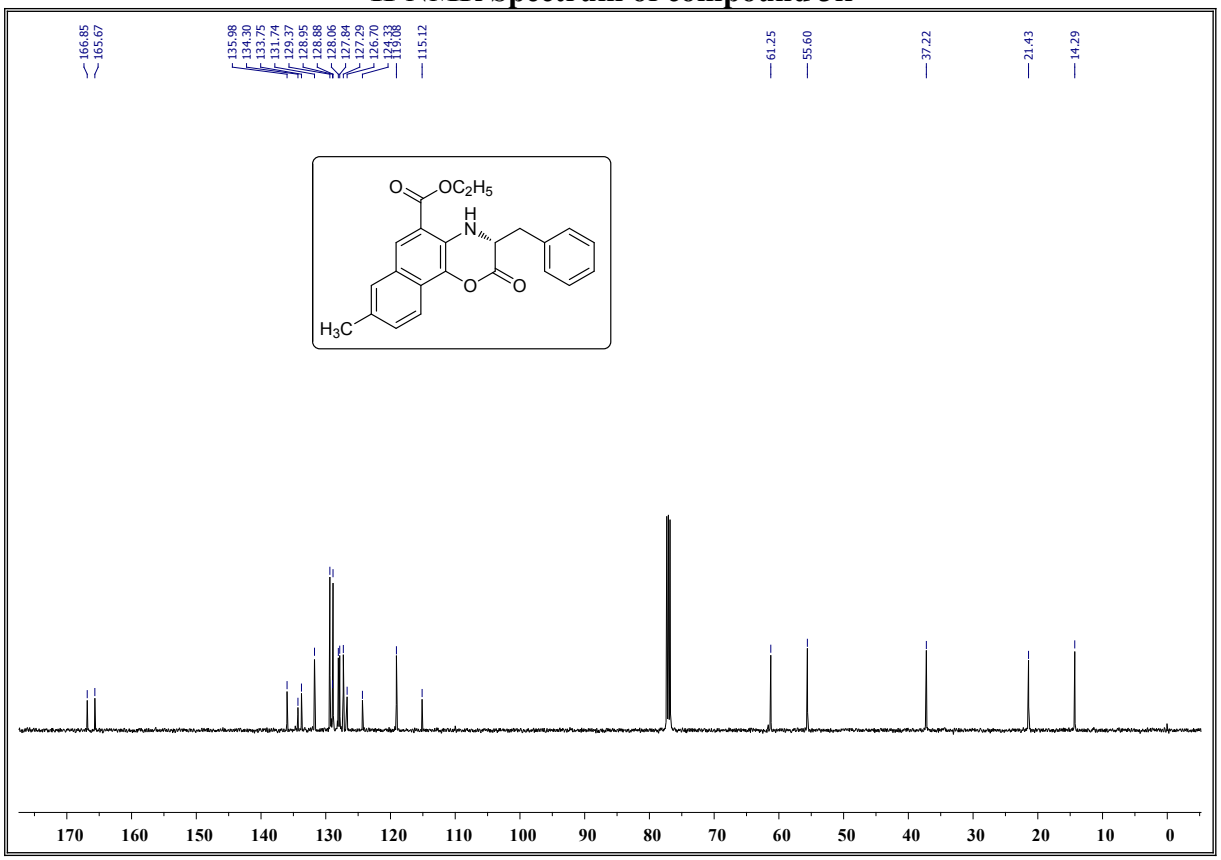
^{13}C-NMR Spectrum of compound 3j



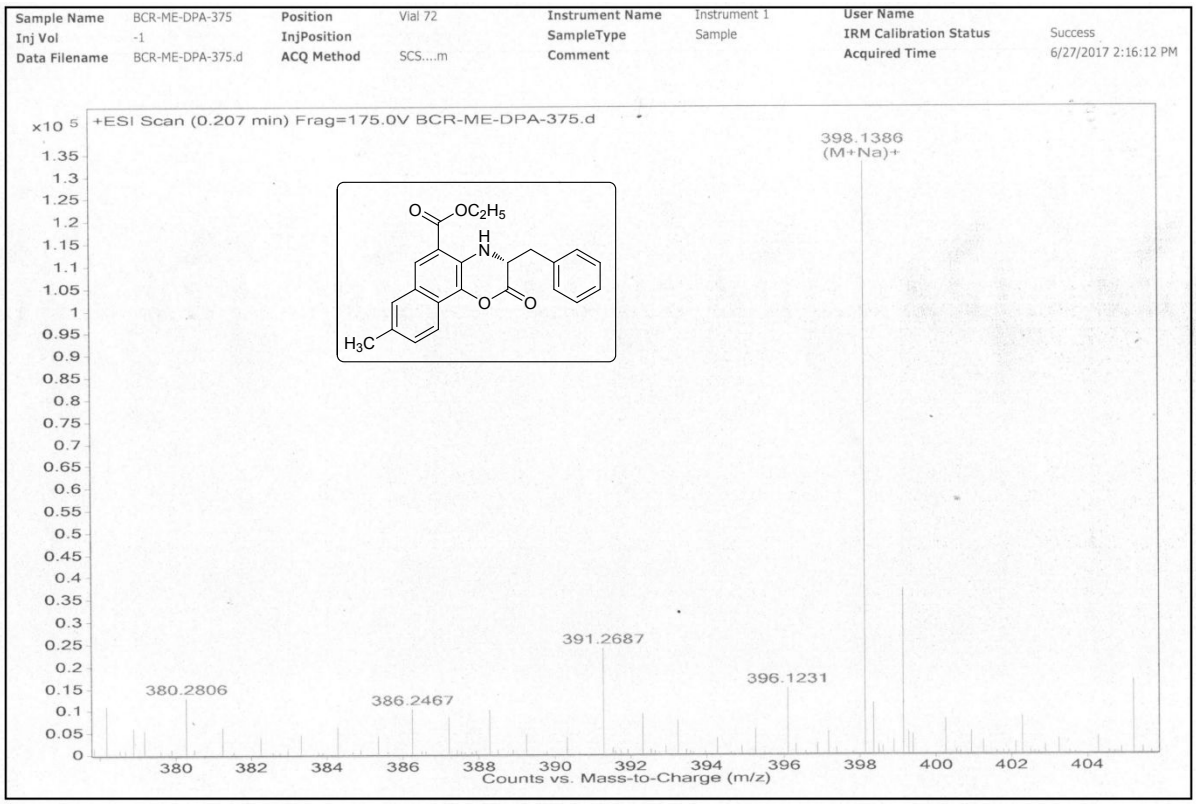
HRMS Spectrum of compound 3j



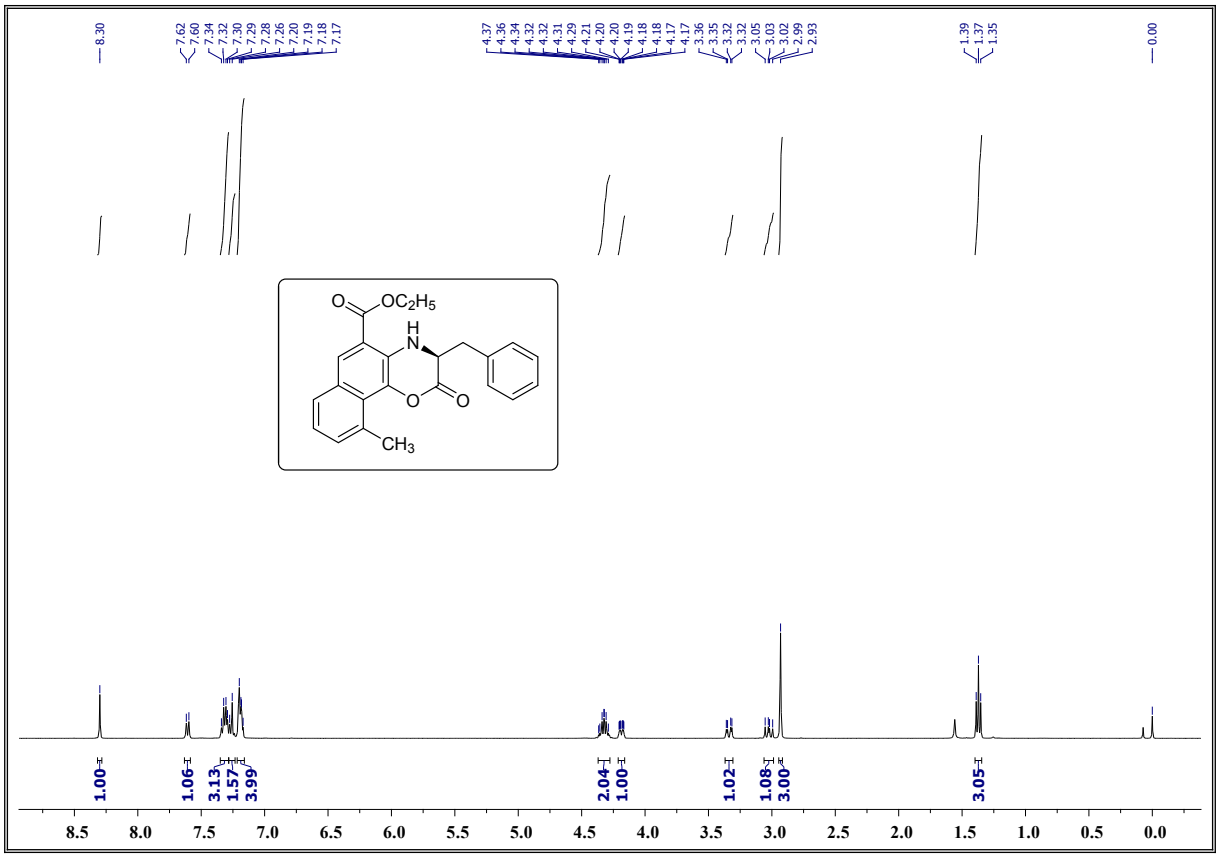
^{1}H-NMR Spectrum of compound 3k



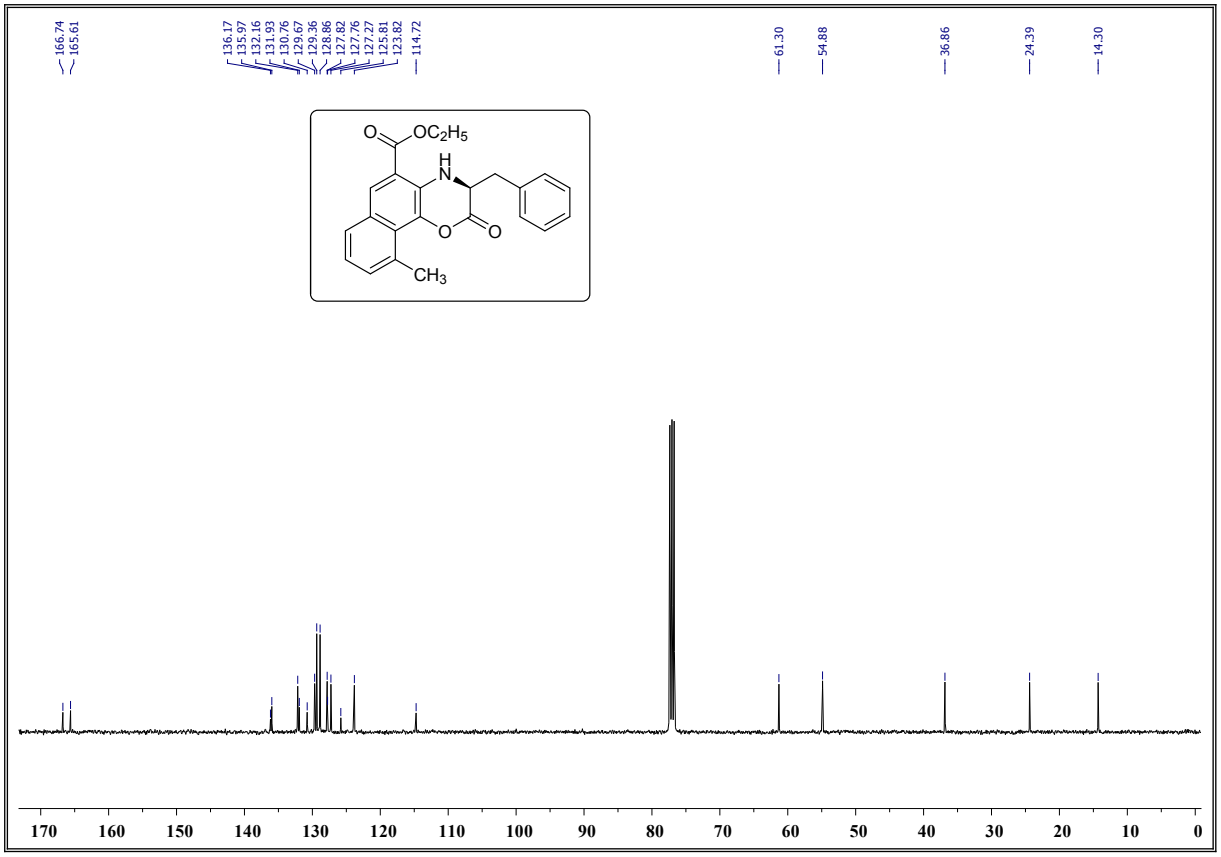
^{13}C-NMR Spectrum of compound 3k



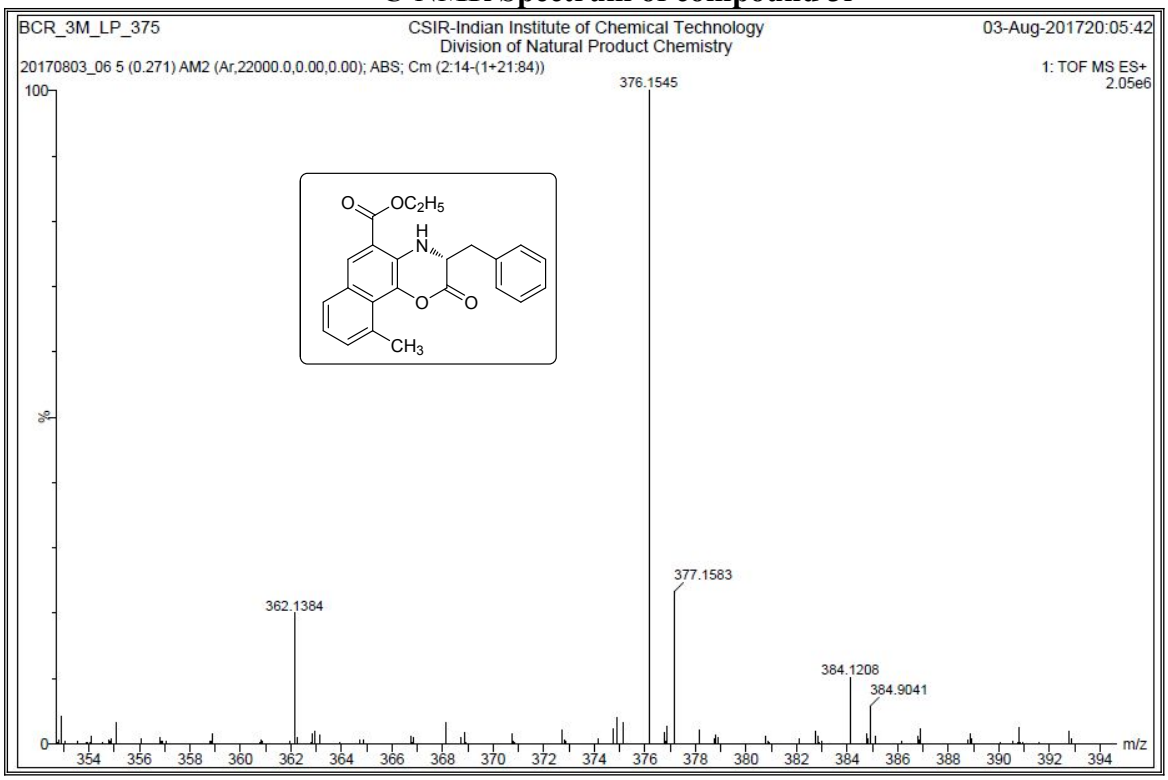
HRMS Spectrum of compound 3k



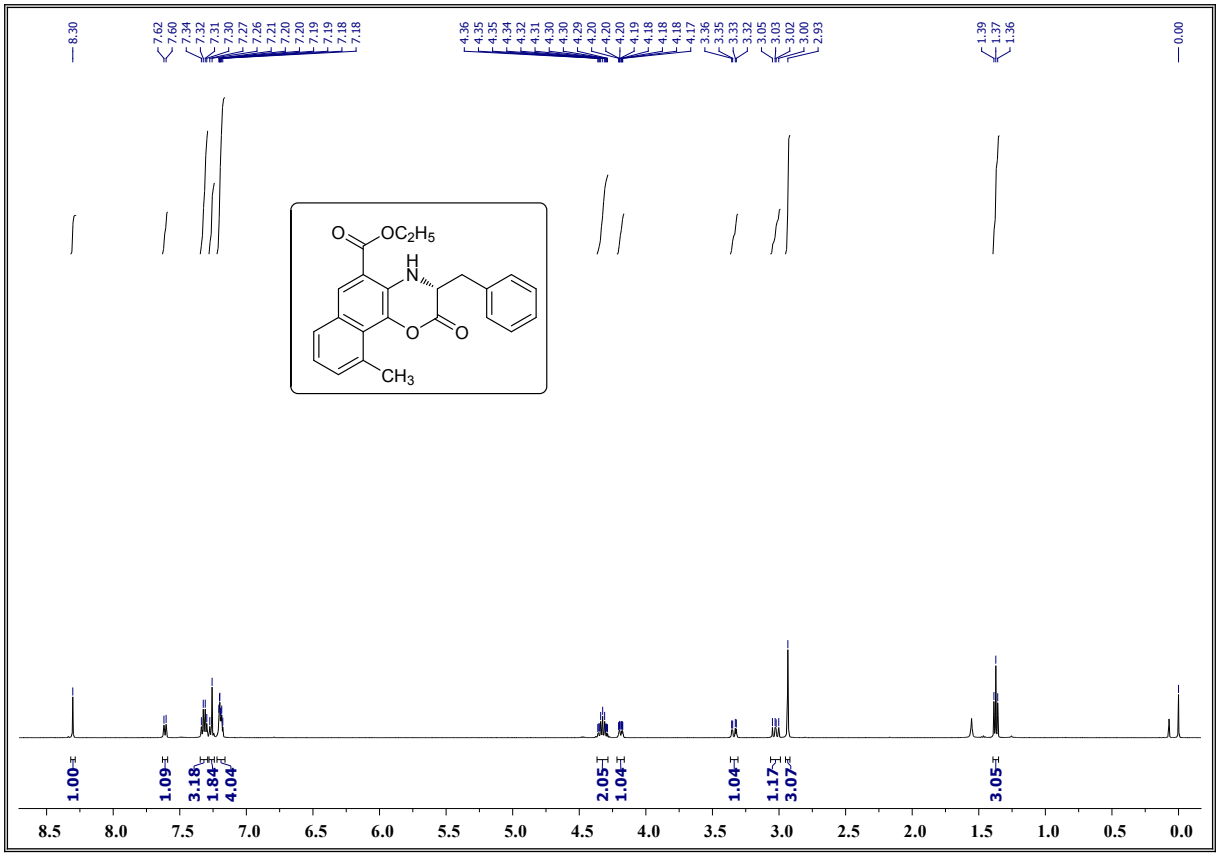
^{1}H-NMR Spectrum of compound 3l



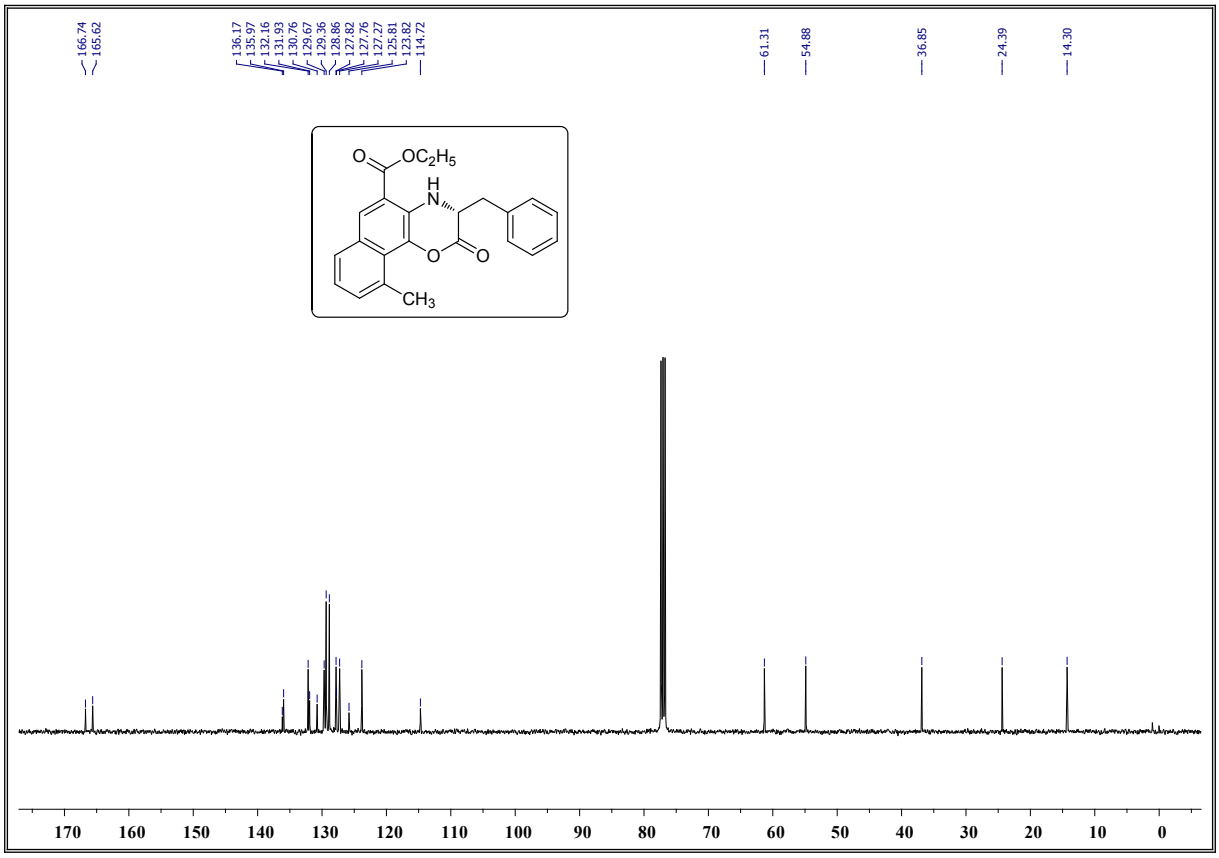
^{13}C-NMR Spectrum of compound 3l



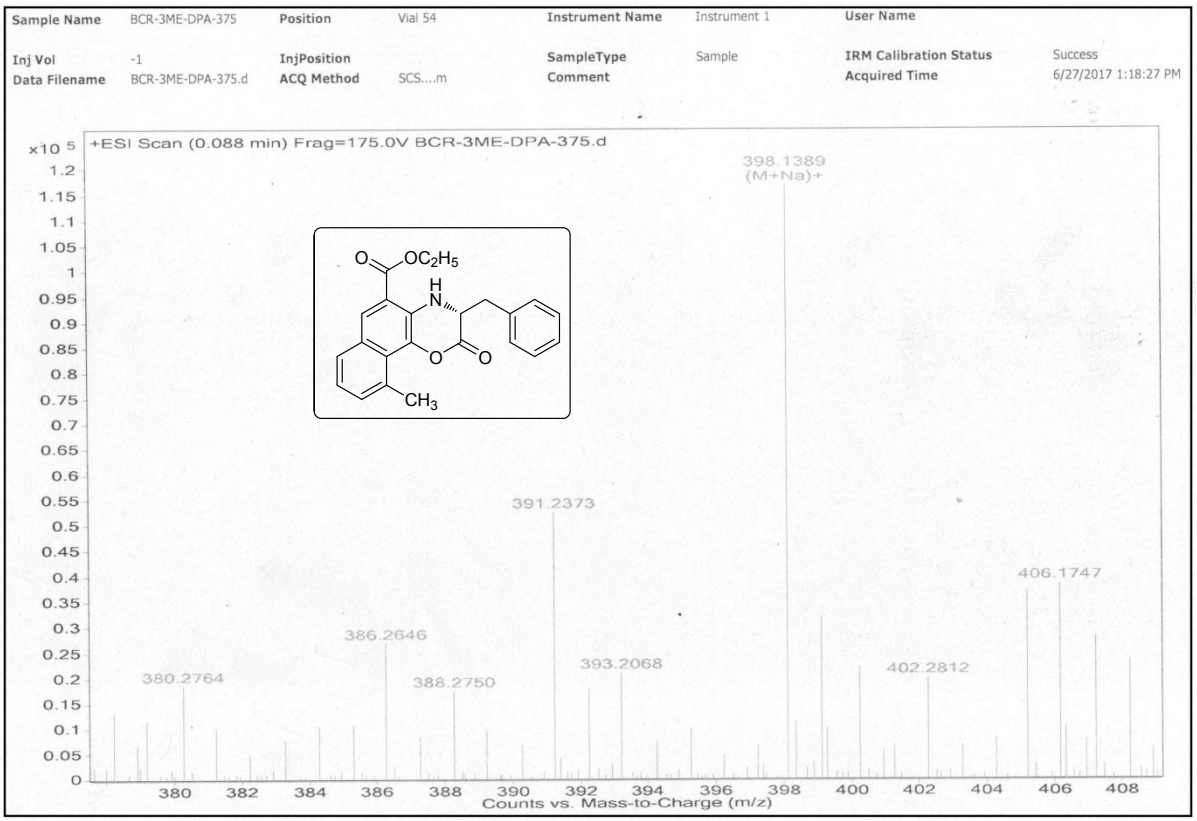
HRMS Spectrum of compound 3l



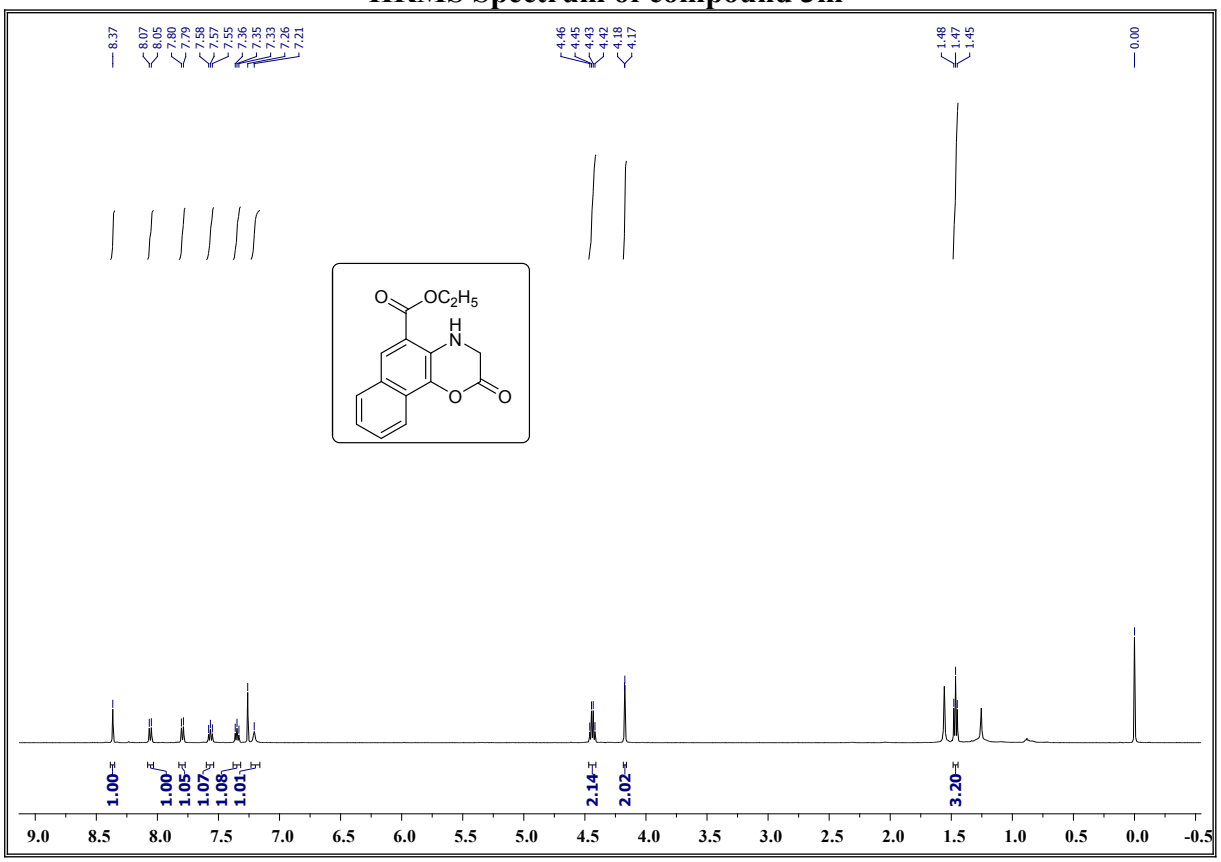
^{1}H-NMR Spectrum of compound 3m



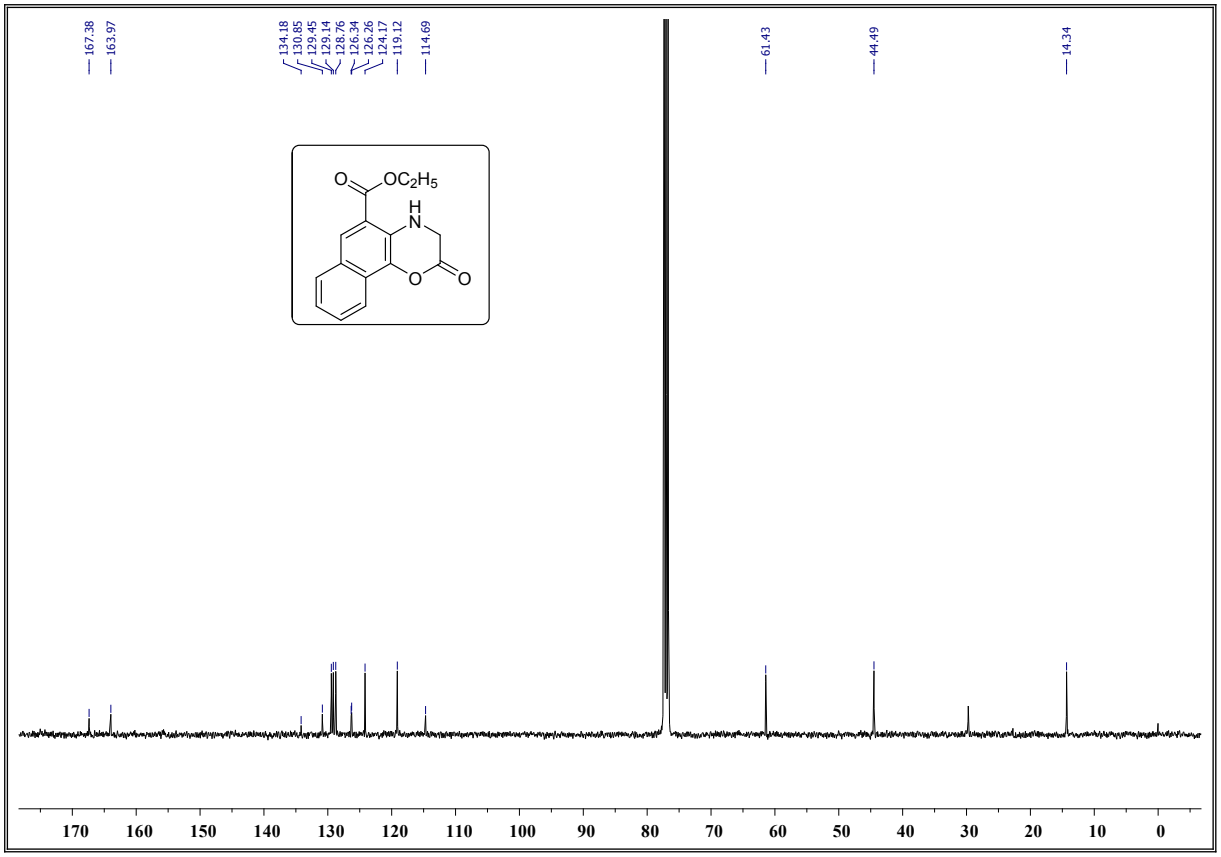
^{13}C-NMR Spectrum of compound 3m



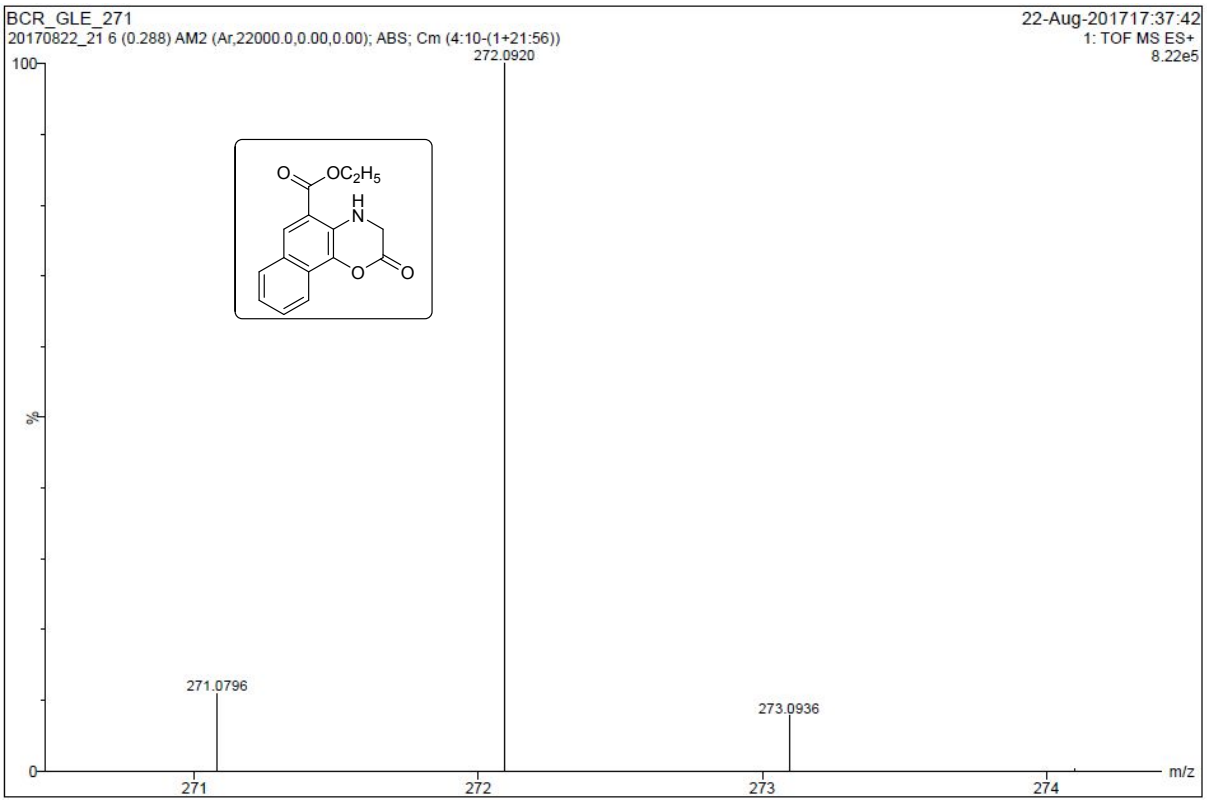
HRMS Spectrum of compound 3m



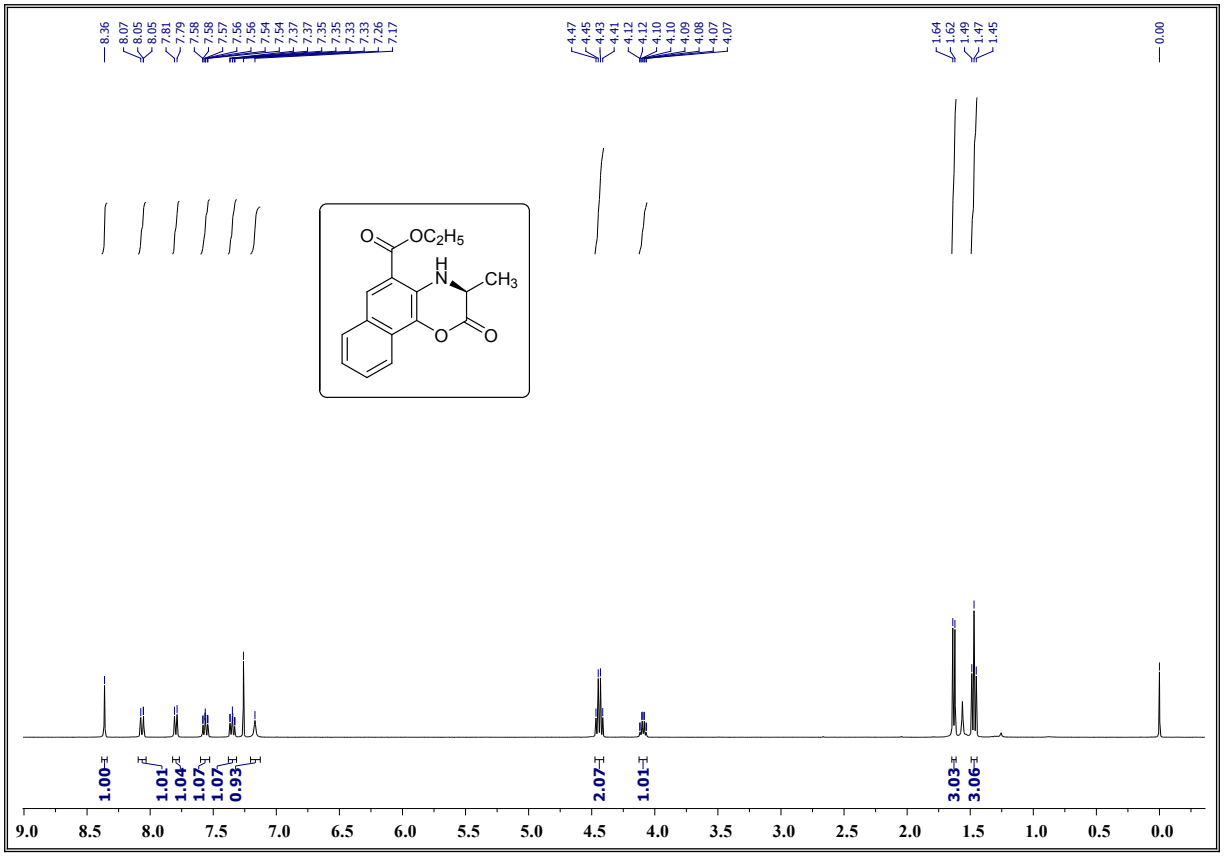
^{1}H-NMR Spectrum of compound 3n



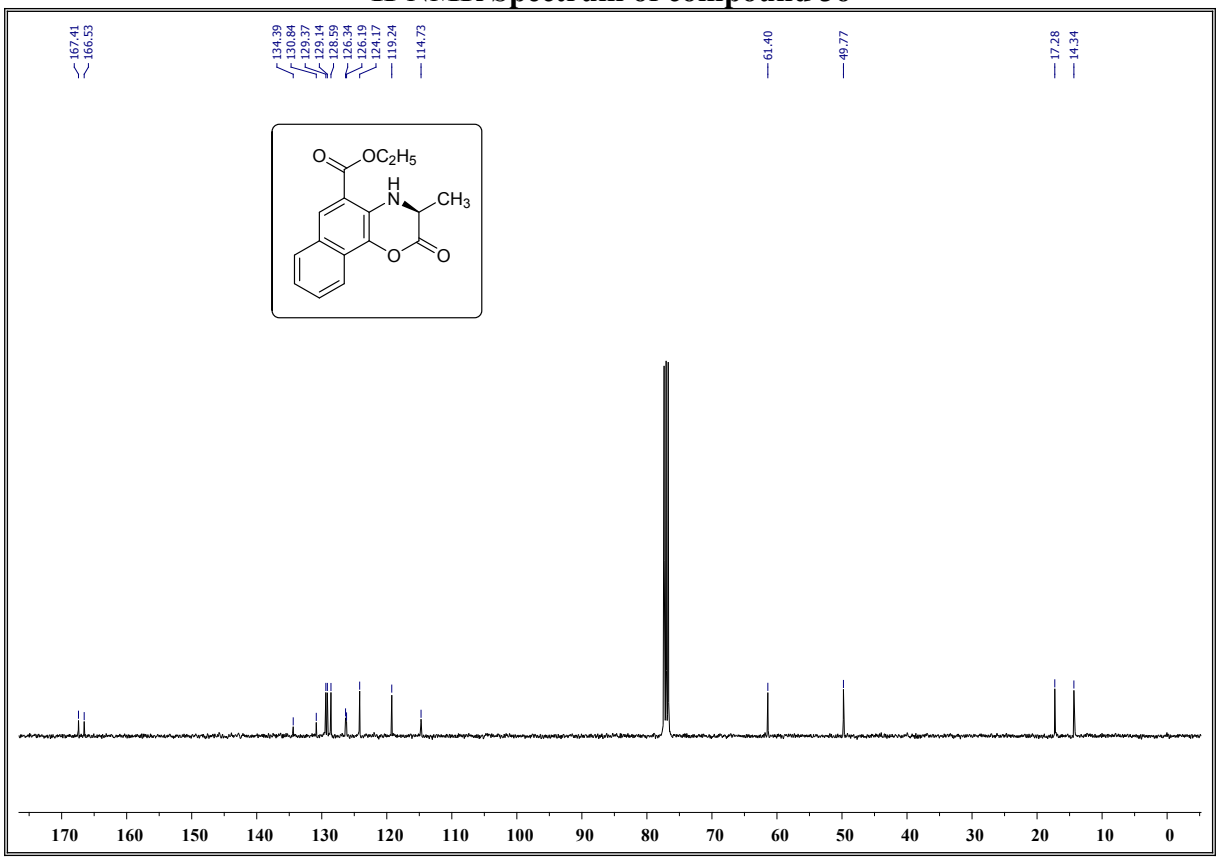
^{13}C-NMR Spectrum of compound 3n



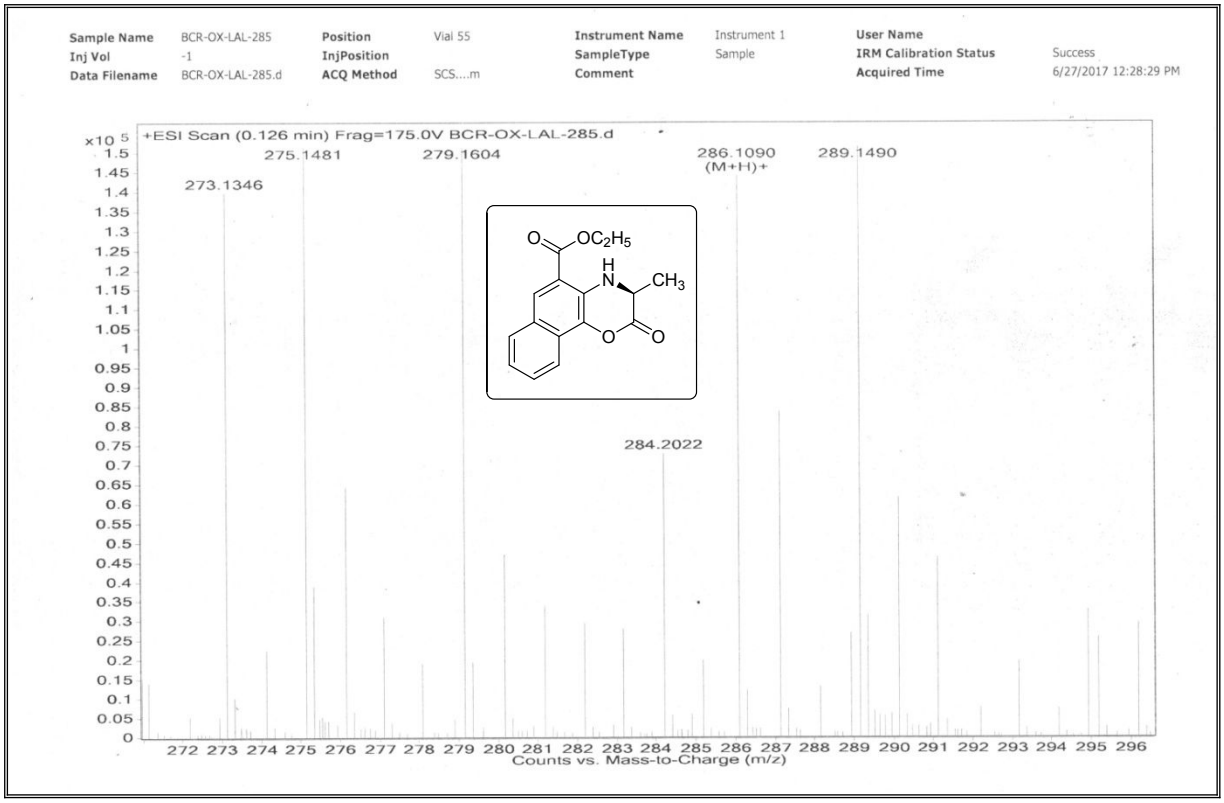
HRMS Spectrum of compound 3n



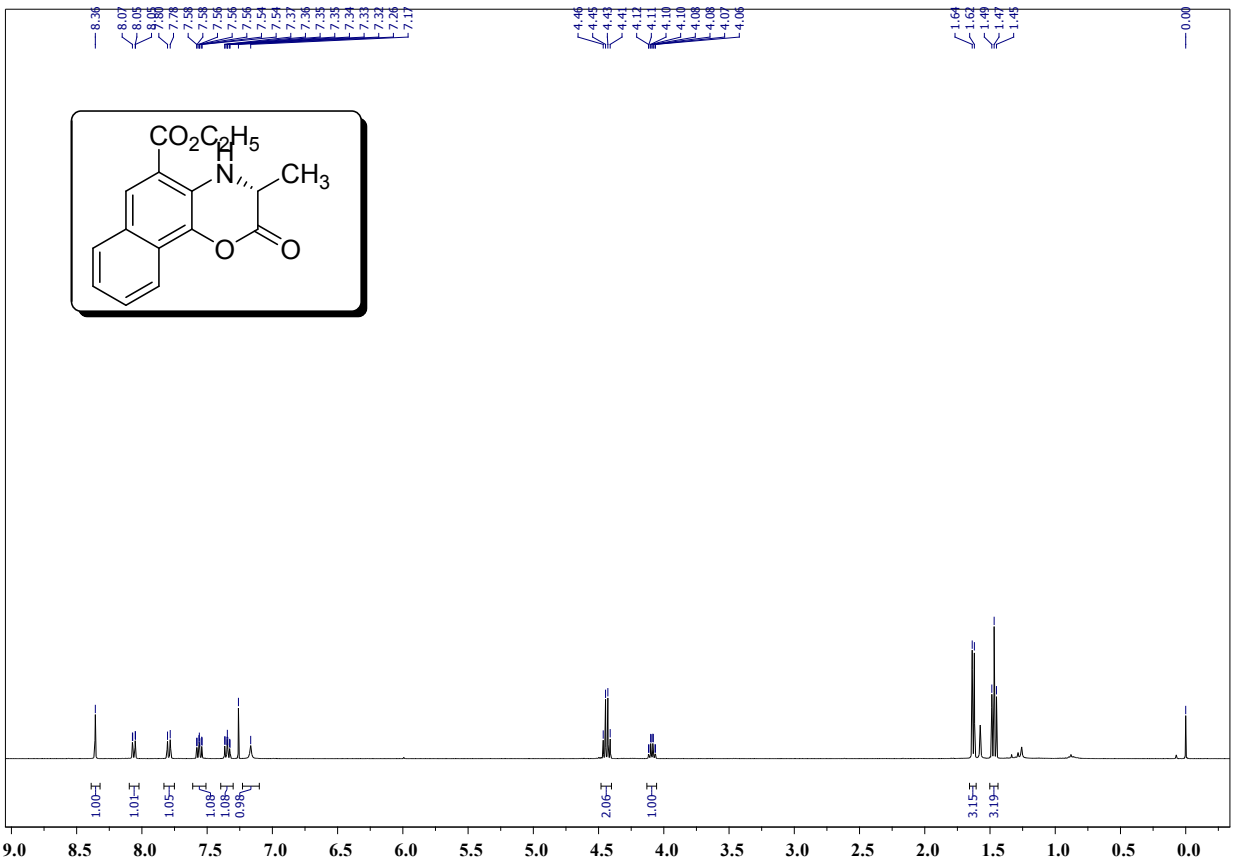
^{1}H-NMR Spectrum of compound 3o



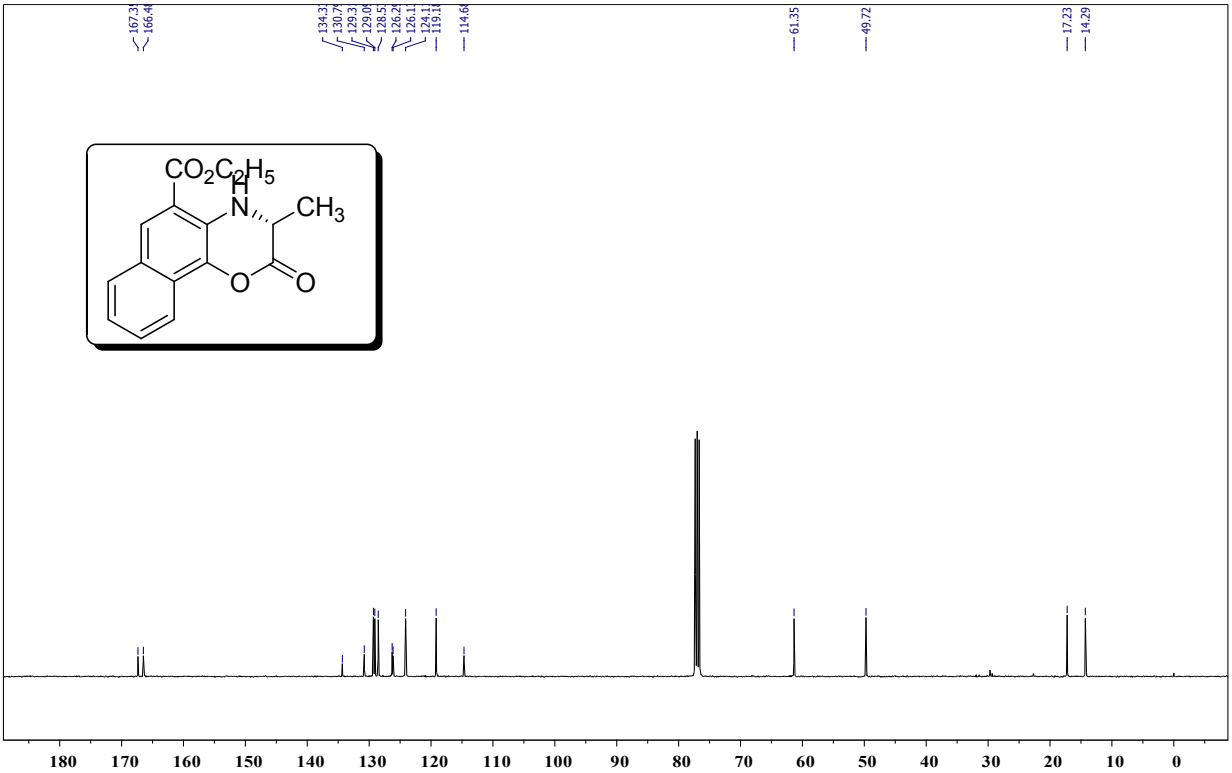
^{13}C-NMR Spectrum of compound 3o



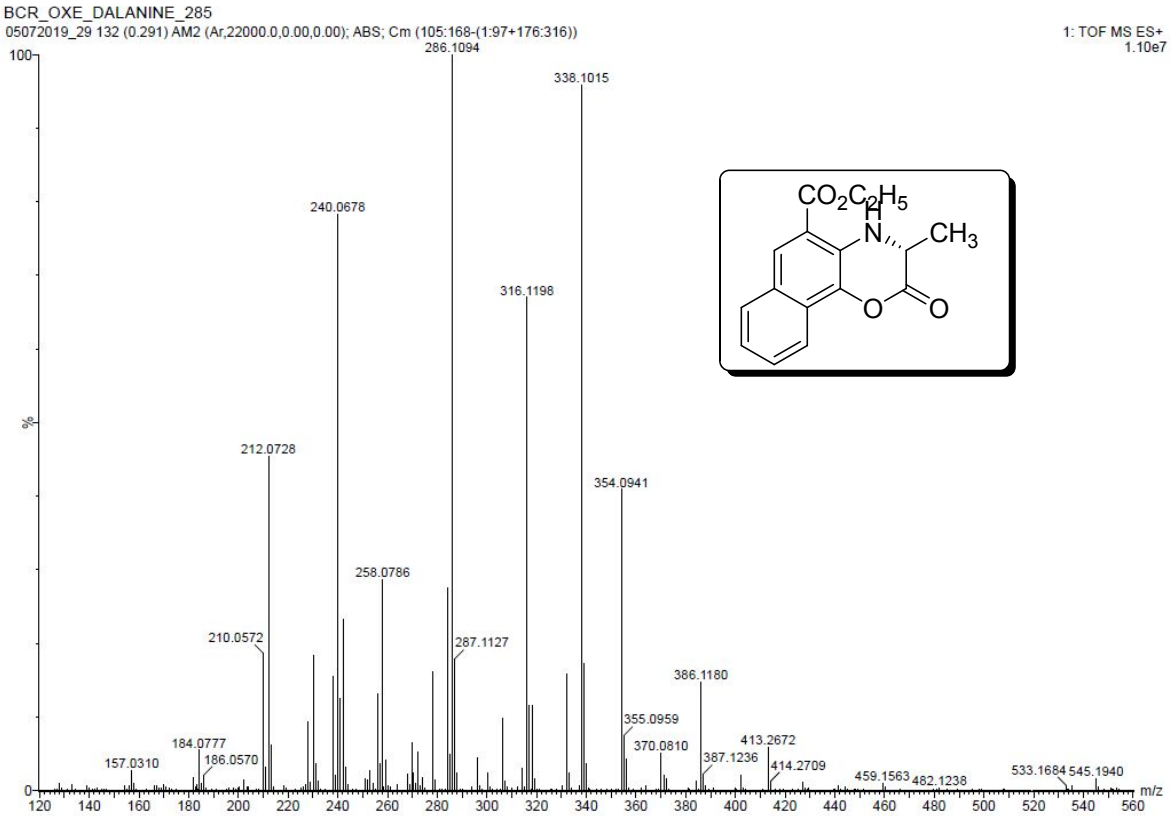
HRMS Spectrum of compound 3o



^{1}H NMR Spectrum of compound 3p



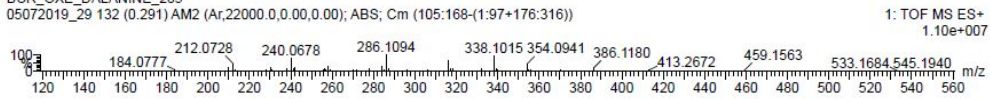
^{13}C NMR Spectrum of compound 3p



Elemental Composition Report **Page 1**

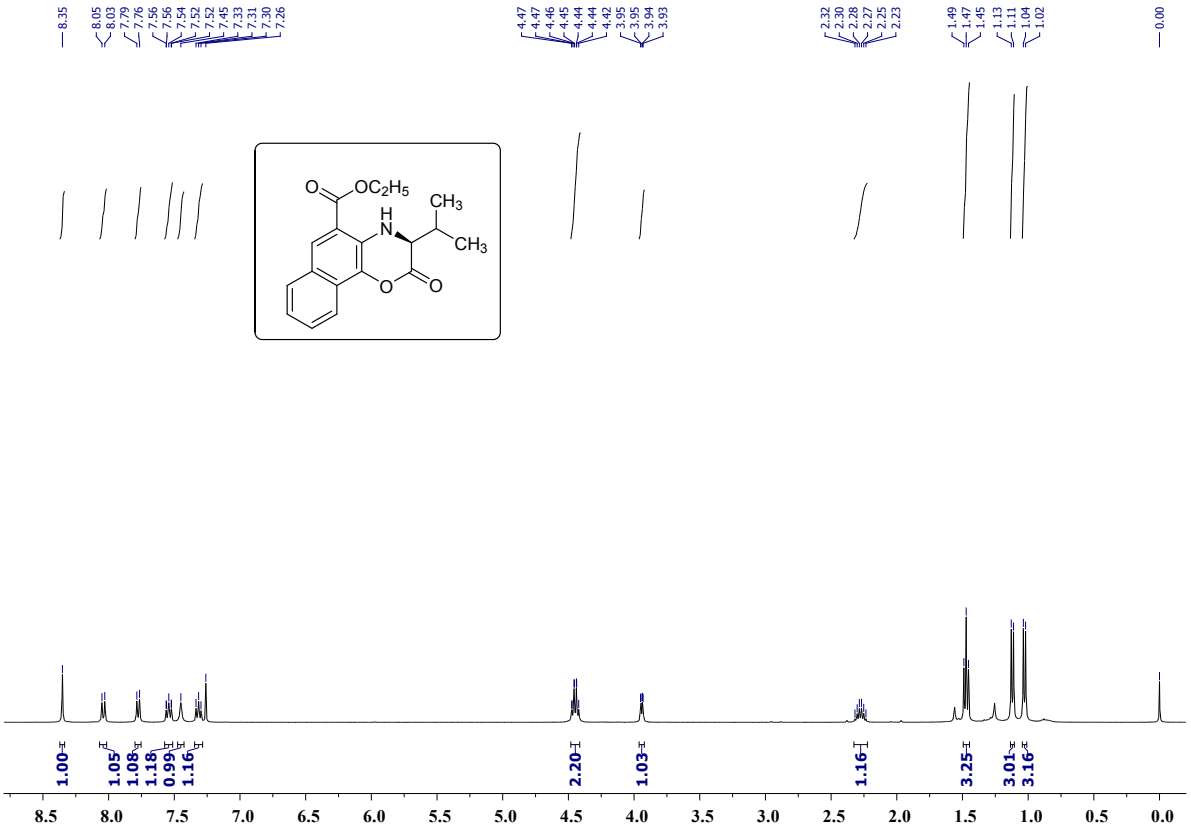
Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: On (Carbon range ± 5) (Set 0 < Cl < 9, 0< Br < 9 and 0 < S < 7 for enhanced filtering)
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
34 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-19 H: 0-22 N: 0-1 O: 0-5 Na: 0-1

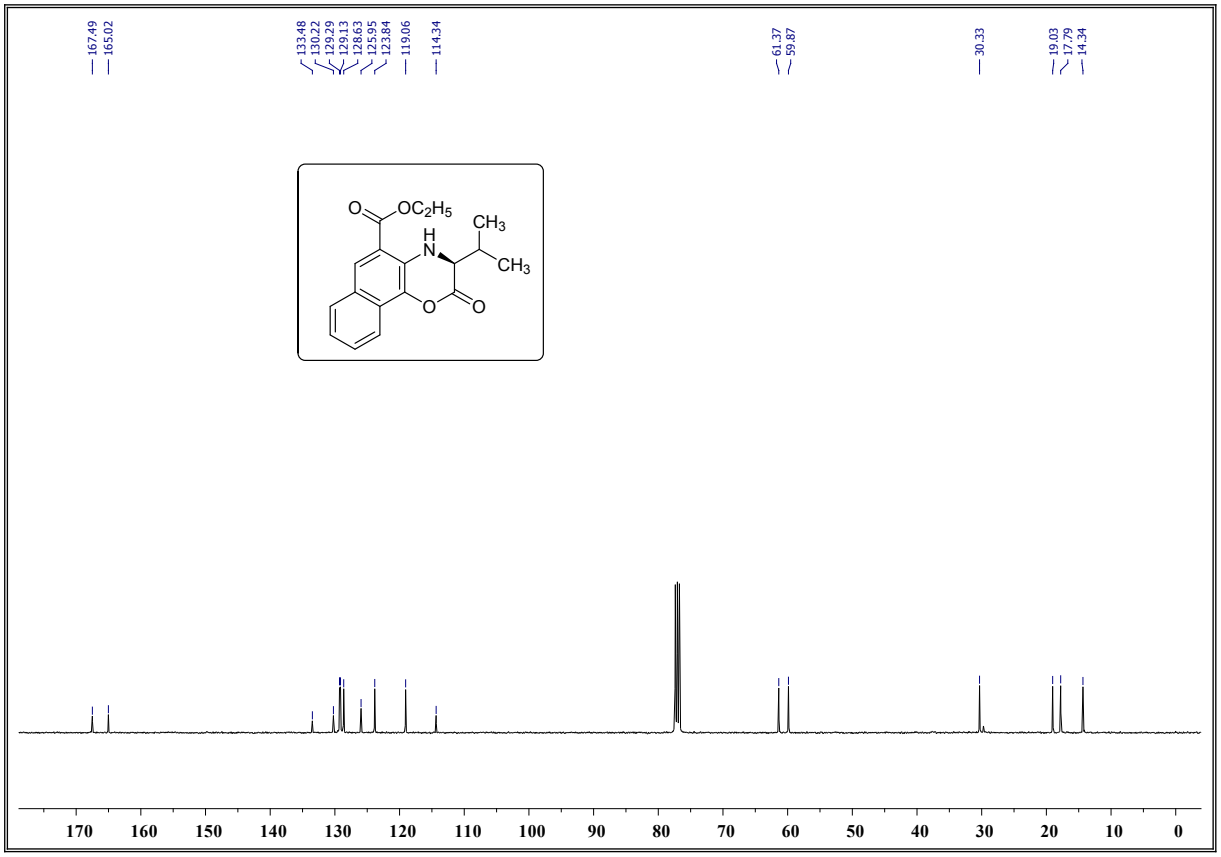


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
286.1094	286.1079	1.5	5.2	9.5	659.8	n/a	n/a	C16 H16 N O4

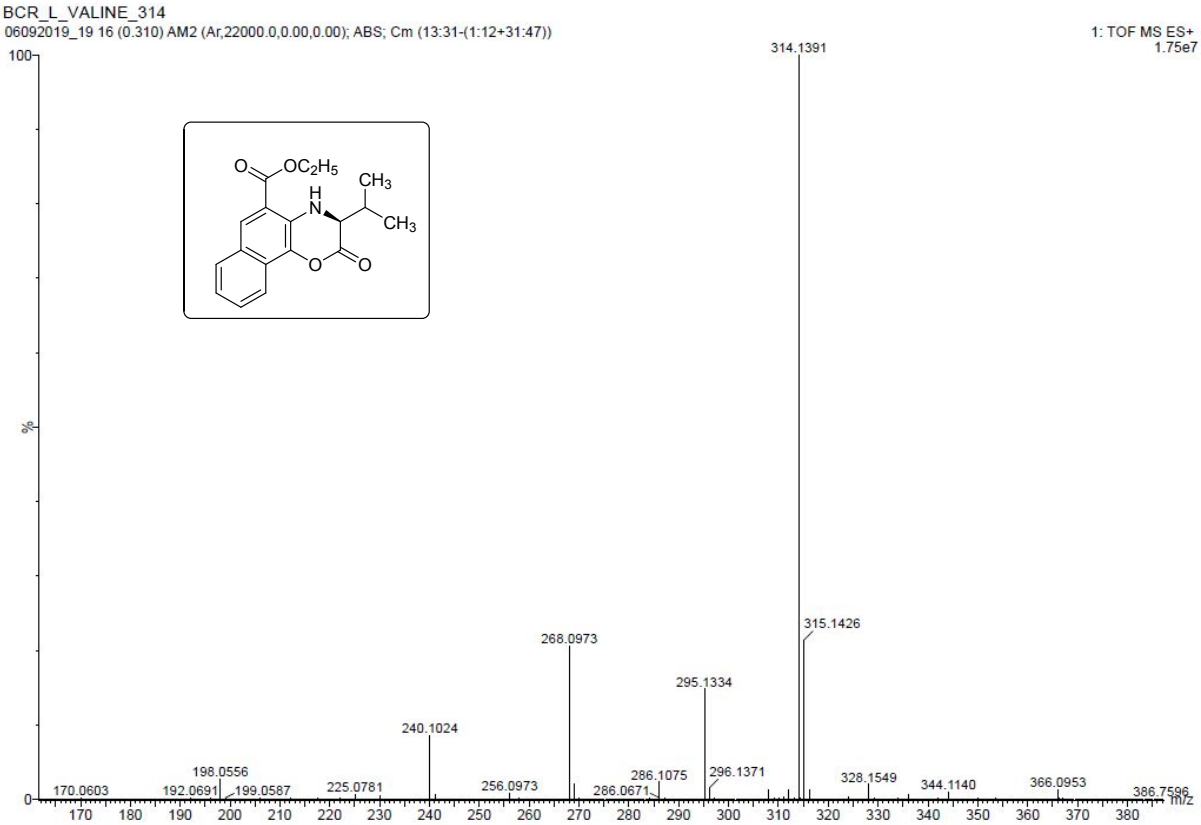
HRMS Spectrum of compound **3p**



^{1}H-NMR Spectrum of compound 3q

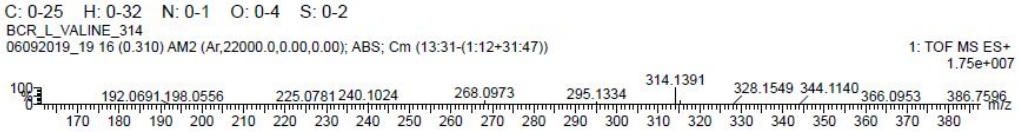


^{13}C-NMR Spectrum of compound 3q



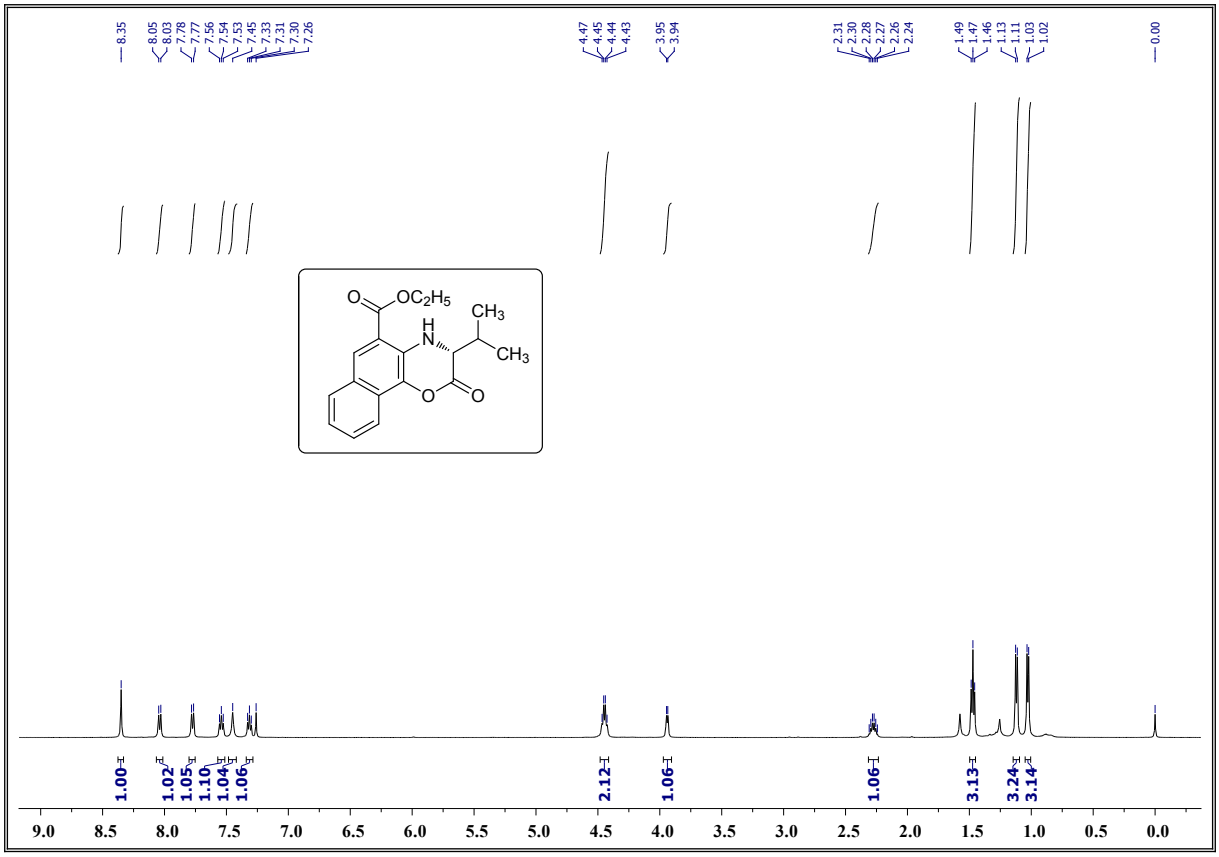
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
84 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-25 H: 0-32 N: 0-1 O: 0-4 S: 0-2

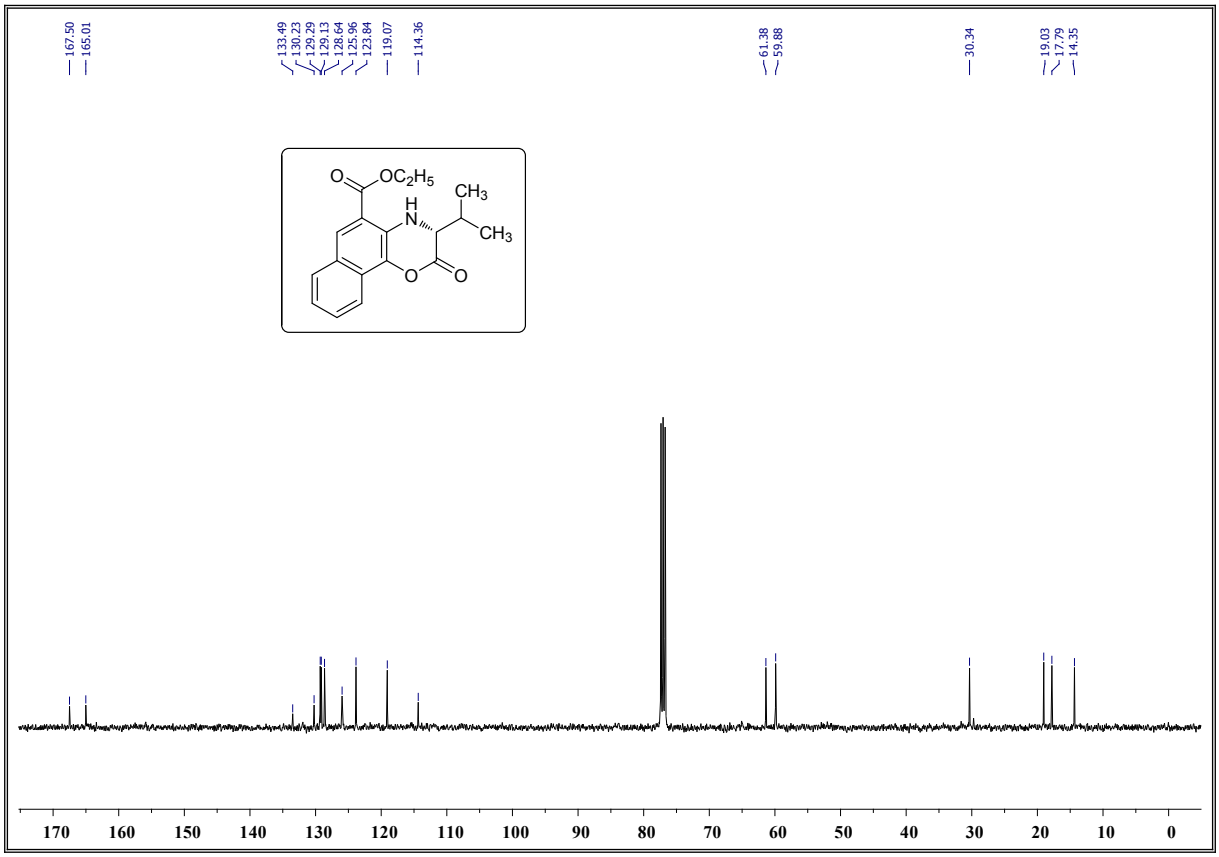


Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
314.1391	314.1392	-0.1	-0.3	9.5	741.9	n/a	n/a	C18 H20 N O4

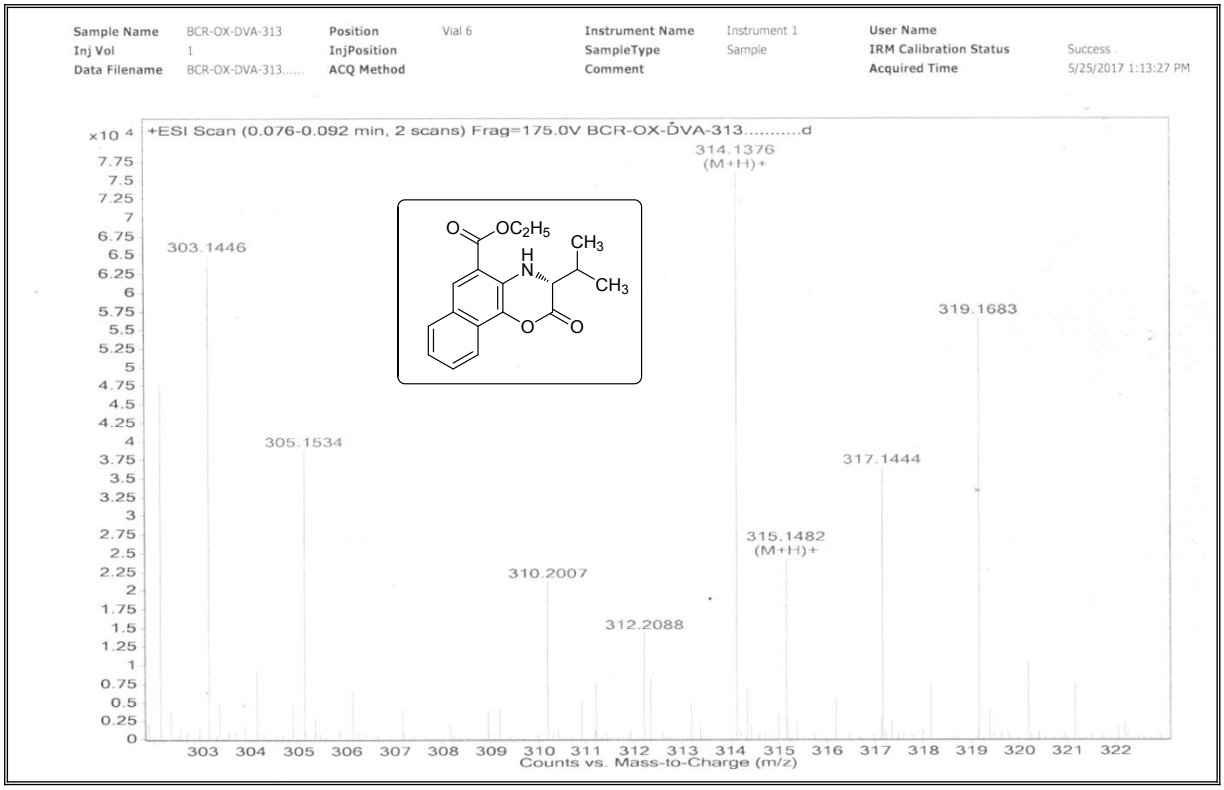
HRMS Spectrum of compound 3q



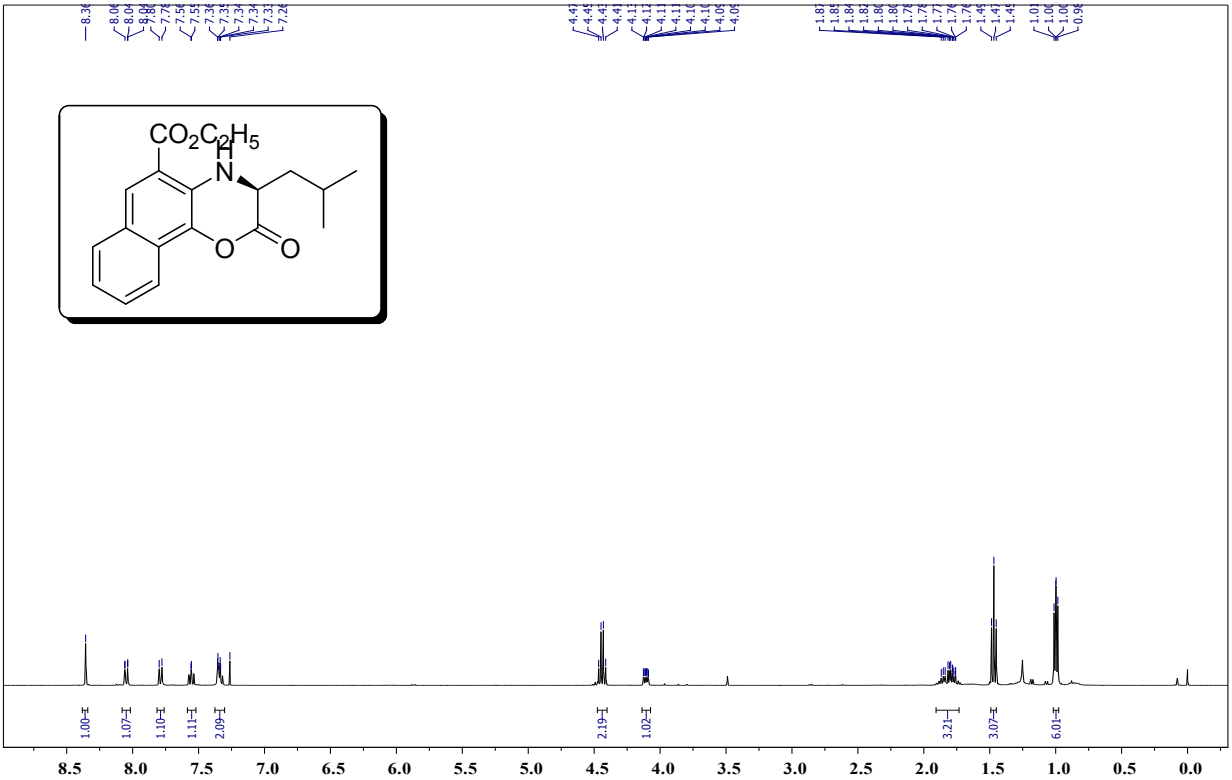
^{1}H-NMR Spectrum of compound 3r



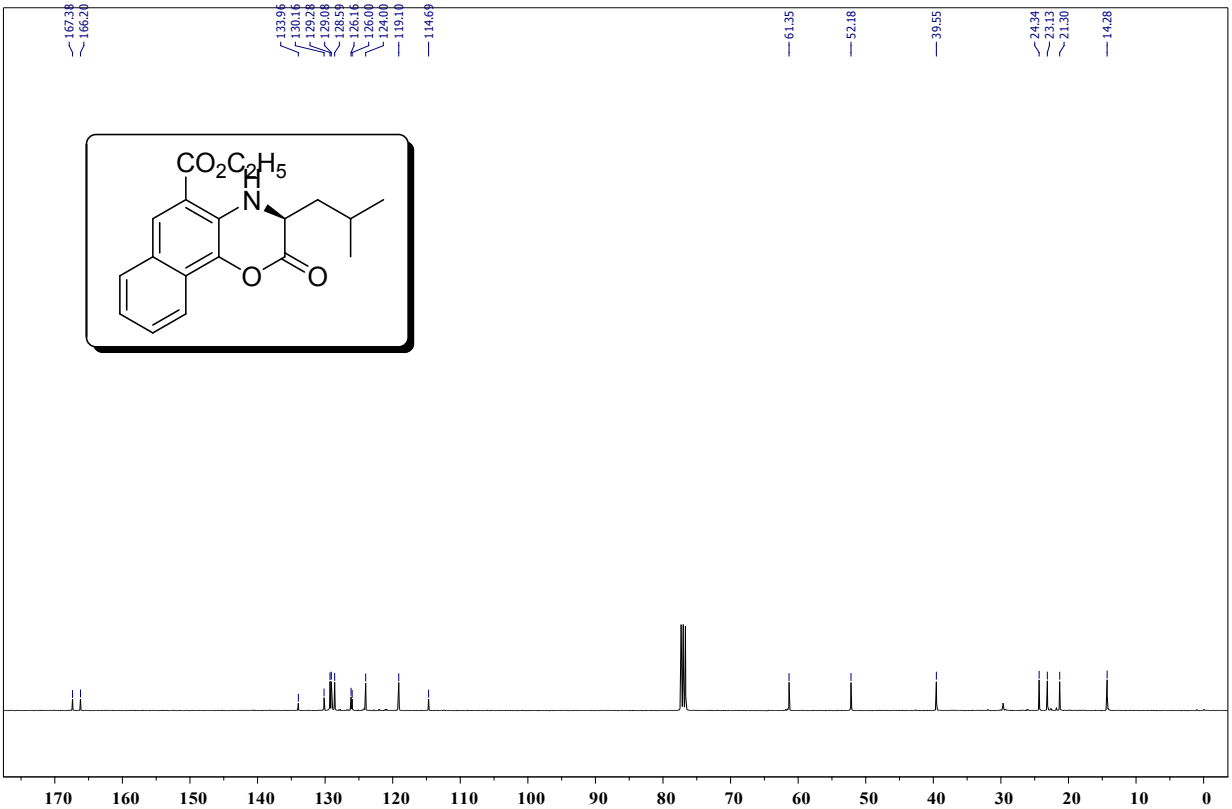
^{13}C-NMR Spectrum of compound 3r



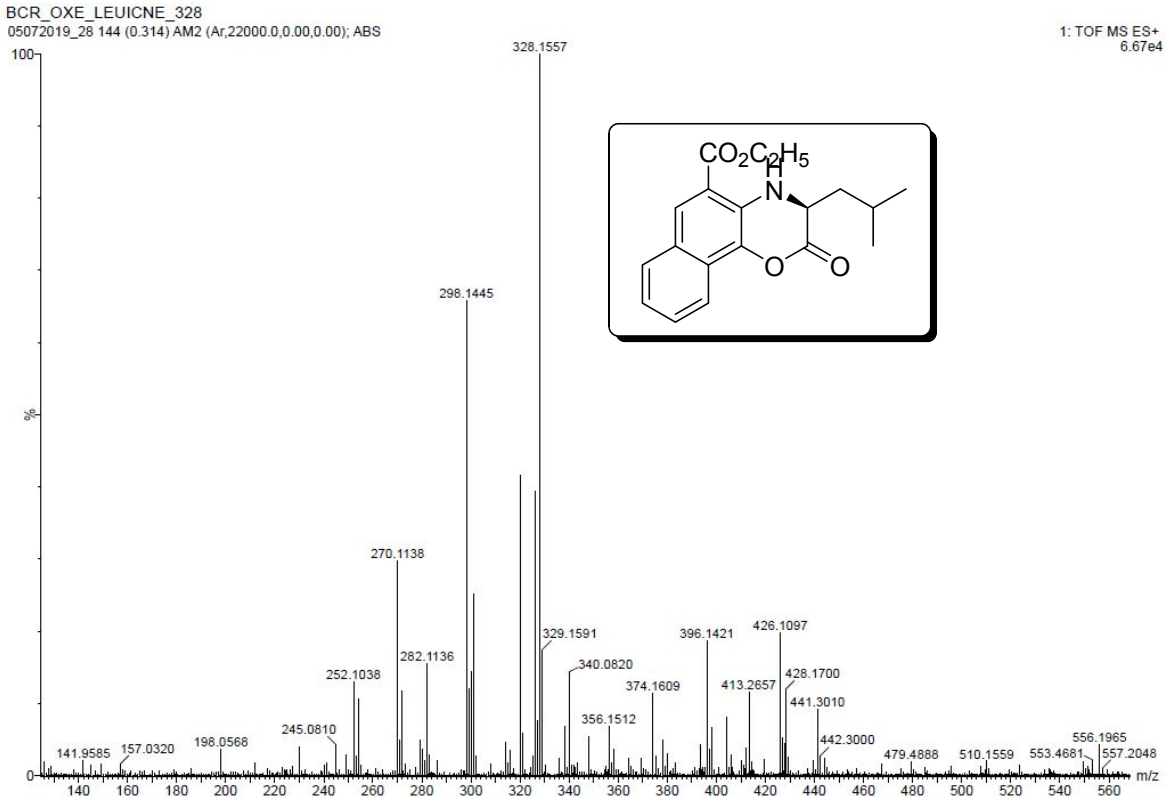
HRMS Spectrum of compound 3r



^{1}H NMR Spectrum of compound 3s



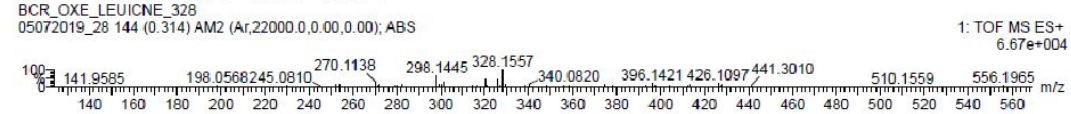
^{13}C NMR Spectrum of compound 3s



Elemental Composition Report **Page 1**

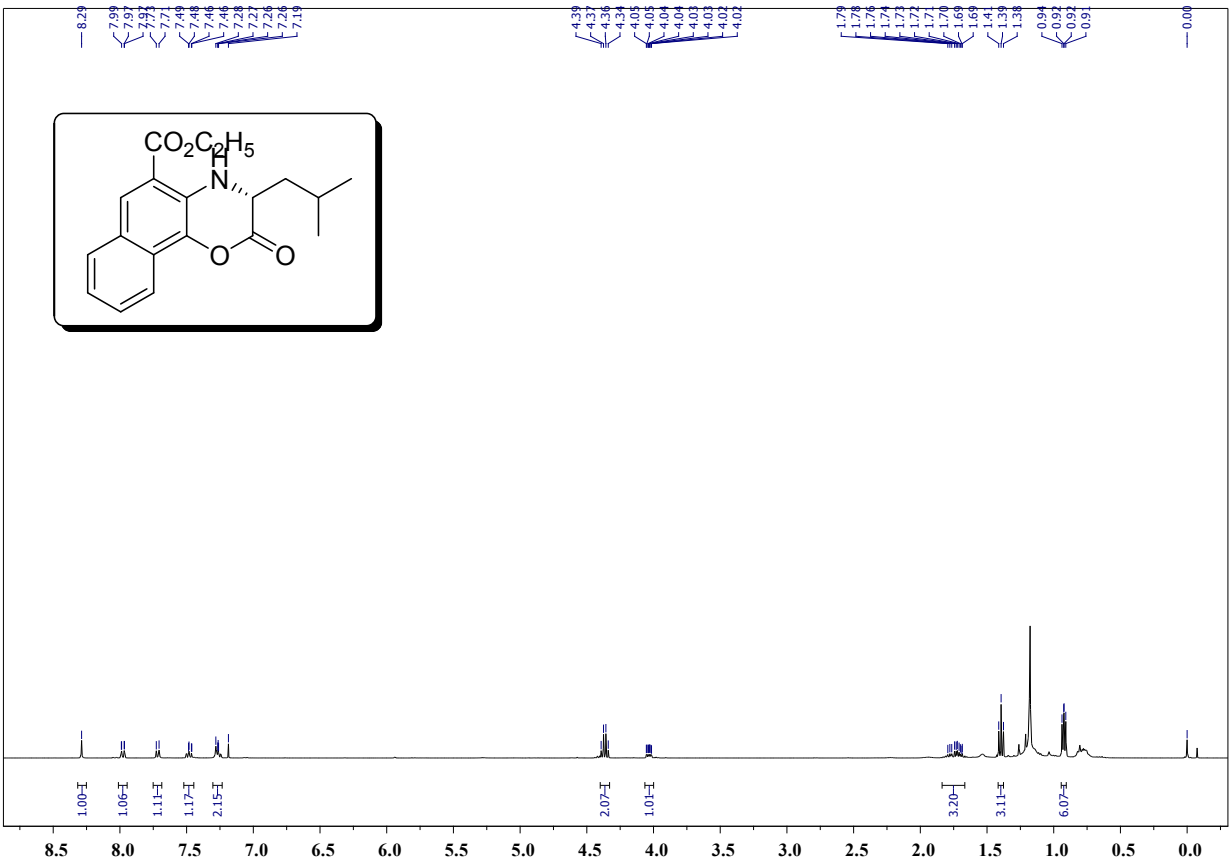
Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: On (Carbon range ± 5) (Set 0 < Cl < 9, 0< Br < 9 and 0 < S < 7 for enhanced filtering)
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
22 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-19 H: 0-22 N: 0-1 O: 0-5 Na: 0-1

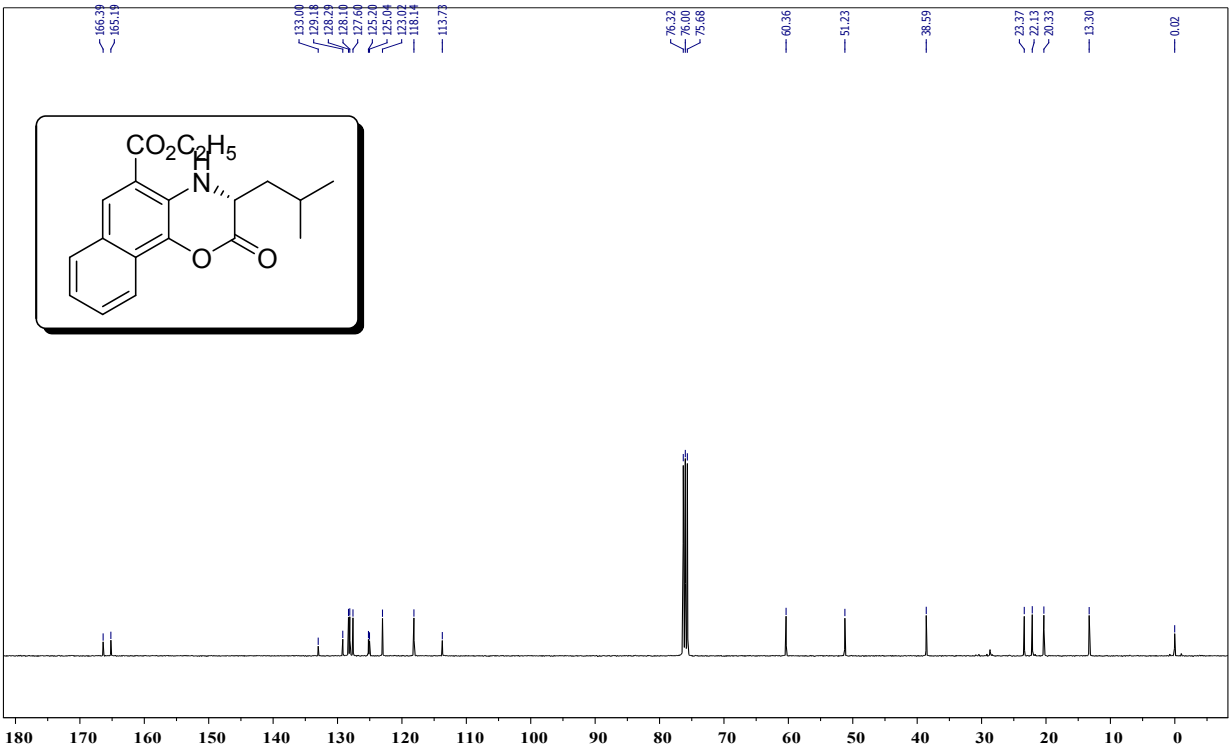


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
328.1557	328.1549	0.8	2.4	9.5	249.0	n/a	n/a	C19 H22 N O4

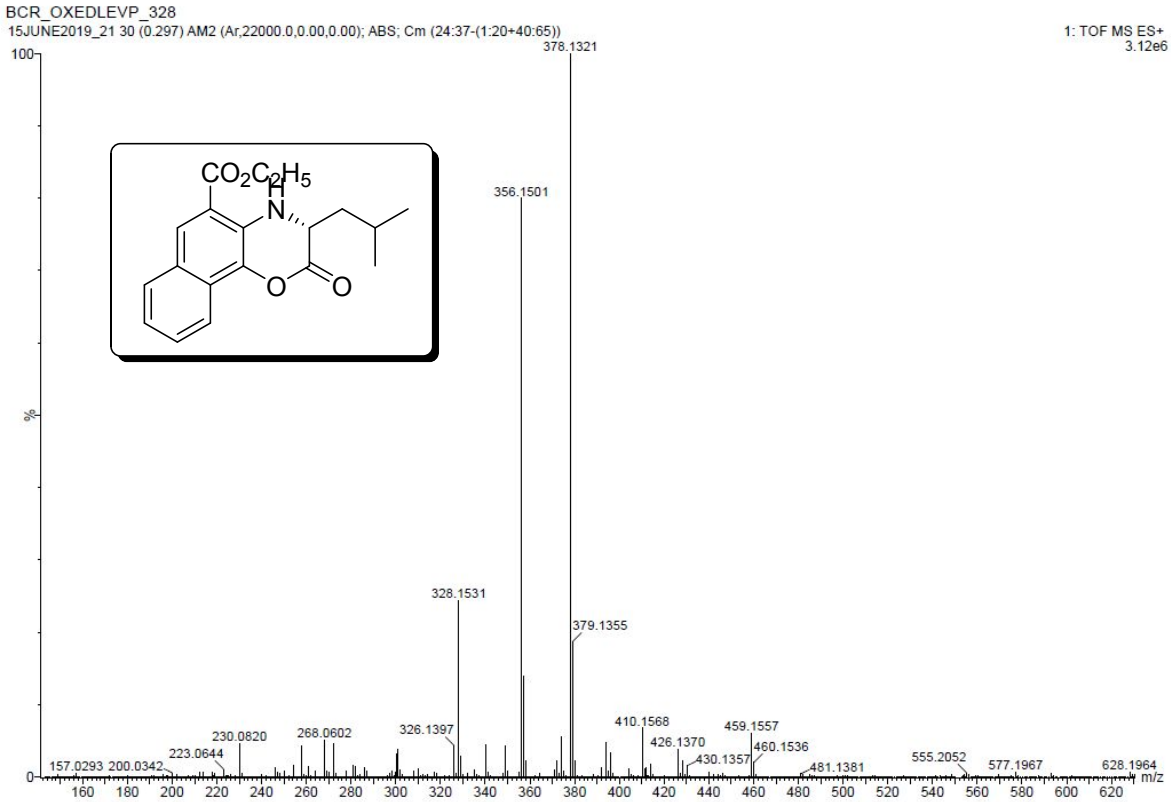
HRMS Spectrum of compound 3s



^{1}H NMR Spectrum of compound 3t



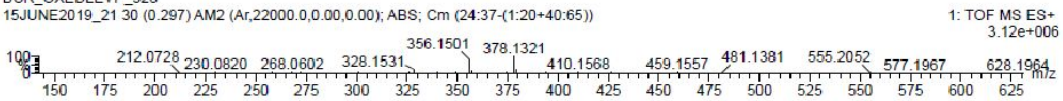
^{13}C NMR Spectrum of compound 3t



Elemental Composition Report **Page 1**

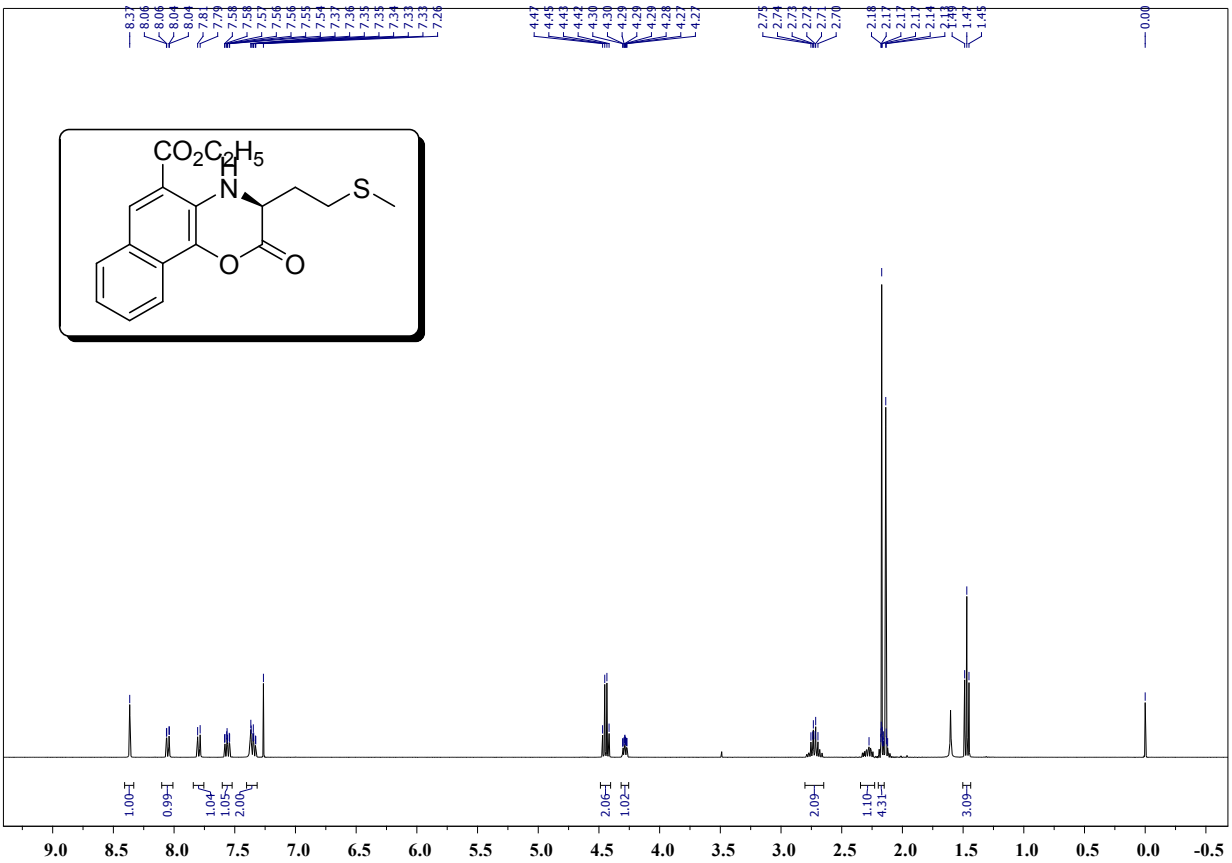
Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
11 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-19 H: 0-25 N: 0-1 O: 0-5

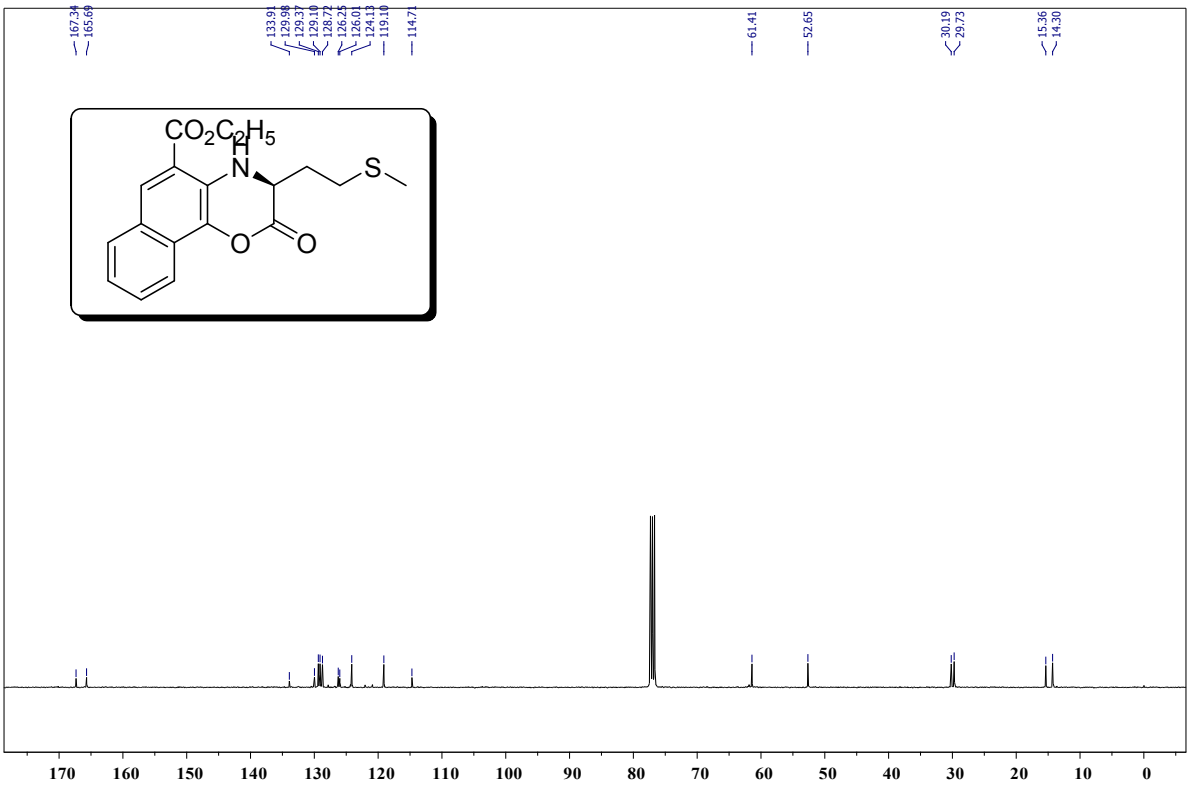


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
328.1531	328.1549	-1.8	-5.5	9.5	306.5	n/a	n/a	C19 H22 N O4

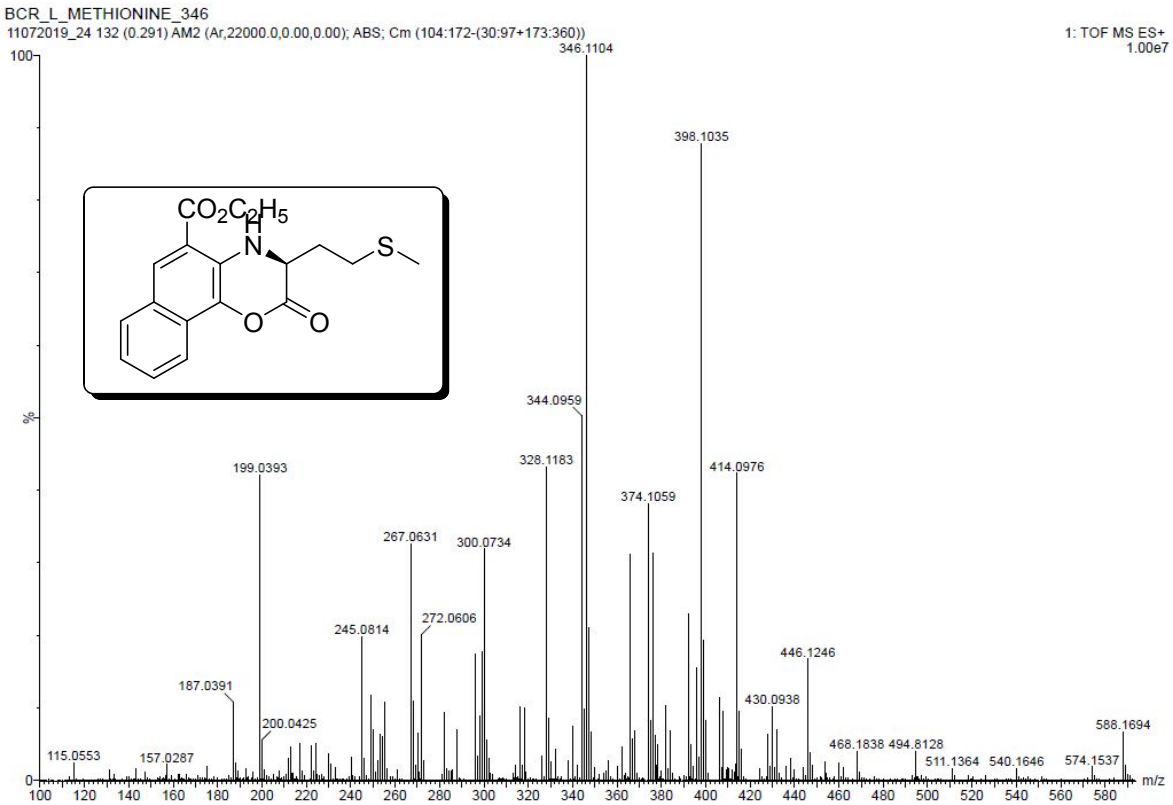
HRMS Spectrum of compound 3t



^{1}H NMR Spectrum of compound 3u



^{13}C NMR Spectrum of compound 3u



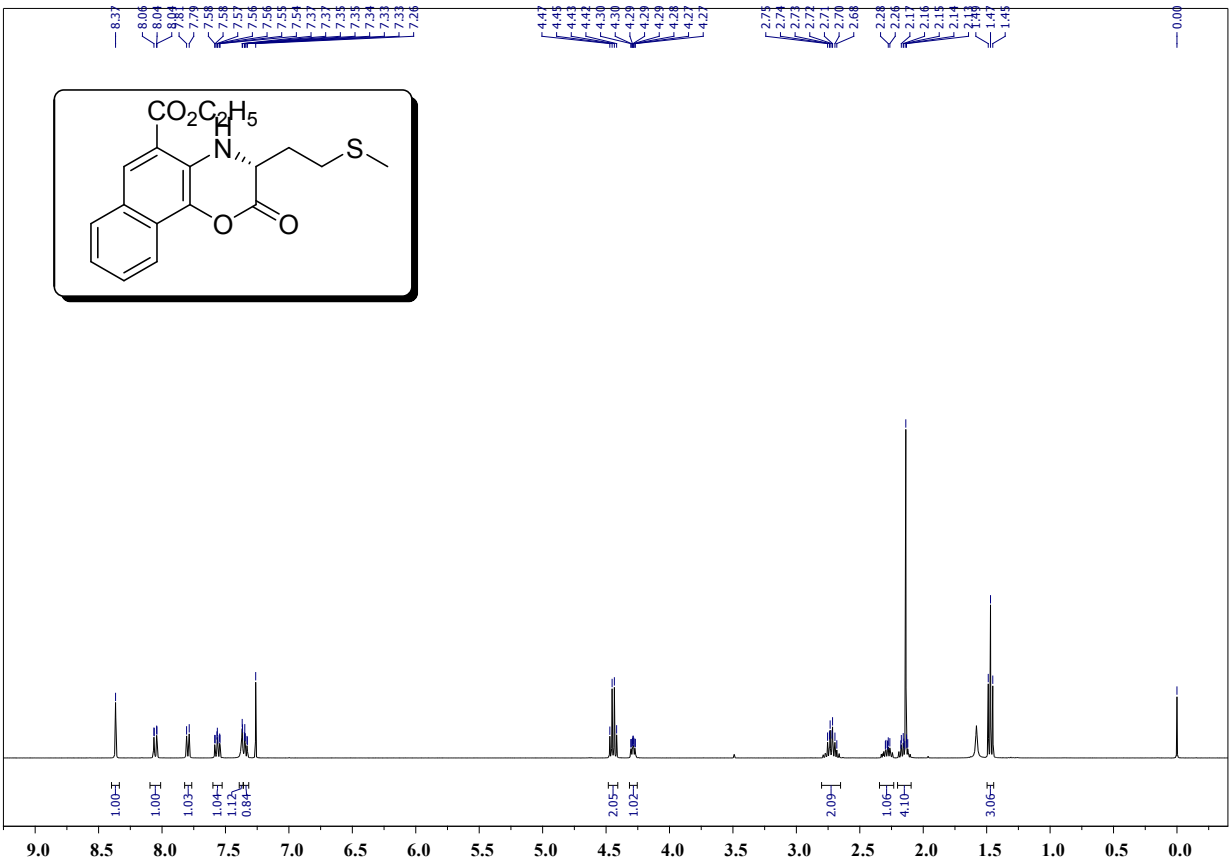
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

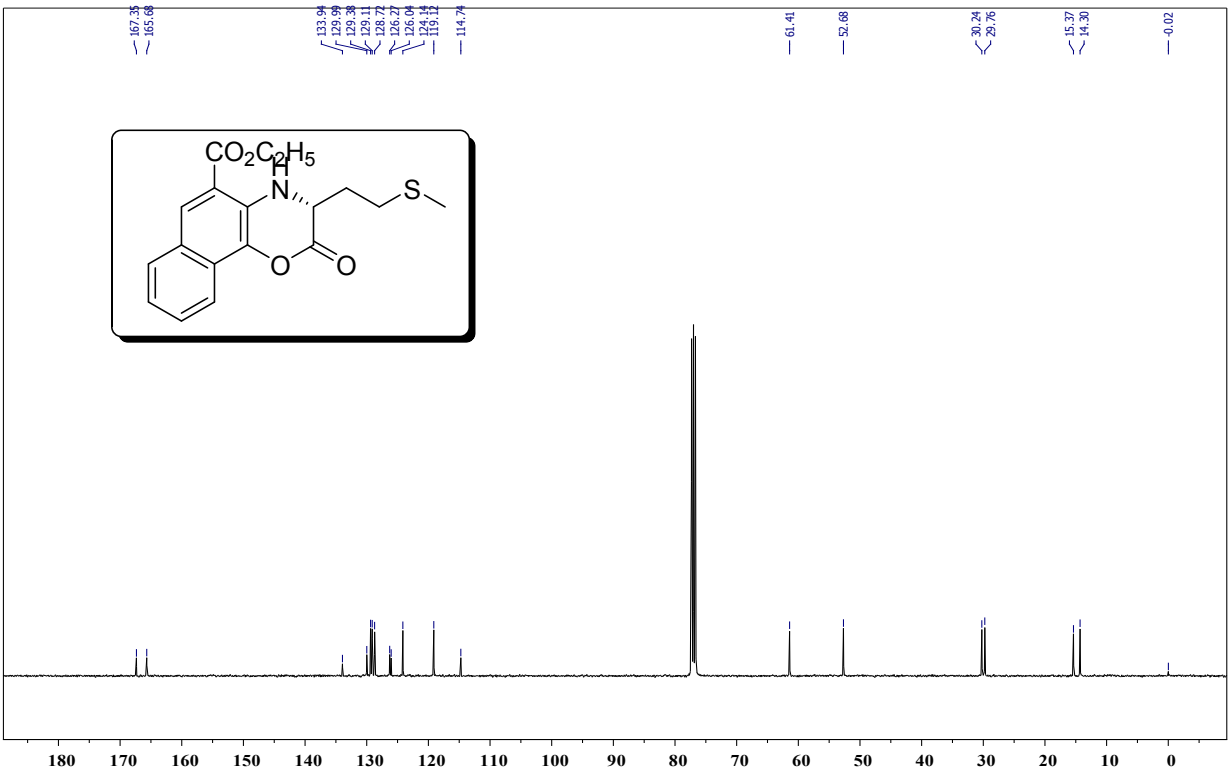
Monoisotopic Mass, Even Electron Ions
36 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-18 H: 0-20 N: 0-1 O: 0-5 S: 0-2

Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
346.1104	346.1113	-0.9	-2.6	9.5	598.9	n/a	n/a	C18 H20 N O4 S

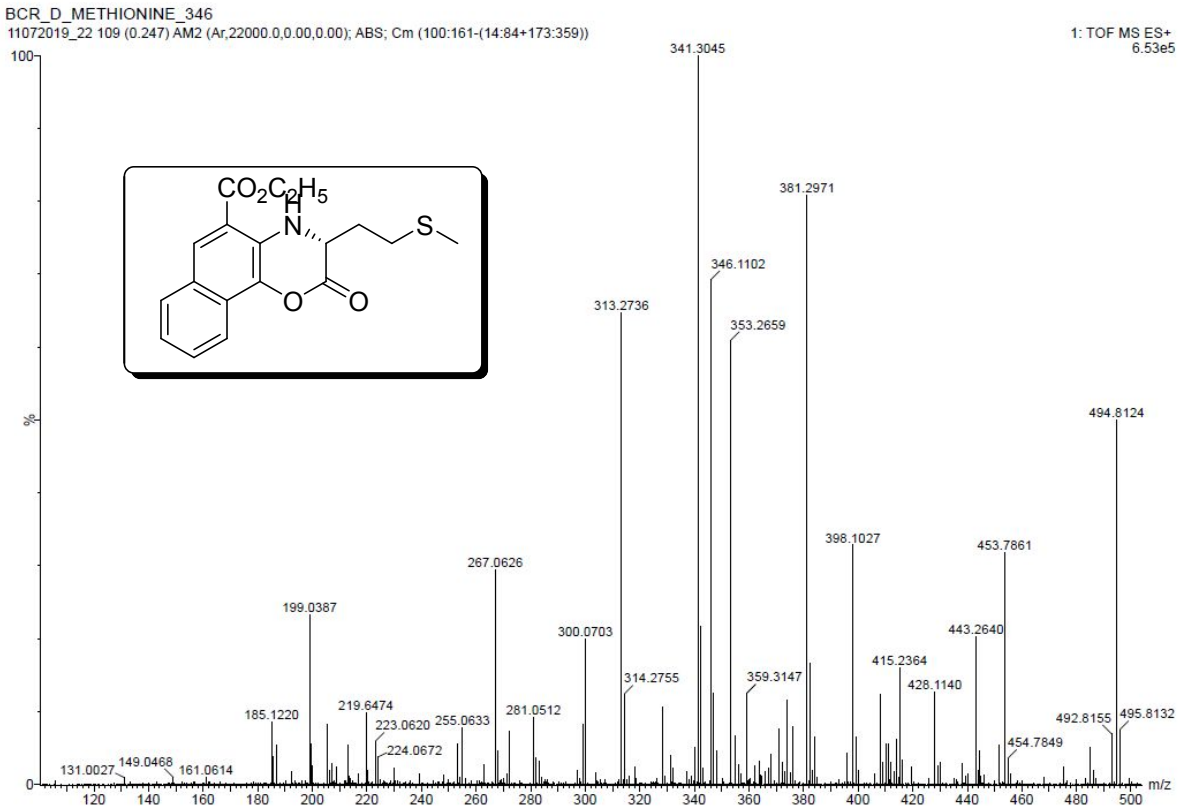
HRMS Spectrum of compound 3u



^{1}H NMR Spectrum of compound 3v



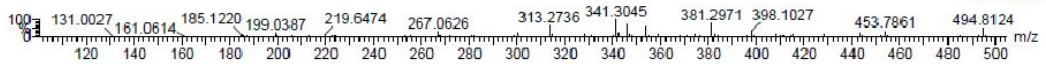
^{13}C NMR Spectrum of compound 3v



Elemental Composition Report **Page 1**

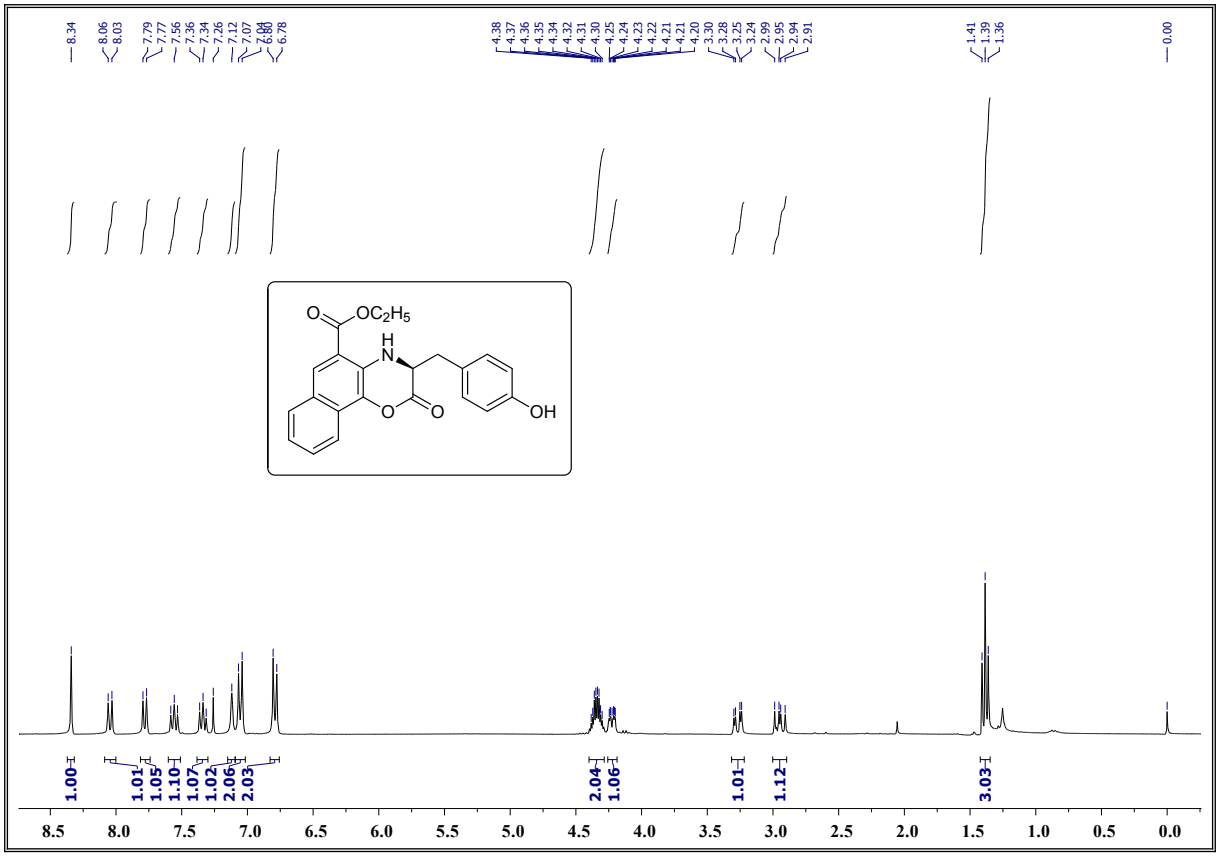
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
29 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-18 H: 0-20 N: 0-1 O: 0-4 S: 0-2
BCR_D_METHIONINE_346
11072019_22 109 (0.247) AM2 (Ar,22000.0,0.00,0.00); ABS; Cm (100:161-(14:84+173:359))
1: TOF MS ES+
6.53e+005

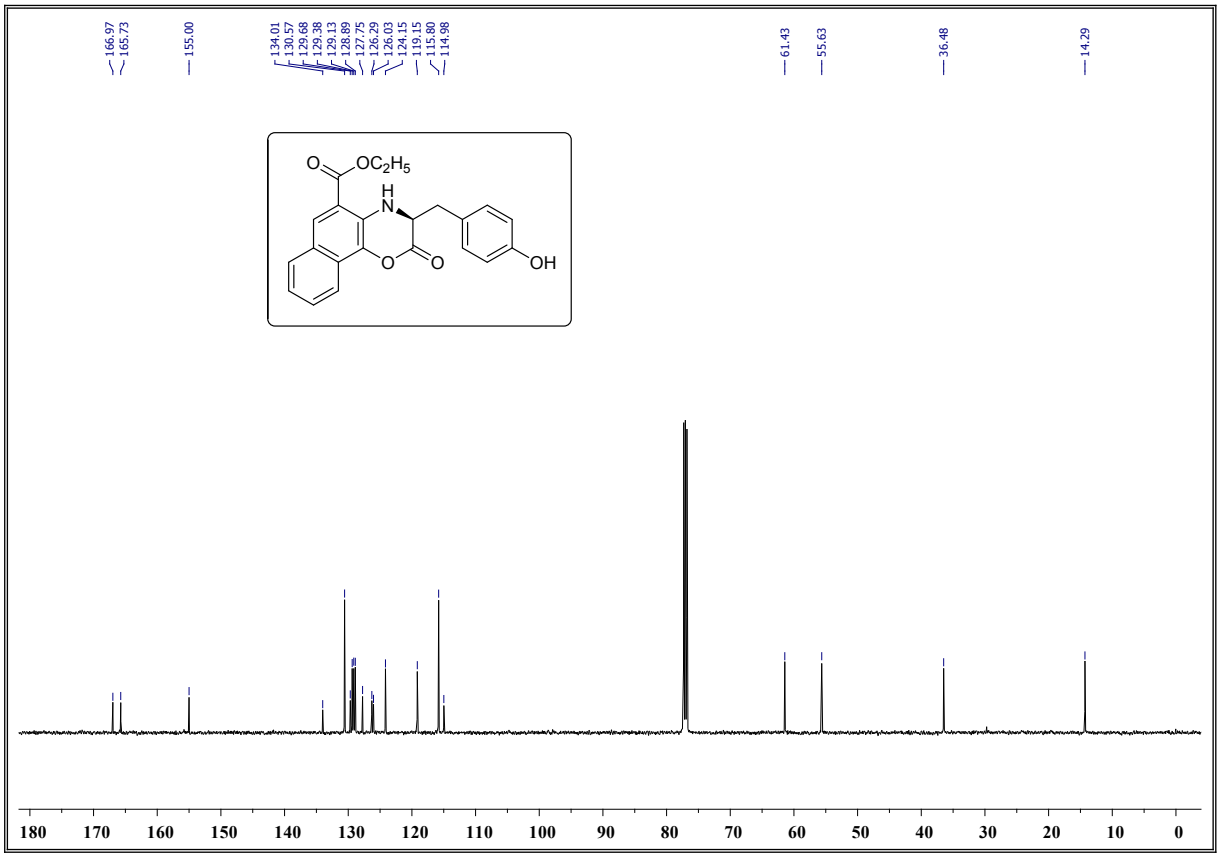


Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
346.1102	346.1113	-1.1	-3.2	9.5	376.6	n/a	n/a	C18 H20 N O4 S

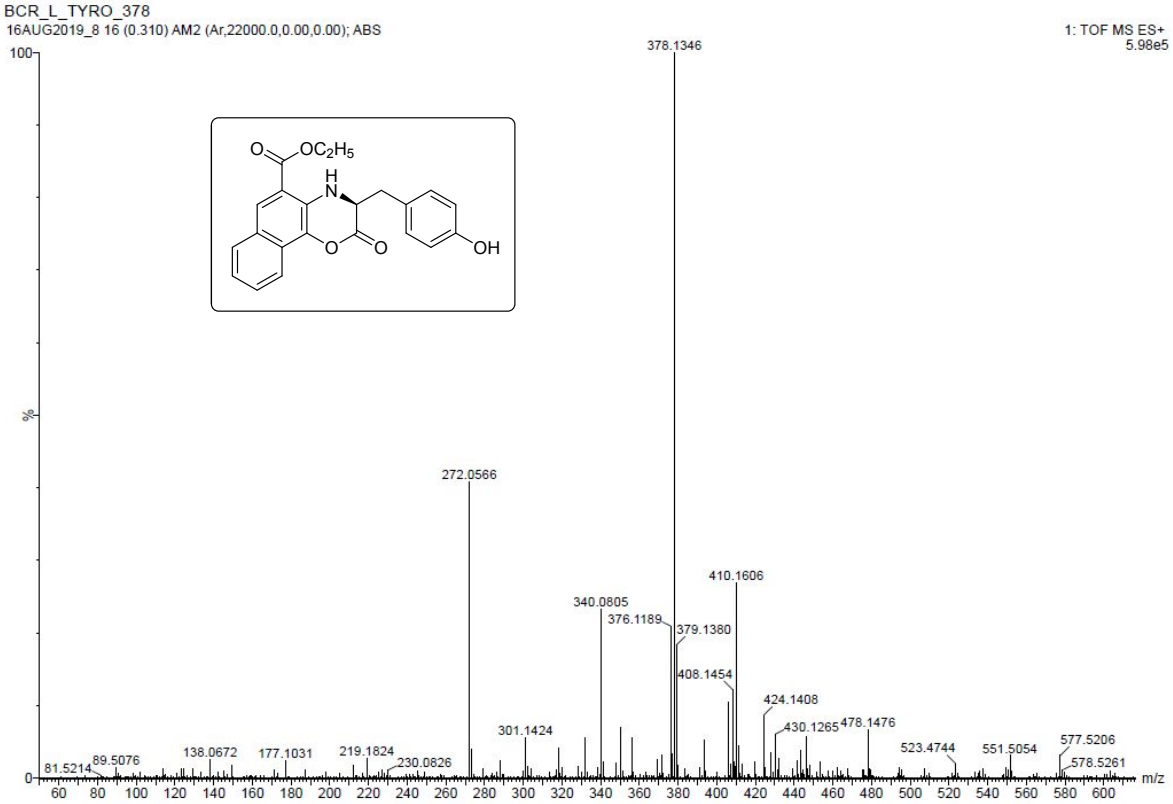
HRMS Spectrum of compound 3v



^{1}H-NMR Spectrum of compound 3x



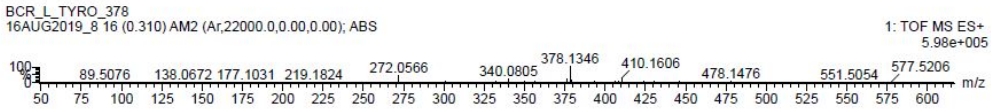
^{13}C-NMR Spectrum of compound 3x



Elemental Composition Report **Page 1**

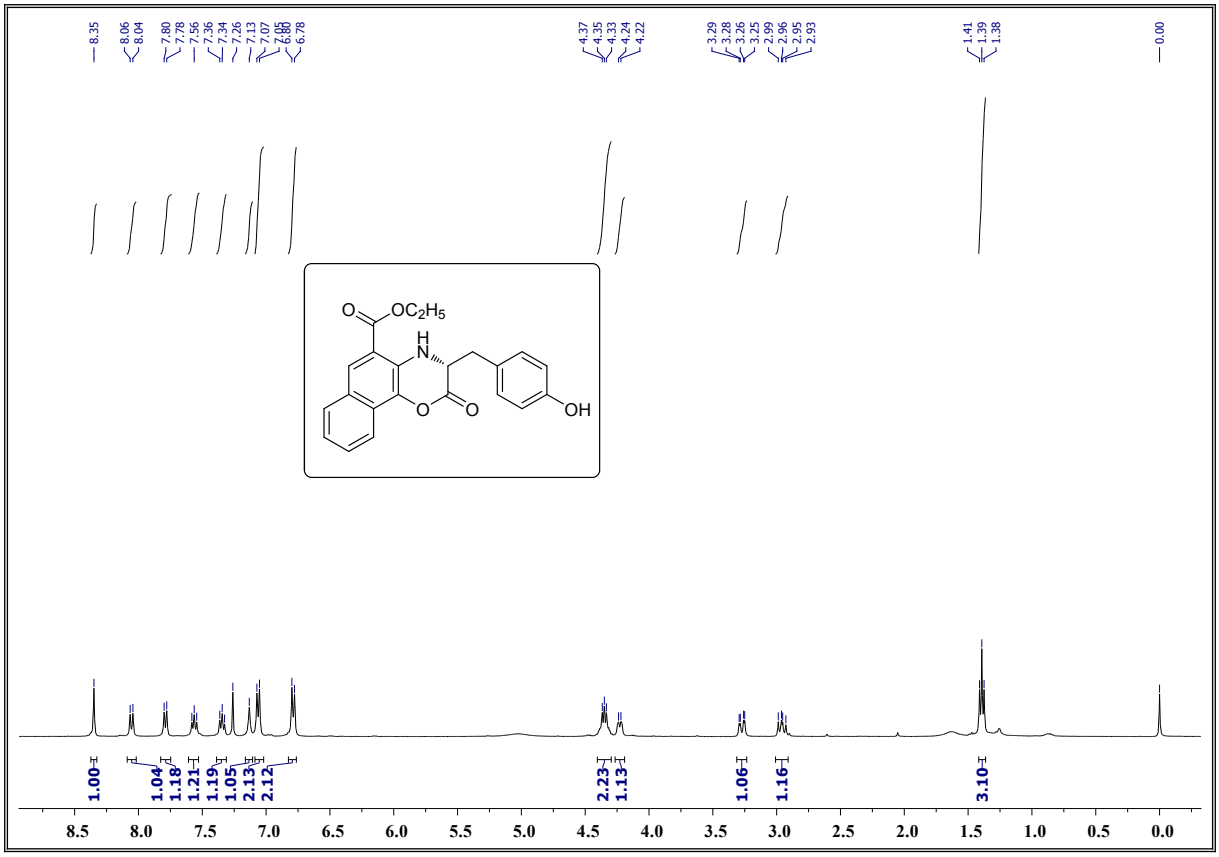
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
61 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-22 H: 0-20 N: 0-3 O: 0-5 I: 0-1

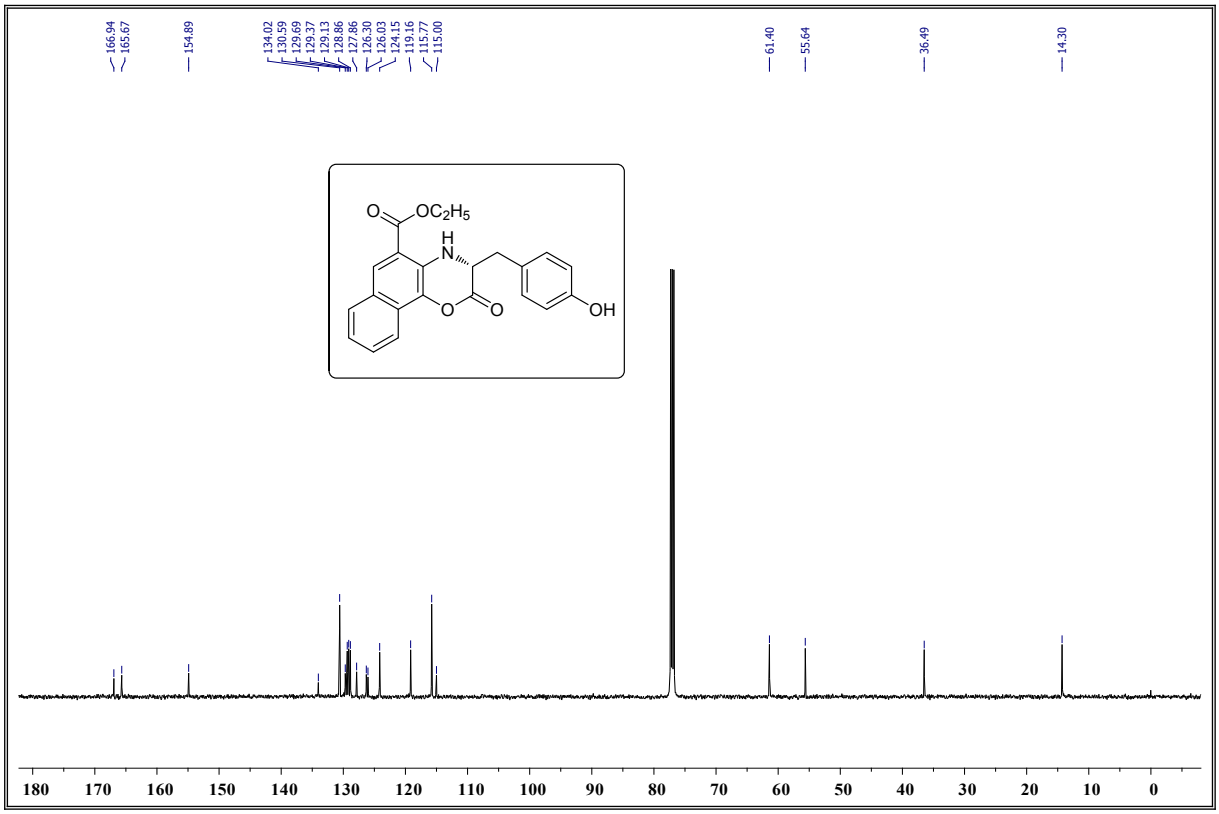


Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
378.1346	378.1341	0.5	1.3	13.5	482.1	n/a	n/a	C22 H20 N O5

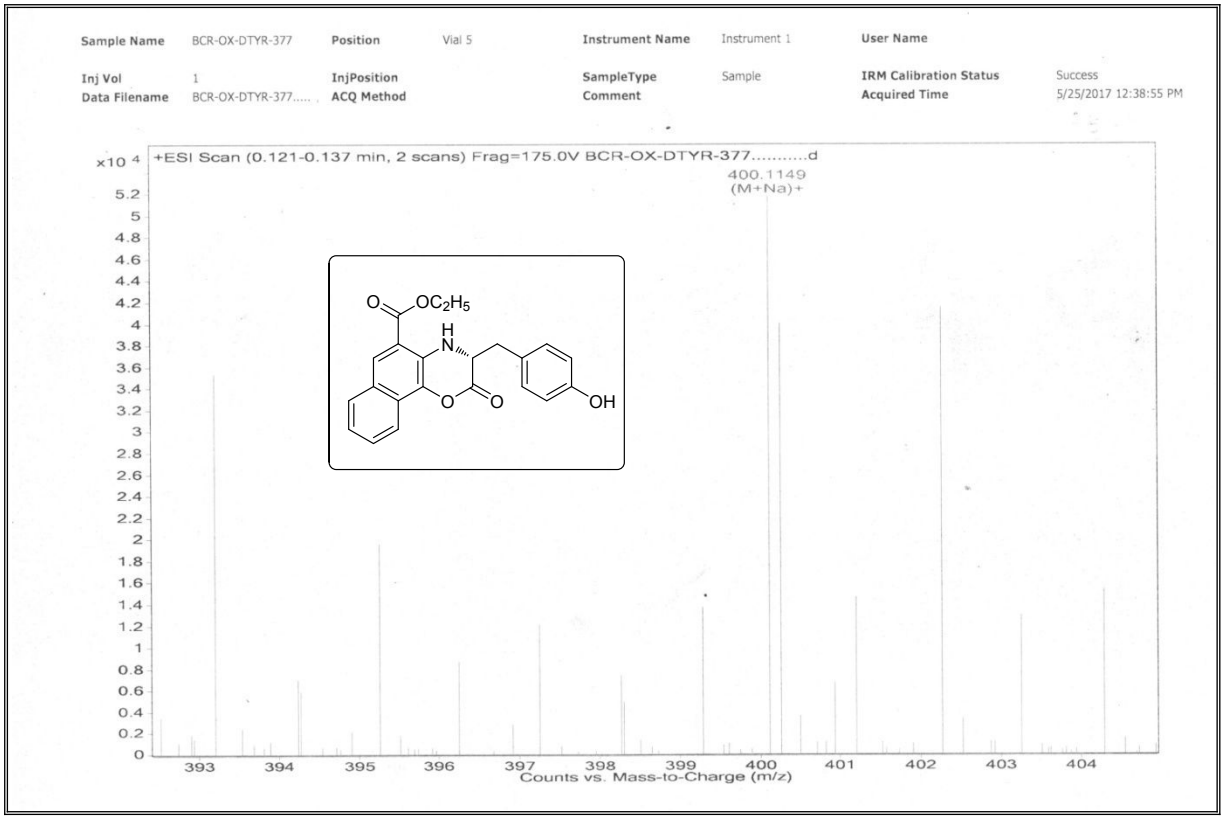
HRMS Spectrum of compound 3x



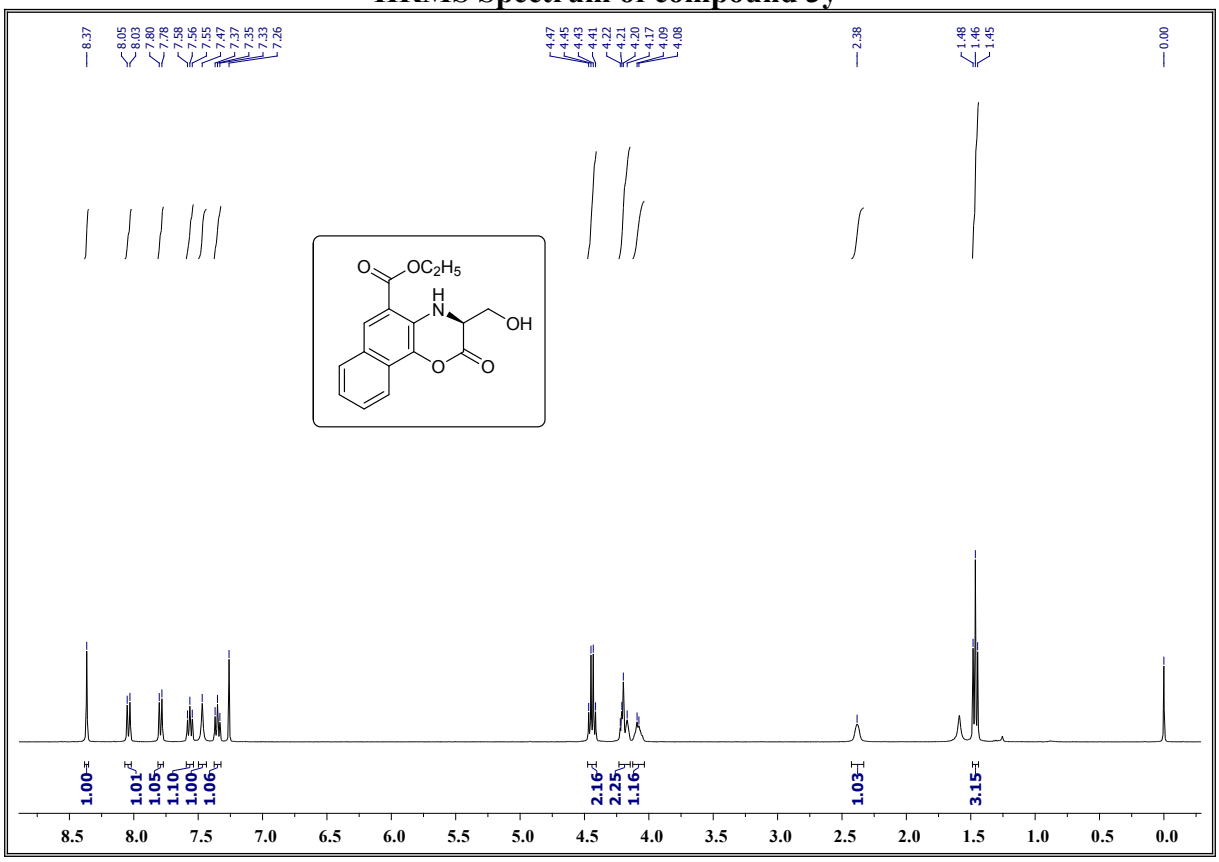
^{1}H-NMR Spectrum of compound 3y



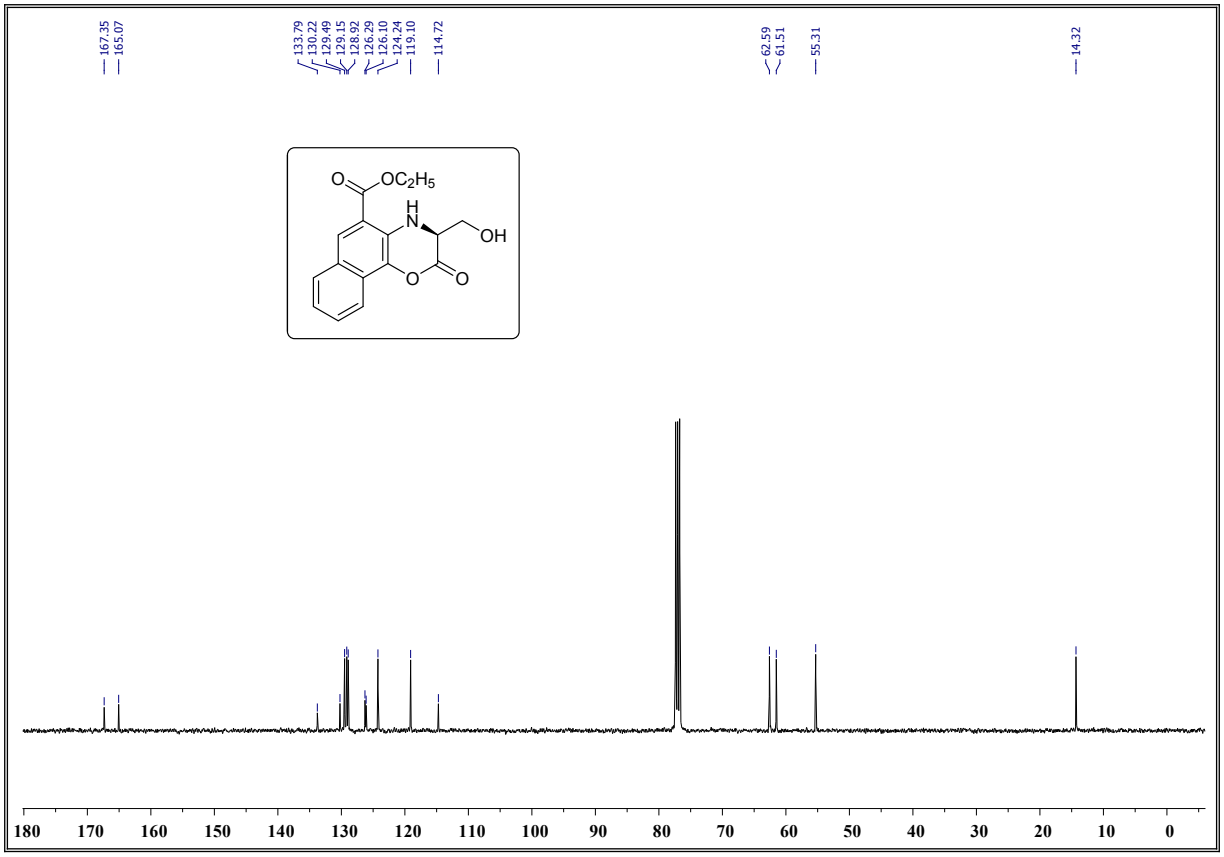
^{13}C-NMR Spectrum of compound 3y



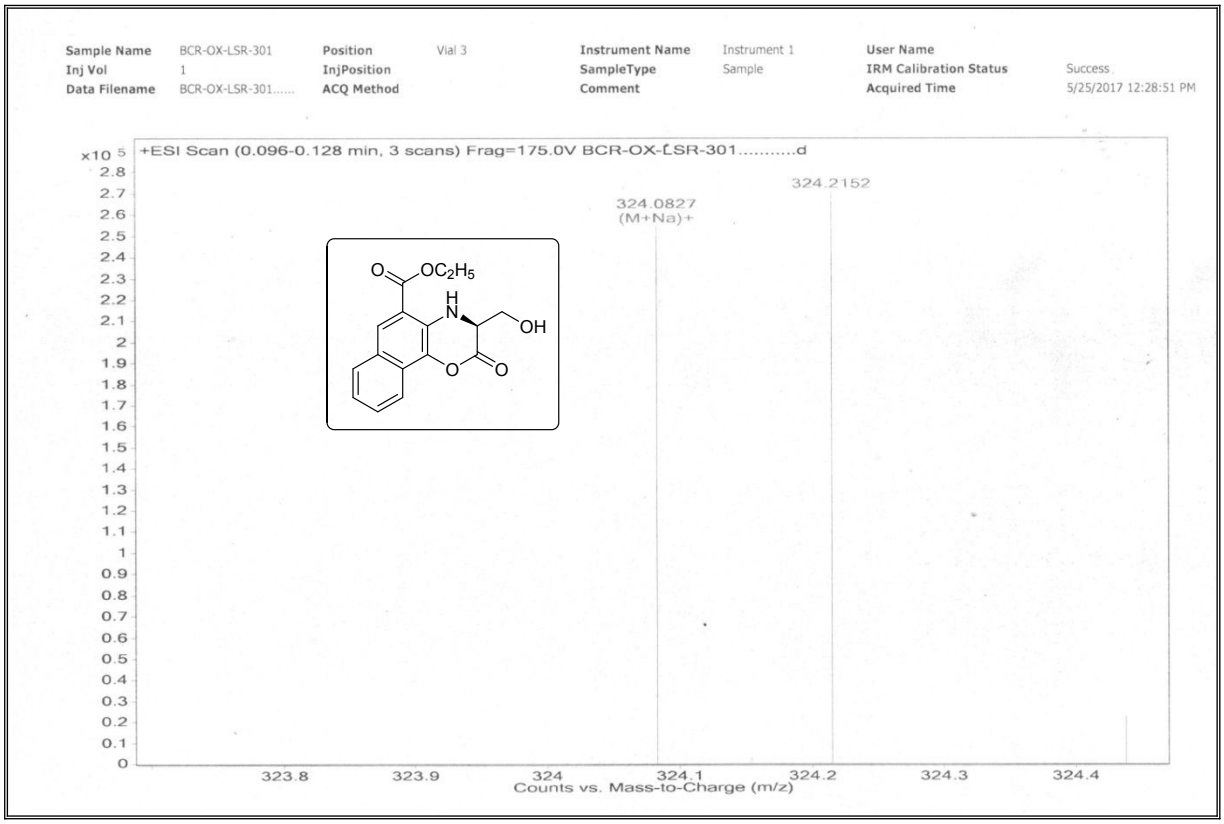
HRMS Spectrum of compound 3y



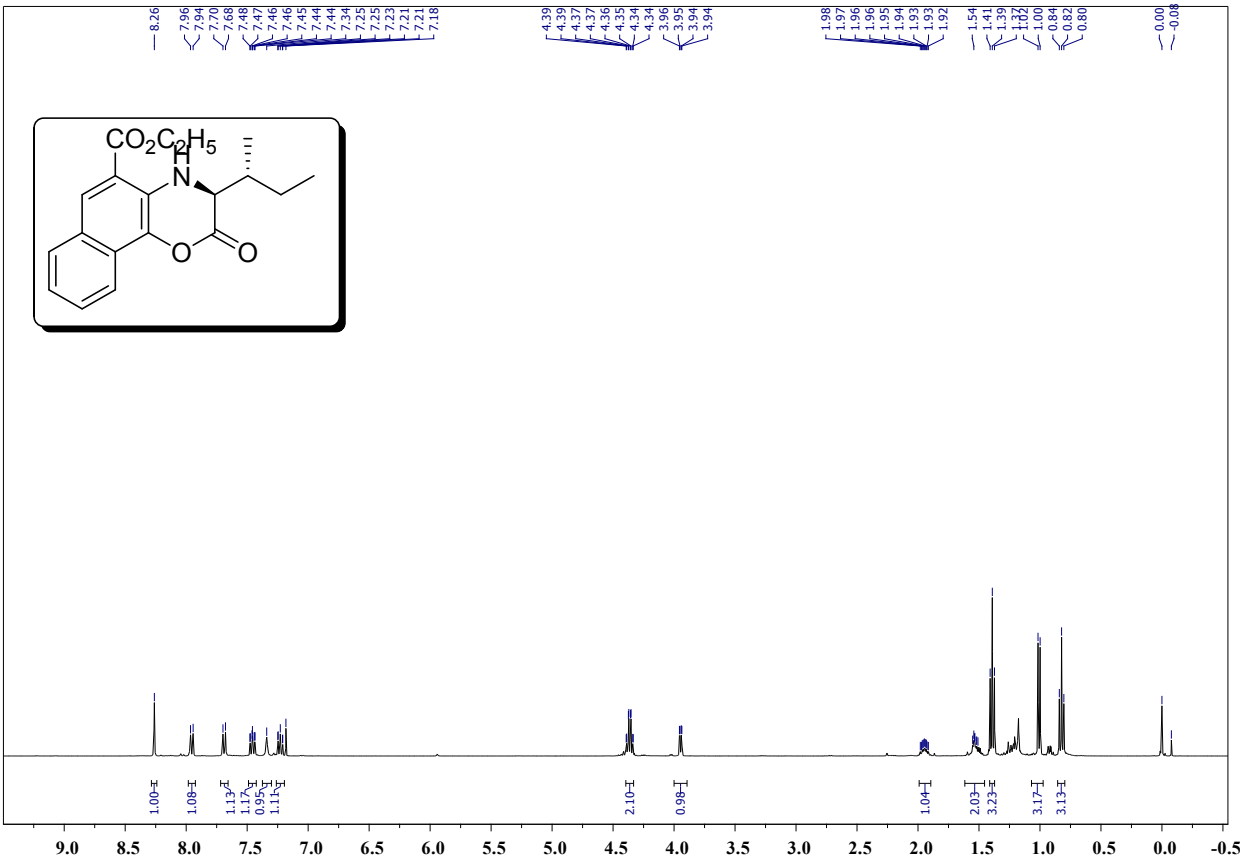
^{1}H-NMR Spectrum of compound 3z



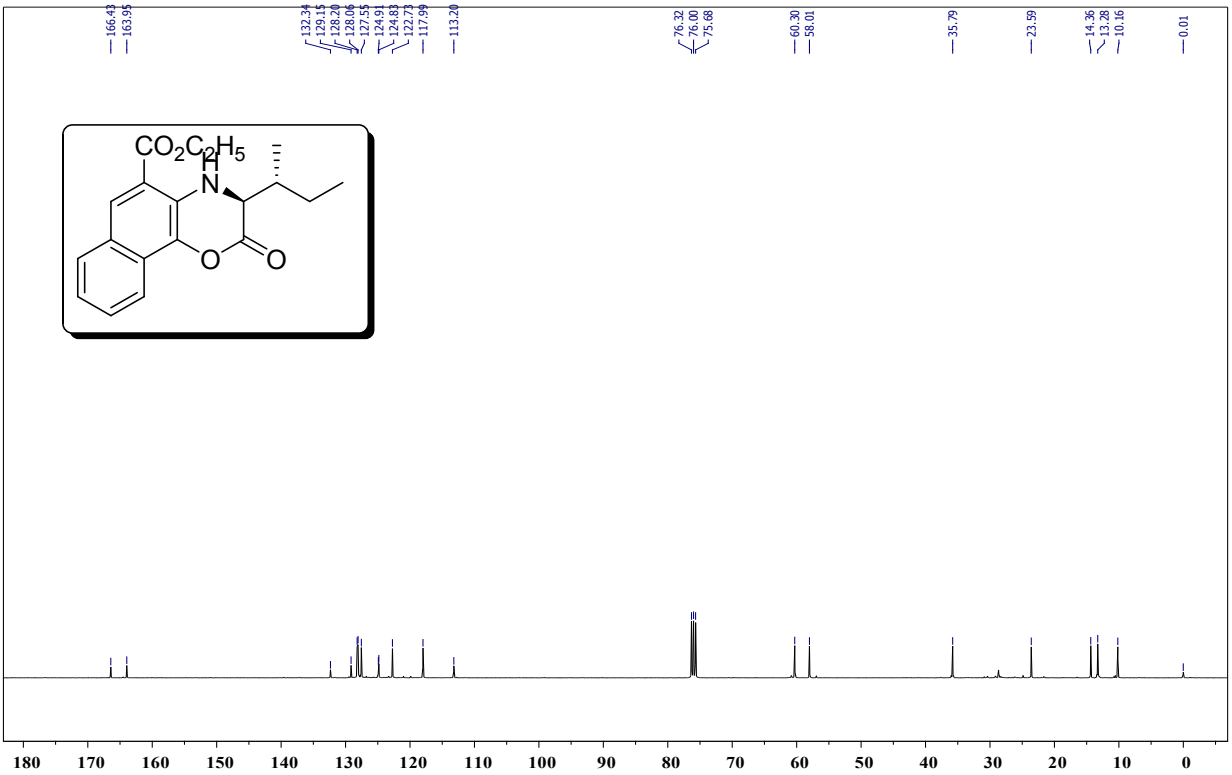
^{13}C-NMR Spectrum of compound 3z



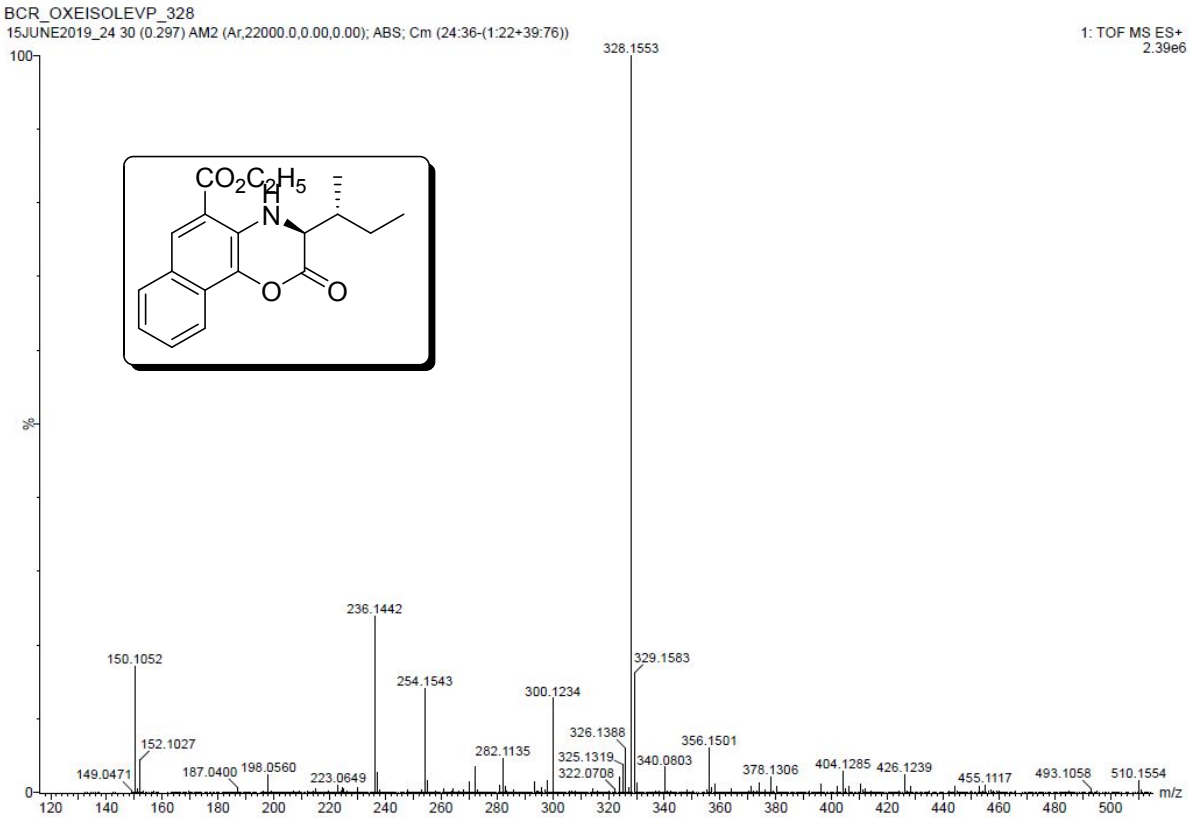
HRMS Spectrum of compound 3z



^{1}H NMR Spectrum of compound 3zb



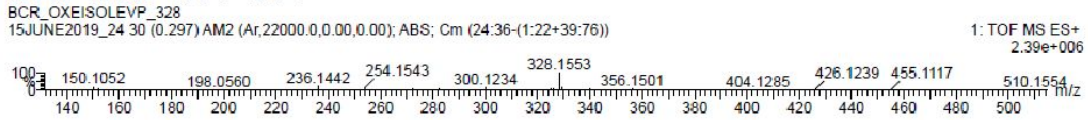
^{13}C NMR Spectrum of compound 3zb



Elemental Composition Report **Page 1**

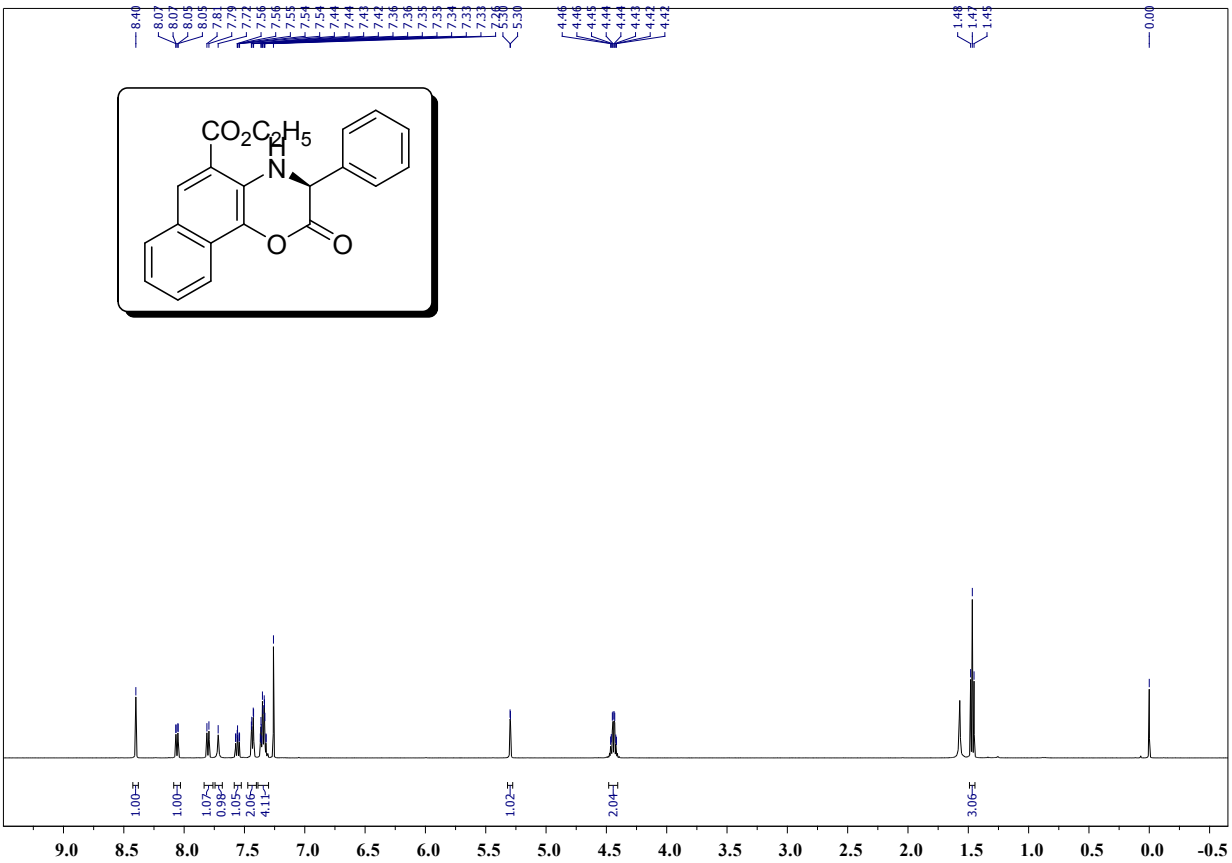
Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
8 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-19 H: 0-22 N: 0-1 O: 0-4

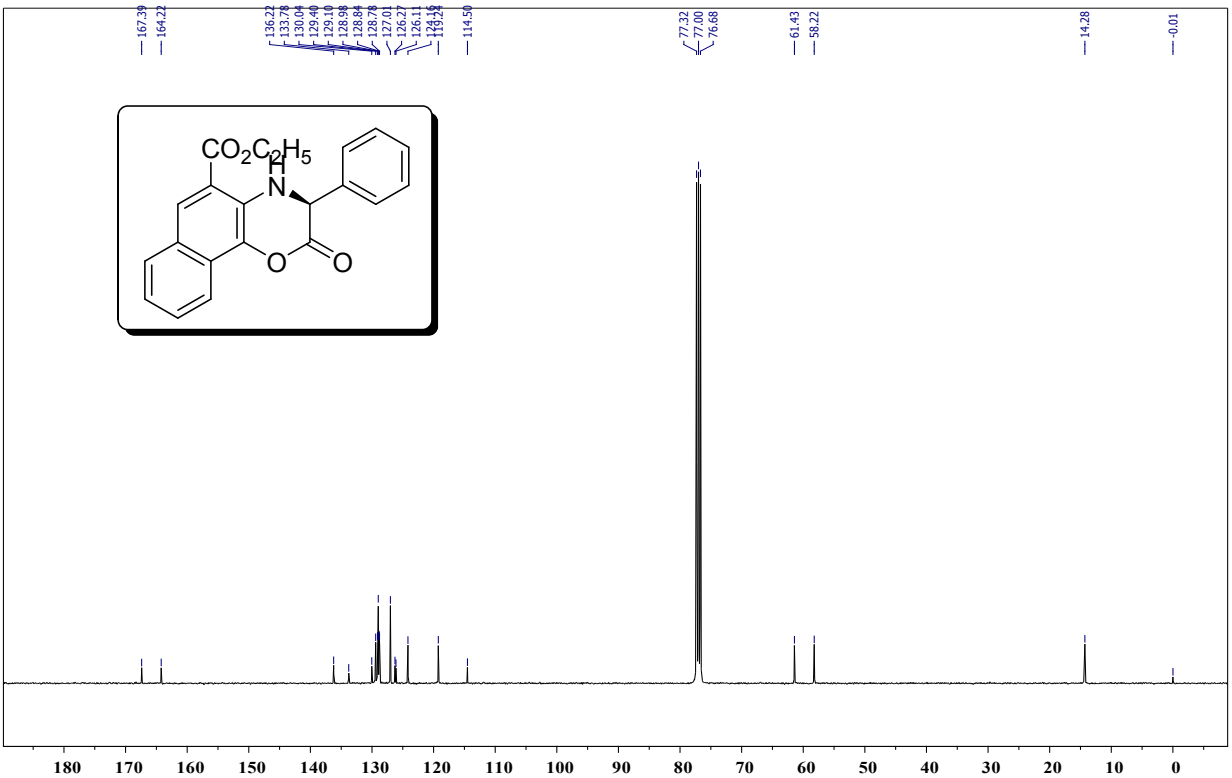


Minimum:				-1.5				
Maximum:		5.0	100.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
328.1553	328.1549	0.4	1.2	9.5	199.1	n/a	n/a	C19 H22 N O4

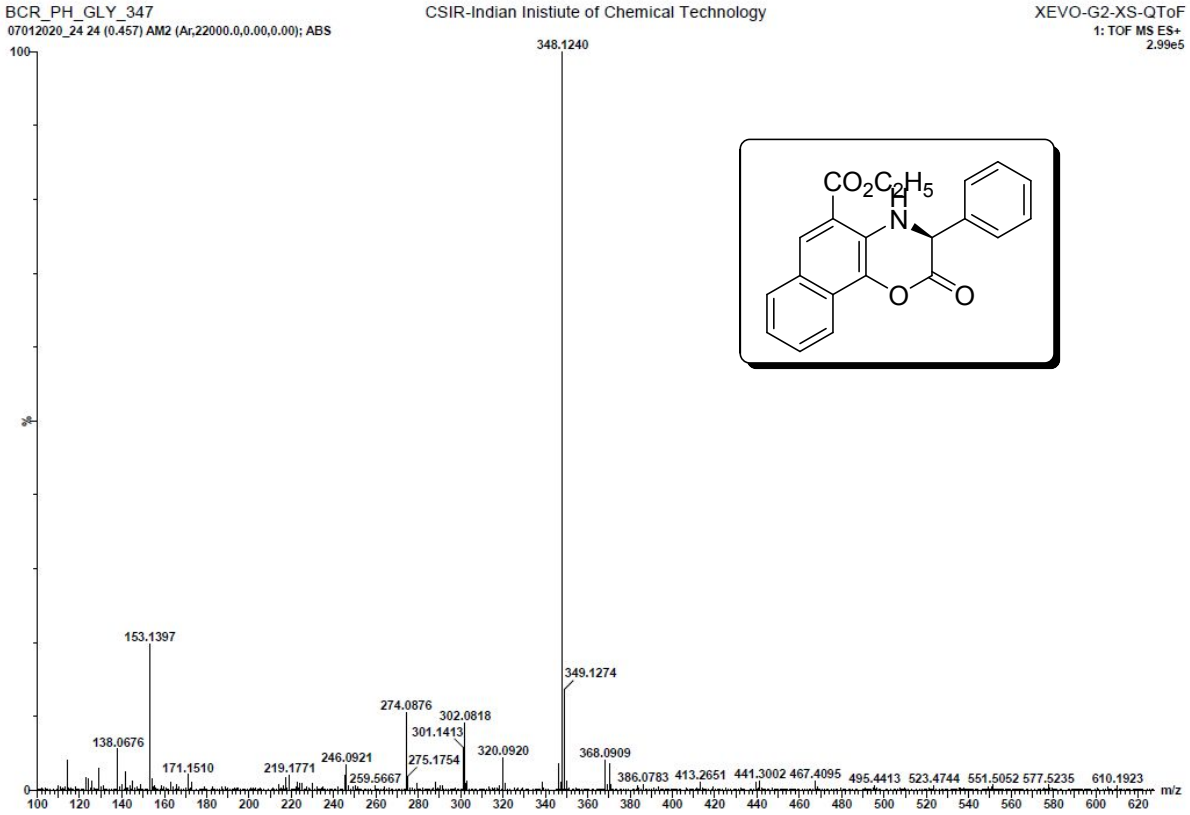
HRMS Spectrum of compound 3zb



^{1}H NMR Spectrum of compound 3ze



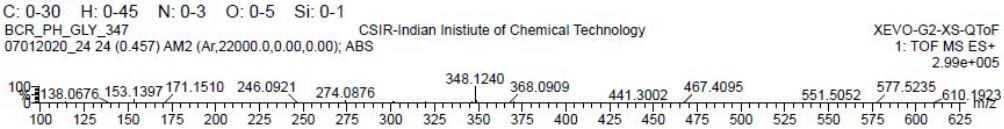
^{13}C NMR Spectrum of compound 3ze



Elemental Composition Report **Page 1**

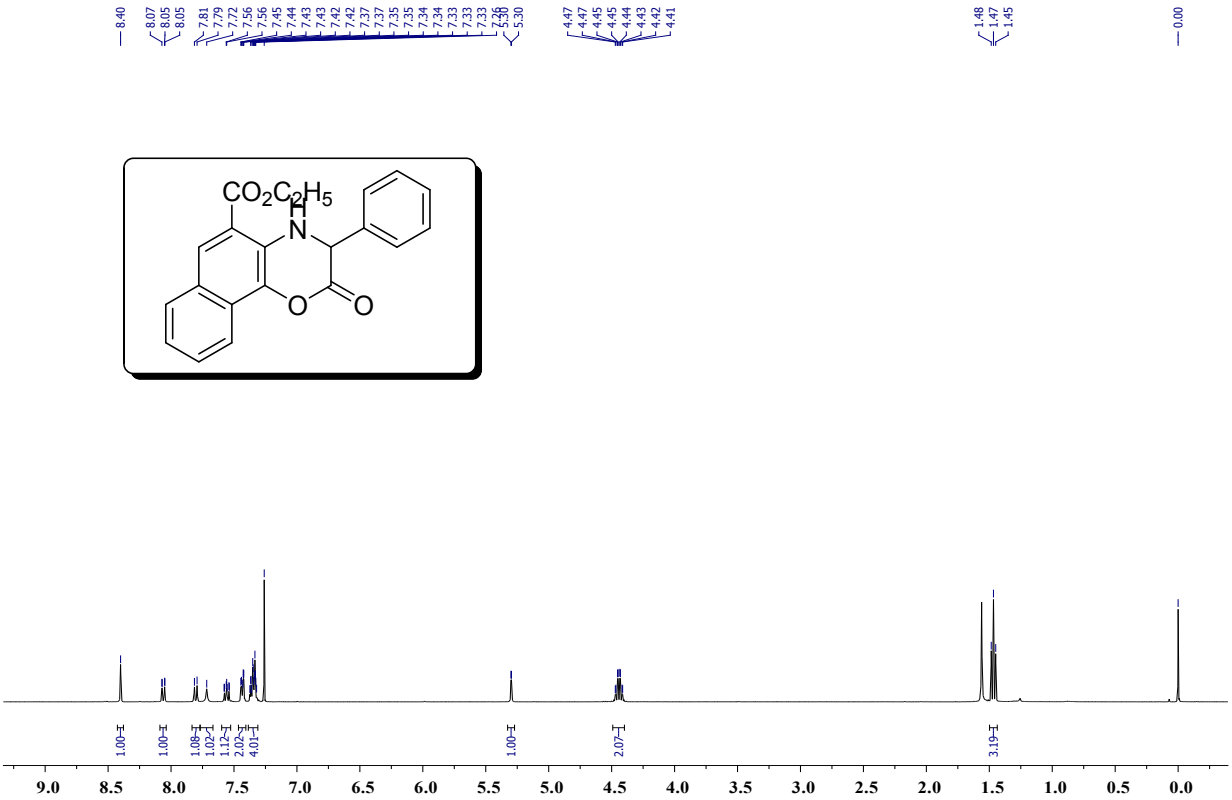
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
184 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-30 H: 0-45 N: 0-3 O: 0-5 Si: 0-1

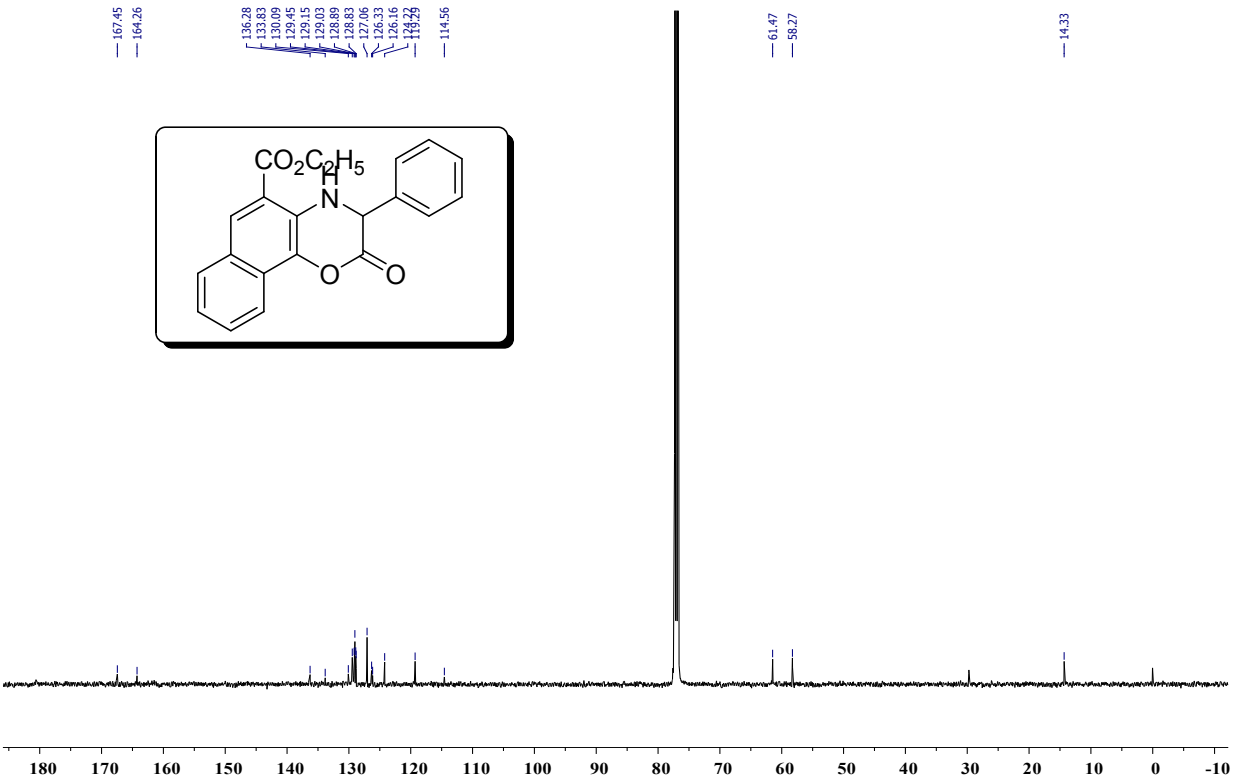


Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
348.1240	348.1236	0.4	1.1	13.5	456.7	n/a	n/a	C21 H18 N O4

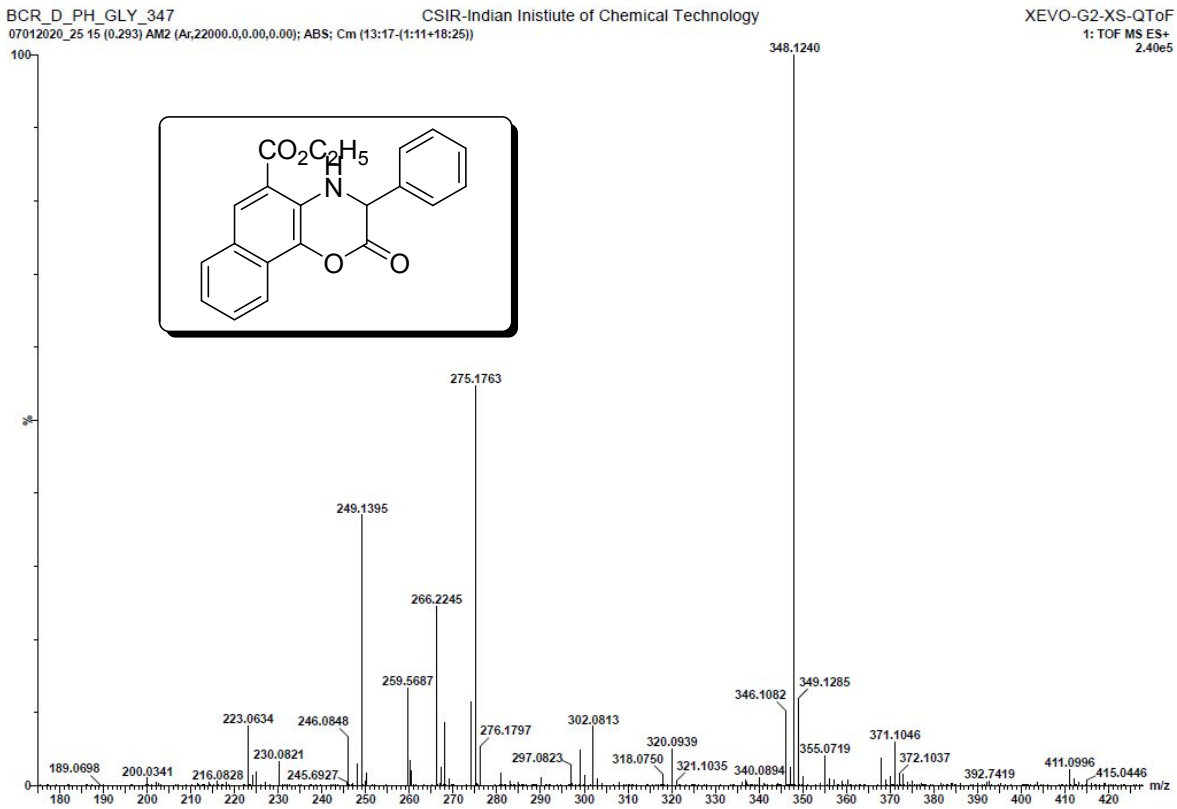
HRMS Spectrum of compound 3ze



^{1}H NMR Spectrum of compound 3zf



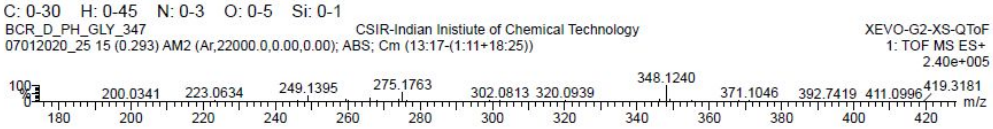
^{13}C NMR Spectrum of compound 3zf



Elemental Composition Report **Page 1**

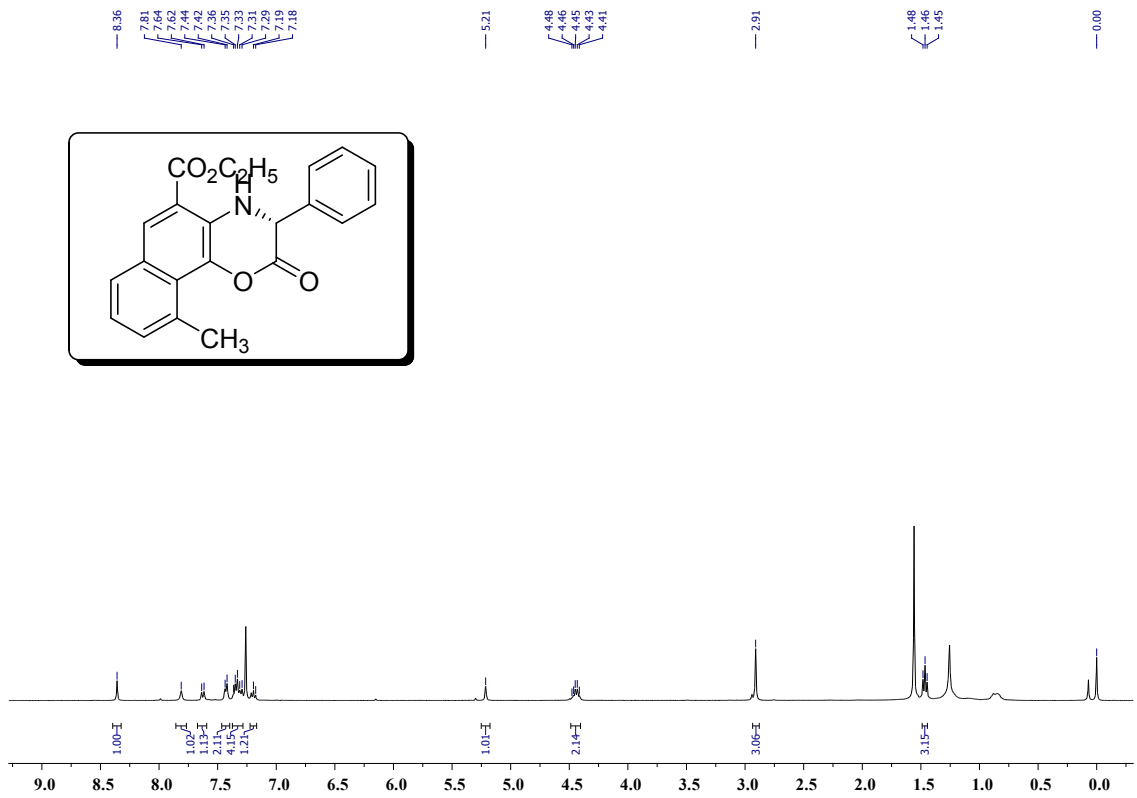
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
184 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-30 H: 0-45 N: 0-3 O: 0-5 Si: 0-1

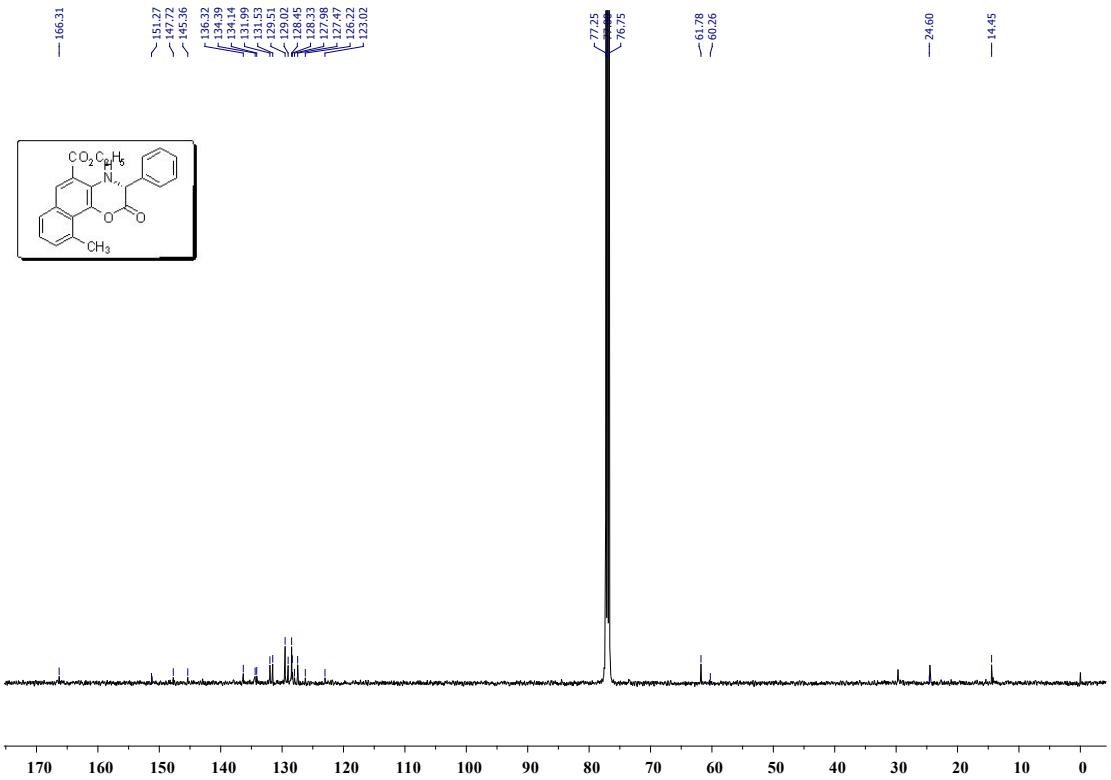


Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
348.1240	348.1236	0.4	1.1	13.5	335.9	n/a	n/a	C21 H18 N O4

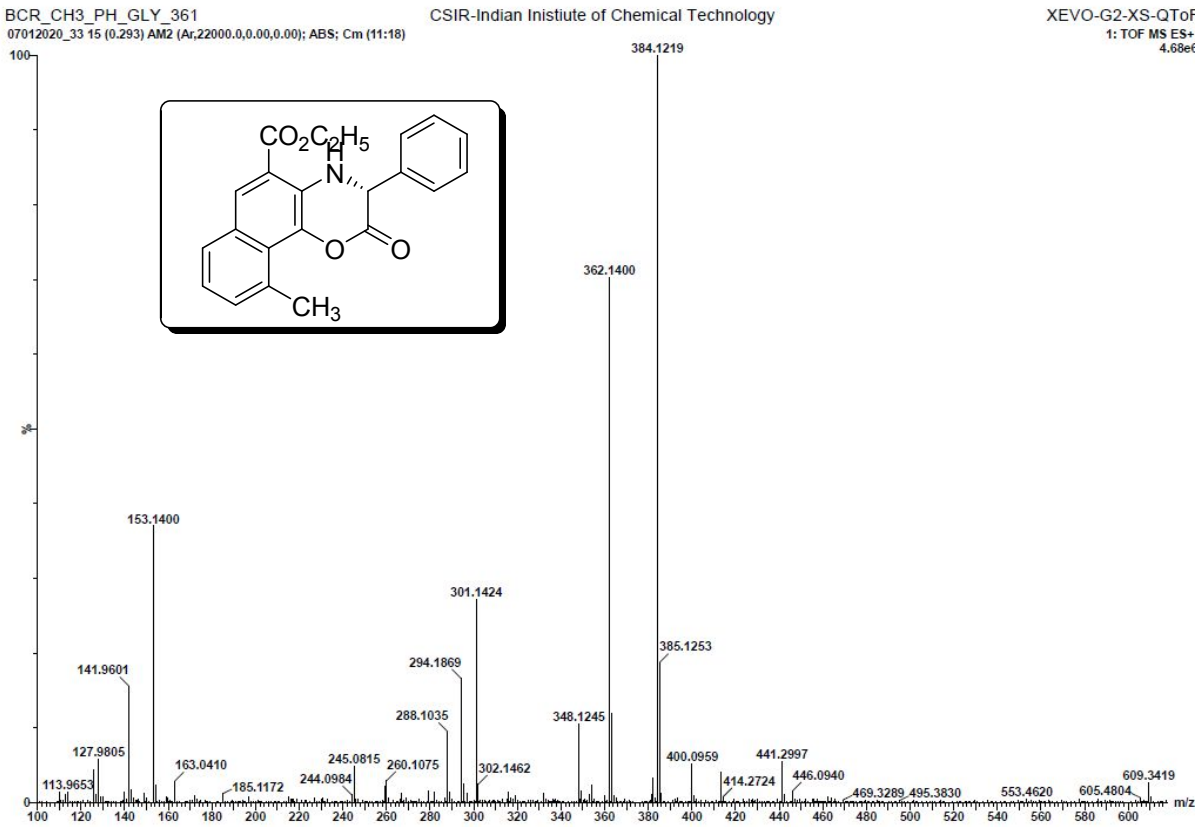
HRMS Spectrum of compound 3zf



^{1}H NMR Spectrum of compound 3zg



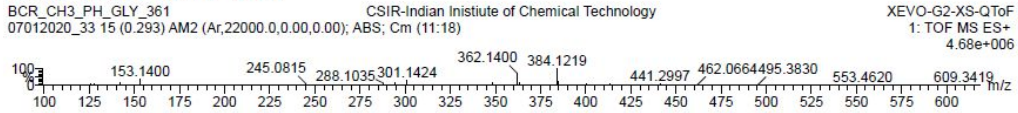
^{13}C NMR Spectrum of compound 3zg



Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

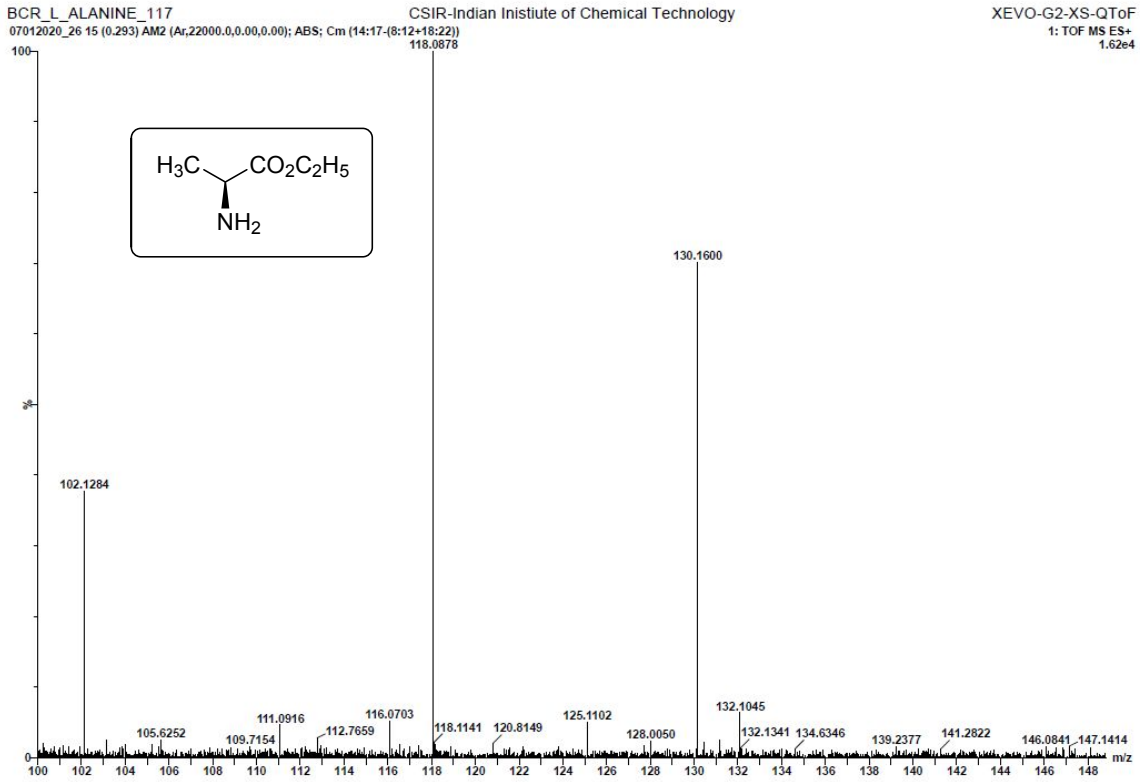
Monoisotopic Mass, Even Electron Ions
22 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-25 H: 0-20 N: 0-3 O: 0-4



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
362.1400	362.1392	0.8	2.2	13.5	563.2	n/a	n/a	C22 H20 N O4

HRMS Spectrum of compound 3zg

S54. HRMS & HPLC Spectrums of Compounds 2e-f and 2p-q

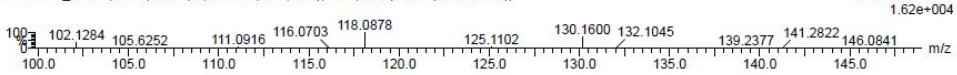


Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

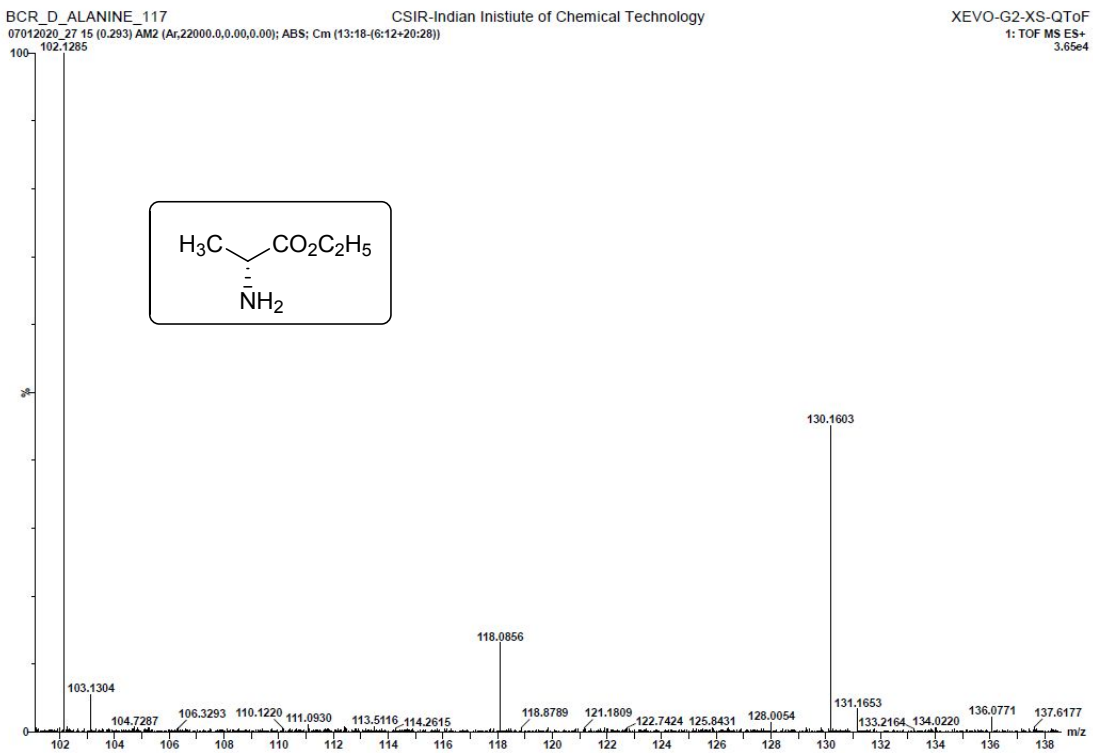
Monoisotopic Mass, Even Electron Ions
39 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-30 H: 0-45 N: 0-3 O: 0-5

BCR_L_ALANINE_117 CSIR-Indian Inistiute of Chemical Technology XEVO-G2-XS-QToF
07012020_26 15 (0.293) AM2 (Ar,22000.0,0.00,0.00); ABS; Cm (14:17-(8:12+18:22)) 1: TOF MS ES+
1.62e+004



Minimum:				-1.5				
Maximum:		5.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
118.0878	118.0868	1.0	8.5	0.5	788.0	n/a	n/a	C5 H12 N O2

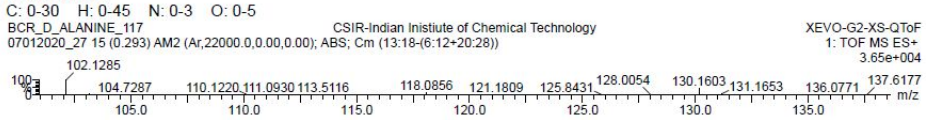
HRMS of Compound 2e



Elemental Composition Report **Page 1**

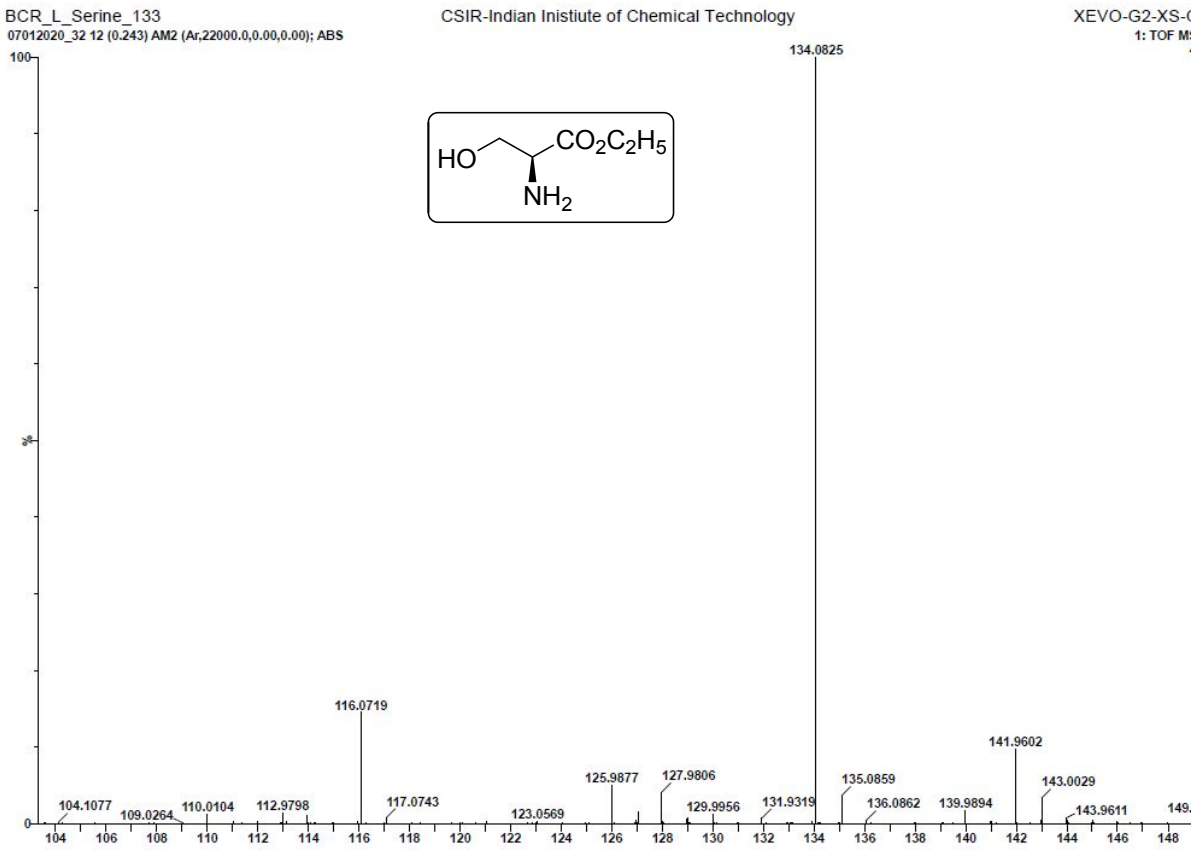
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
39 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-30 H: 0-45 N: 0-3 O: 0-5



Minimum:				-1.5				
Maximum:		5.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
118.0856	118.0868	-1.2	-10.2	0.5	576.7	n/a	n/a	C5 H12 N O2

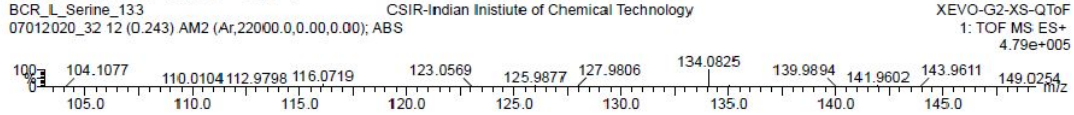
HRMS of Compound 2f



Elemental Composition Report **Page 1**

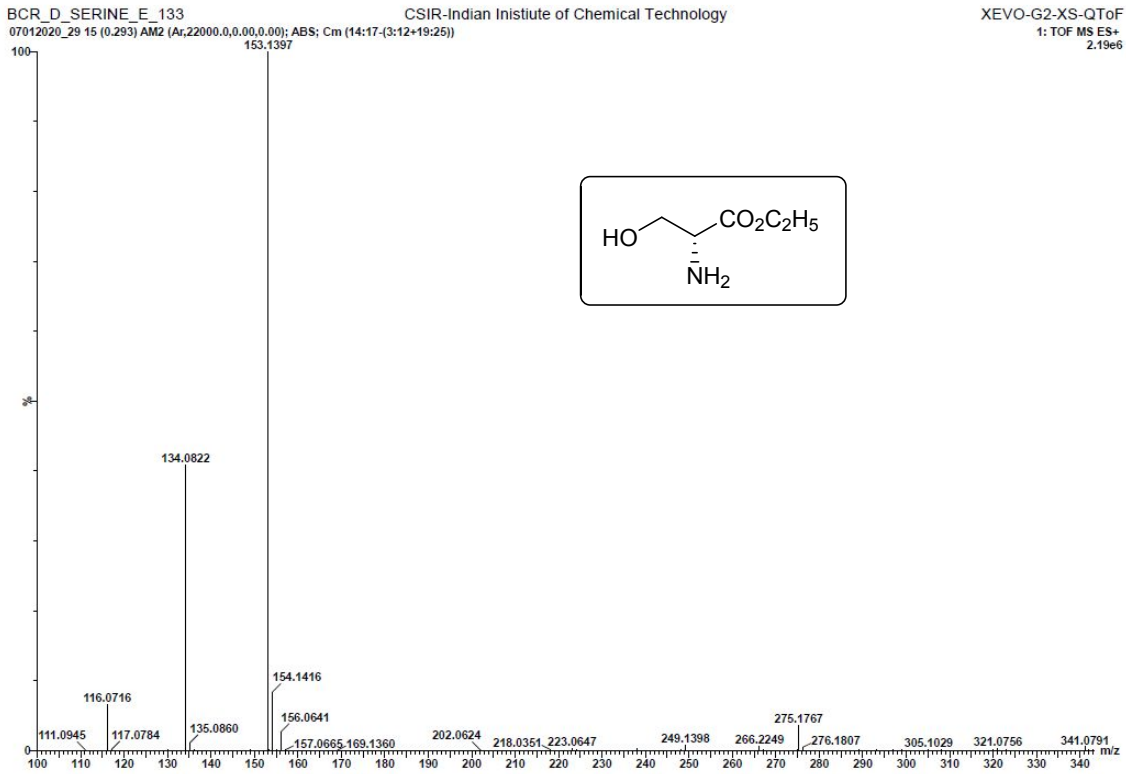
Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
54 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-25 H: 0-30 N: 0-5 O: 0-4



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
134.0825	134.0817	0.8	6.0	0.5	814.3	n/a	n/a	C5 H12 N O3

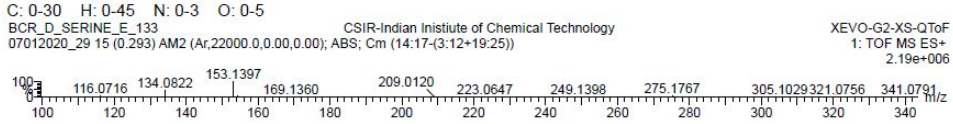
HRMS of Compound 2p



Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
44 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-30 H: 0-45 N: 0-3 O: 0-5



Minimum:				-1.5				
Maximum:		5.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
134.0822	134.0817	0.5	3.7	0.5	397.1	n/a	n/a	C5 H12 N O3

HRMS of Compound 2q

==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\Data\Project1\DR.B.CHINNA RAJU\L-ALANINE-ESTER-R2.lcd

Acquired by	: Admin
Sample Name	: L-ALANINE-ESTER-R
Sample ID	: L-ALANINE-ESTER-R
Tray#	: 1
Vail #	: 0
Injection Volume	: 10 uL
Data File Name	: L-ALANINE-ESTER-R2.lcd
Method File Name	: IC-3-CHIRAL.lcm
Batch File Name	:
Report File Name	: Default.lcr
Data Acquired	: 12/16/2019 5:42:42 AM
Data Processed	: 12/16/2019 6:02:46 AM

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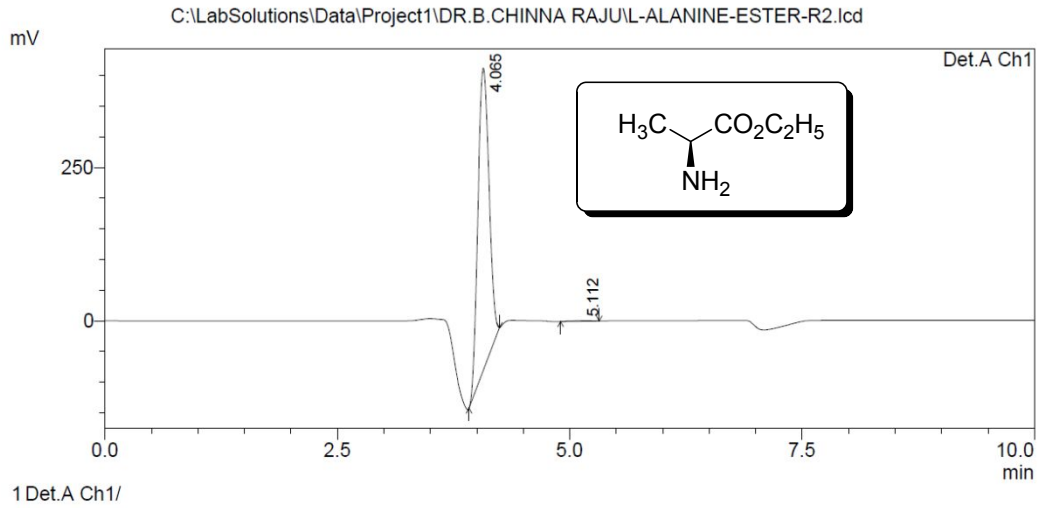


PeakTable

Detector A Ch1

Peak#	Ret. Time	Area	Height	Area %
1	4.065	4123098	494891	99.779
2	5.112	9136	538	0.221
Total		4132233	495429	100.000

HPLC of compound **2e**

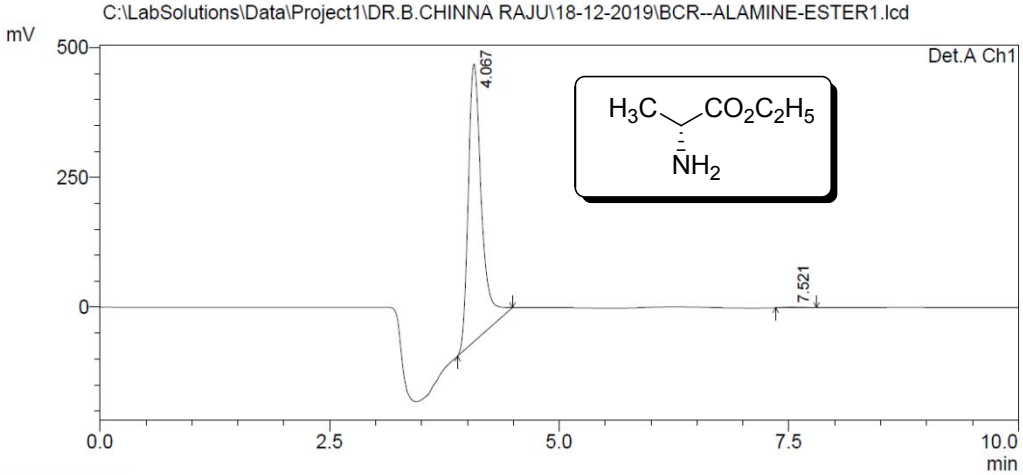
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\Data\Project1\DR.B.CHINNA RAJU\18-12-2019\BCR--ALAMINE-ESTER1.lcd

Acquired by	: Admin
Sample Name	: BCR--ALAMINE-ESTER
Sample ID	: BCR--ALAMINE-ESTER
Tray#	: 1
Vail #	: 0
Injection Volume	: 20 uL
Data File Name	: BCR--ALAMINE-ESTER1.lcd
Method File Name	: IC-3-CHIRAL.lcm
Batch File Name	:
Report File Name	: Default.lcr
Data Acquired	: 12/18/2019 6:17:33 PM
Data Processed	: 12/19/2019 11:30:10 AM

<Chromatogram>

C:\LabSolutions\Data\Project1\DR.B.CHINNA RAJU\18-12-2019\BCR--ALAMINE-ESTER1.lcd



1 Det.A Ch1/

PeakTable

Detector A Ch1

Peak#	Ret. Time	Area	Height	Area %
1	4.067	5432753	535069	99.784
2	7.521	11772	986	0.216
Total		5444525	536055	100.000

HPLC of compound **2f**

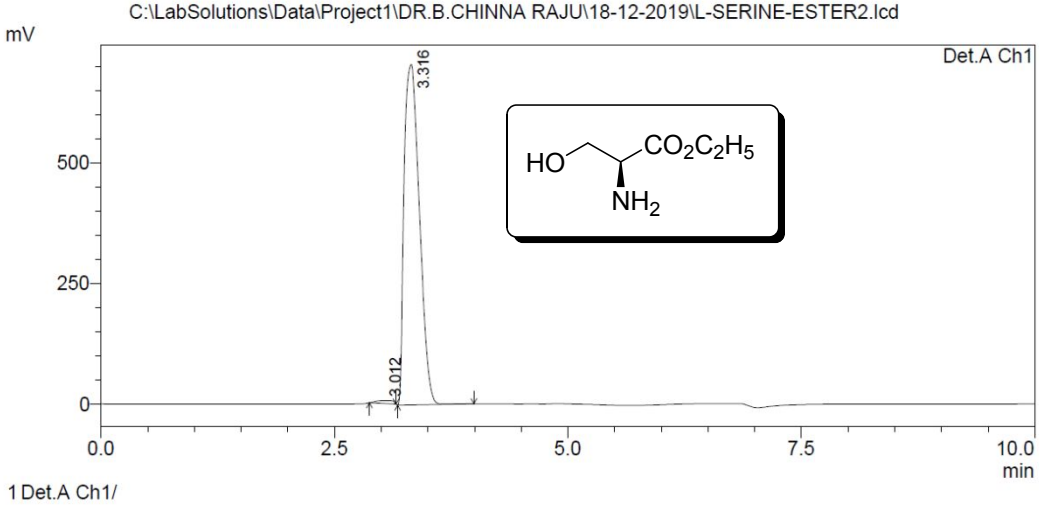
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\Data\Project1\DR.B.CHINNA RAJU\18-12-2019\L-SERINE-ESTER2.lcd

Acquired by	: Admin
Sample Name	: L-SERINE-ESTER
Sample ID	: L-SERINE-ESTER
Tray#	: 1
Vail #	: 0
Injection Volume	: 20 uL
Data File Name	: L-SERINE-ESTER2.lcd
Method File Name	: IC-3-CHIRAL.lcm
Batch File Name	:
Report File Name	: Default.lcr
Data Acquired	: 12/18/2019 5:51:54 PM
Data Processed	: 12/19/2019 4:55:12 PM

<Chromatogram>

C:\LabSolutions\Data\Project1\DR.B.CHINNA RAJU\18-12-2019\L-SERINE-ESTER2.lcd



1 Det.A Ch1/

PeakTable

Detector A Ch1

Peak#	Ret. Time	Area	Height	Area %
1	3.012	74505	5665	0.920
2	3.316	8025627	705744	99.080
Total		8100133	711409	100.000

HPLC of compound **2p**

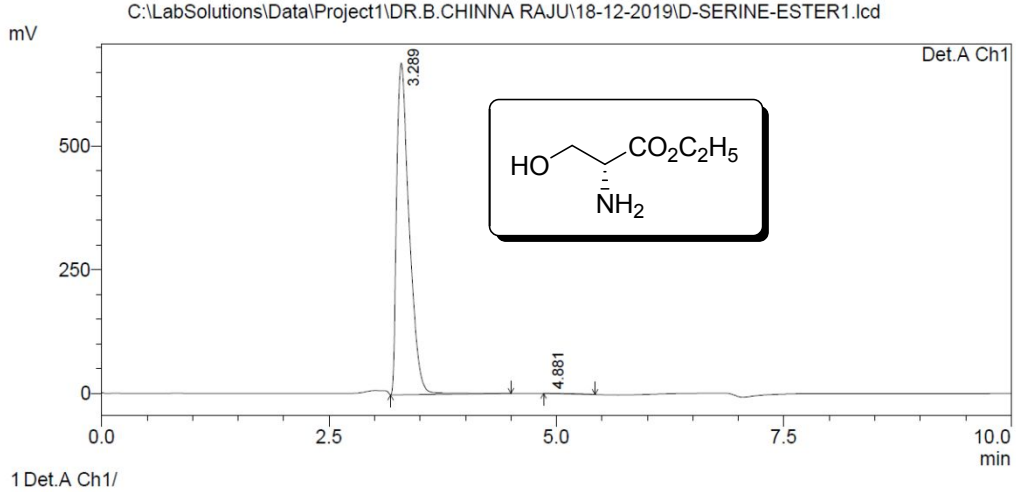
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\Data\Project1\DR.B.CHINNA RAJU\18-12-2019\D-SERINE-ESTER1.lcd

Acquired by	: Admin
Sample Name	: D-SERINE-ESTER
Sample ID	: D-SERINE-ESTER
Tray#	: 1
Vail #	: 0
Injection Volume	: 20 uL
Data File Name	: D-SERINE-ESTER1.lcd
Method File Name	: IC-3-CHIRAL.lcm
Batch File Name	:
Report File Name	: Default.lcr
Data Acquired	: 12/18/2019 5:26:35 PM
Data Processed	: 12/18/2019 5:36:40 PM

<Chromatogram>

C:\LabSolutions\Data\Project1\DR.B.CHINNA RAJU\18-12-2019\D-SERINE-ESTER1.lcd



PeakTable

Detector A Ch1

Peak#	Ret. Time	Area	Height	Area %
1	3.289	6438301	671641	99.813
2	4.881	12045	141	0.187
Total		6450345	671782	100.000

HPLC of compound **2q**

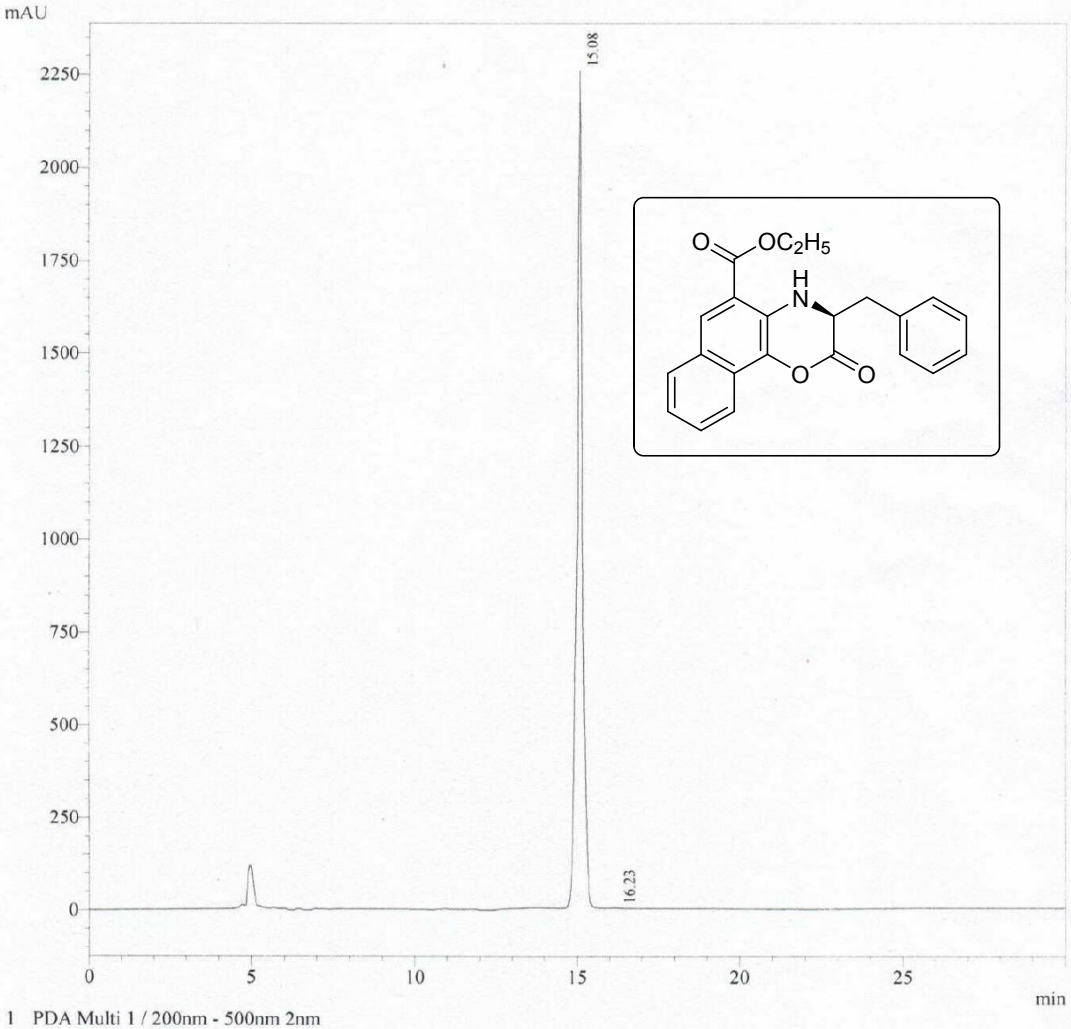
HPLC spectrums of the target compounds 3a-v, 3x-z, 3zb and 3ze-zg

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
CROP PROTECTION CHEMICALS DIVISION

Acquired by : T RAMESH BABU
Sample Name : NAPHTHOXINONE
Sample ID : BCR-L-PA 85:15
Data Filename : NAPHTHO-11.lcd
Method Filename : ramesh.lcm
Date Acquired : 18/07/2019

3a

D:\BCR\NAPHTHO-11.lcd



1 PDA Multi 1 / 200nm - 500nm 2nm

PDA Ch1 200nm - 500nm 2nm

Peak#	Ret. Time	Area	Area %
1	15.08	28638753	99.89
2	16.23	32525	0.11
Total		28671279	100.00

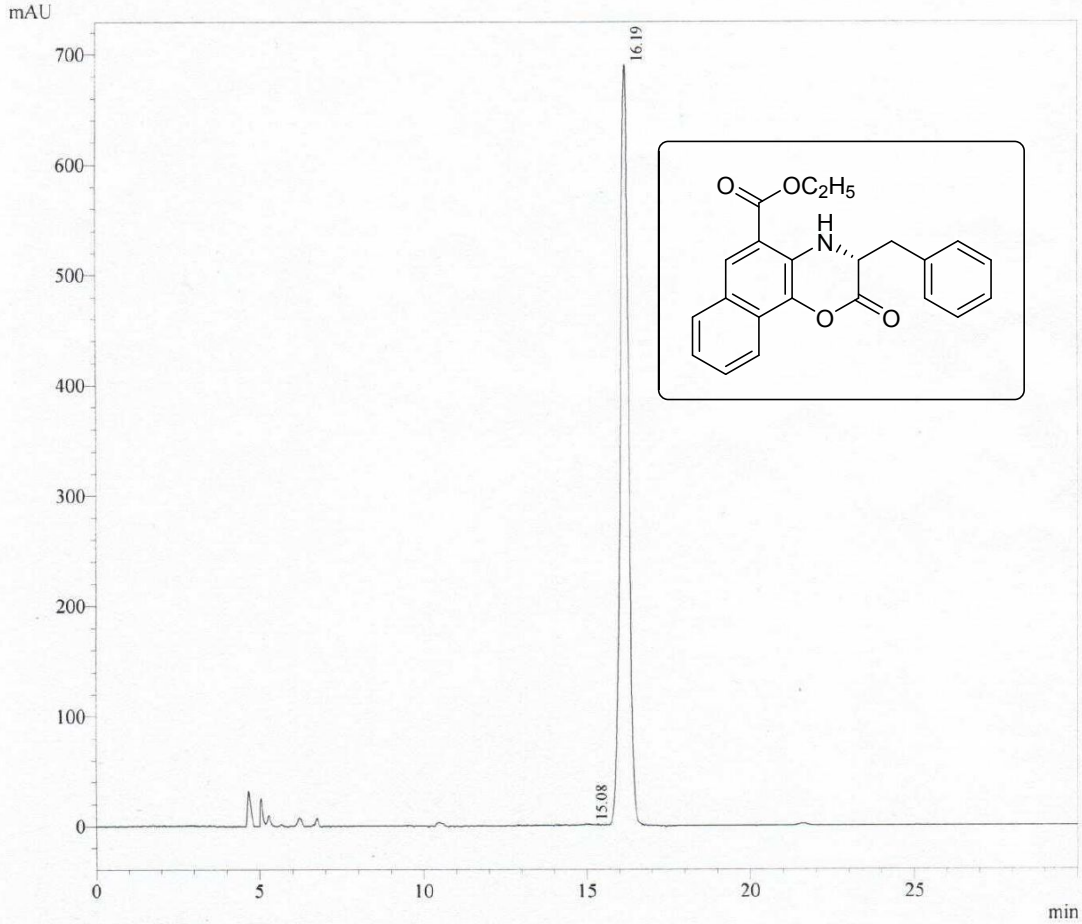
HPLC Spectrum of compound 3a

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
CROP PROTECTION CHEMICALS DIVISION

3b

Acquired by : T RAMESH BABU
Sample Name : NAPHTHOXINONE
Sample ID : BCR-D-PA 85:15
Data Filename : NAPHTHO-10.lcd
Method Filename : ramesh.lcm
Date Acquired : 18/07/2019

D:\BCR\NAPHTHO-10.lcd



1 PDA Multi 1 / 200nm - 500nm 2nm

PDA Ch1 200nm - 500nm 2nm

Peak#	Ret. Time	Area	Area %
1	15.08	6324	0.05
2	16.19	12399144	99.95
Total		12405468	100.00

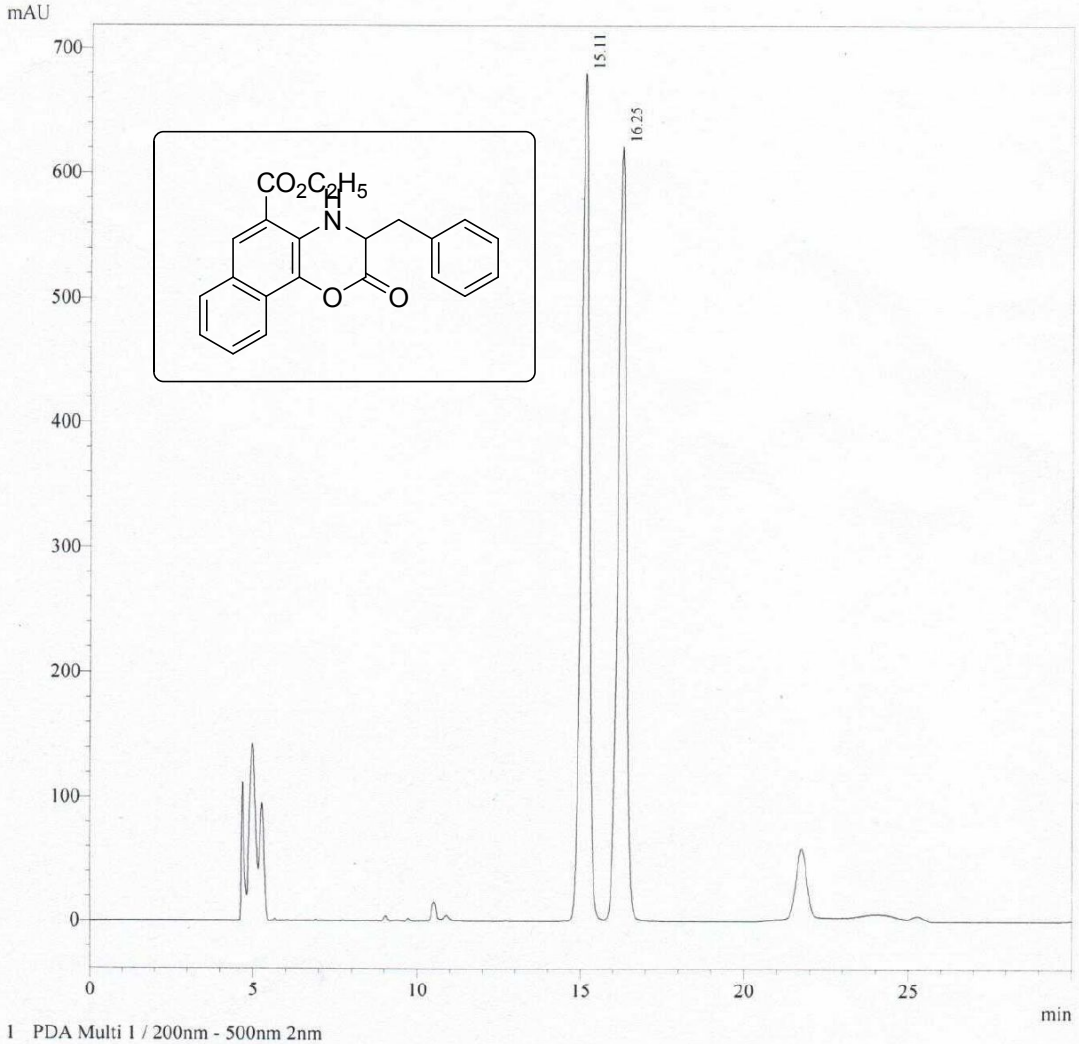
HPLC Spectrum of compound 3b

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
CROP PROTECTION CHEMICALS DIVISION

Acquired by : T RAMESH BABU
Sample Name : NAPHTHOXINONE
Sample ID : BCR-DL-PA 85:15
Data Filename : NAPHTHO-14.lcd
Method Filename : ramesh.lcm
Date Acquired : 18/07/2019

3c

D:\BCR\NAPHTHO-14.lcd



1 PDA Multi 1 / 200nm - 500nm 2nm

PDA Ch1 200nm - 500nm 2nm

Peak#	Ret. Time	Area	Area %
1	15.11	11628652	50.61
2	16.25	11350082	49.39
Total		22978734	100.00

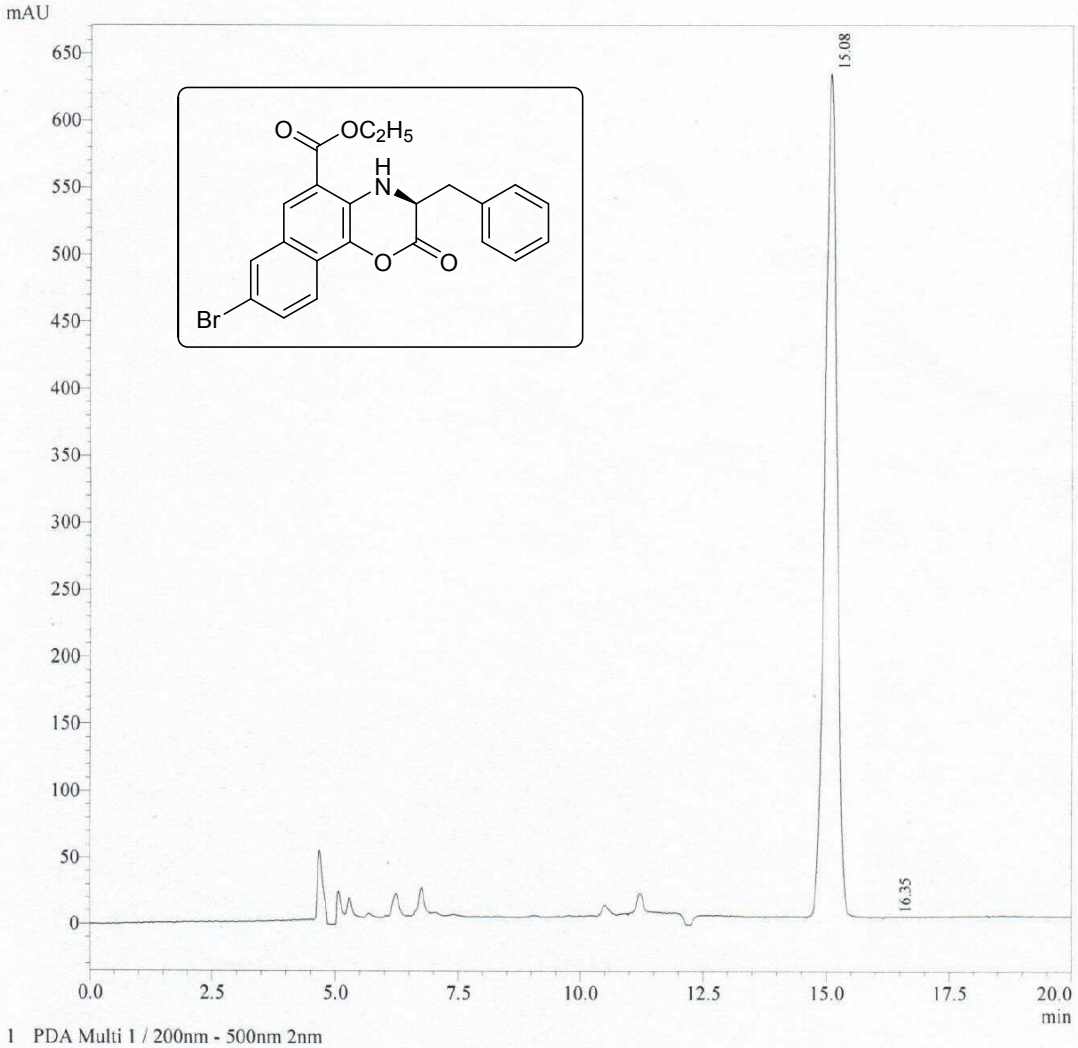
HPLC Spectrum of compound 3c

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
CROP PROTECTION CHEMICALS DIVISION

Acquired by : T RAMESH BABU
Sample Name : NAPHTHOXINONE
Sample ID : BCR-Br-L-PA
Data Filename : NAPHTHO-18.lcd
Method Filename : ramesh.lcm
Date Acquired : 19/07/2019

3d

D:\BCR\NAPHTHO-18.lcd



1 PDA Multi 1 / 200nm - 500nm 2nm

PDA Ch1 200nm - 500nm 2nm

Peak#	Ret. Time	Area	Area %
1	15.08	10562341	99.76
2	16.35	24918	0.24
Total		10587259	100.00

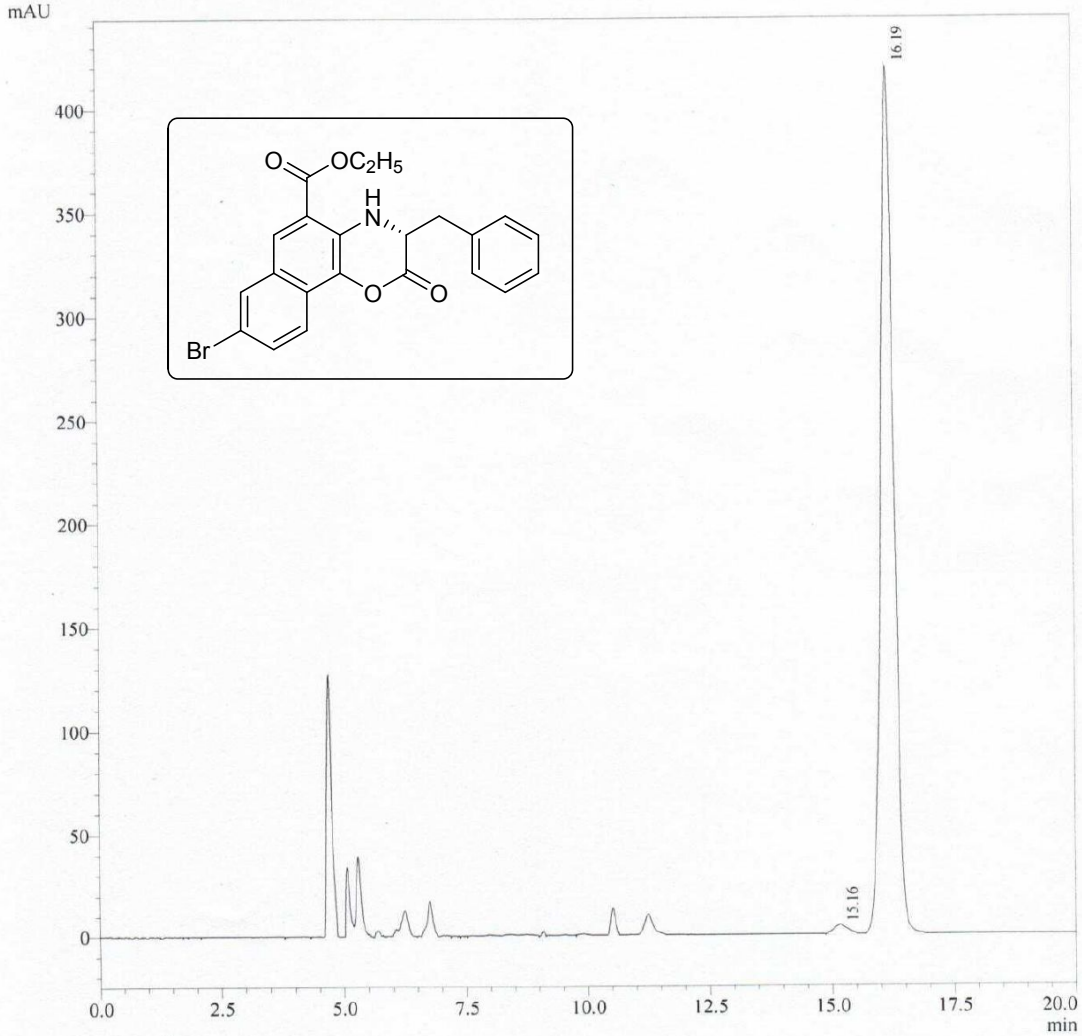
HPLC Spectrum of compound 3d

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
CROP PROTECTION CHEMICALS DIVISION

Acquired by : T RAMESH BABU
Sample Name : NAPHTHOXINONE
Sample ID : BCR-Br-D-PA
Data Filename : NAPHTHO-19.lcd
Method Filename : ramesh.lcm
Date Acquired : 19/07/2019

3e.

D:\BCR\NAPHTHO-19.lcd



1 PDA Multi 1 / 200nm - 500nm 2nm

PDA Ch1 200nm - 500nm 2nm

Peak#	Ret. Time	Area	Area %
1	15.16	108859	1.37
2	16.19	7845797	98.63
Total		7954655	100.00

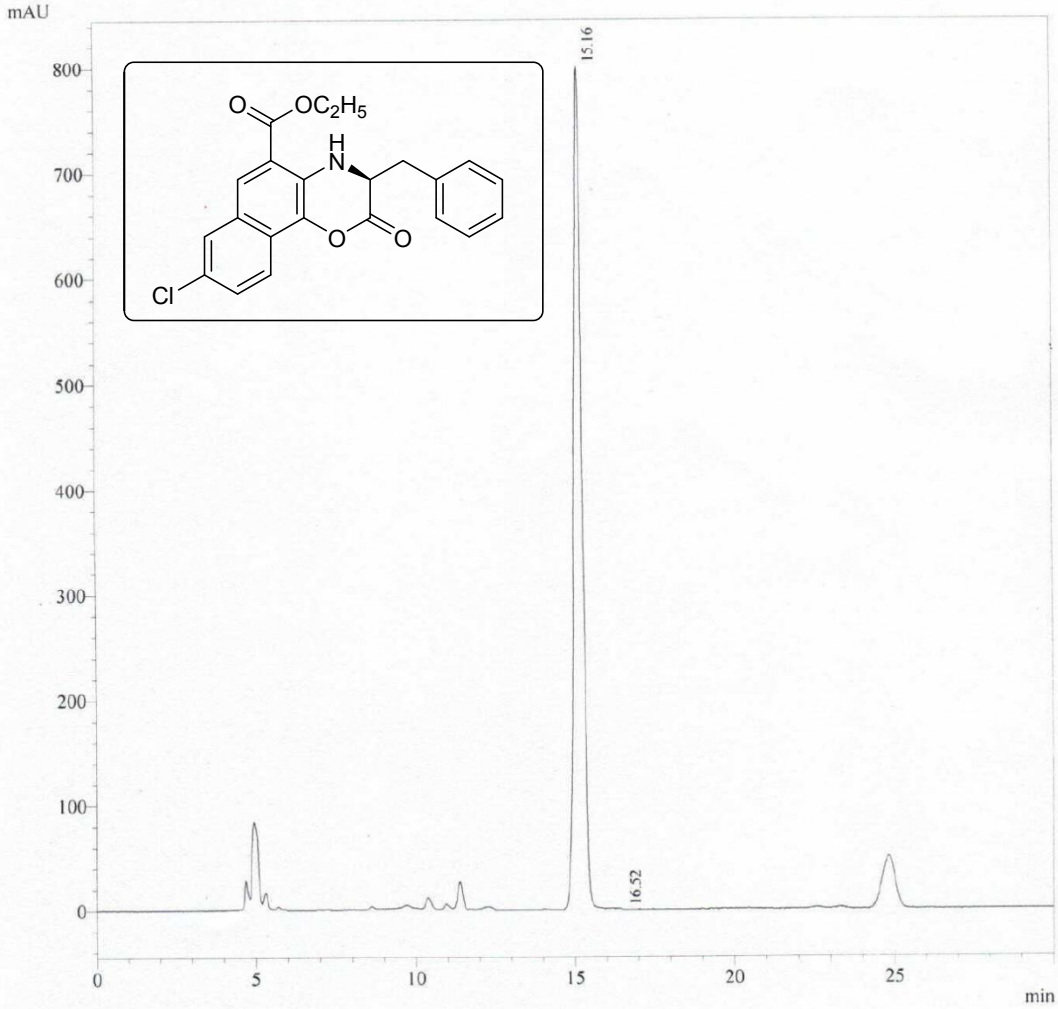
HPLC Spectrum of compound 3e

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
CROP PROTECTION CHEMICALS DIVISION

Acquired by : T RAMESH BABU
Sample Name : NAPHTHOXINONE
Sample ID : BCR-Cl-L-PA
Data Filename : NAPHTHO-28.lcd
Method Filename : ramesh.lcm
Date Acquired : 23/07/2019

D:\BCR\NAPHTHO-28.lcd

3f



1 PDA Multi 1 / 200nm - 500nm 2nm

PDA Ch1 200nm - 500nm 2nm

Peak#	Ret. Time	Area	Area %
1	15.16	14300643	99.99
2	16.52	916	0.01
Total		14301559	100.00

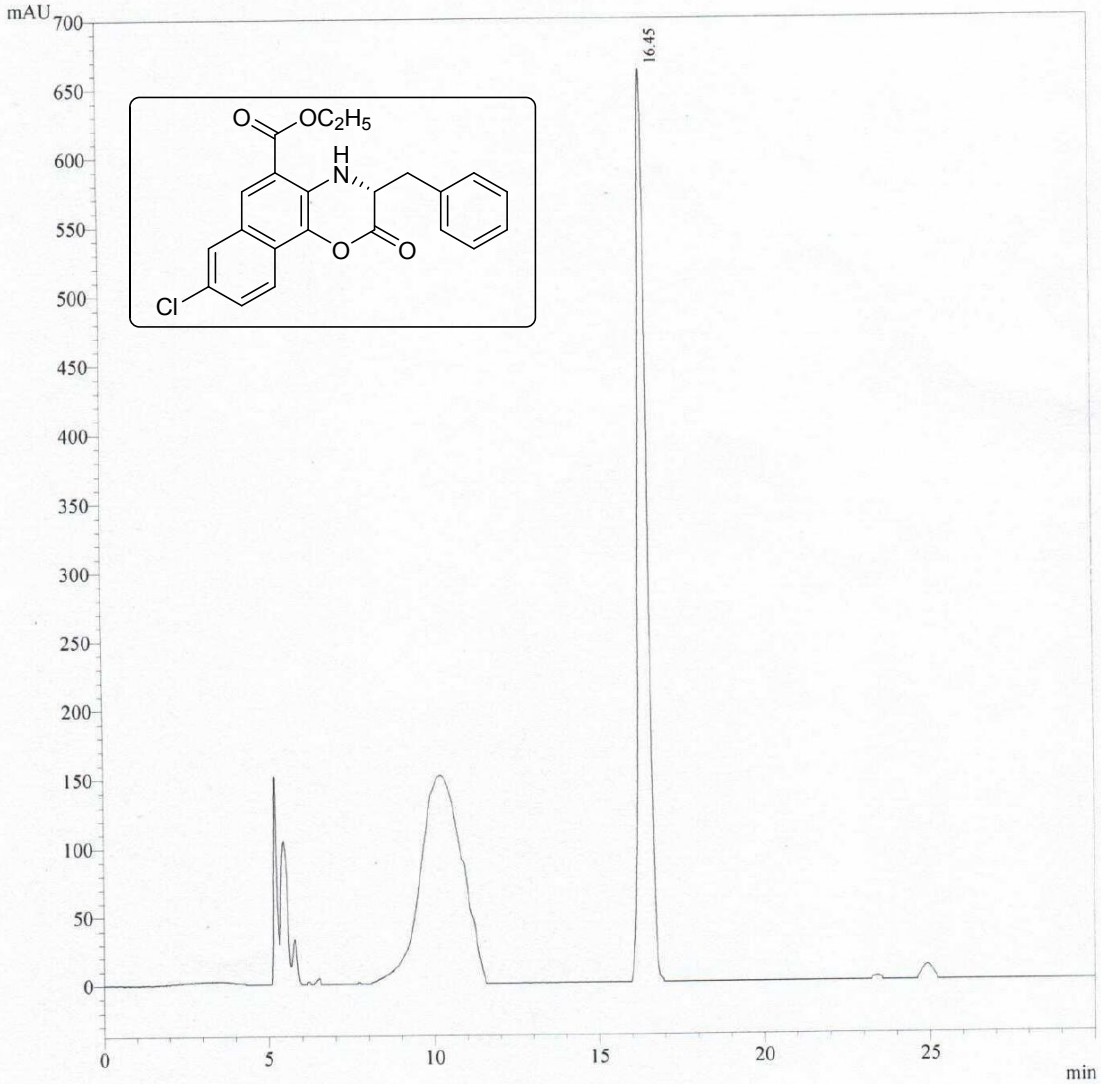
HPLC Spectrum of compound 3f

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
CROP PROTECTION CHEMICALS DIVISION

Acquired by : T RAMESH BABU
Sample Name : NAPHTHOXINONE
Sample ID : BCR-Cl- D-PA
Data Filename : NAPHTHO-29.lcd
Method Filename : ramesh.lcm
Date Acquired : 23/07/2019

39

D:\BCR\NAPHTHO-29.lcd



1 PDA Multi 1 / 200nm - 500nm 2nm

PDA Ch1 200nm - 500nm 2nm

Peak#	Ret. Time	Area	Area %
1	16.45	12991219	100.00
Total		12991219	100.00

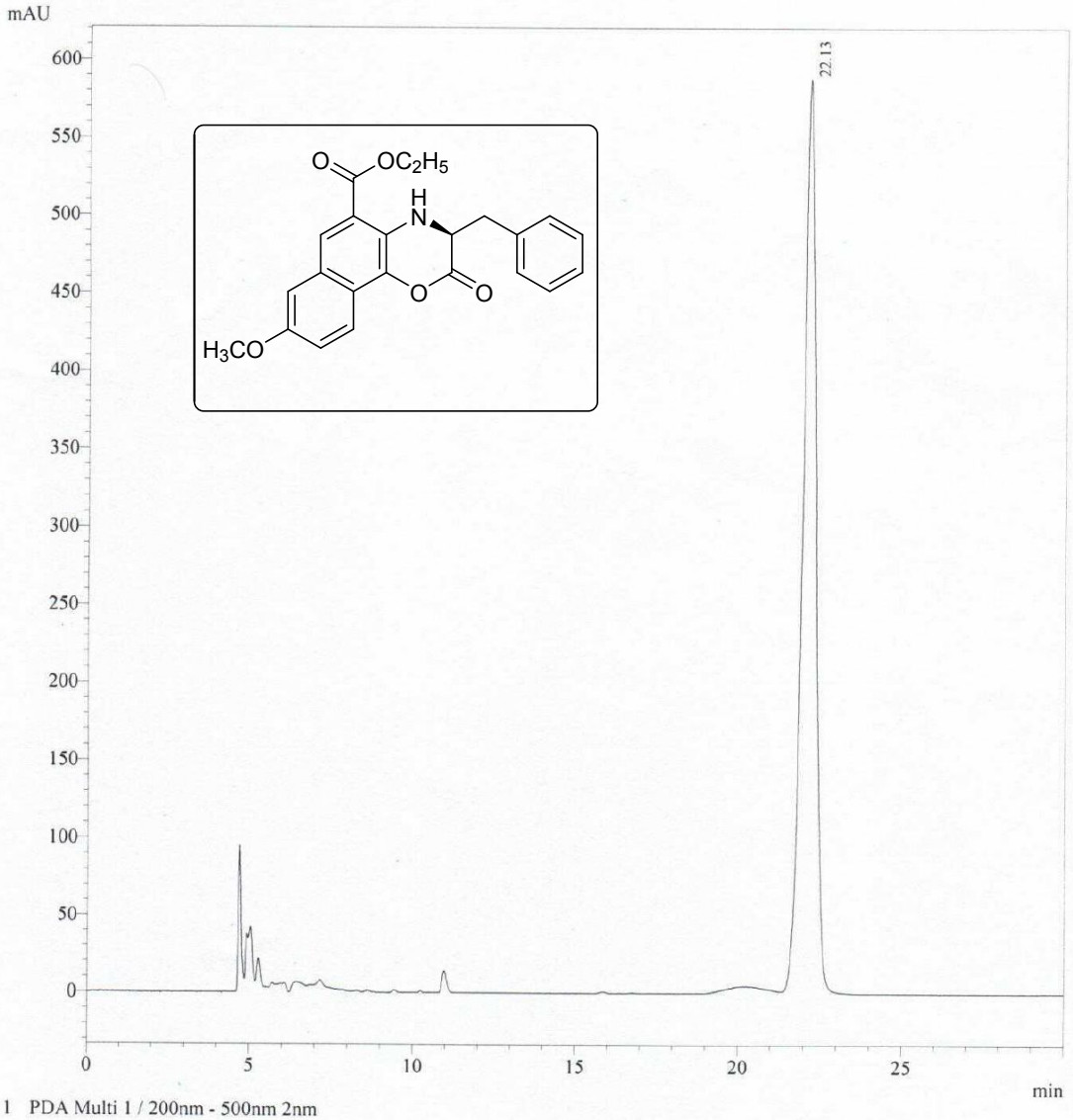
HPLC Spectrum of compound 3g

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
CROP PROTECTION CHEMICALS DIVISION

Acquired by : T RAMESH BABU
Sample Name : NAPHTHOXINONE
Sample ID : BCR-OMe-L-PA
Data Filename : NAPHTHO-25.lcd
Method Filename : ramesh.lcm
Date Acquired : 22/07/2019

3h.

D:\BCR\NAPHTHO-25.lcd



1 PDA Multi 1 / 200nm - 500nm 2nm

PDA Ch1 200nm - 500nm 2nm

Peak#	Ret. Time	Area	Area %
1	22.13	16536011	100.00
Total		16536011	100.00

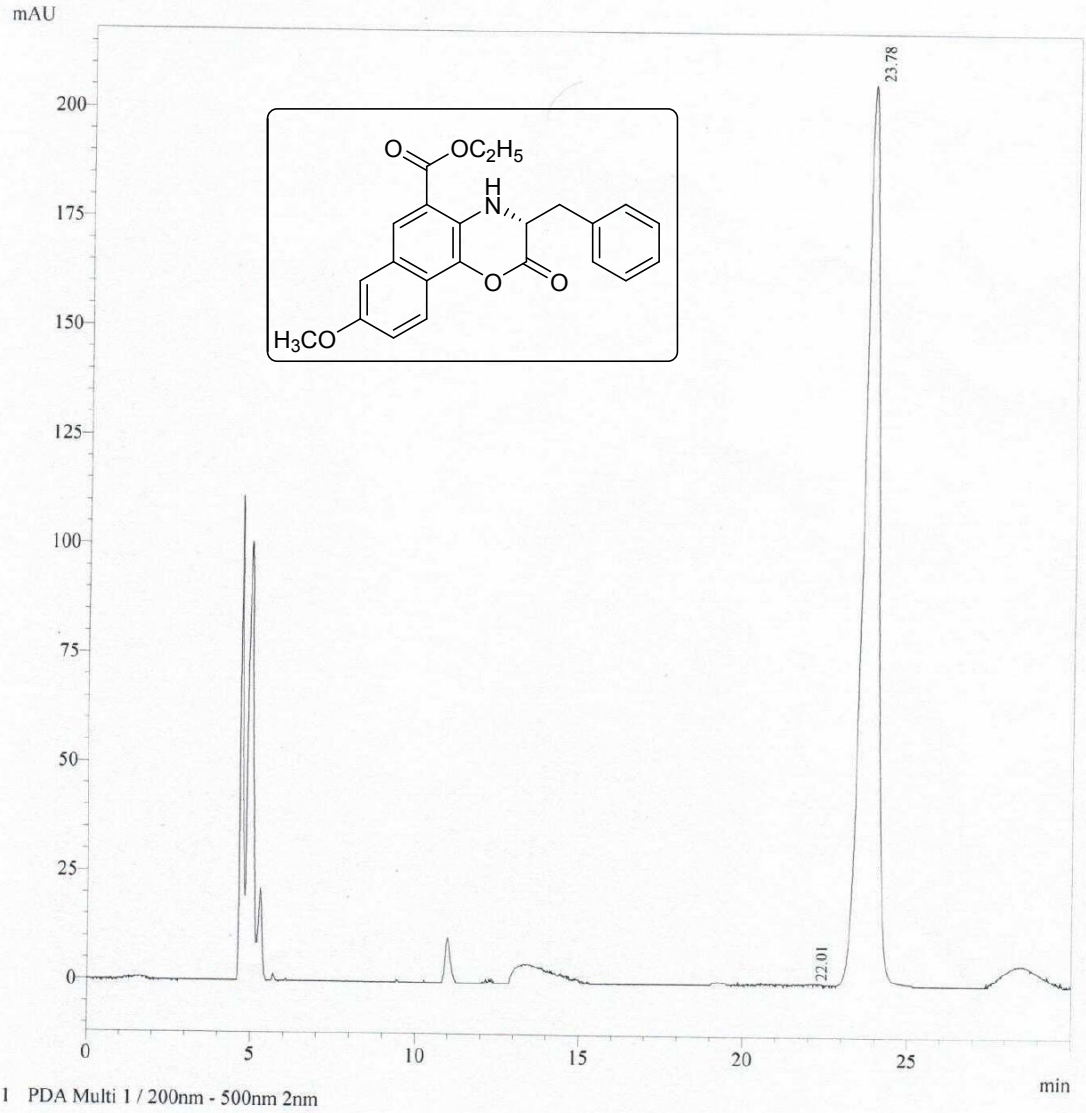
HPLC Spectrum of compound 3h

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
CROP PROTECTION CHEMICALS DIVISION

Acquired by : T RAMESH BABU
Sample Name : NAPHTHOXINONE
Sample ID : BCR-OMe-D-PA
Data Filename : NAPHTHO-26.lcd
Method Filename : ramesh.lcm
Date Acquired : 22/07/2019

D:\BCR\NAPHTHO-26.lcd

3i



1 PDA Multi 1 / 200nm - 500nm 2nm

PDA Ch1 200nm - 500nm 2nm

Peak#	Ret. Time	Area	Area %
1	22.01	1331	0.02
2	23.78	6495197	99.98
Total		6496528	100.00

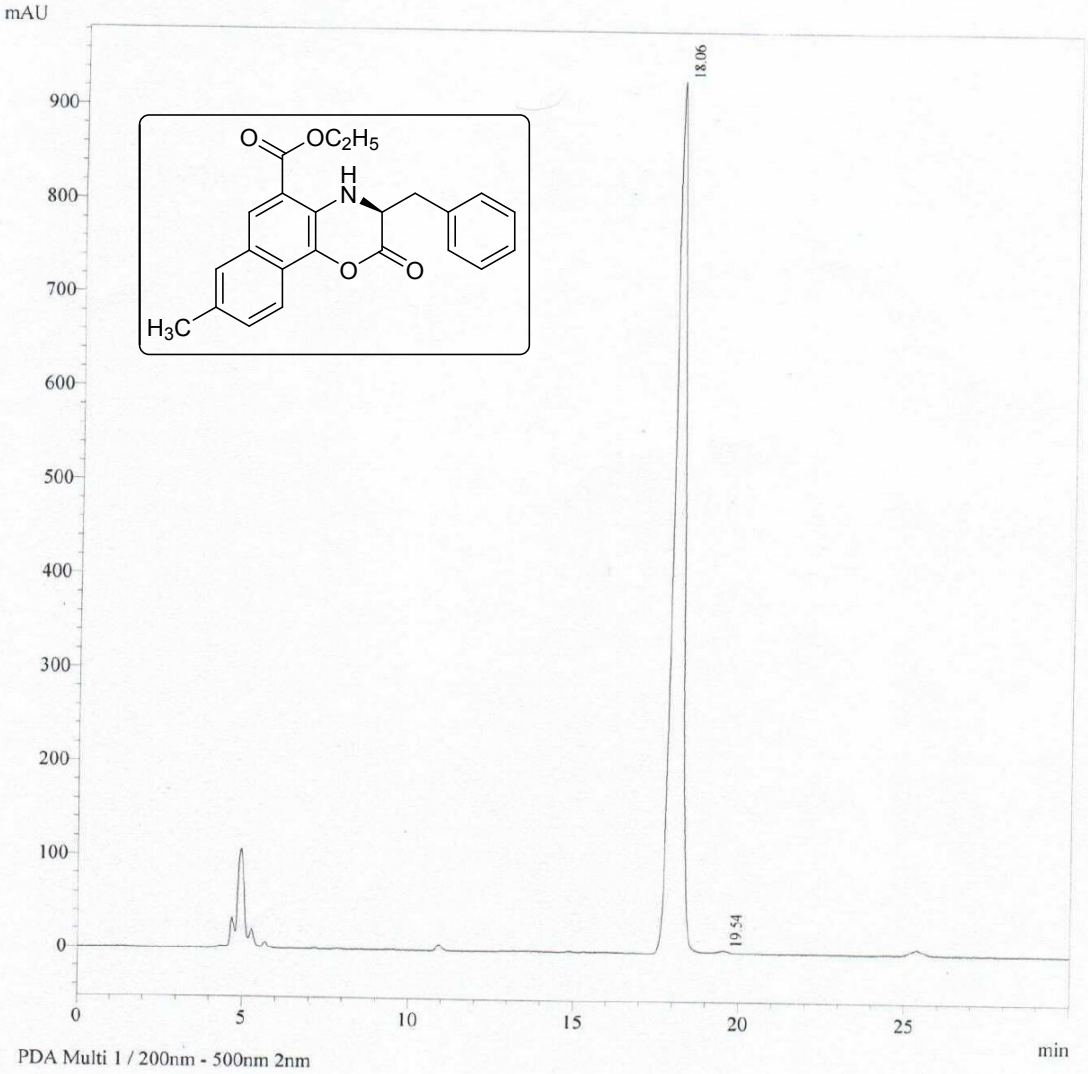
HPLC Spectrum of compound 3i

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
CROP PROTECTION CHEMICALS DIVISION

Acquired by : T RAMESH BABU
Sample Name : NAPHTHOXINONE
Sample ID : BCR-Me- L- PA
Data Filename : NAPHTHO-32.lcd
Method Filename : ramesh.lcm
Date Acquired : 23/07/2019

D:\BCR\NAPHTHO-32.lcd

3J



1 PDA Multi 1 / 200nm - 500nm 2nm

PDA Ch1 200nm - 500nm 2nm

Peak#	Ret. Time	Area	Area %
1	18.06	20616846	99.56
2	19.54	91109	0.44
Total		20707954	100.00

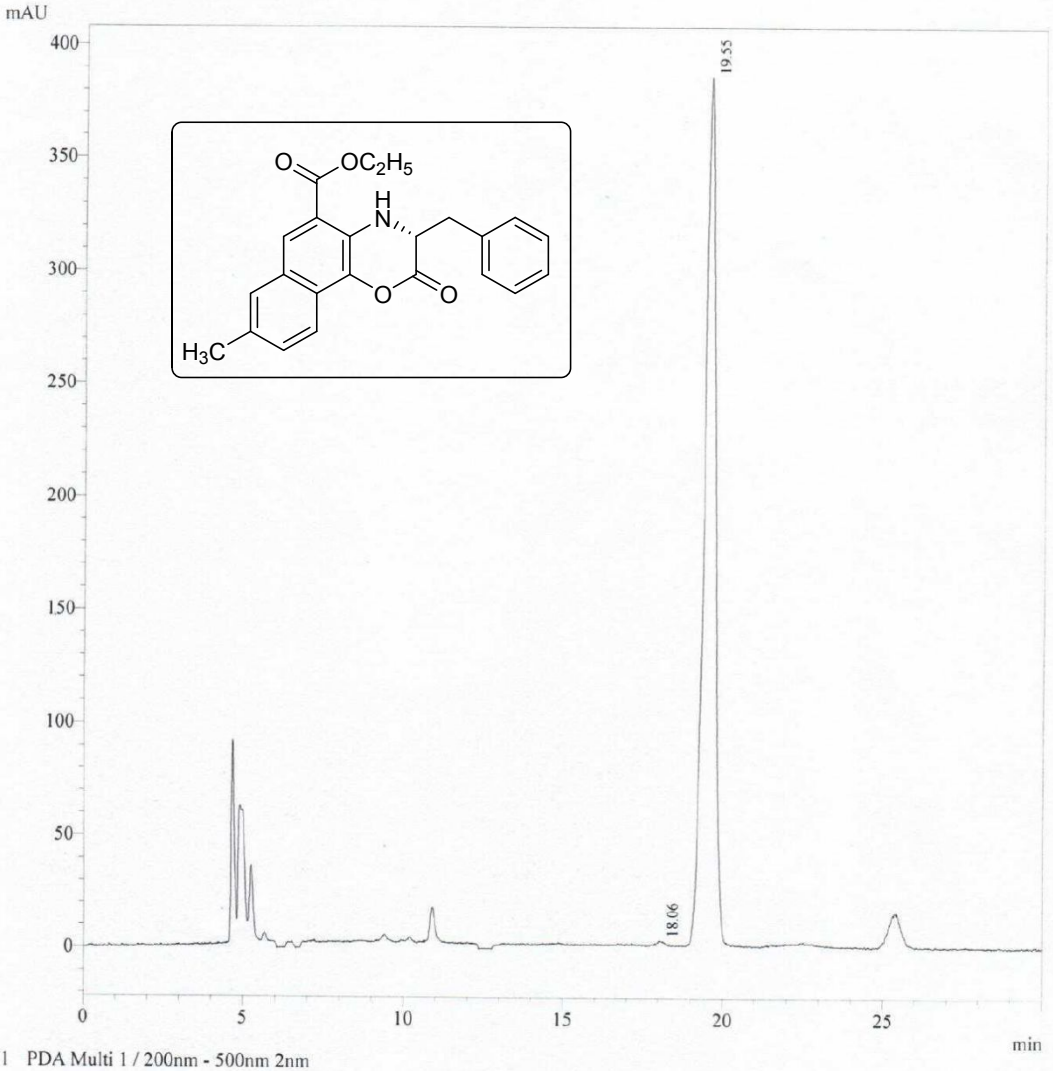
HPLC Spectrum of compound 3j

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
CROP PROTECTION CHEMICALS DIVISION

Acquired by : T RAMESH BABU
Sample Name : NAPHTHOXINONE
Sample ID : BCR-Me- D- PA
Data Filename : NAPHTHO-33.lcd
Method Filename : ramesh.lcm
Date Acquired : 23/07/2019

3K

D:\BCR\NAPHTHO-33.lcd



1 PDA Multi 1 / 200nm - 500nm 2nm

PDA Ch1 200nm - 500nm 2nm

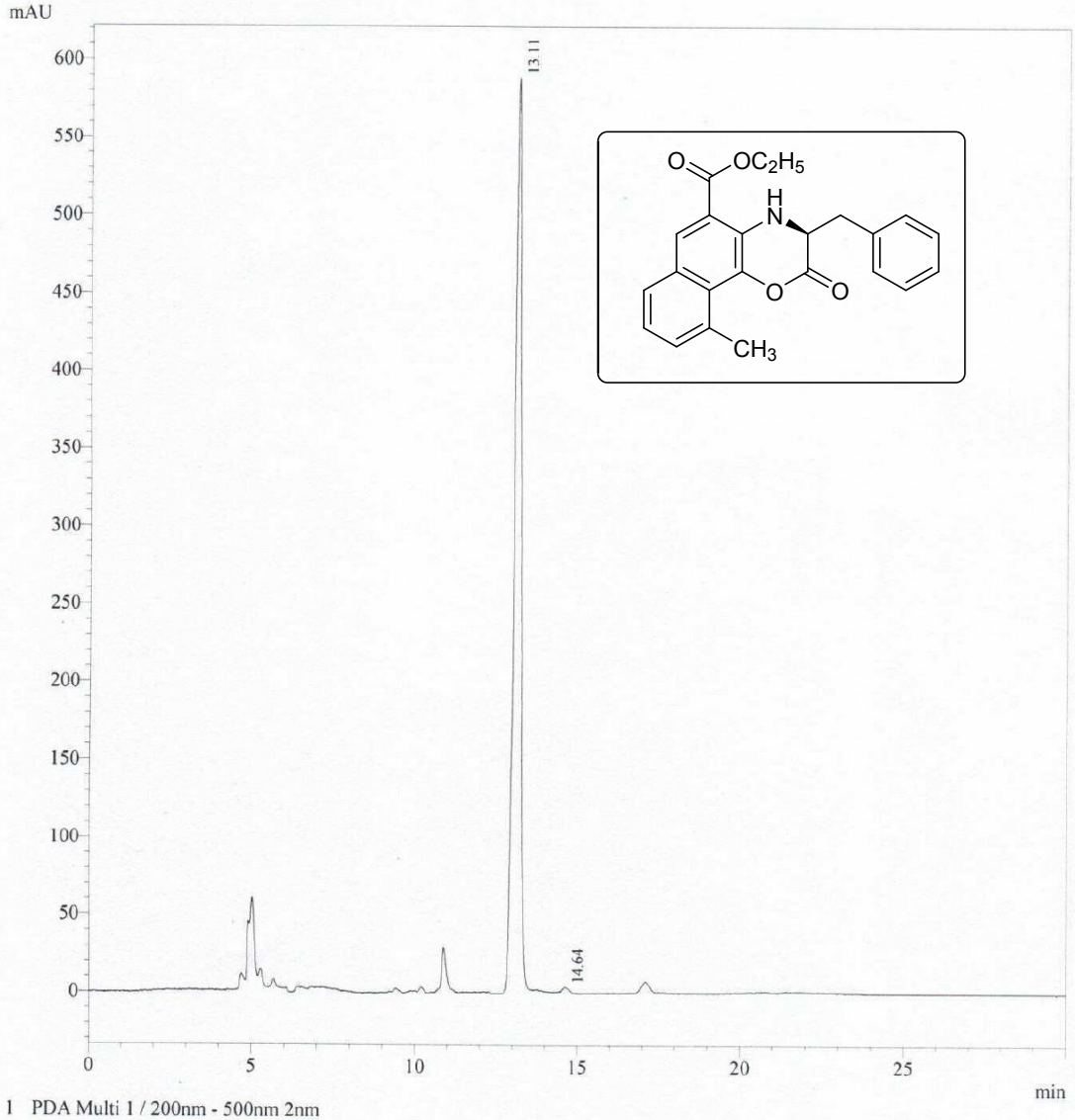
Peak#	Ret. Time	Area	Area %
1	18.06	39311	0.41
2	19.55	9536473	99.59
Total		9575784	100.00

HPLC Spectrum of compound 3k

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
CROP PROTECTION CHEMICALS DIVISION

Acquired by : T RAMESH BABU
Sample Name : NAPHTHOXINONE
Sample ID : BCR-3Me- L- PA
Data Filename : NAPHTHO-35.lcd
Method Filename : ramesh.lcm
Date Acquired : 23/07/2019

D:\BCR\NAPHTHO-35.lcd 3l



1 PDA Multi 1 / 200nm - 500nm 2nm

PDA Ch1 200nm - 500nm 2nm

Peak#	Ret. Time	Area	Area %
1	13.11	8677337	99.30
2	14.64	61523	0.70

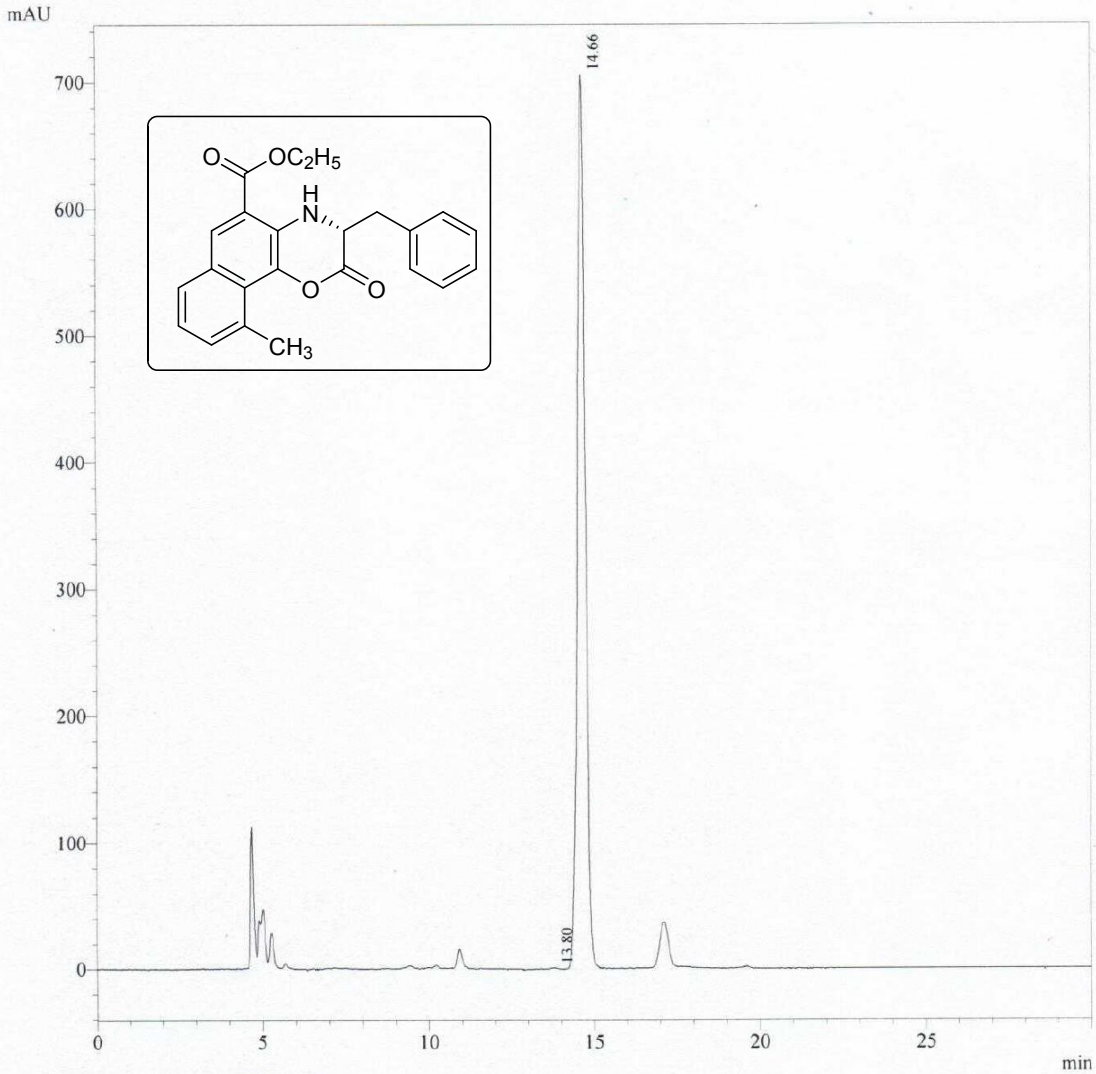
HPLC Spectrum of compound 3l

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
CROP PROTECTION CHEMICALS DIVISION

Acquired by : T RAMESH BABU
Sample Name : NAPHTHOXINONE
Sample ID : BCR-3Me- D- PA
Data Filename : NAPHTHO-34.lcd
Method Filename : ramesh.lcm
Date Acquired : 23/07/2019

3m

D:\BCR\NAPHTHO-34.lcd



1 PDA Multi 1 / 200nm - 500nm 2nm

PDA Ch1 200nm - 500nm 2nm

Peak#	Ret. Time	Area	Area %
1	13.80	20649	0.17
2	14.66	11890771	99.83
Total		11911420	100.00

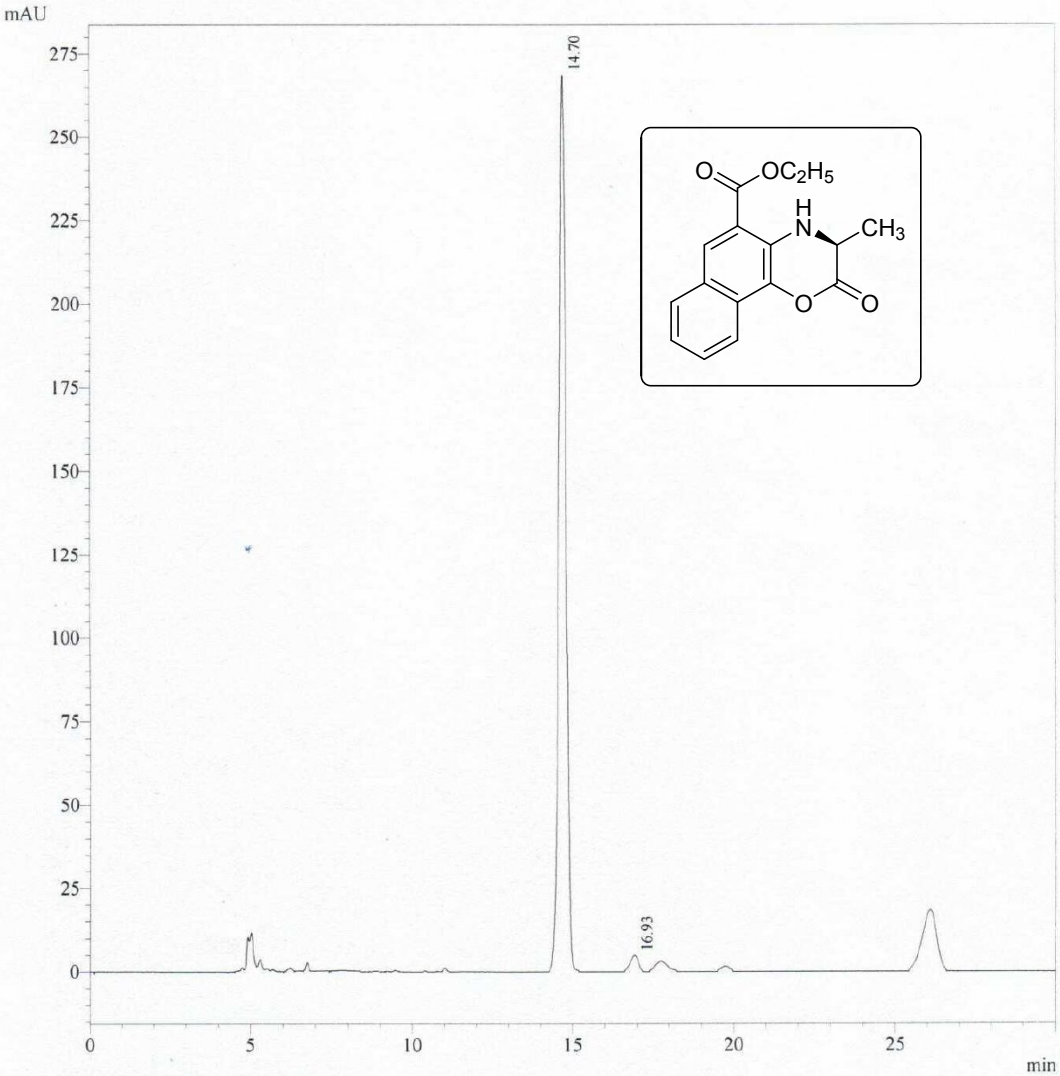
HPLC Spectrum of compound 3m

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
CROP PROTECTION CHEMICALS DIVISION

Acquired by : T RAMESH BABU
Sample Name : NAPHTHOXINONE
Sample ID : BCR-L-ALA
Data Filename : NAPHTHO-38.lcd
Method Filename : ramesh.lcm
Date Acquired : 24/07/2019

30

D:\BCR\NAPHTHO-38.lcd



1 PDA Multi 1 / 200nm - 500nm 2nm

PDA Ch1 200nm - 500nm 2nm

Peak#	Ret. Time	Area	Area %
1	14.70	4142303	97.84
2	16.93	91619	2.16
Total		4233922	100.00

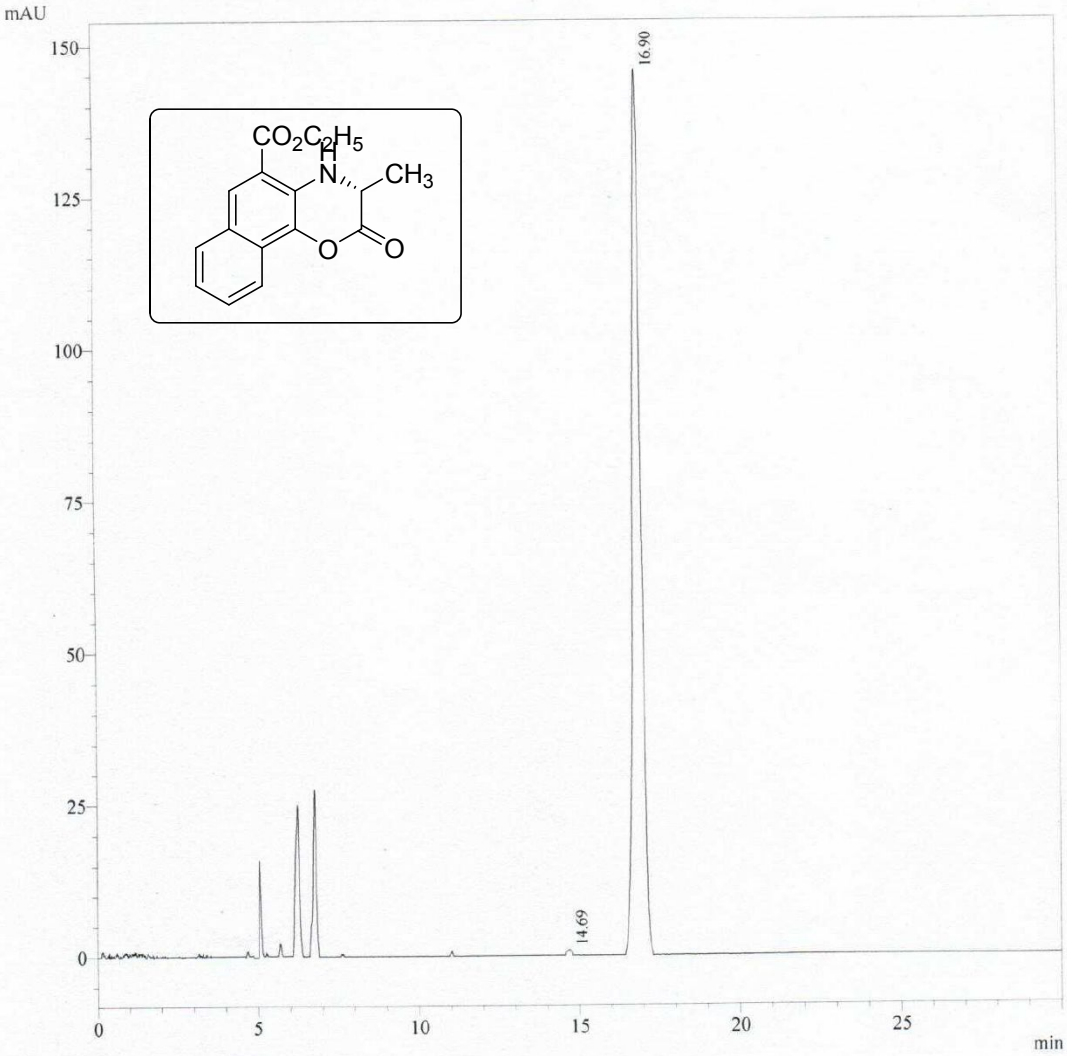
HPLC Spectrum of compound 3o

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
CROP PROTECTION CHEMICALS DIVISION

Acquired by : T RAMESH BABU
Sample Name : NAPHTHOXINONE
Sample ID : BCR-D-ALA
Data Filename : NAPHTHO-37.lcd
Method Filename : ramesh.lcm
Date Acquired : 24/07/2019

3P

D:\BCR\NAPHTHO-37.lcd



1 PDA Multi 1 / 200nm - 500nm 2nm

PDA Ch1 200nm - 500nm 2nm

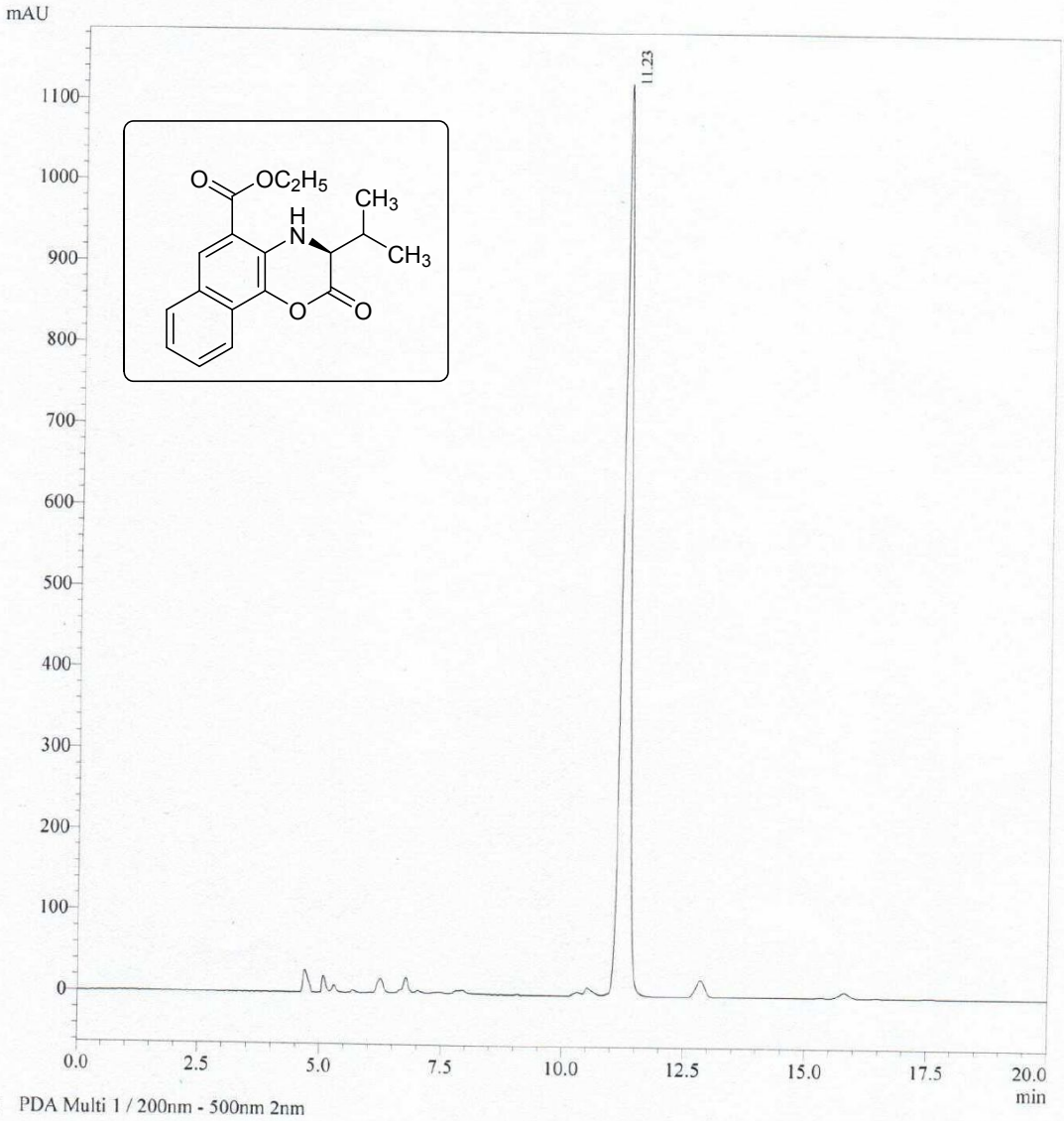
Peak#	Ret. Time	Area	Area %
1	14.69	9977	0.37
2	16.90	2702298	99.63
Total		2712275	100.00

HPLC Spectrum of compound 3p

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
CROP PROTECTION CHEMICALS DIVISION

Acquired by : T RAMESH BABU
Sample Name : NAPHTHOXINONE
Sample ID : BCR-L-VAL
Data Filename : NAPHTHO-17.lcd
Method Filename : ramesh.lcm
Date Acquired : 19/07/2019

D:\BCR\NAPHTHO-17.lcd 3q



1 PDA Multi 1 / 200nm - 500nm 2nm

PDA Ch1 200nm - 500nm 2nm

Peak#	Ret. Time	Area	Area %
1	11.23	12843476	100.00
Total		12843476	100.00

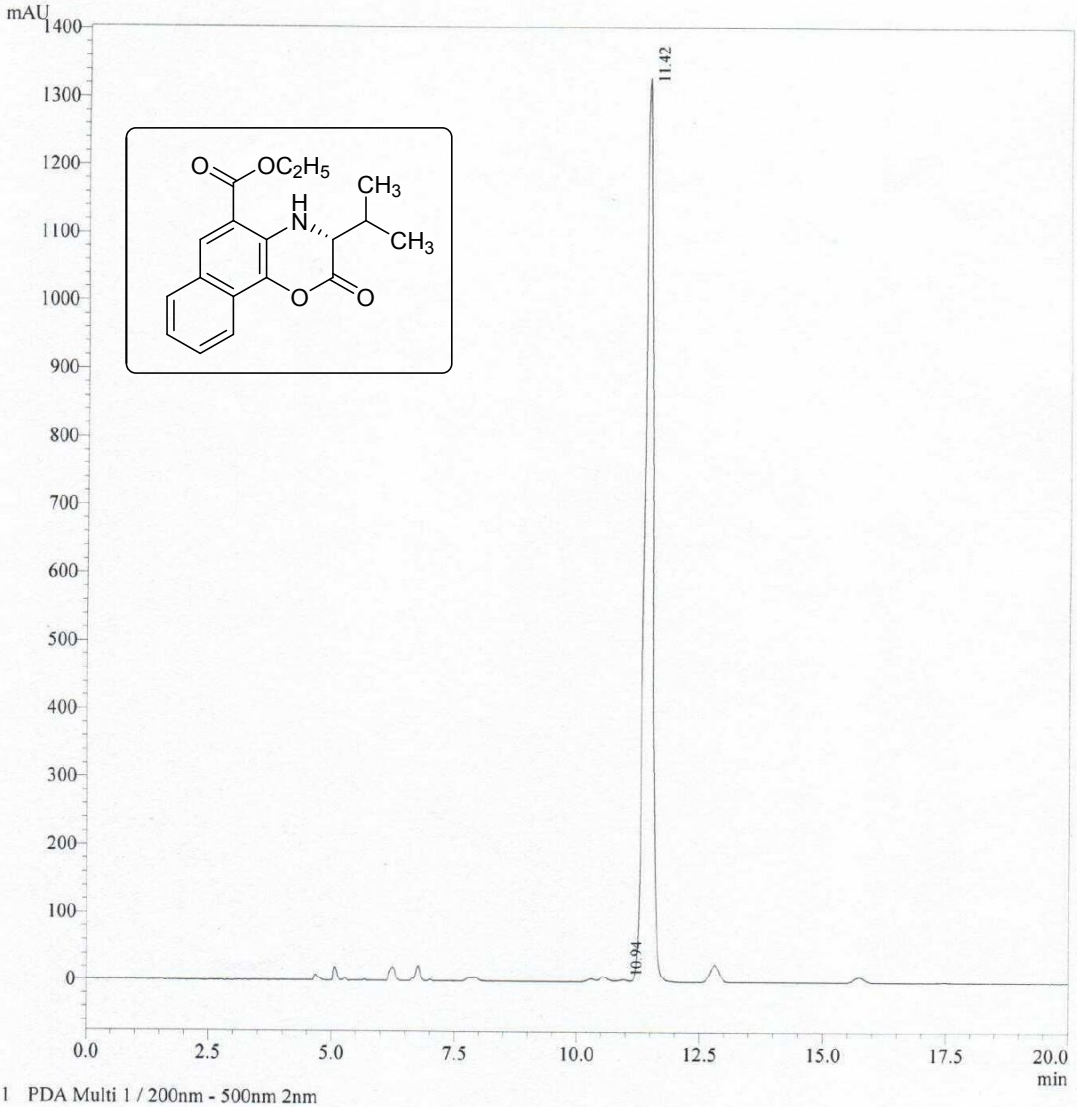
HPLC Spectrum of compound 3q

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
CROP PROTECTION CHEMICALS DIVISION

Acquired by : T RAMESH BABU
Sample Name : NAPHTHOXINONE
Sample ID : BCR-D-VAt
Data Filename : NAPHTHO-15.lcd
Method Filename : ramesh.lcm
Date Acquired : 19/07/2019

3r

D:\BCR\NAPHTHO-15.lcd



1 PDA Multi 1 / 200nm - 500nm 2nm

PDA Ch1 200nm - 500nm 2nm

Peak#	Ret. Time	Area	Area %
1	10.94	17950	0.12
2	11.42	15474286	99.88
Total		15492236	100.00

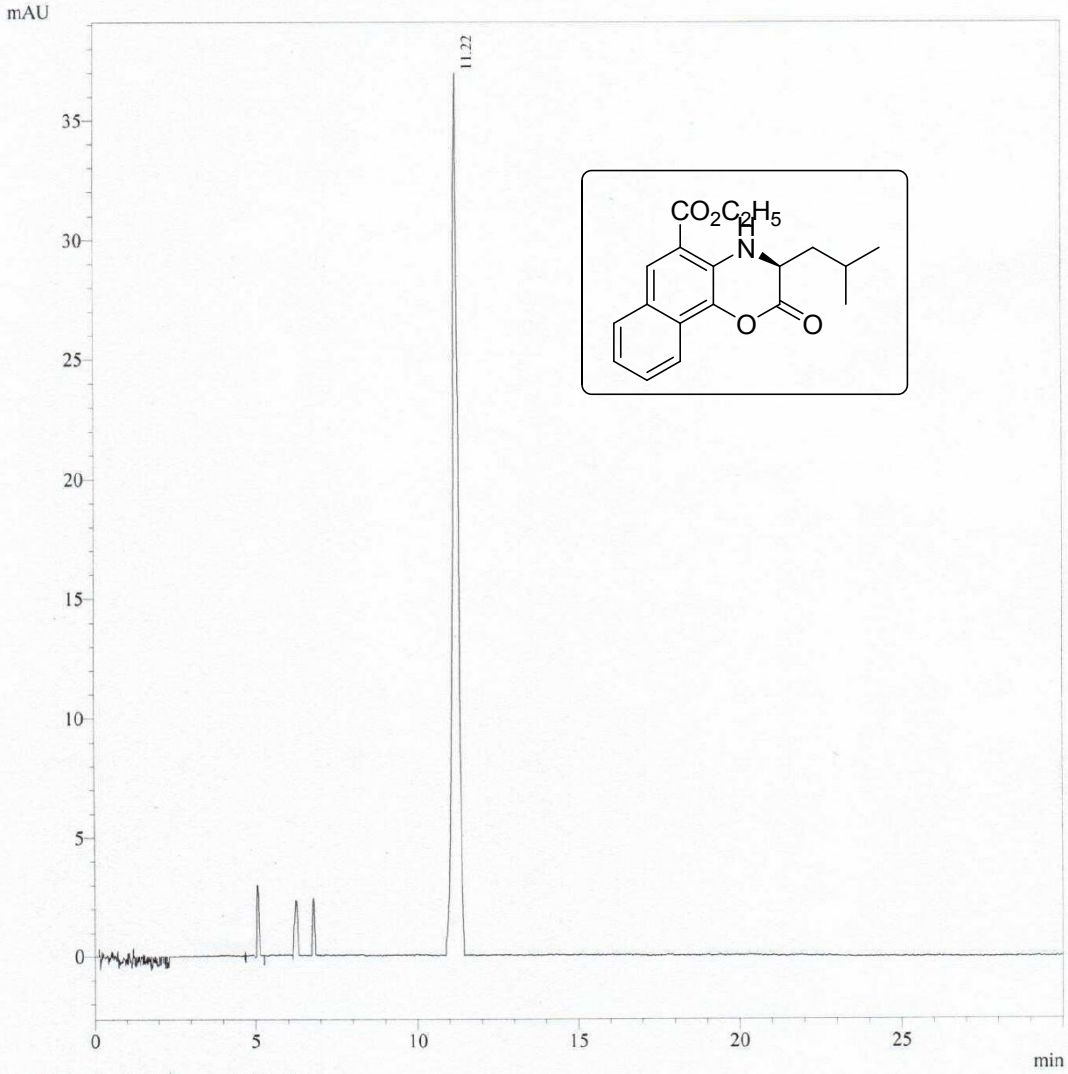
HPLC Spectrum of compound 3r

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
CROP PROTECTION CHEMICALS DIVISION

Acquired by : T RAMESH BABU
Sample Name : NAPHTHOXINONE
Sample ID : BCR-L-Leucine
Data Filename : NAPHTHO-44.lcd
Method Filename : ramesh.lcm
Date Acquired : 25/07/2019

3s

D:\BCR\NAPHTHO-44.lcd



1 PDA Multi 1 / 200nm - 500nm 2nm

PDA Ch1 200nm - 500nm 2nm

Peak#	Ret. Time	Area	Area %
1	11.22	464145	100.00
Total		464145	100.00

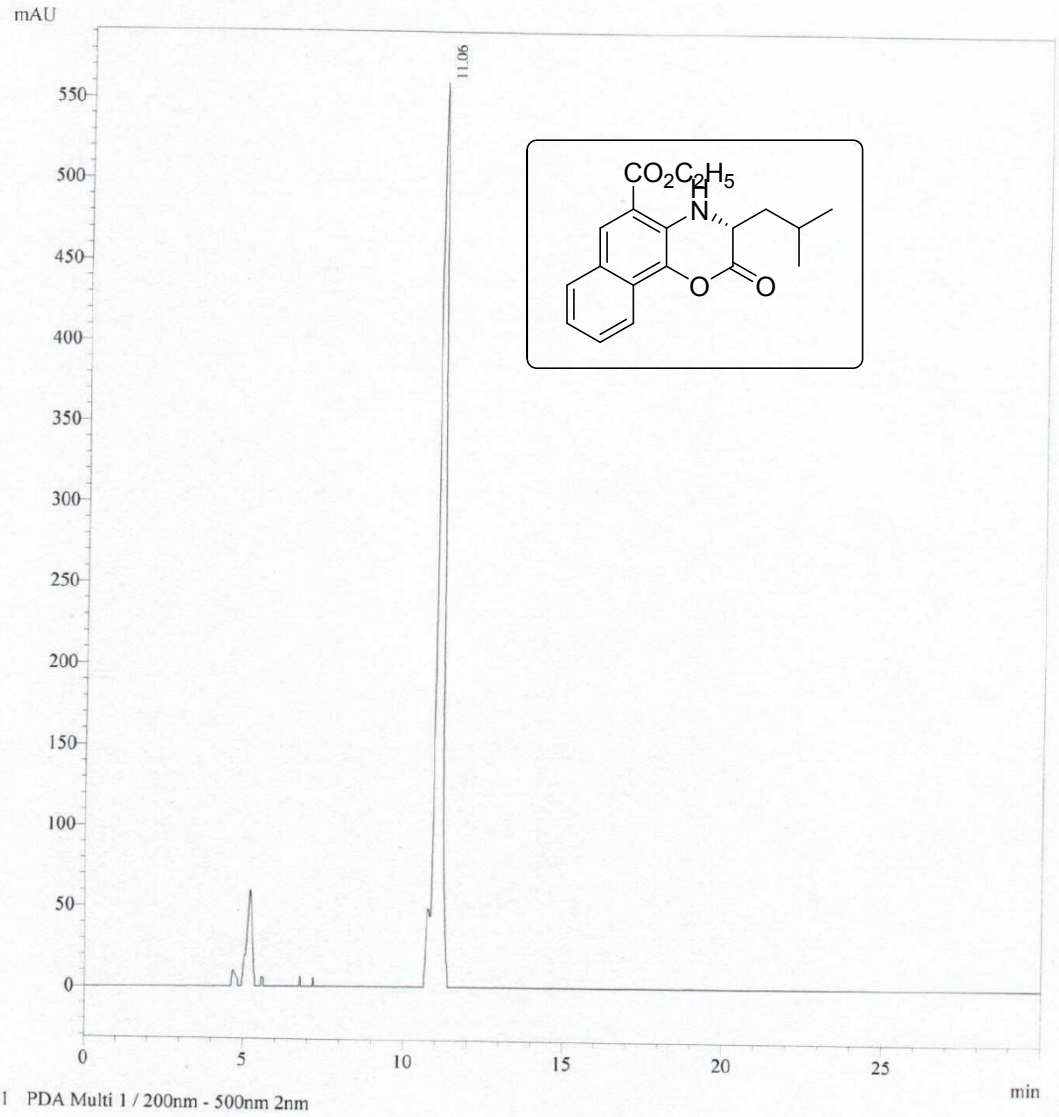
HPLC Spectrum of compound 3s

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
CROP PROTECTION CHEMICALS DIVISION

Acquired by : T RAMESH BABU
Sample Name : NAPHTHOXINONE
Sample ID : BCR-D-Leucine
Data Filename : NAPHTHO-45.lcd
Method Filename : ramesh.lcm
Date Acquired : 26/07/2019

3t

D:\BCR\NAPHTHO-45.lcd



1 PDA Multi 1 / 200nm - 500nm 2nm

PDA Ch1 200nm - 500nm 2nm

Peak#	Ret. Time	Area	Area %
1	11.06	7189186	100.00
Total		7189186	100.00

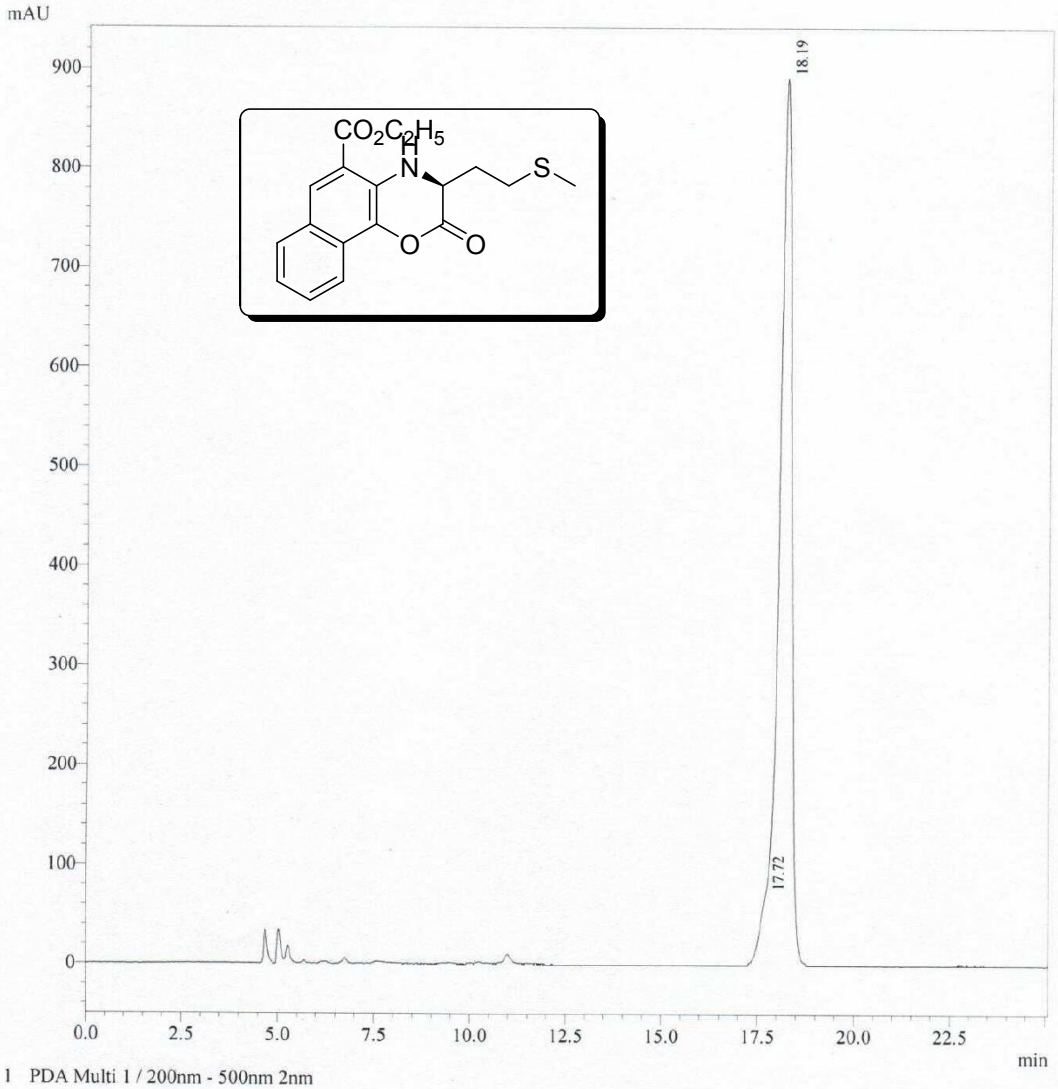
HPLC Spectrum of compound 3t

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
CROP PROTECTION CHEMICALS DIVISION

Acquired by : T RAMESH BABU
Sample Name : NAPHTHOXINONE
Sample ID : BCR-L-Meth
Data Filename : NAPHTHO-22.lcd
Method Filename : ramesh.lcm
Date Acquired : 22/07/2019

3u

D:\BCR\NAPHTHO-22.lcd



1 PDA Multi 1 / 200nm - 500nm 2nm

PDA Ch1 200nm - 500nm 2nm

Peak#	Ret. Time	Area	Area %
1	17.72	793463	3.89
2	18.19	19613922	96.11
Total		20407385	100.00

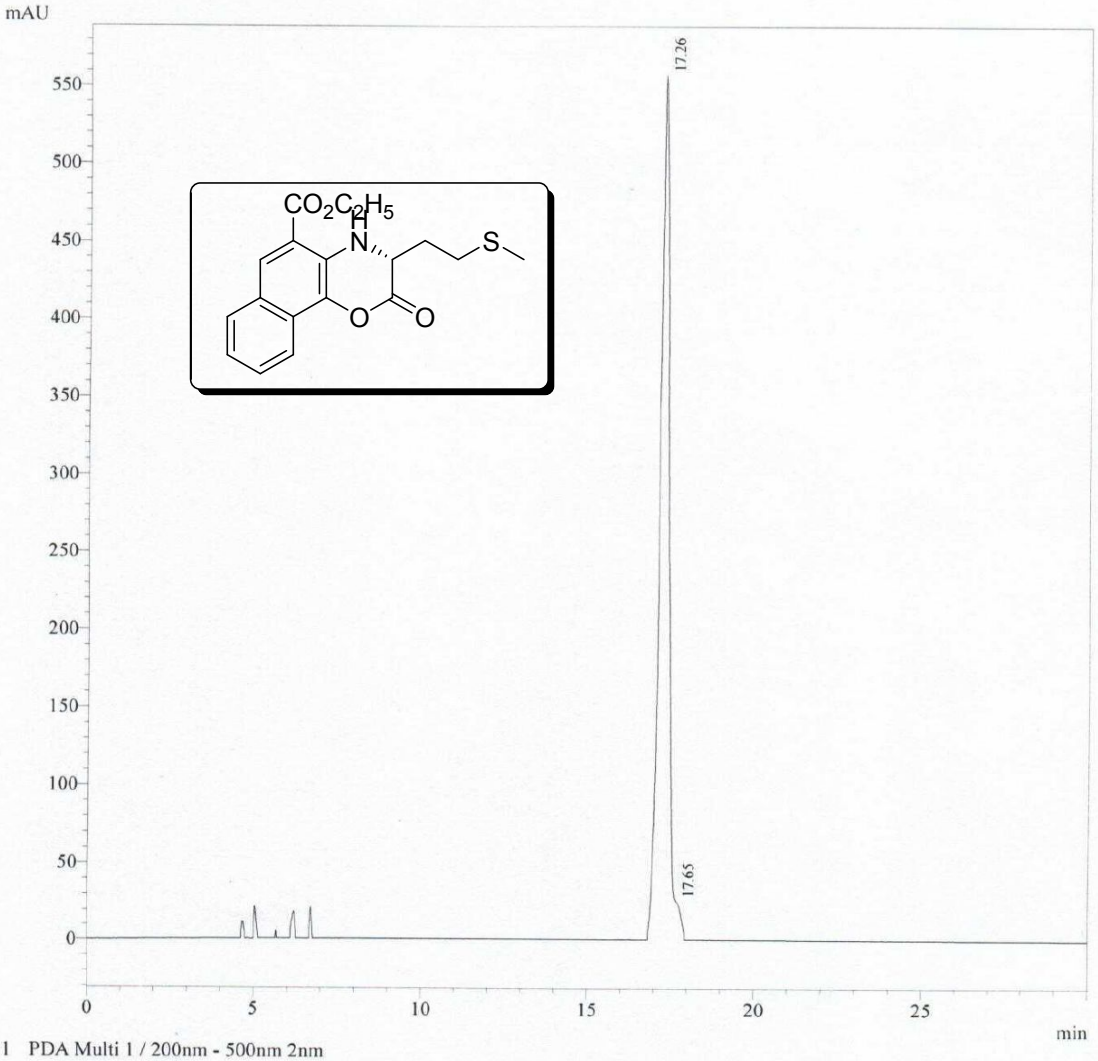
HPLC Spectrum of compound 3u

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
CROP PROTECTION CHEMICALS DIVISION

Acquired by : T RAMESH BABU
Sample Name : NAPHTHOXINONE
Sample ID : BCR-D-Meth
Data Filename : NAPHTHO-21.lcd
Method Filename : ramesh.lcm
Date Acquired : 22/07/2019

3V

D:\BCR\NAPHTHO-21.lcd



1 PDA Multi 1 / 200nm - 500nm 2nm

PDA Ch1 200nm - 500nm 2nm

Peak#	Ret. Time	Area	Area %
1	17.26	11071680	97.28
2	17.65	310111	2.72
Total		11381791	100.00

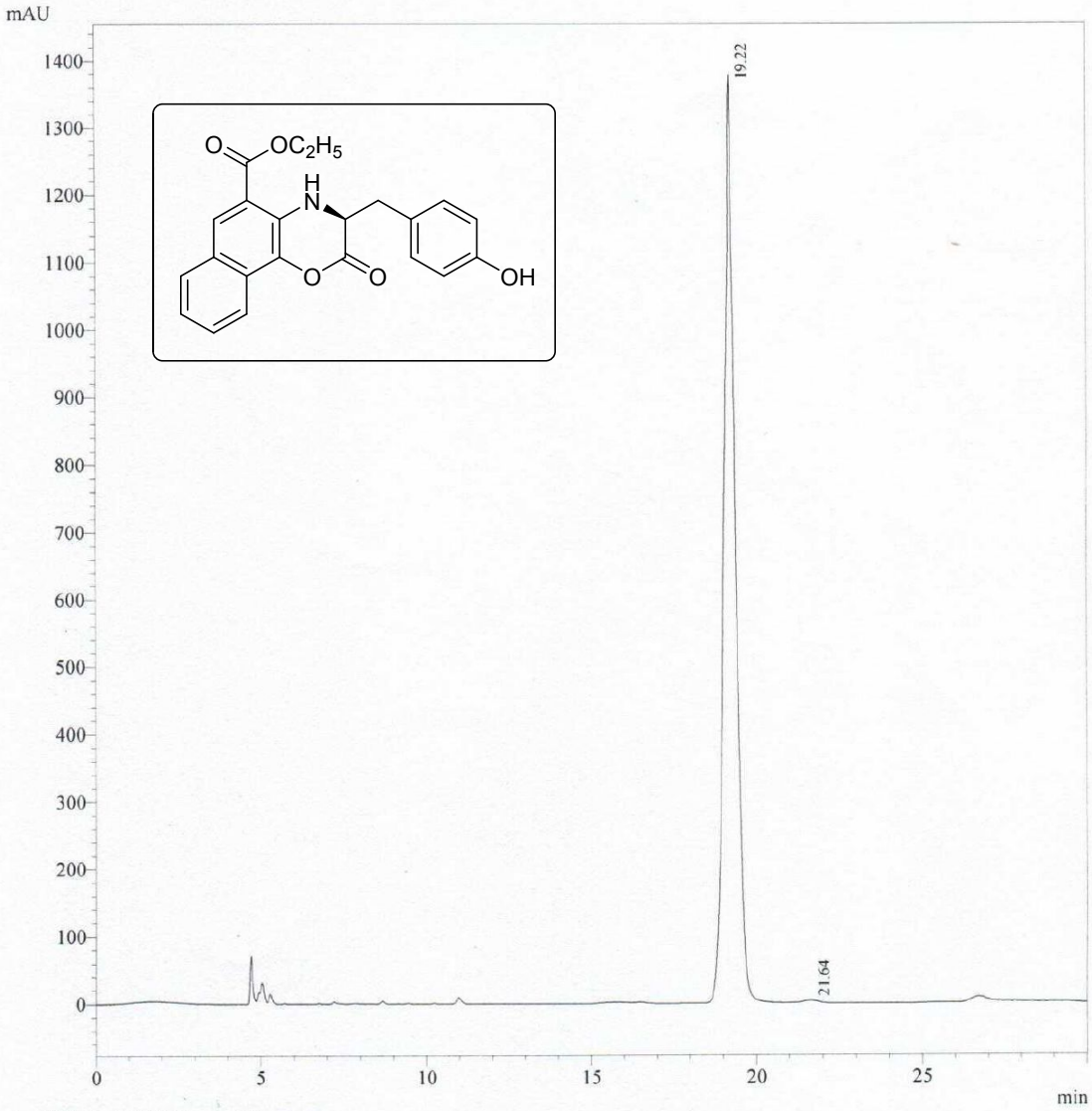
HPLC Spectrum of compound 3v

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
CROP PROTECTION CHEMICALS DIVISION

Acquired by : T RAMESH BABU
Sample Name : NAPHTHOXINONE
Sample ID : BCR-L-Tyro
Data Filename : NAPHTHO-24.lcd
Method Filename : ramesh.lcm
Date Acquired : 22/07/2019

D:\BCR\NAPHTHO-24.lcd

3w



1 PDA Multi 1 / 200nm - 500nm 2nm

PDA Ch1 200nm - 500nm 2nm

Peak#	Ret. Time	Area	Area %
1	19.22	32355989	99.79
2	21.64	67912	0.21

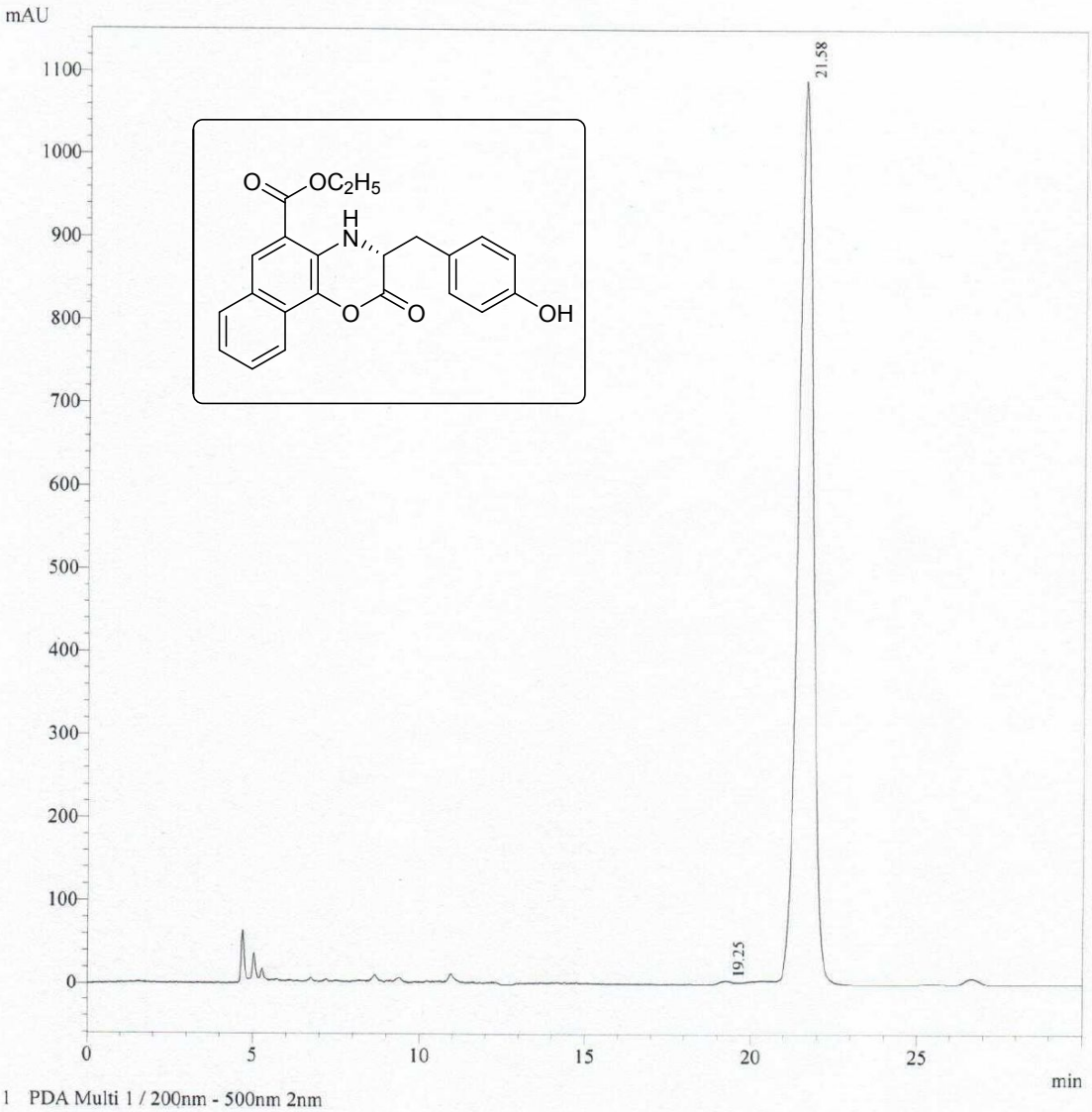
HPLC Spectrum of compound 3x

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
CROP PROTECTION CHEMICALS DIVISION

Acquired by : T RAMESH BABU
Sample Name : NAPHTHOXINONE
Sample ID : BCR-D-Tyro
Data Filename : NAPHTHO-23.lcd
Method Filename : ramesh.lcm
Date Acquired : 22/07/2019

3x

D:\BCR\NAPHTHO-23.lcd



1 PDA Multi 1 / 200nm - 500nm 2nm

PDA Ch1 200nm - 500nm 2nm

Peak#	Ret. Time	Area	Area %
1	19.25	71646	0.21
2	21.58	33705259	99.79
Total		33776905	100.00

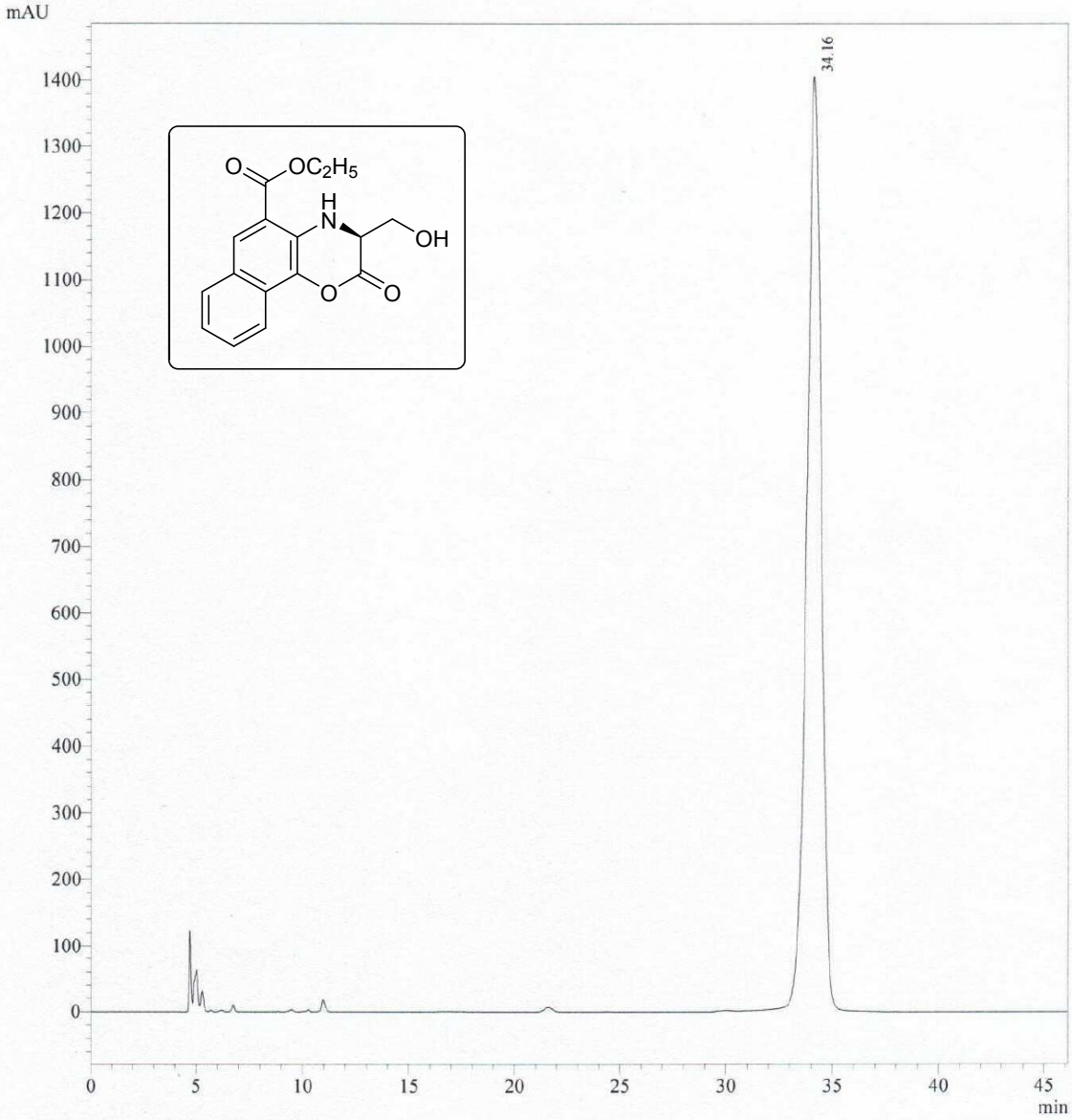
HPLC Spectrum of compound 3y

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
CROP PROTECTION CHEMICALS DIVISION

Acquired by : T RAMESH BABU
Sample Name : NAPHTHOXINONE
Sample ID : BCR-L-Serine
Data Filename : NAPHTHO-40.lcd
Method Filename : ramesh.lcm
Date Acquired : 24/07/2019

3y

D:\BCR\NAPHTHO-40.lcd



1 PDA Multi 1 / 200nm - 500nm 2nm

PDA Ch1 200nm - 500nm 2nm

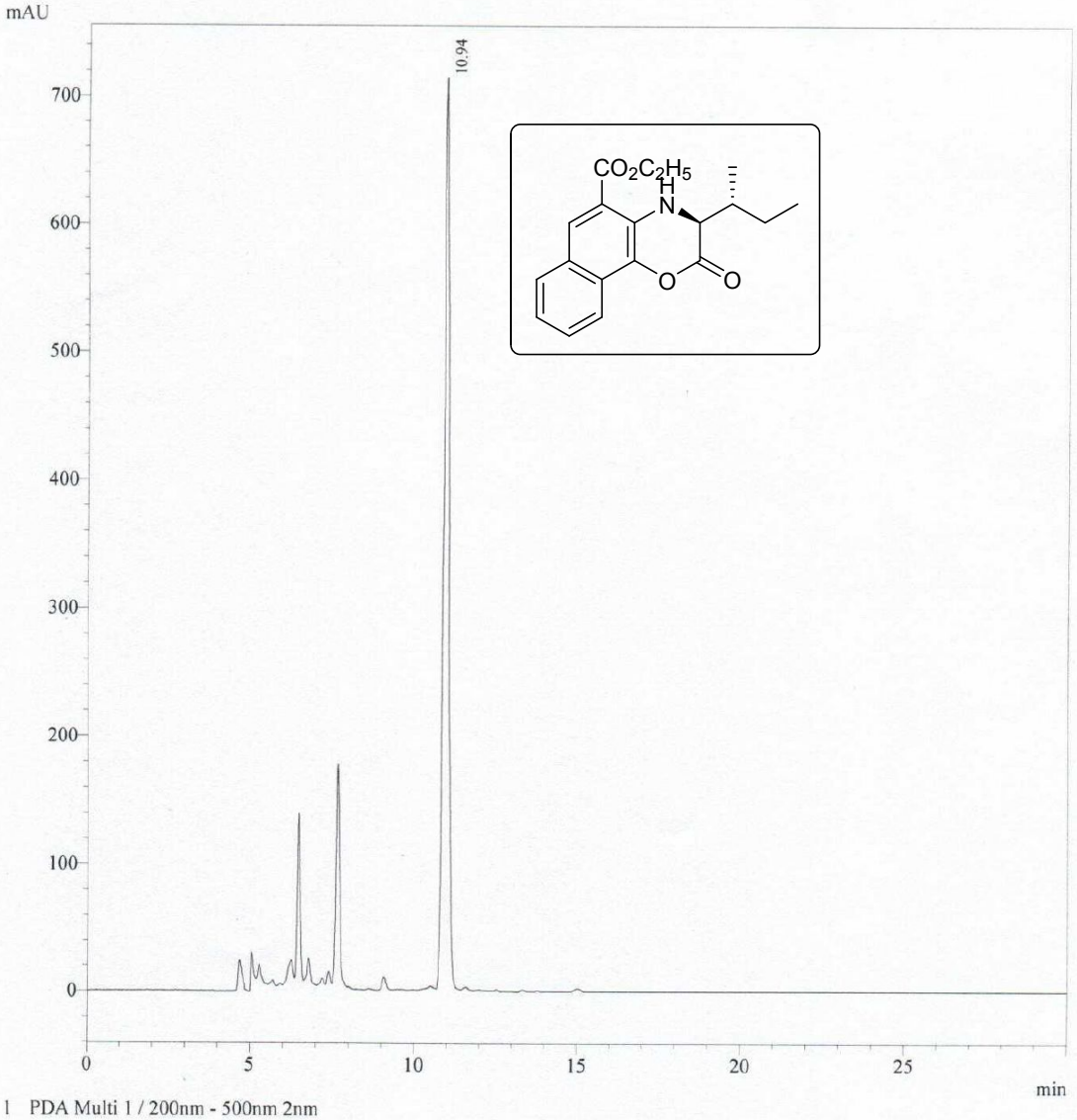
Peak#	Ret. Time	Area	Area %
1	34.16	67010675	100.00

HPLC Spectrum of compound 3z

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
CROP PROTECTION CHEMICALS DIVISION

Acquired by : T RAMESH BABU
Sample Name : NAPHTHOXINONE
Sample ID : BCR-L-Iso Leucine
Data Filename : NAPHTHO-46.lcd
Method Filename : ramesh.lcm
Date Acquired : 26/07/2019

D:\BCR\NAPHTHO-46.lcd 32



1 PDA Multi 1 / 200nm - 500nm 2nm

PDA Ch1 200nm - 500nm 2nm

Peak#	Ret. Time	Area	Area %
1	10.94	8321058	100.00
Total		8321058	100.00

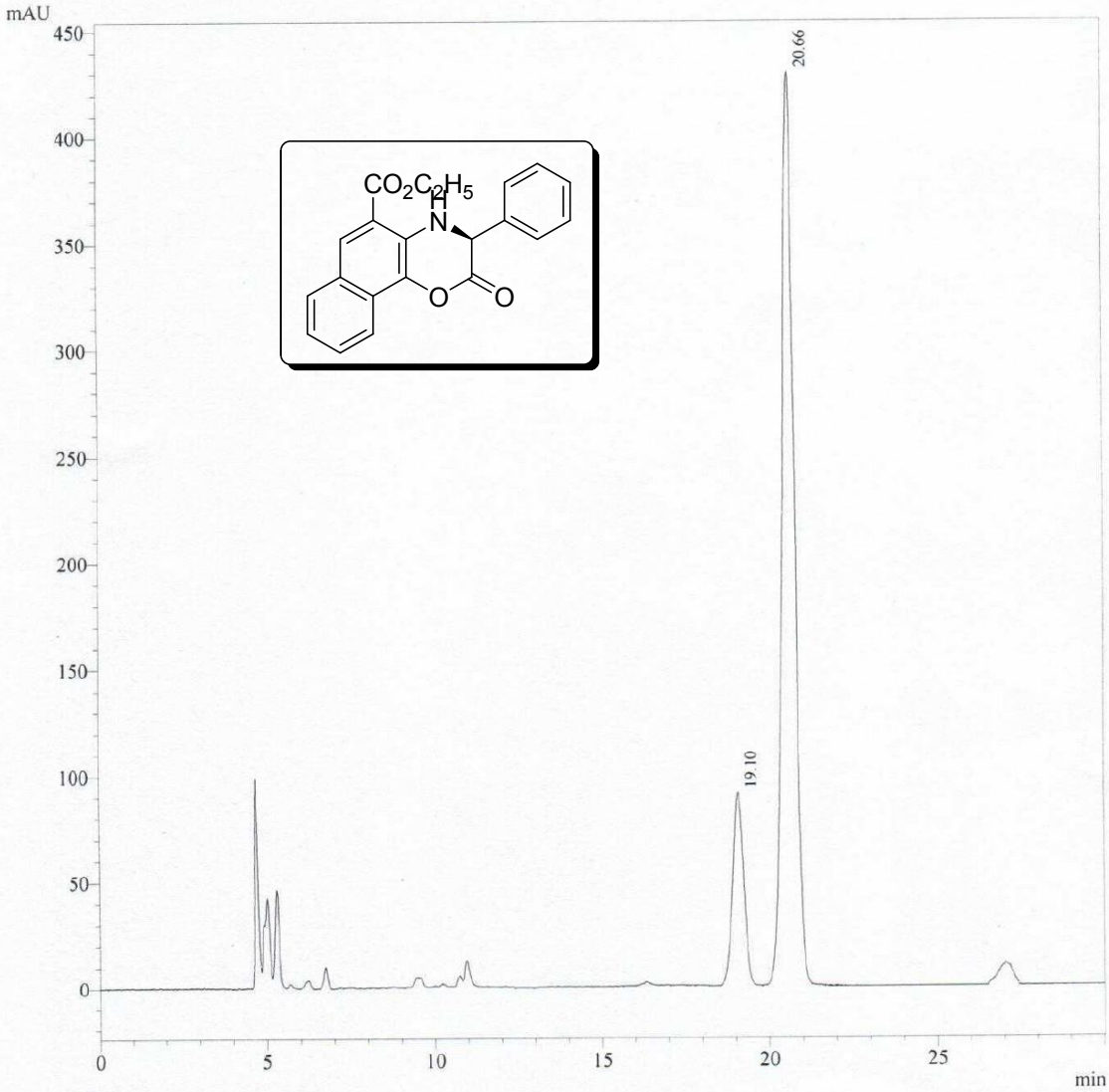
HPLC Spectrum of compound 3zb

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
CROP PROTECTION CHEMICALS DIVISION

Acquired by : T RAMESH BABU
Sample Name : NAPHTHOXINONE
Sample ID : BCR-D-Ph-Gly
Data Filename : NAPHTHO-41.lcd
Method Filename : ramesh.lcm
Date Acquired : 24/07/2019

3za

D:\BCR\NAPHTHO-41.lcd



1 PDA Multi 1 / 200nm - 500nm 2nm

PDA Ch1 200nm - 500nm 2nm

Peak#	Ret. Time	Area	Area %
1	19.10	2120846	16.25
2	20.66	10930469	83.75
Total		13051316	100.00

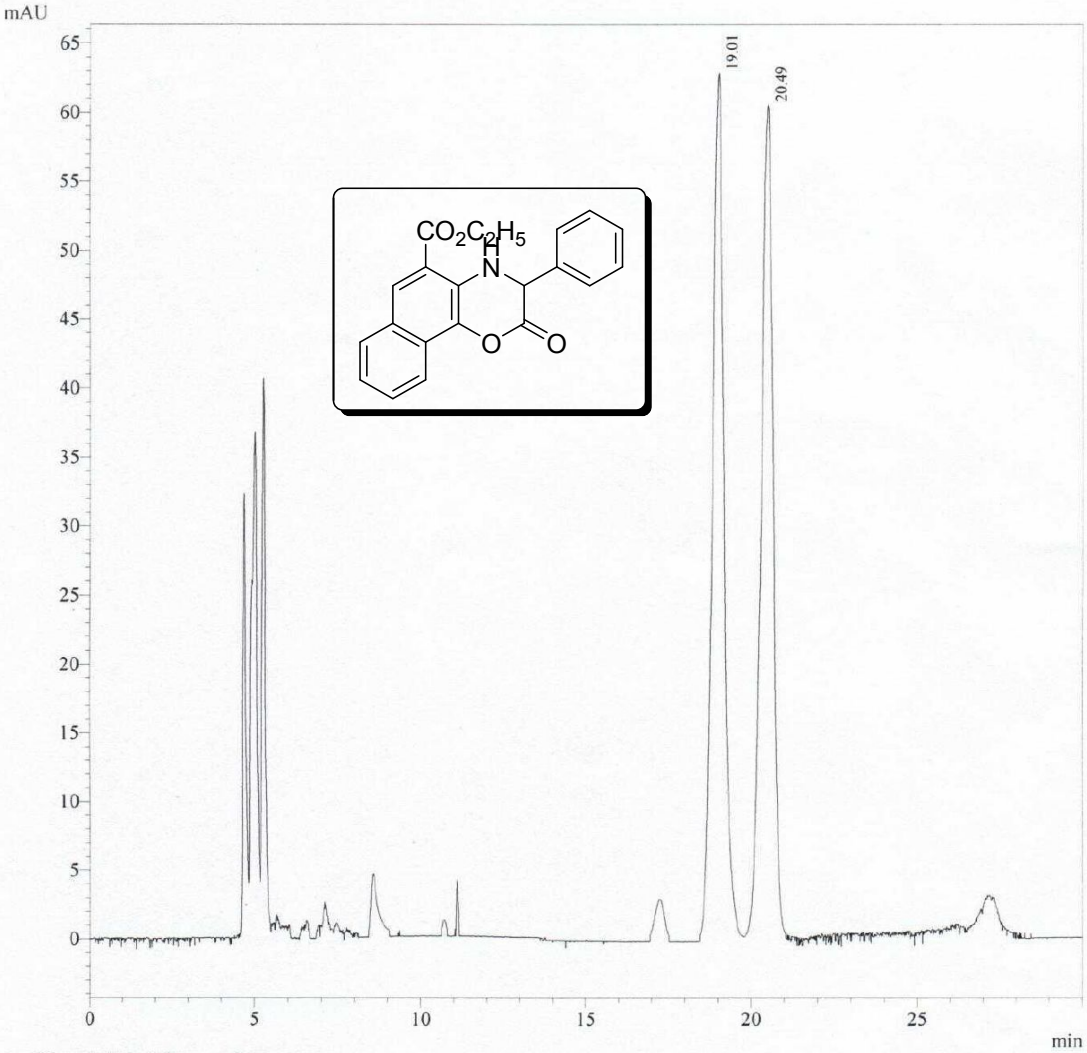
HPLC Spectrum of compound 3ze

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
CROP PROTECTION CHEMICALS DIVISION

Acquired by : T RAMESH BABU
Sample Name : BCR
Sample ID : L-Phenyl Glycine
Data Filename : NAPHTHO-51.lcd
Method Filename : ramesh.lcm
Date Acquired : 07/08/2019

D:\BCR\NAPHTHO-51.lcd

3zb



1 PDA Multi 1 / 200nm - 500nm 2nm

PDA Ch1 200nm - 500nm 2nm

Peak#	Ret. Time	Area	Area %
1	19.01	1543799	49.79
2	20.49	1556804	50.21
Total		3100603	100.00

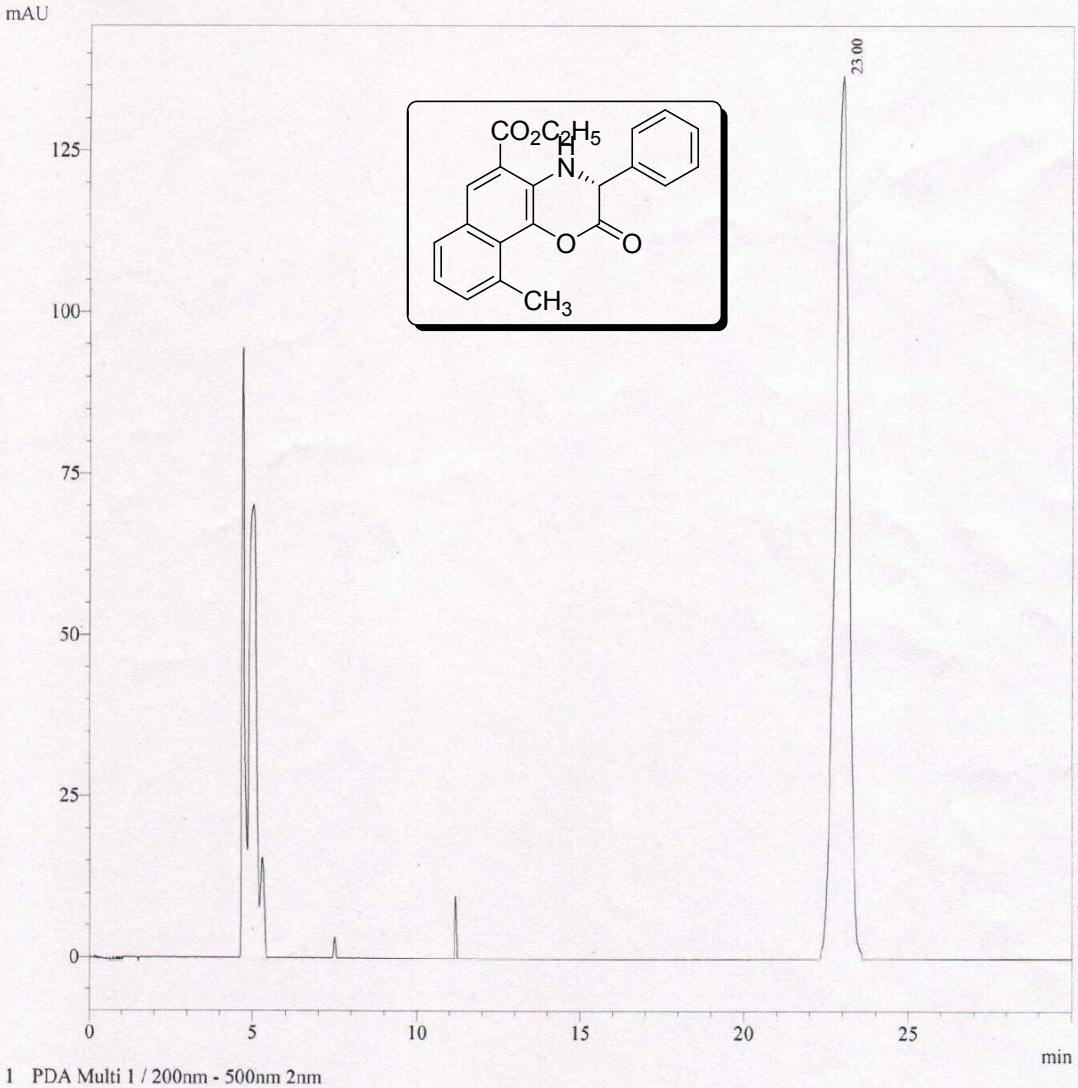
HPLC Spectrum of compound 3zf

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
CROP PROTECTION CHEMICALS DIVISION

Acquired by : T RAMESH BABU
Sample Name : BCR
Sample ID : 3-CH3-L-Phenyl Glycine
Data Filename : NAPHTHO-54.lcd
Method Filename : ramesh.lcm
Date Acquired : 08/08/2019

3zC

D:\BCR\NAPHTHO-54.lcd



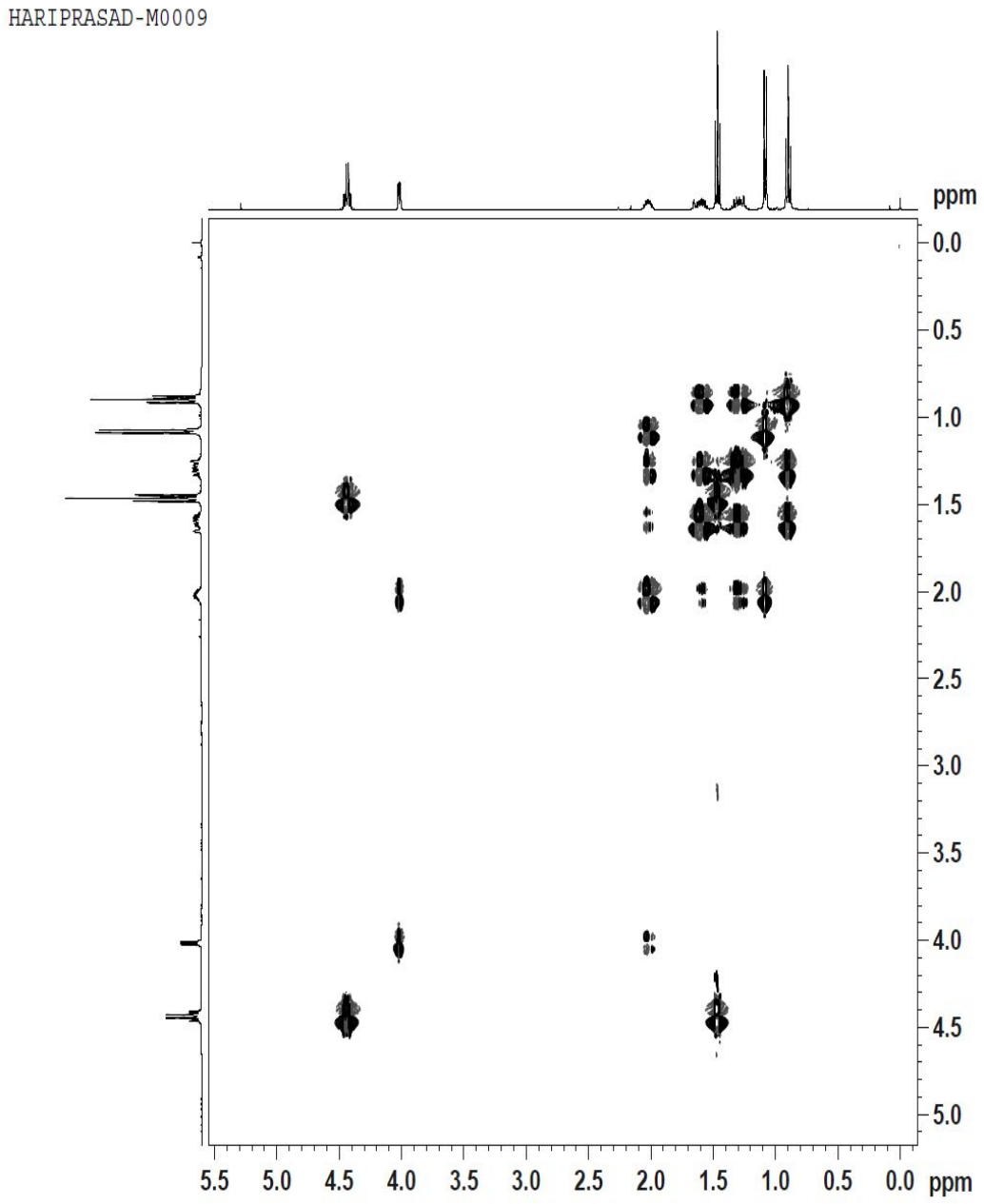
1 PDA Multi 1 / 200nm - 500nm 2nm

PDA Ch1 200nm - 500nm 2nm

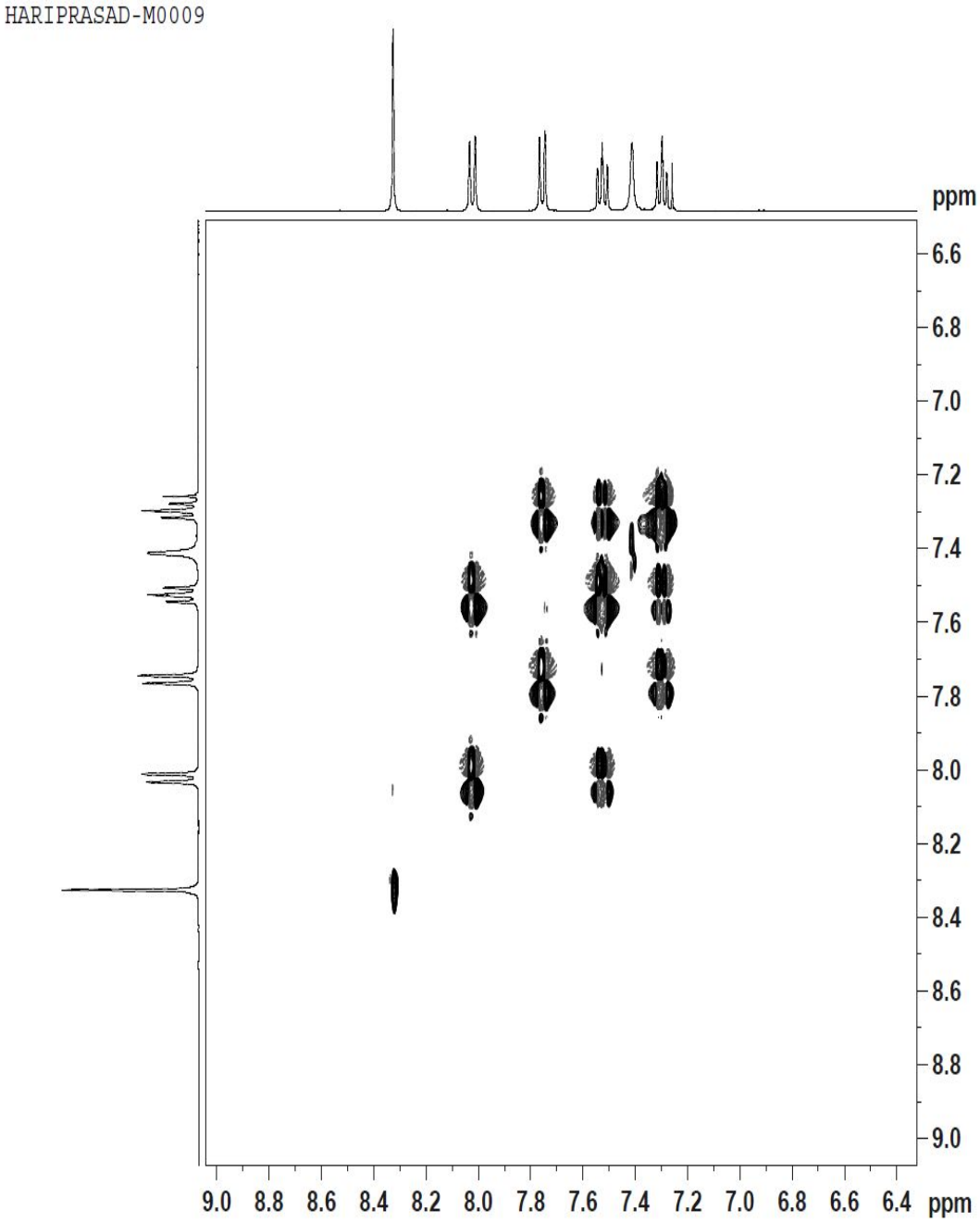
Peak#	Ret. Time	Area	Area %
1	23.00	3873576	100.00
Total		3873576	100.00

HPLC Spectrum of compound 3zg

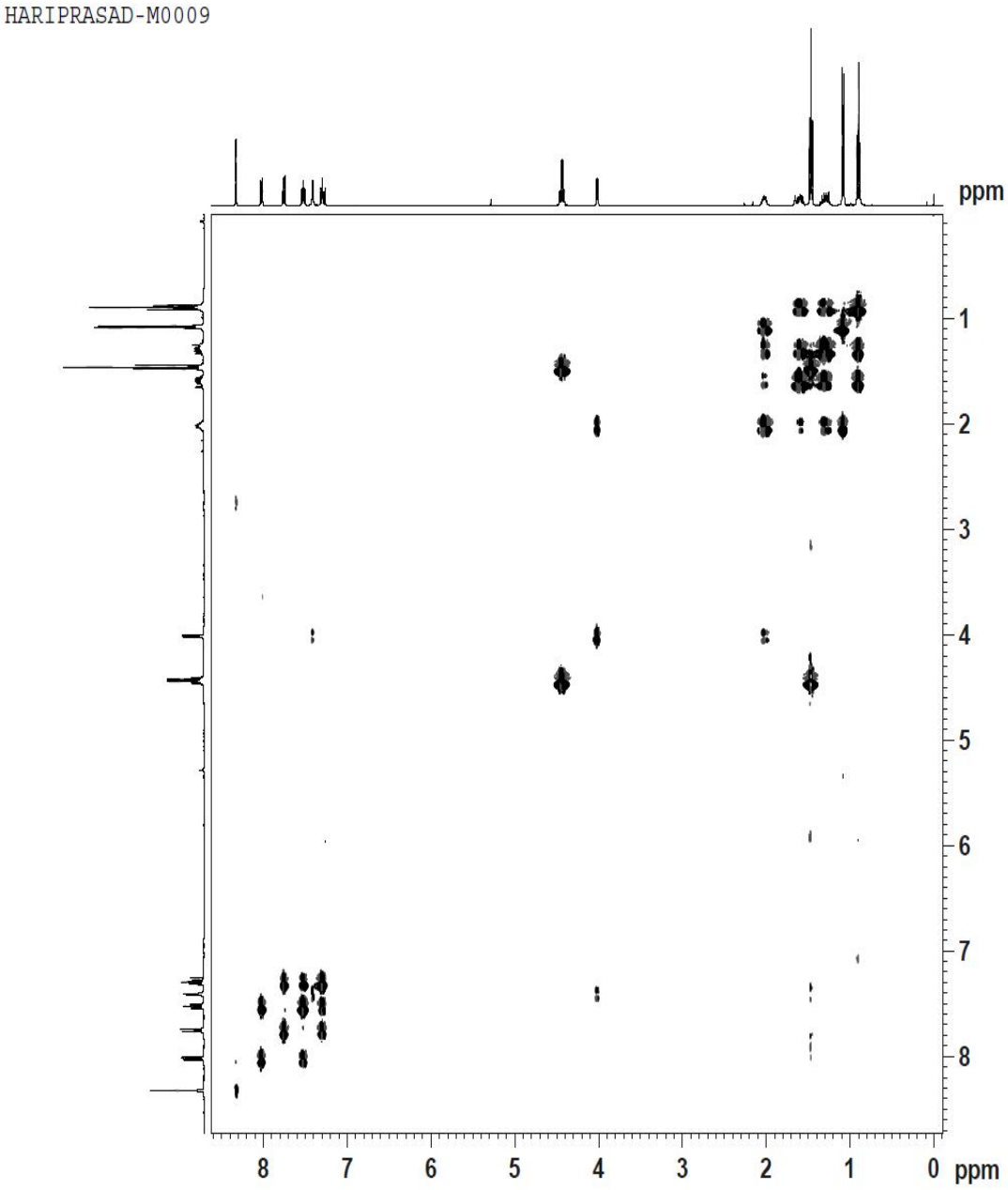
S90. 2D NMR Spectrums of compounds 3zb, 3ze and 3zg



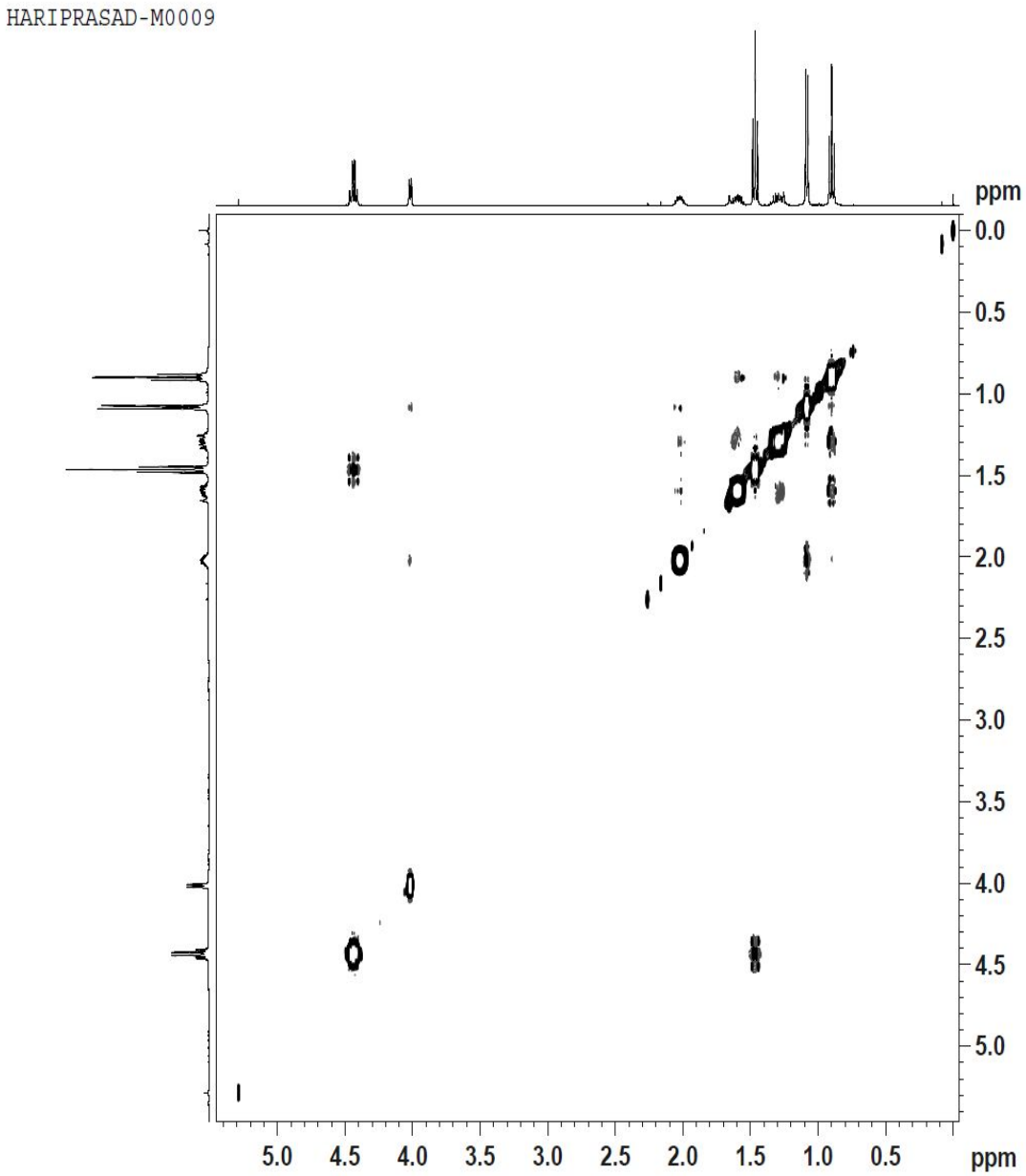
COSY spectrum of compound 3zb



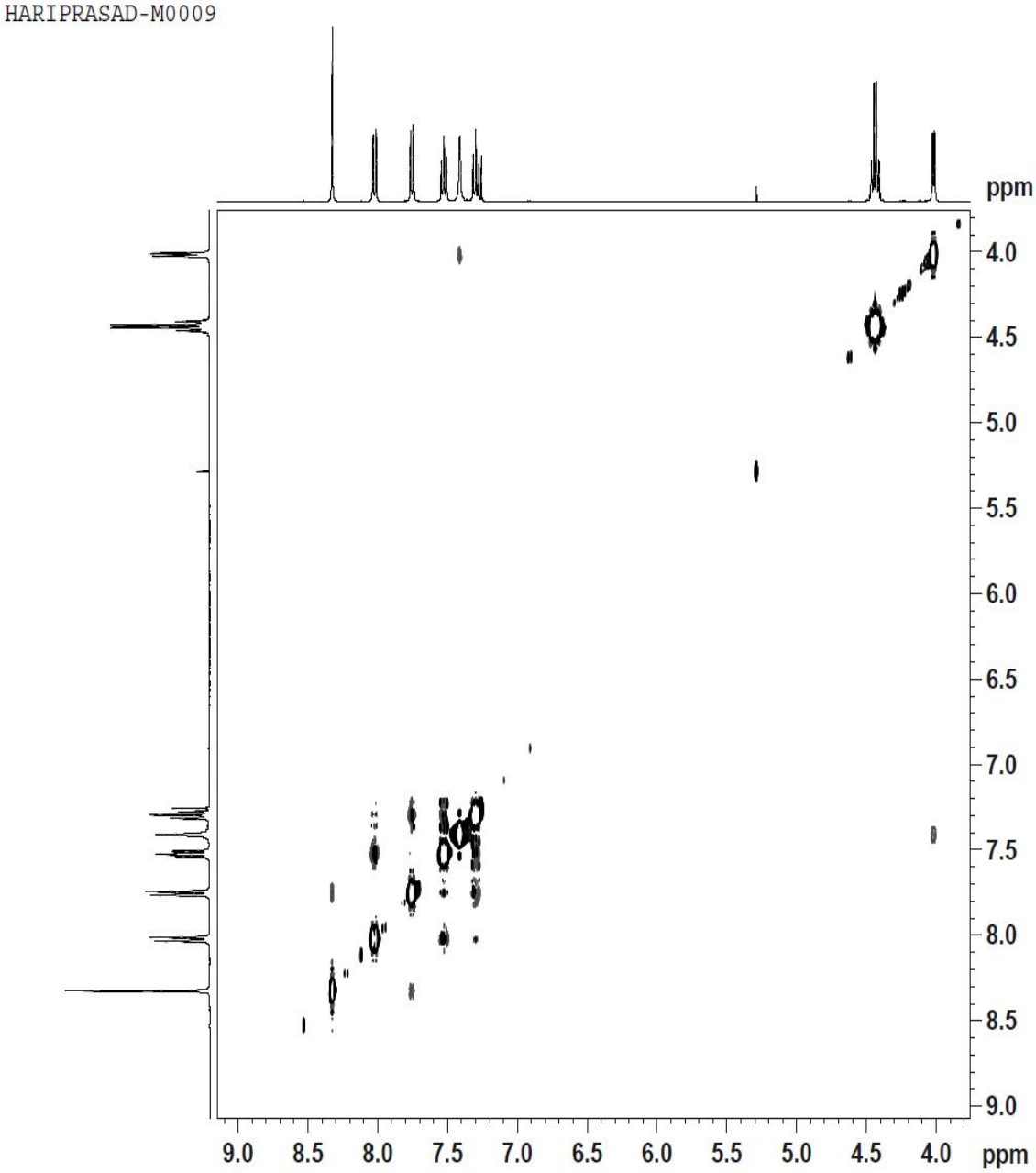
COSY spectrum of compound 3zb



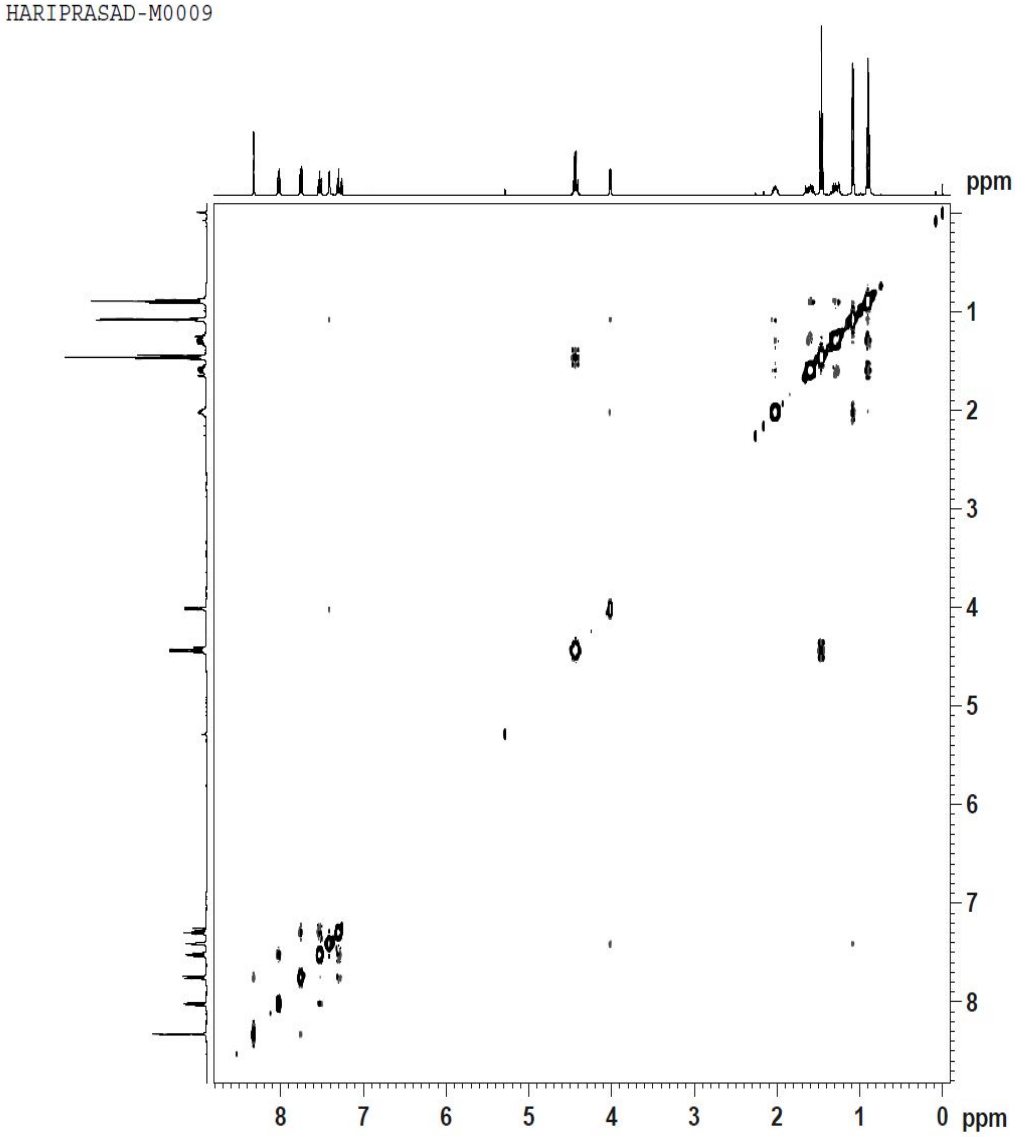
COSY spectrum of compound 3zb



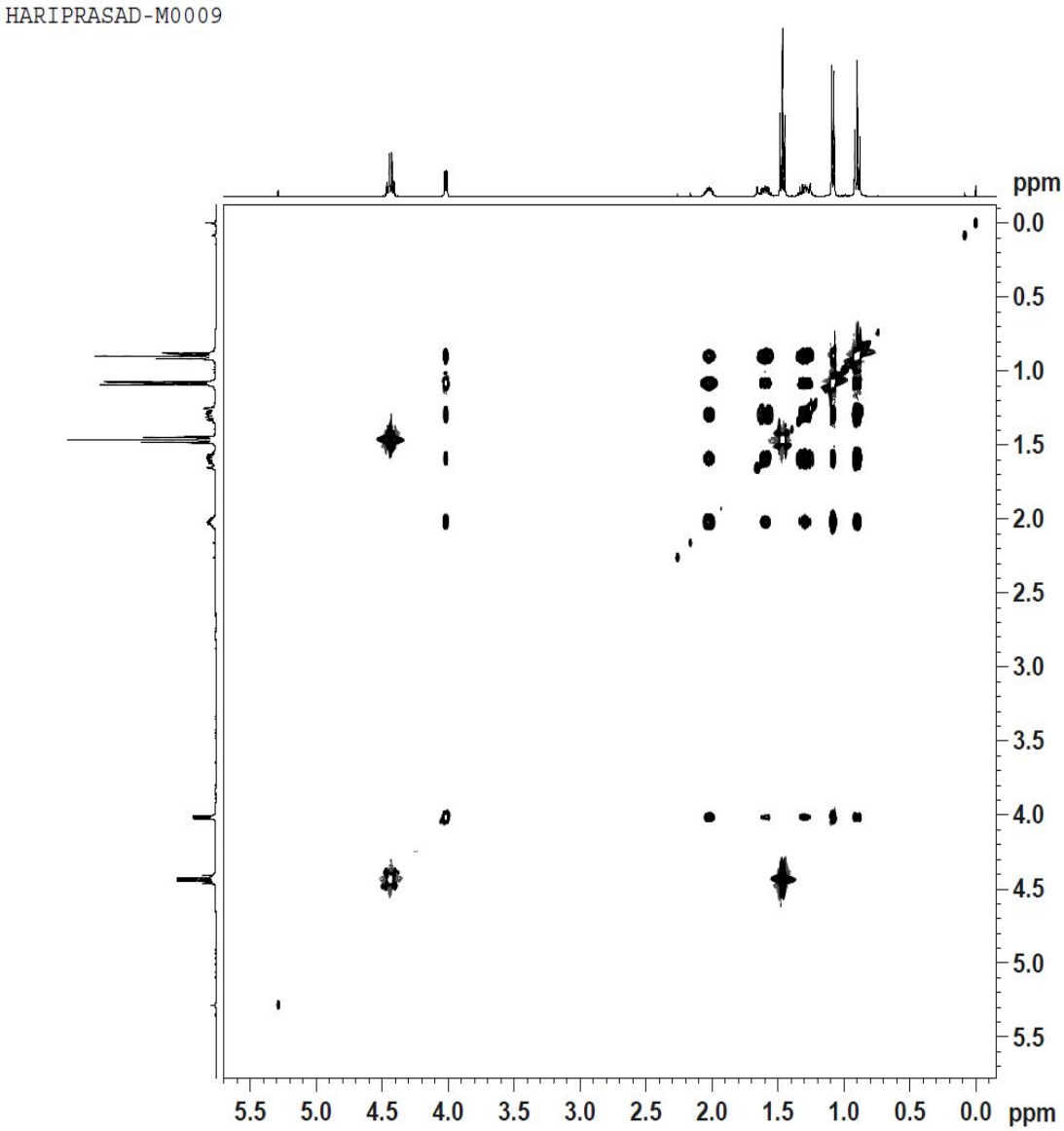
NOESY spectrum of compound 3zb



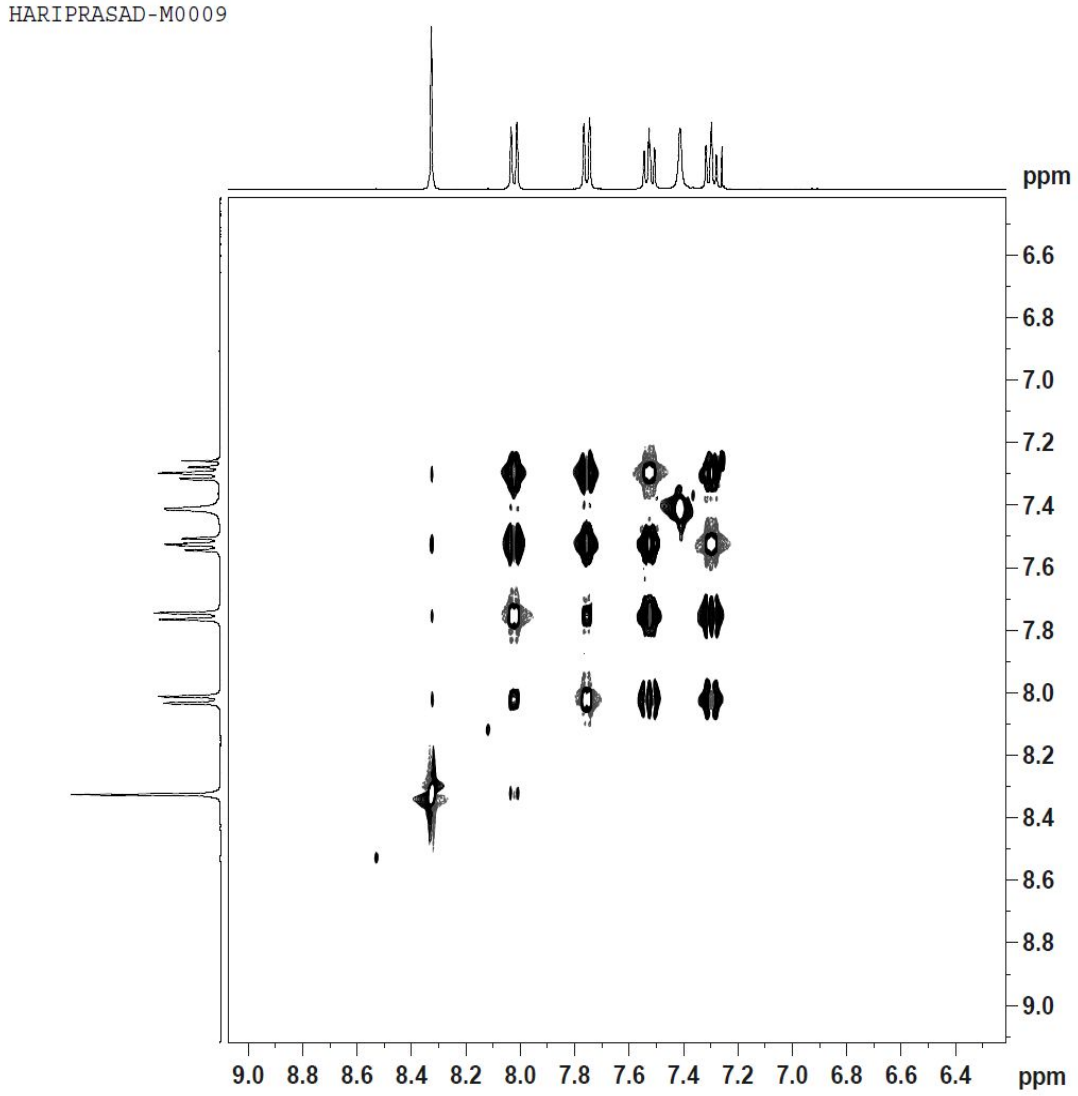
NOESY spectrum of compound 3zb



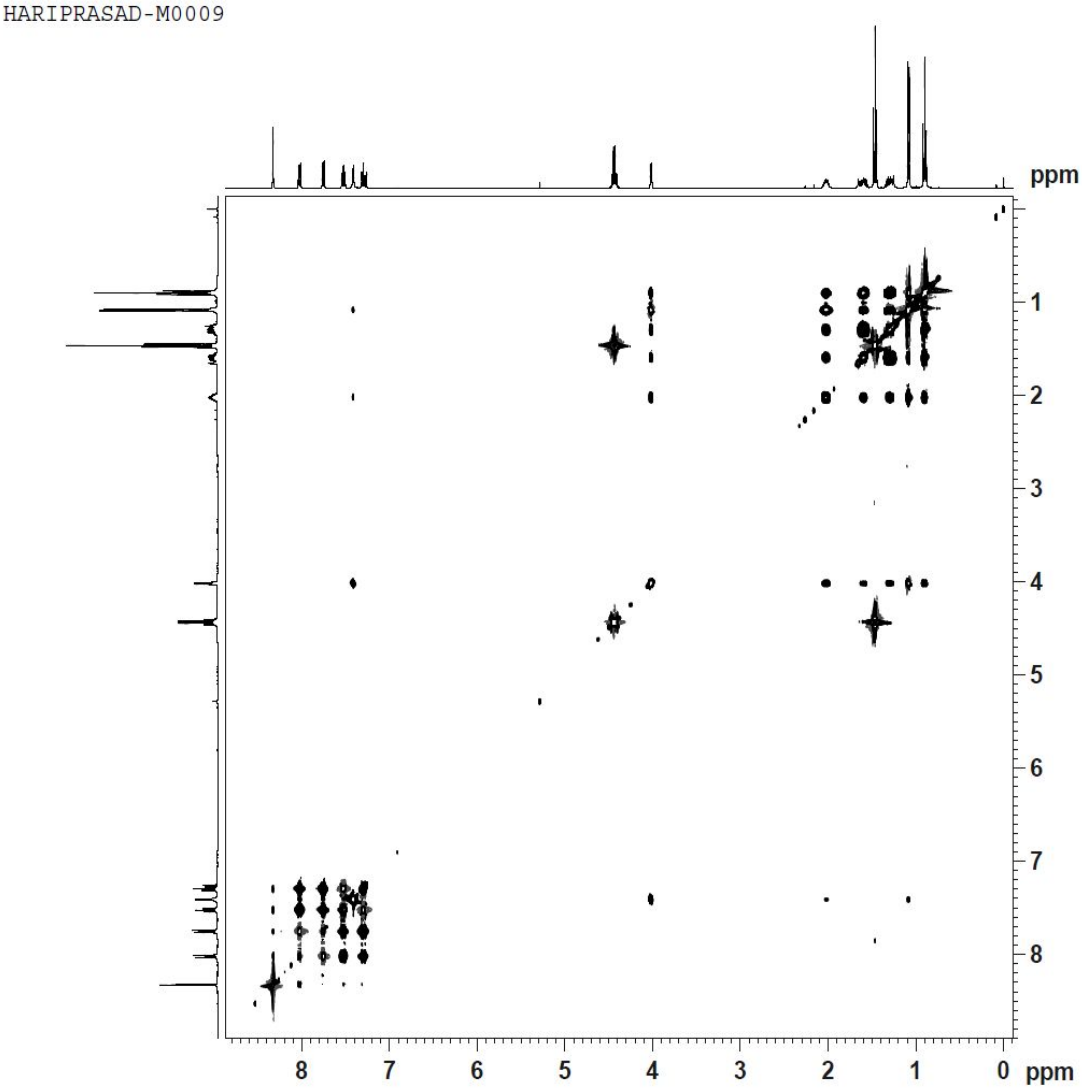
NOESY spectrum of compound 3zb



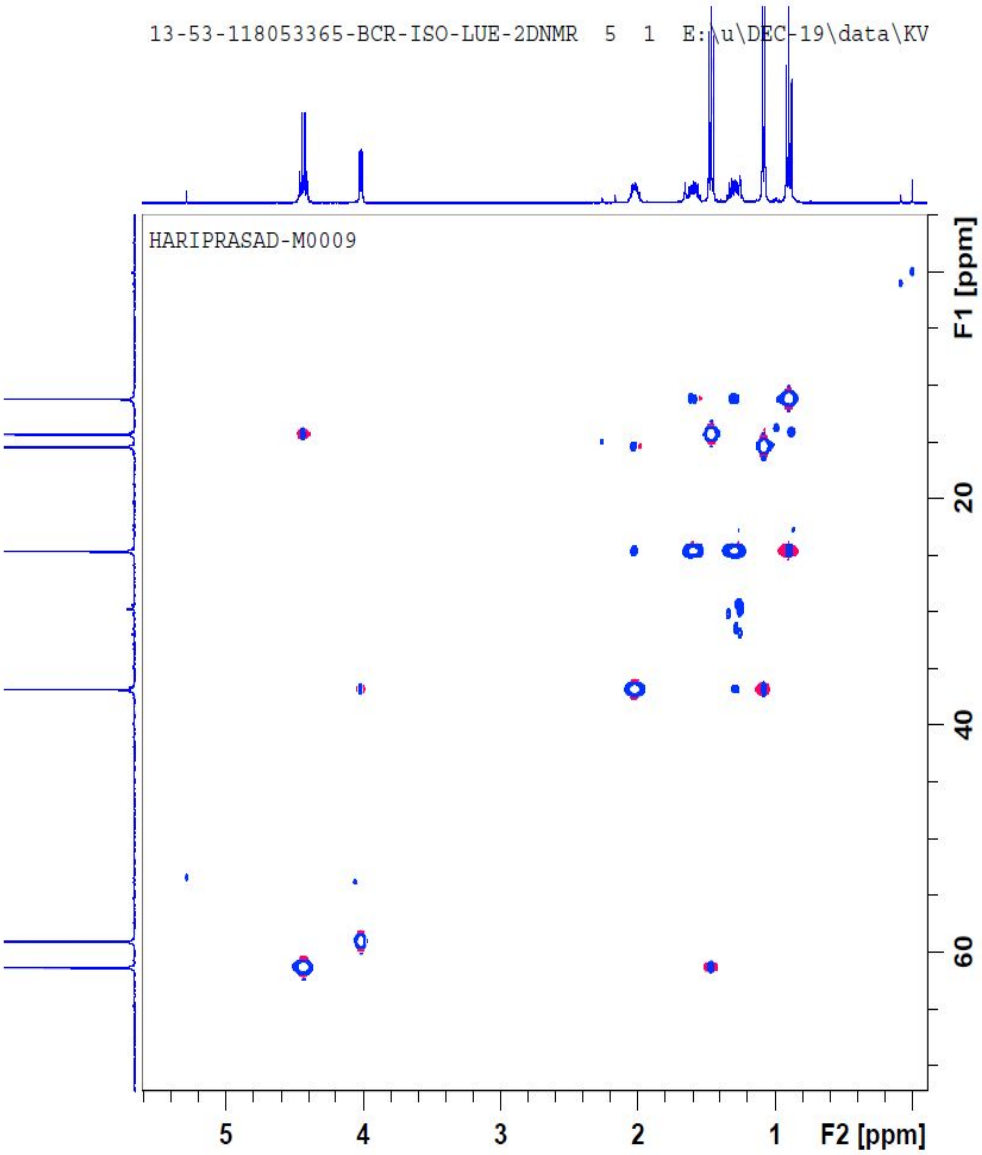
TOCSY spectrum of compound 3zb



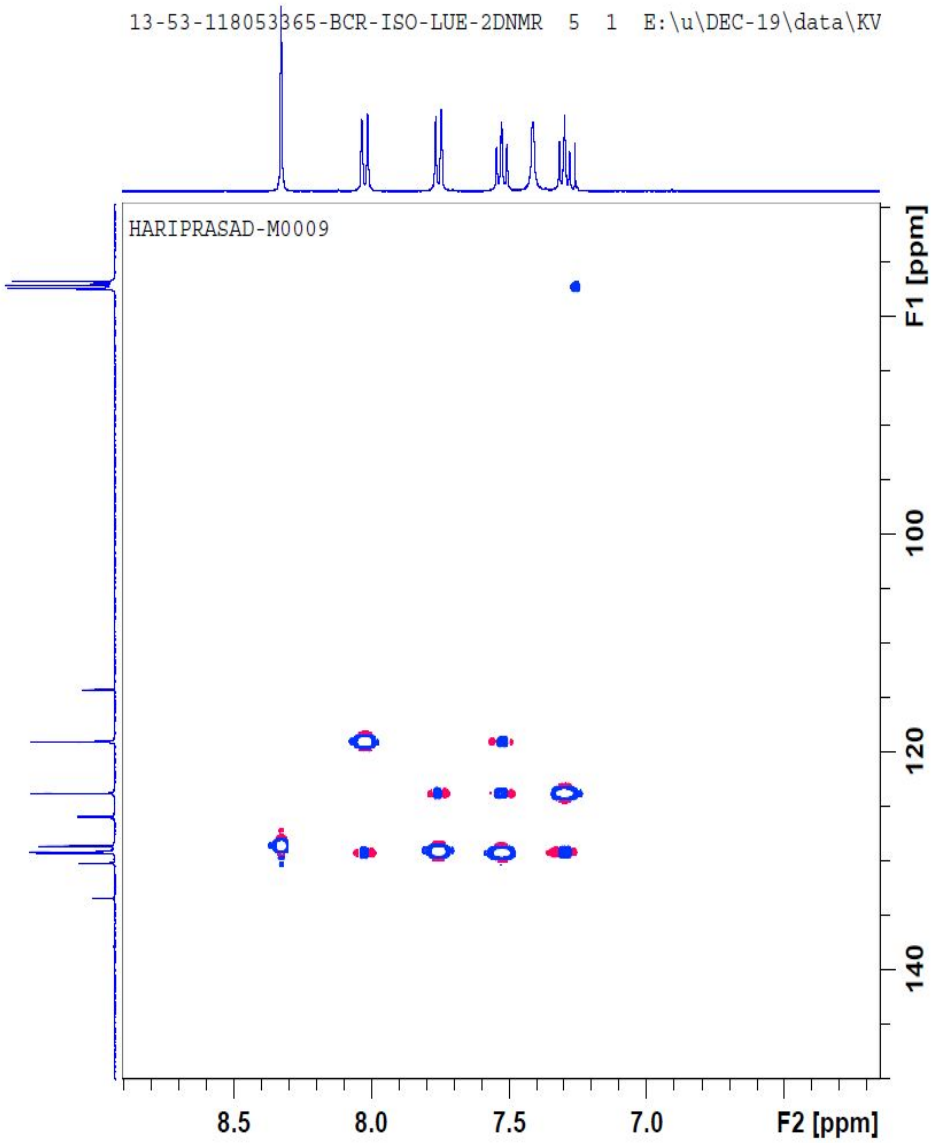
TOCSY spectrum of compound 3zb



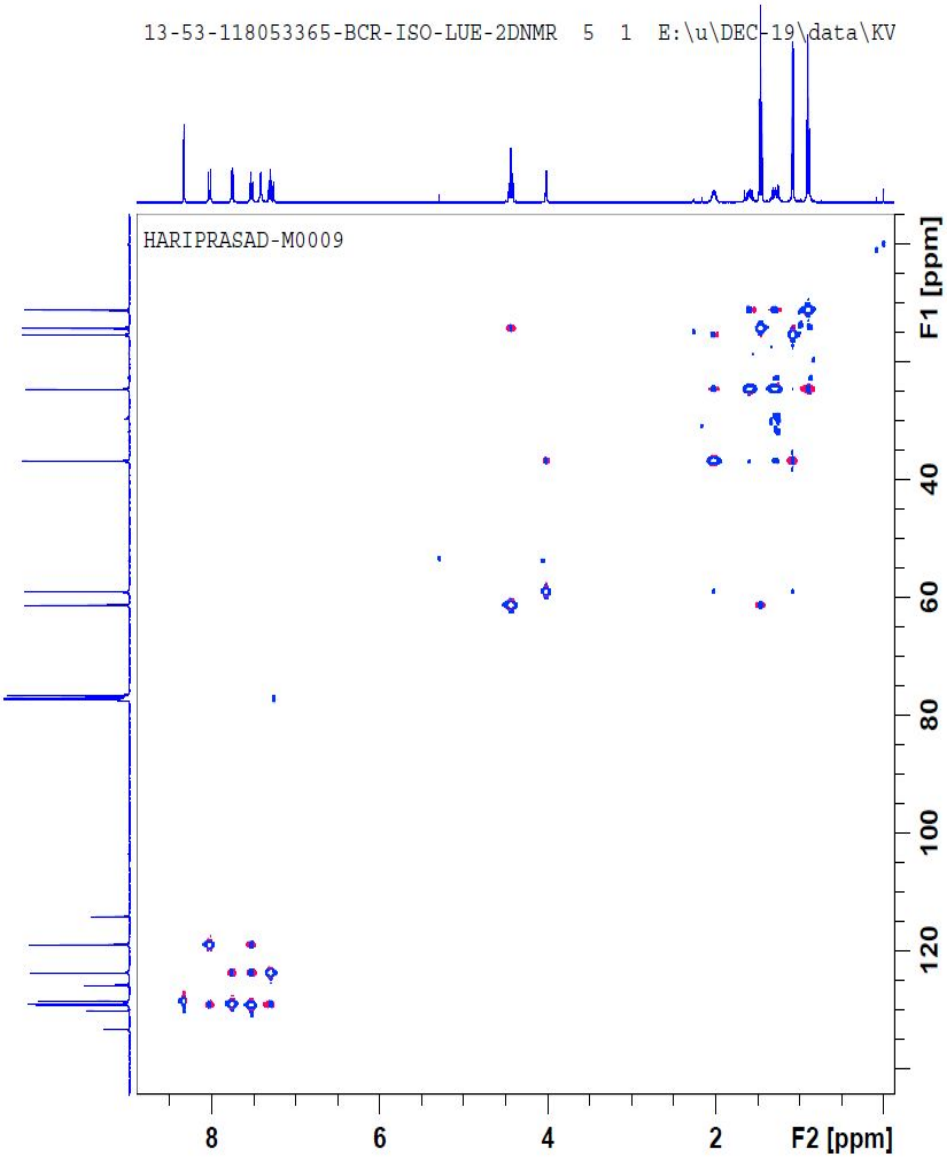
TOCSY spectrum of compound 3zb



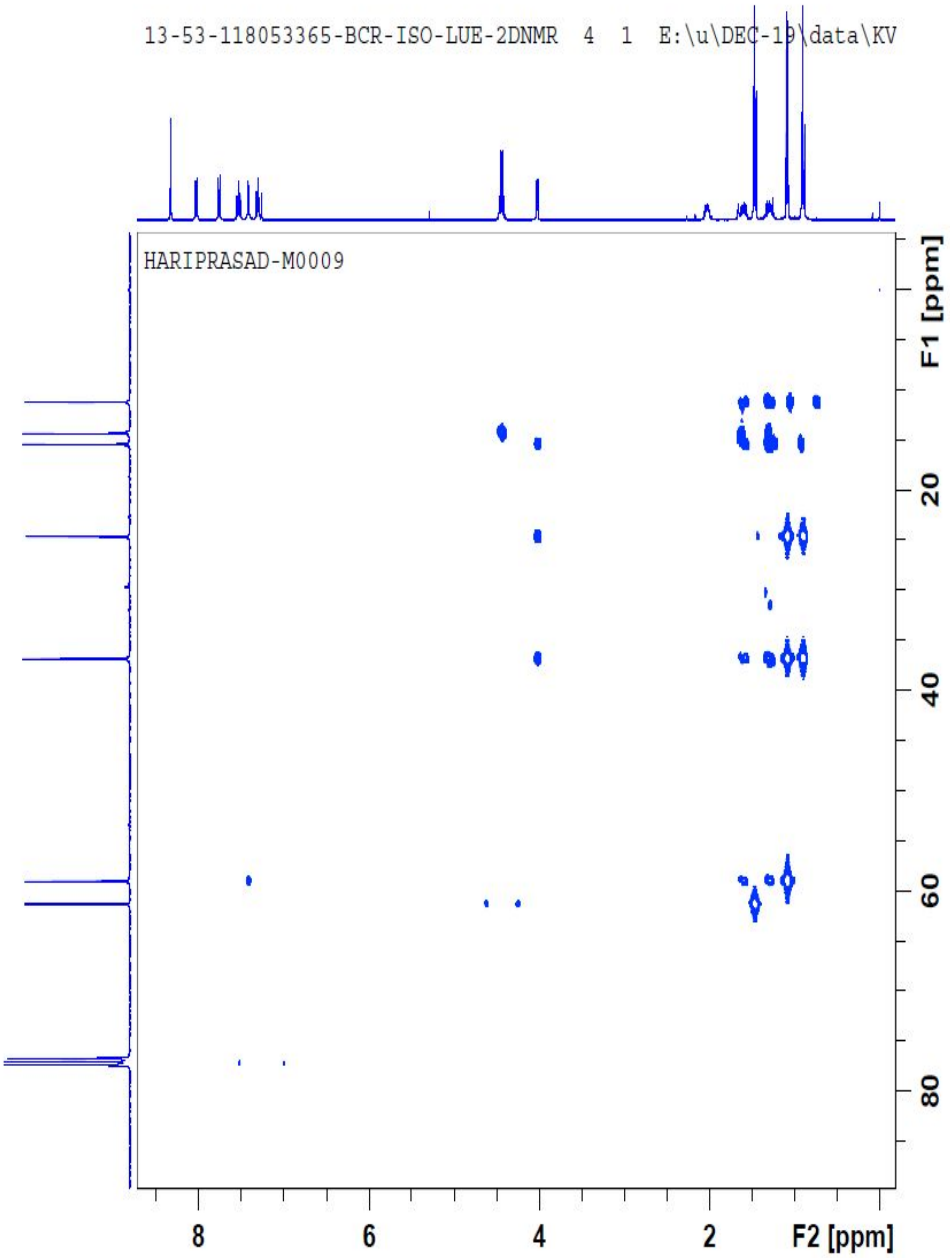
HSQC spectrum of compound 3zb



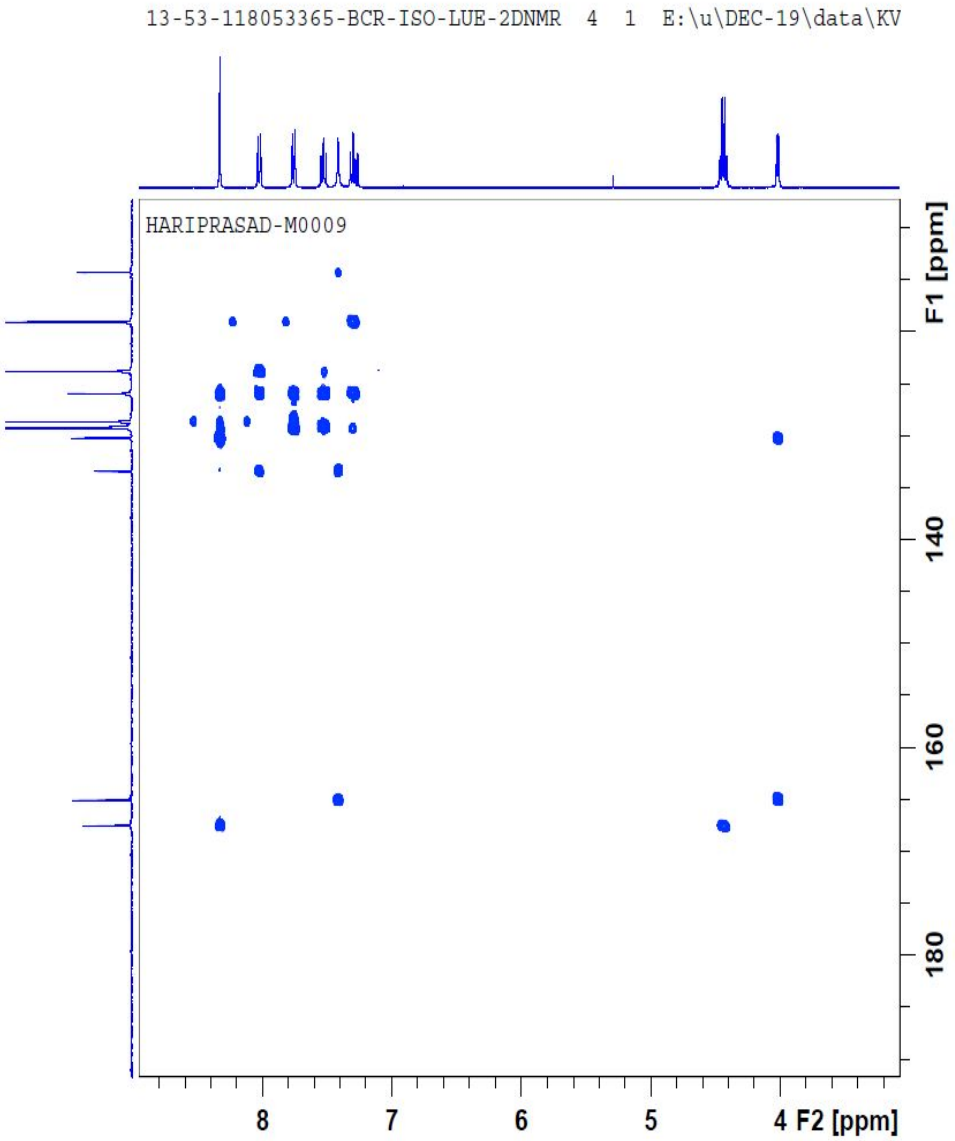
HSQC spectrum of compound 3zb



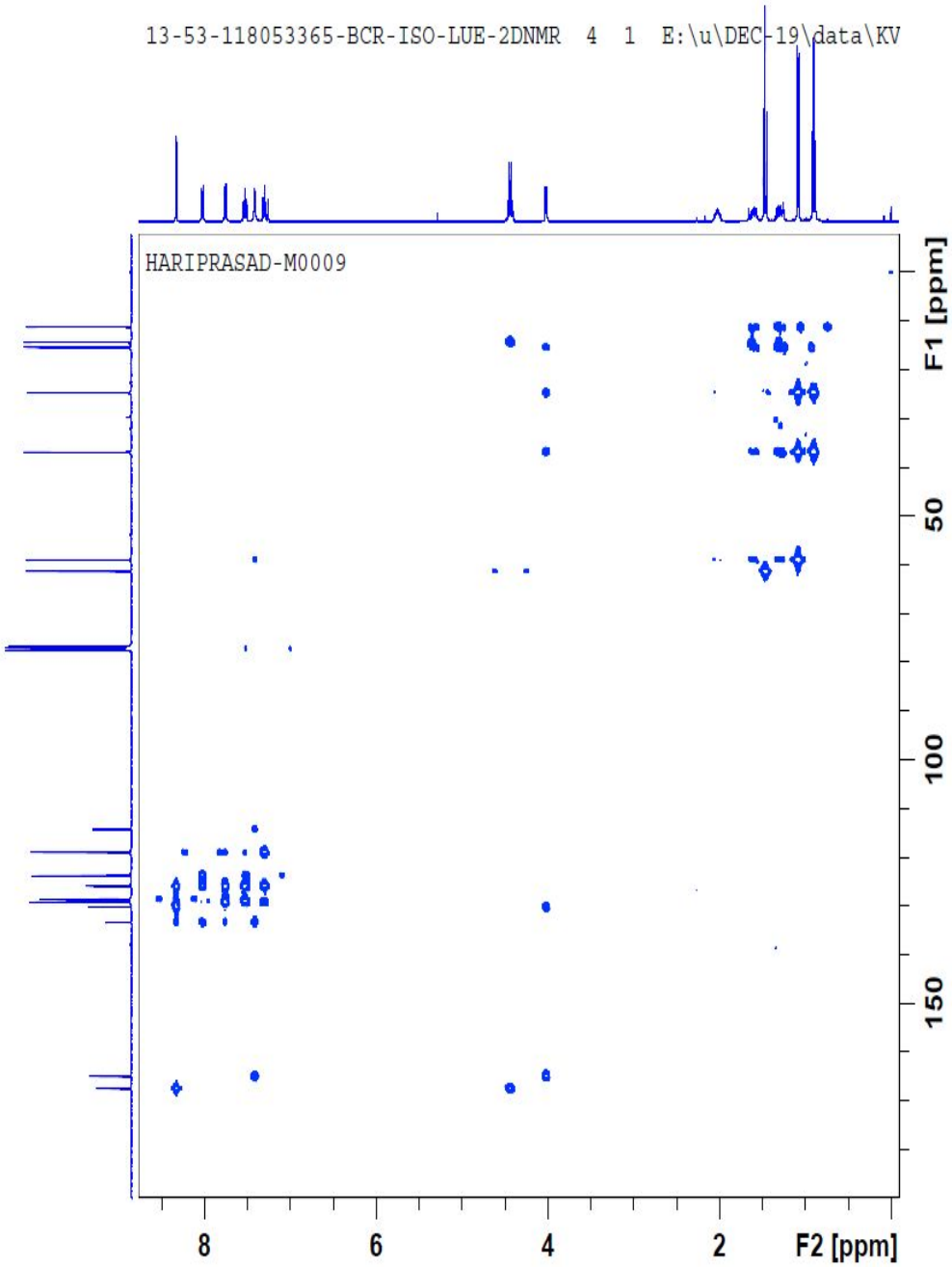
HSQC spectrum of compound 3zb



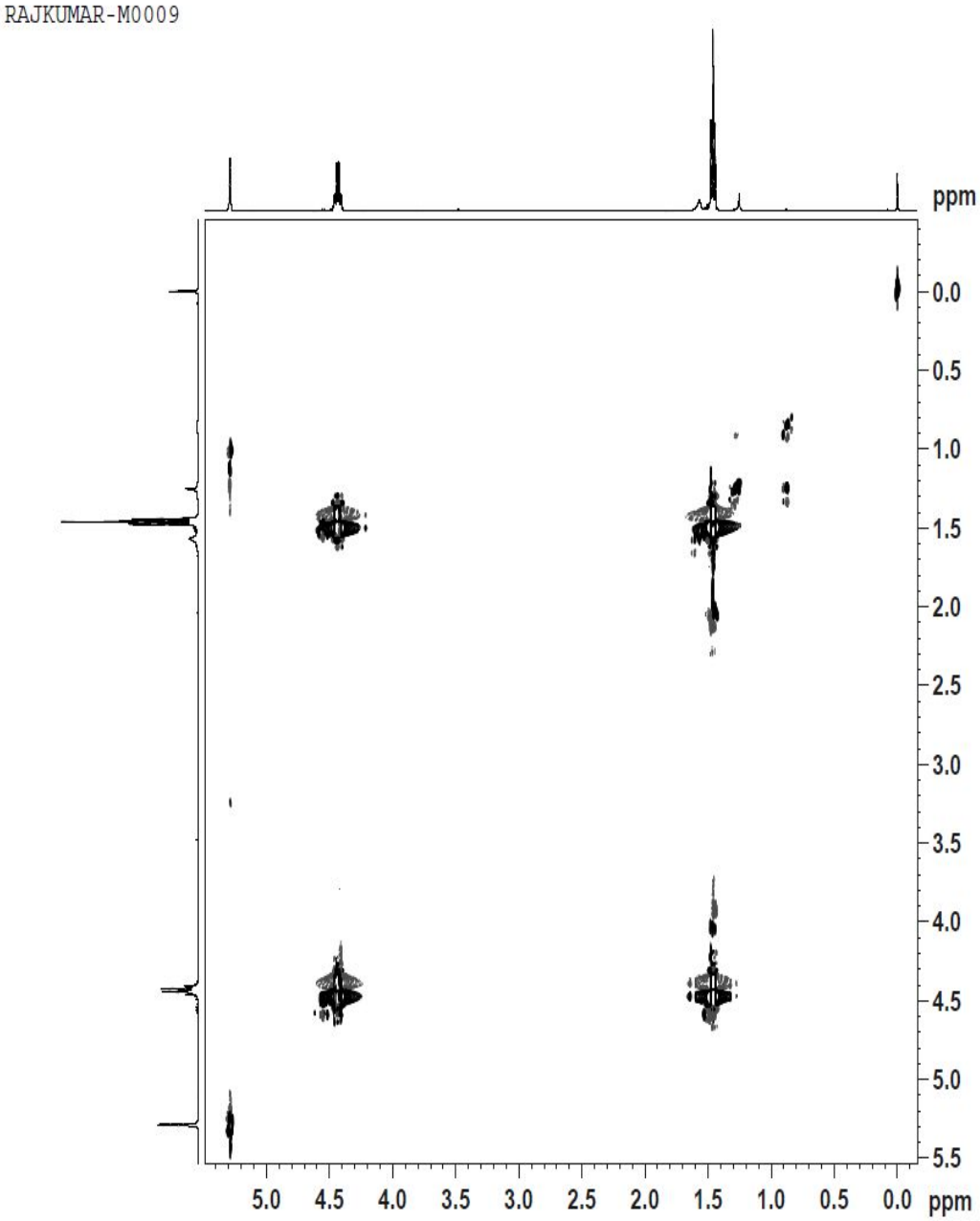
HMBC spectrum of compound 3zb



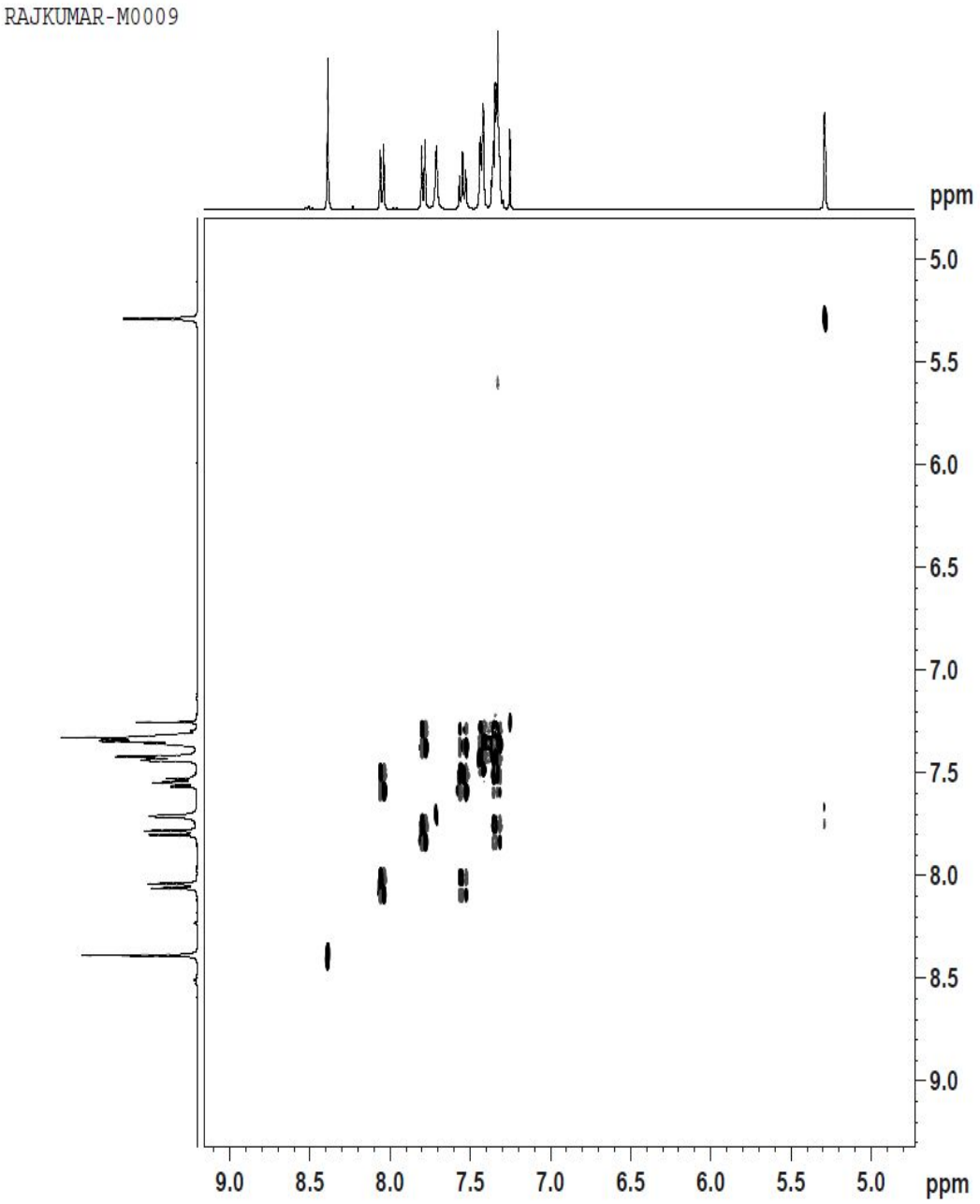
HMBC spectrum of compound 3zb



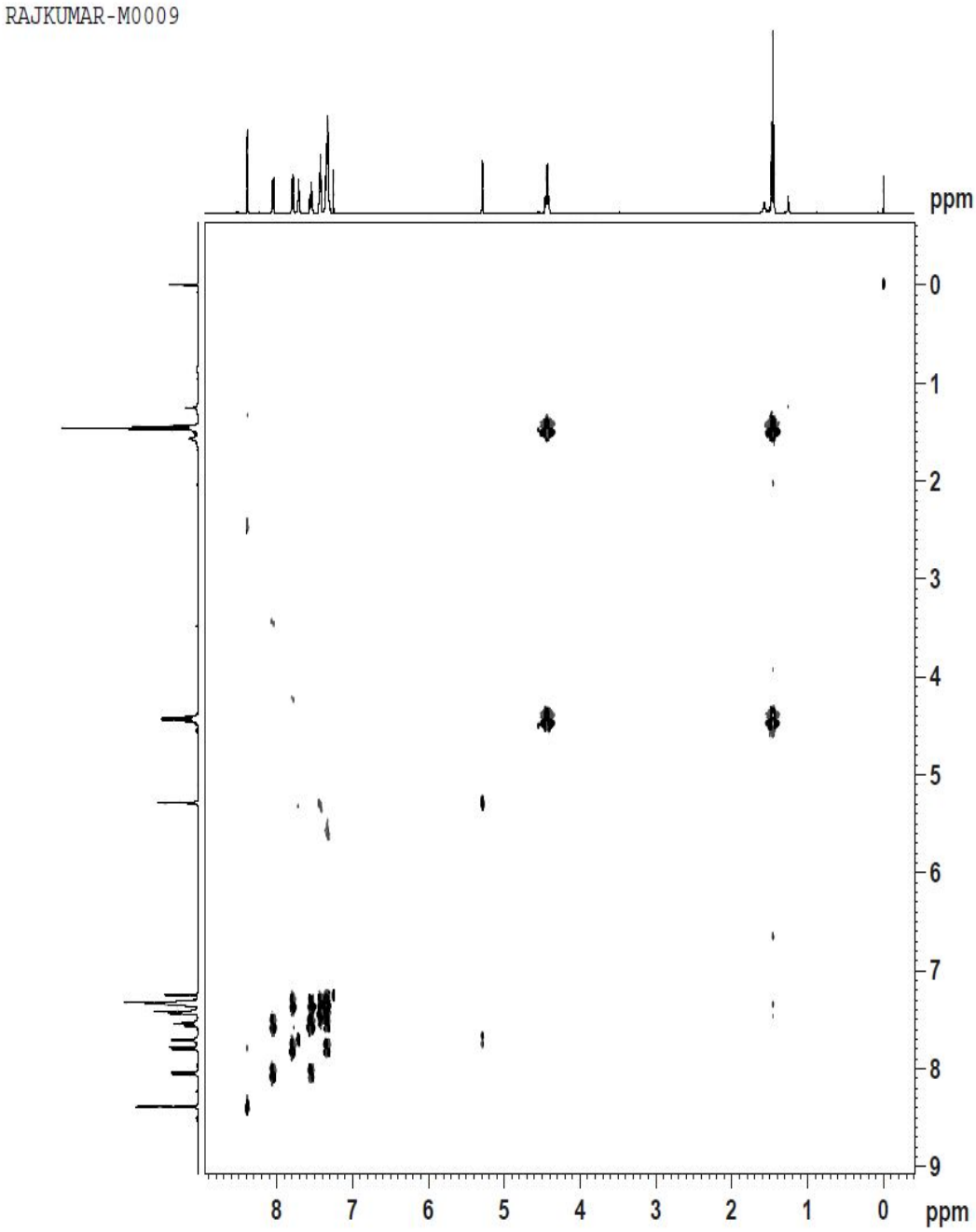
HMBC spectrum of compound 3zb



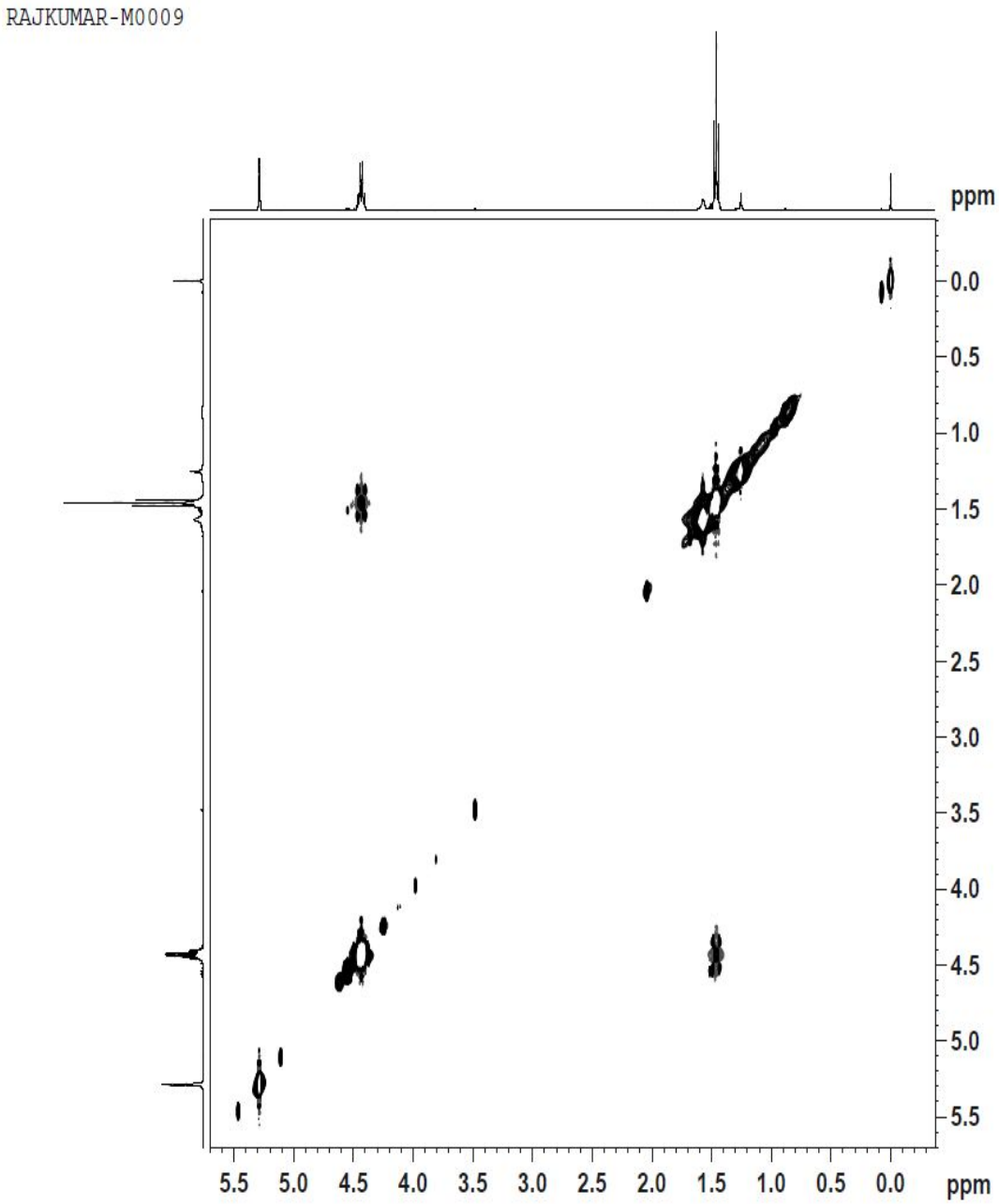
COSY spectrum of compound 3ze



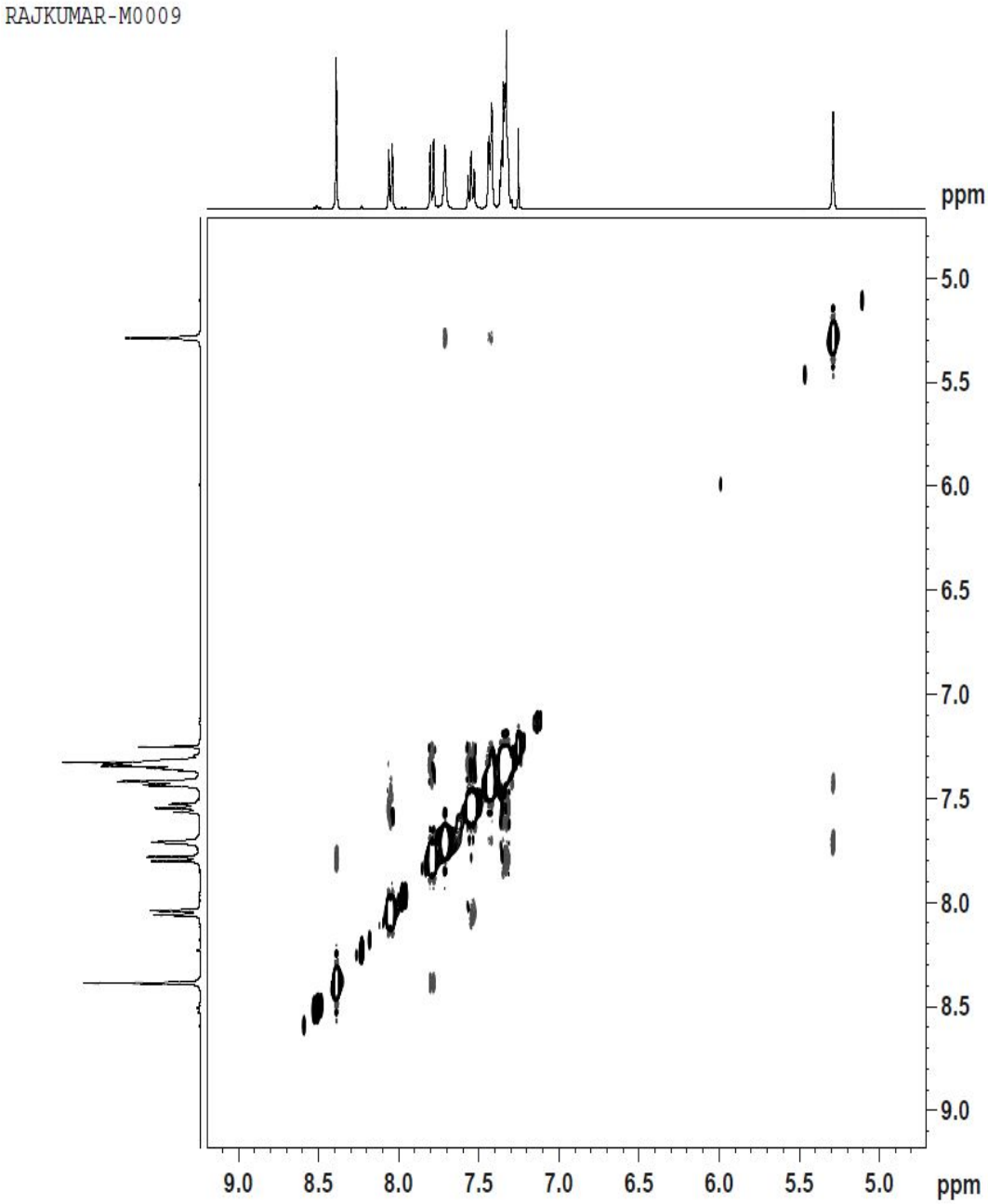
COSY spectrum of compound 3ze



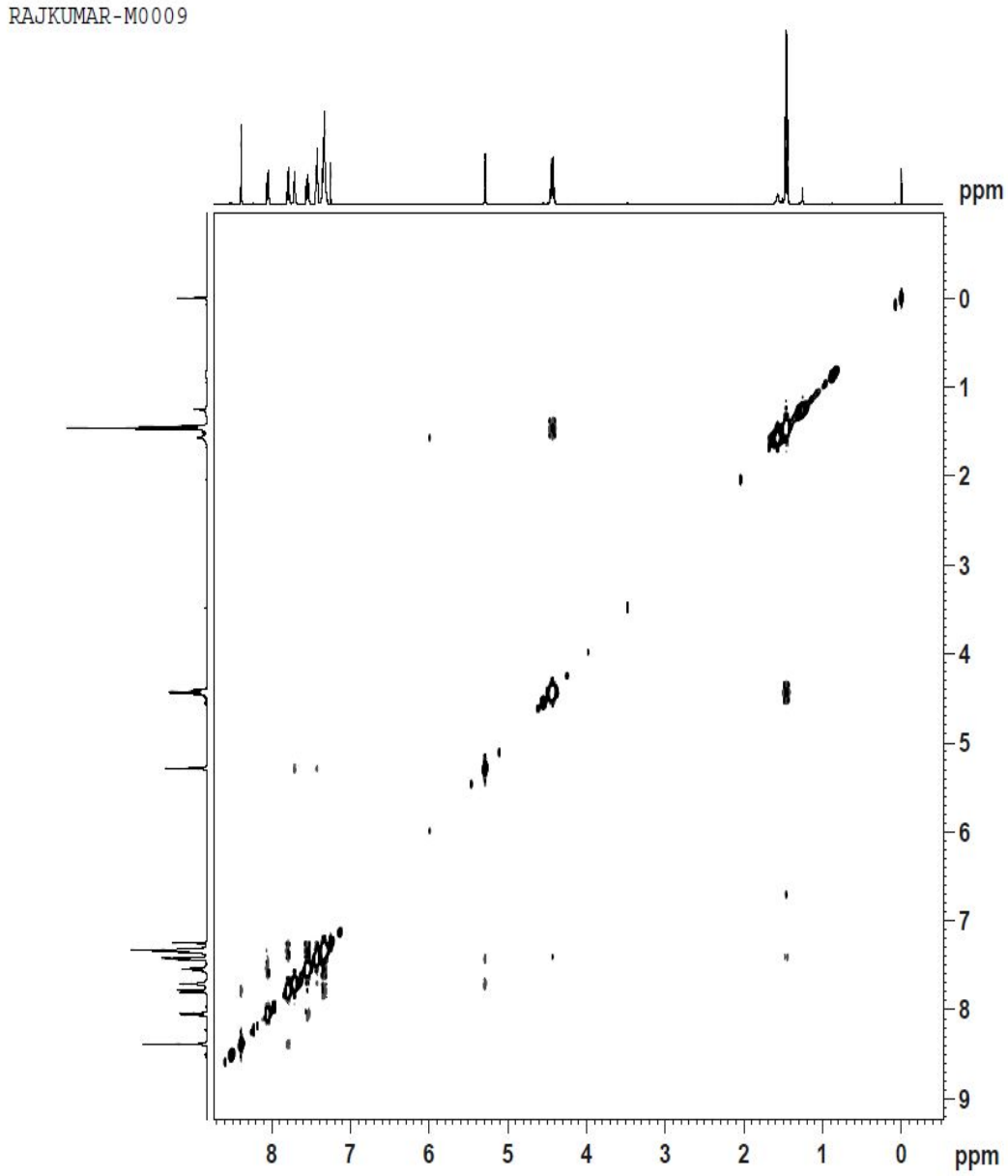
COSY spectrum of compound 3ze



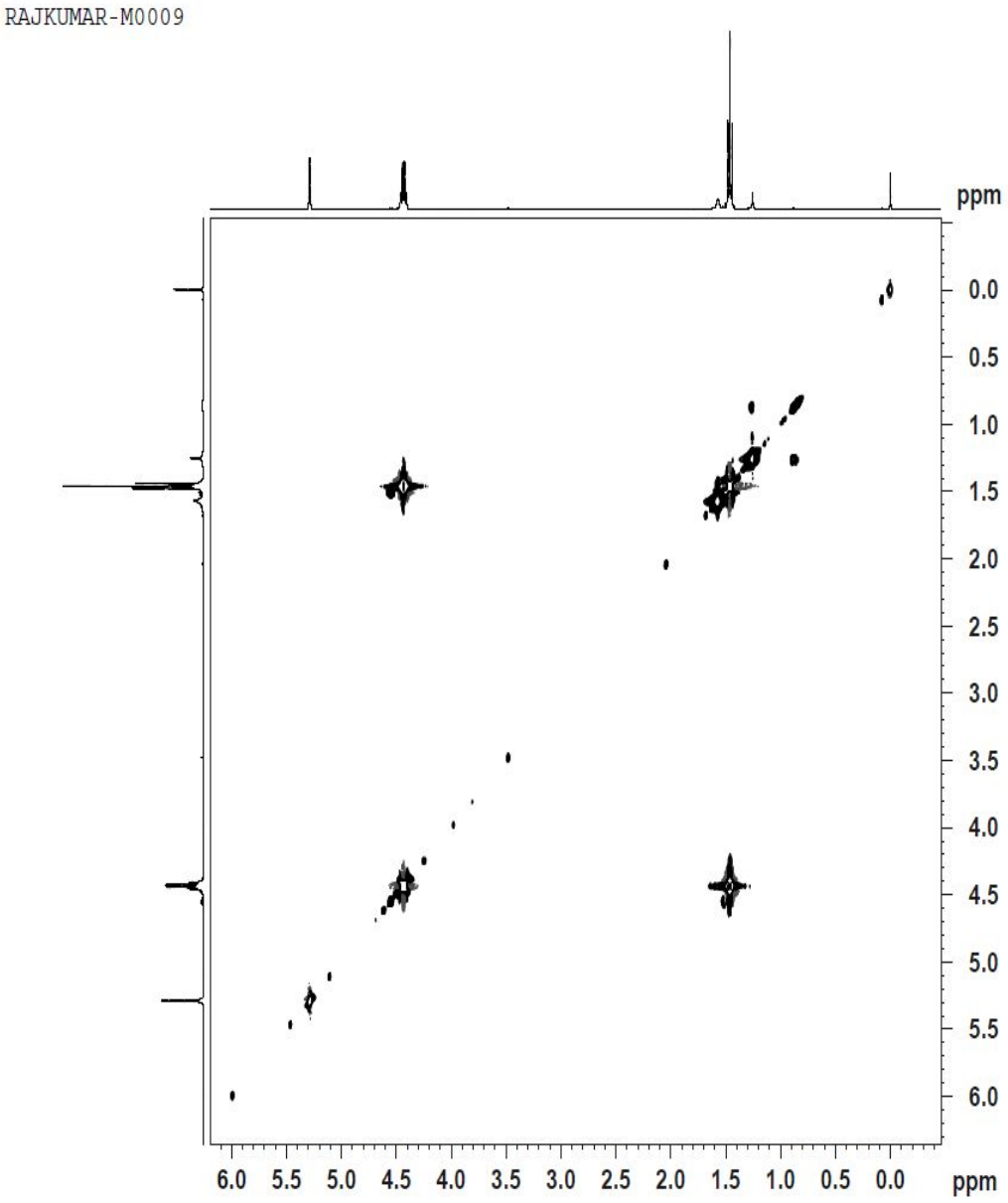
NOESY spectrum of compound 3ze



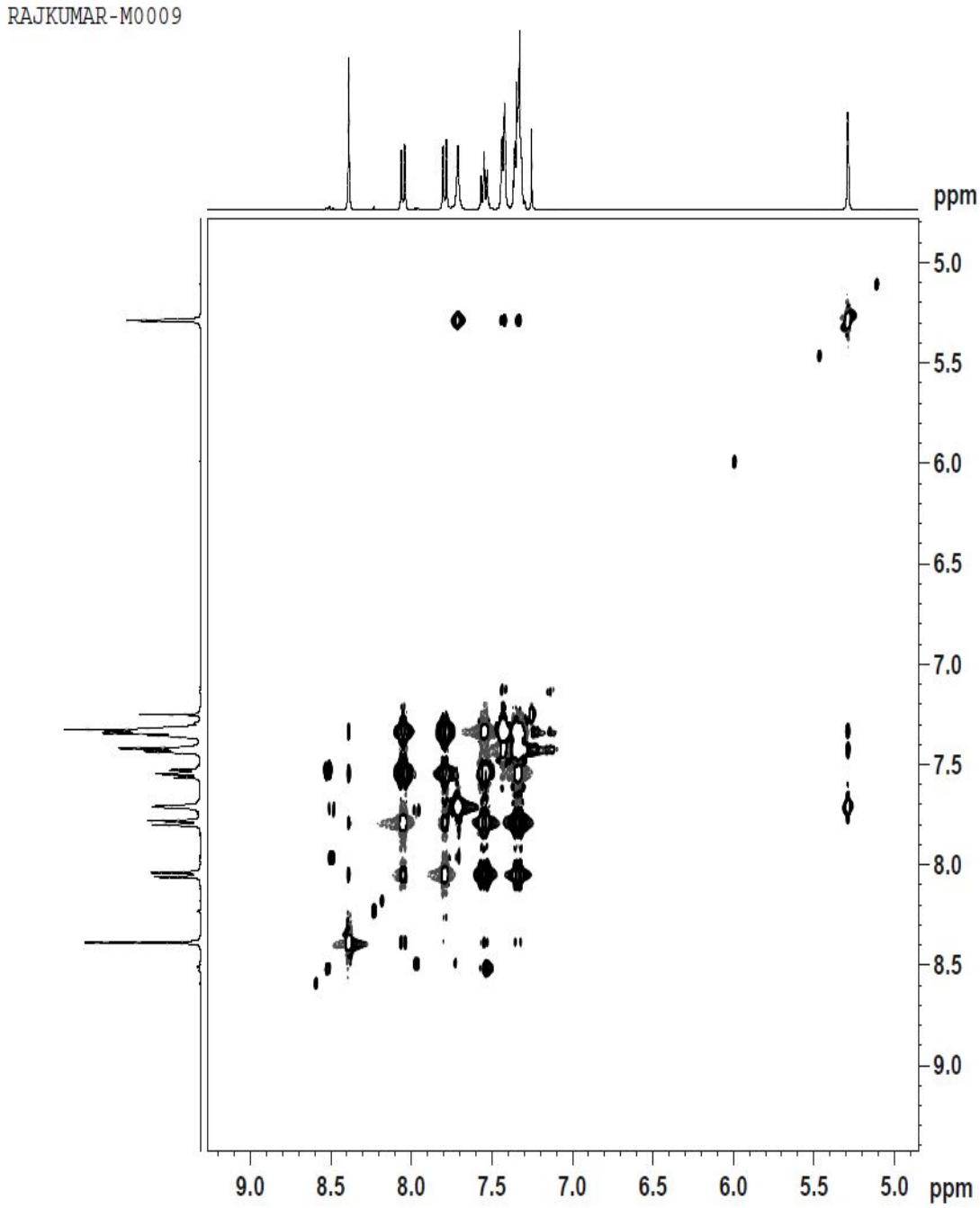
NOESY spectrum of compound 3ze



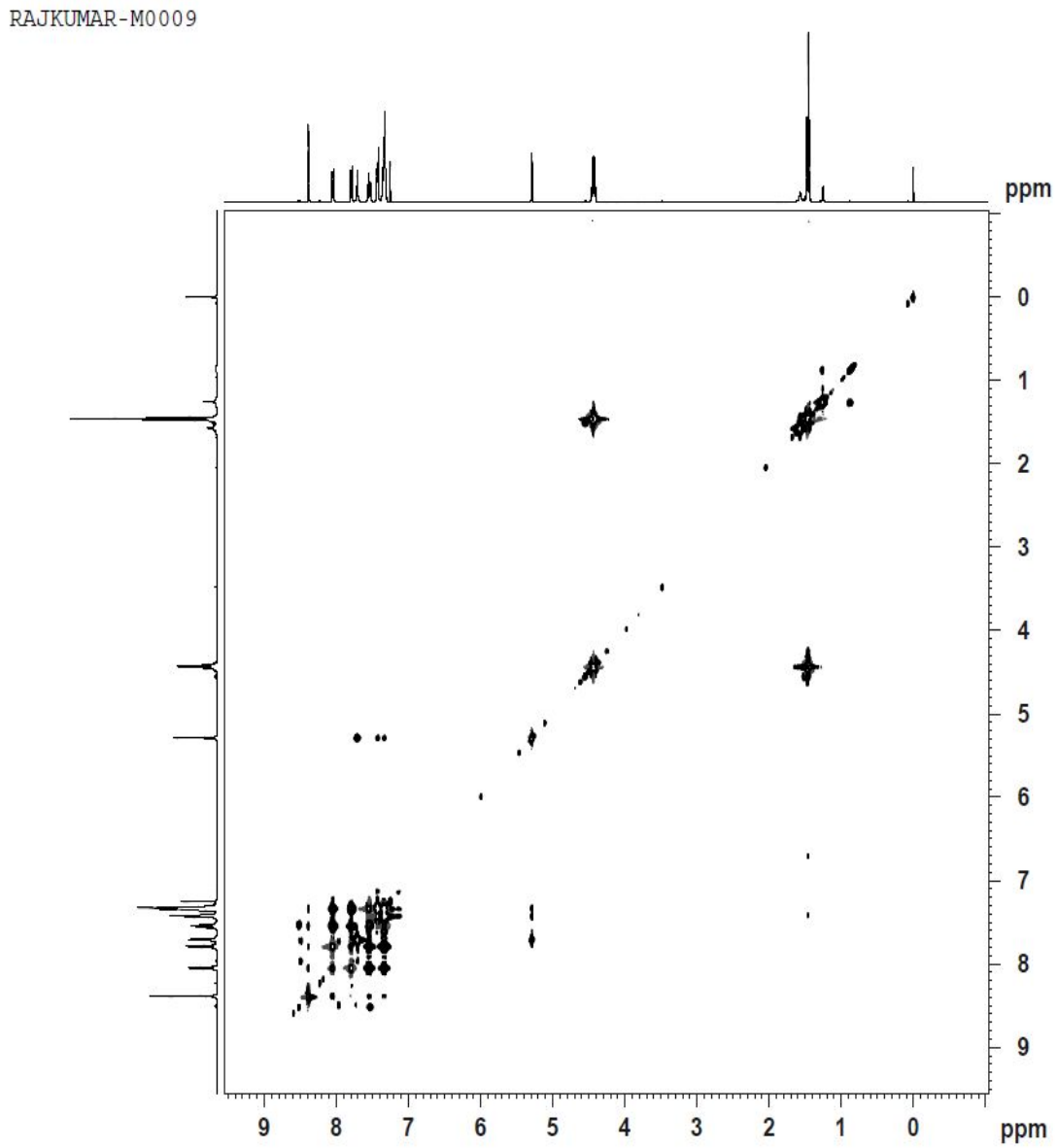
NOESY spectrum of compound 3ze



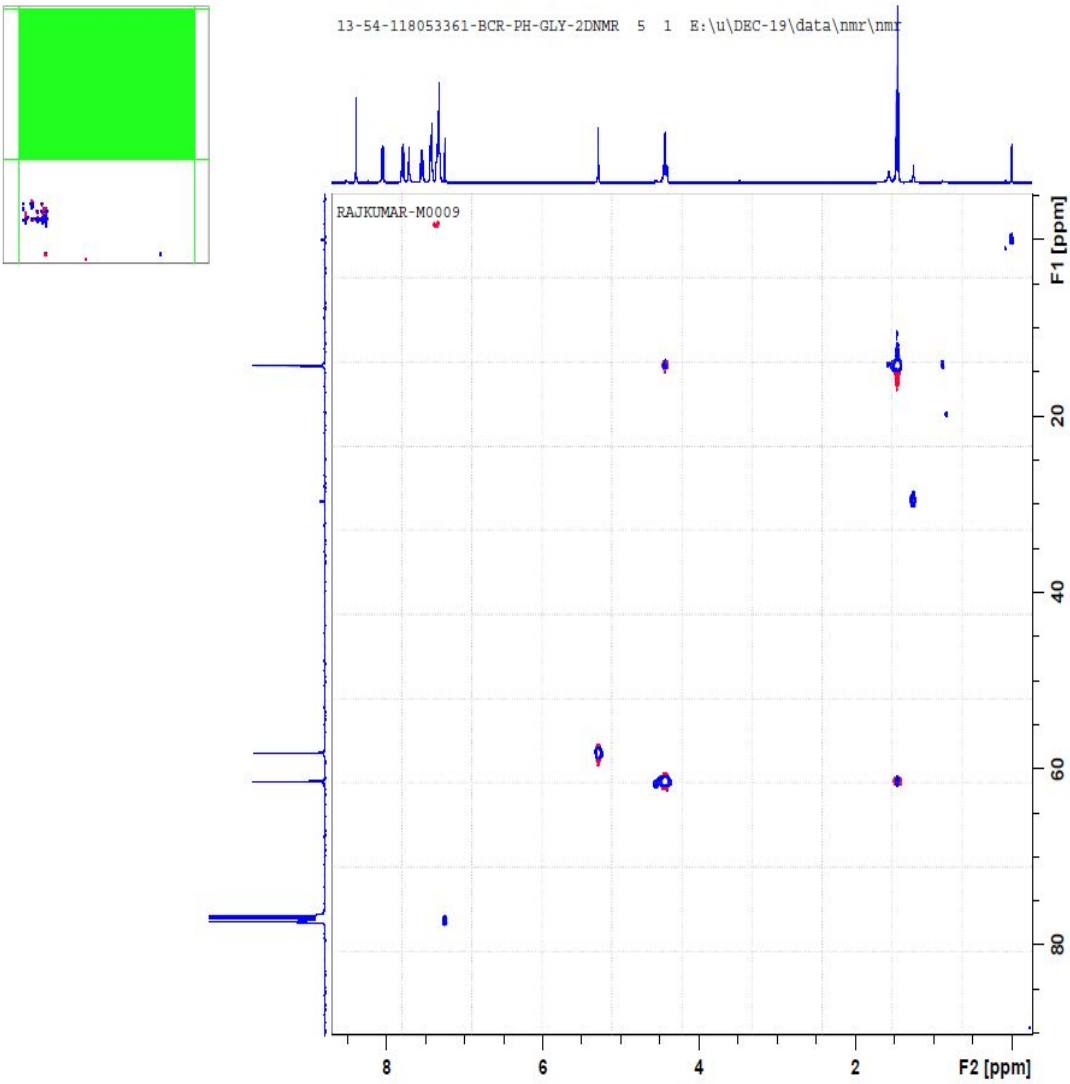
TOCSY spectrum of compound 3ze



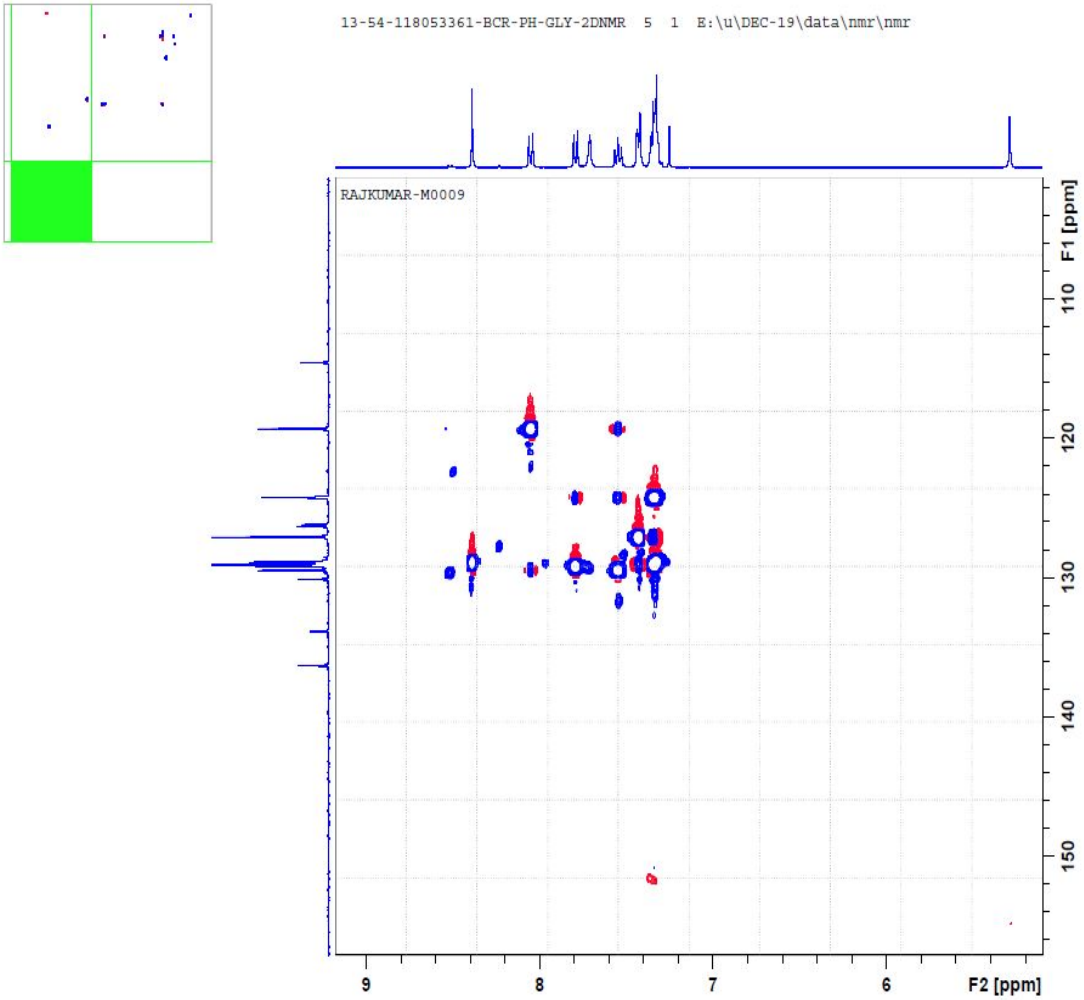
TOCSY spectrum of compound 3ze



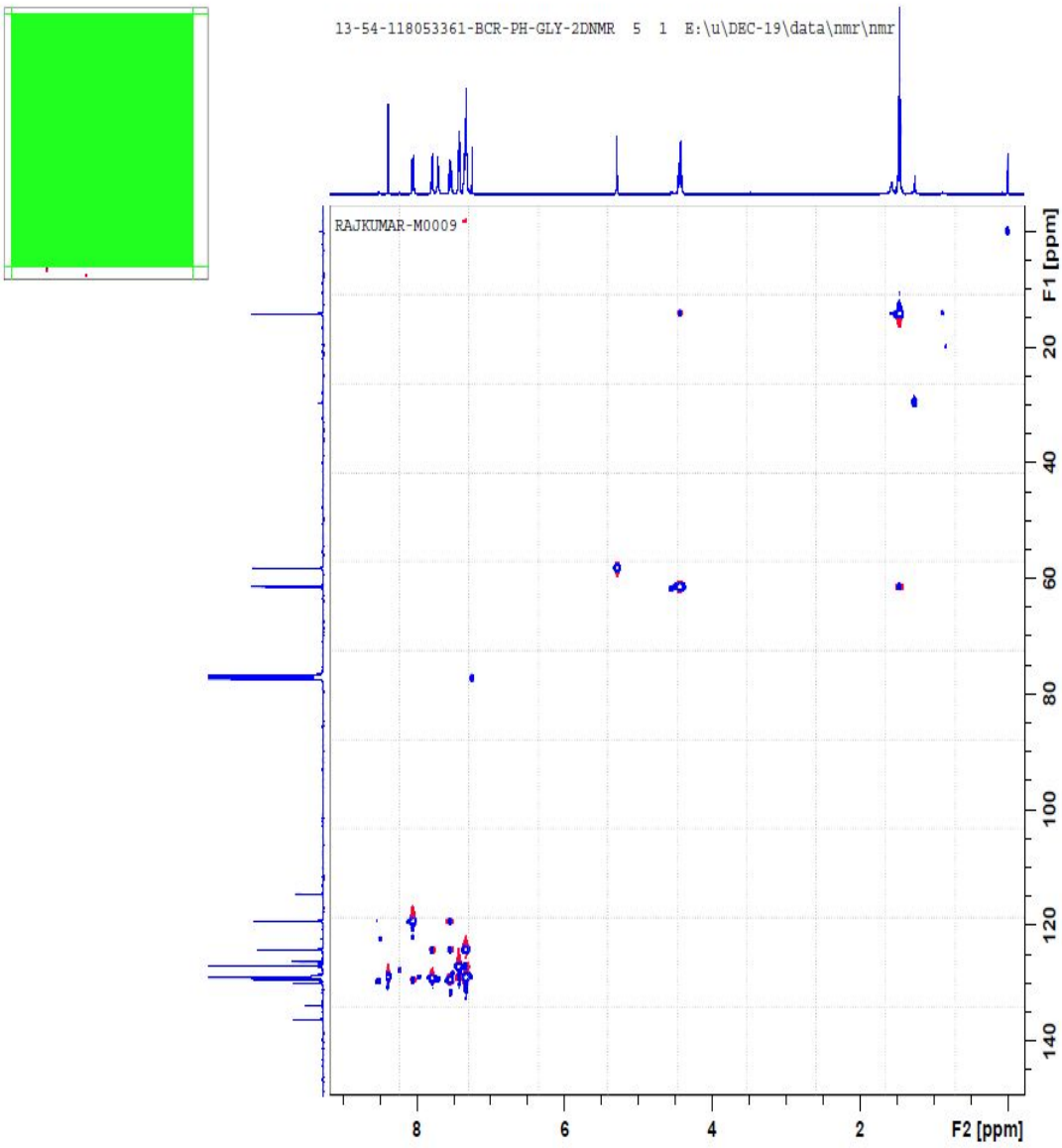
TOCSY spectrum of compound 3ze



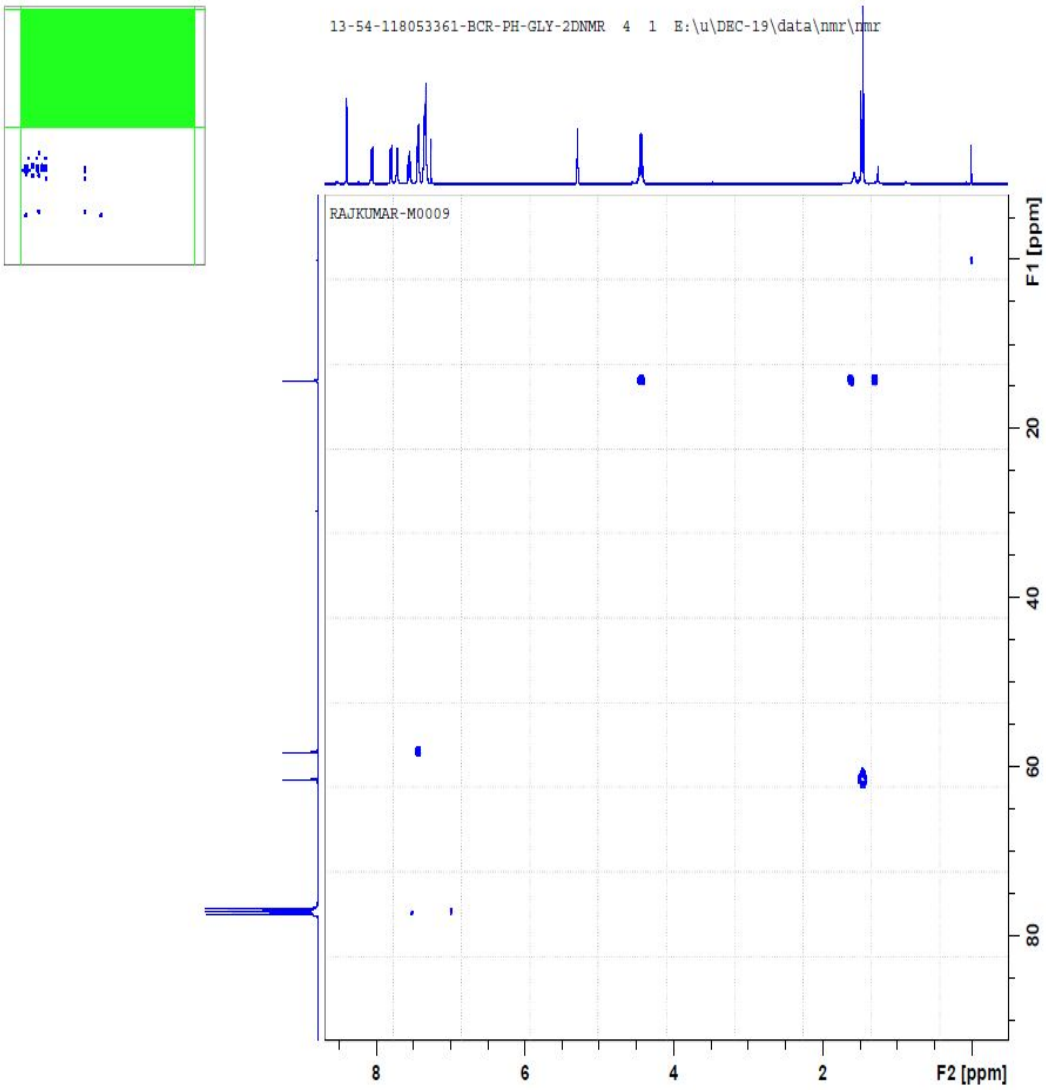
HSQC spectrum of compound 3ze



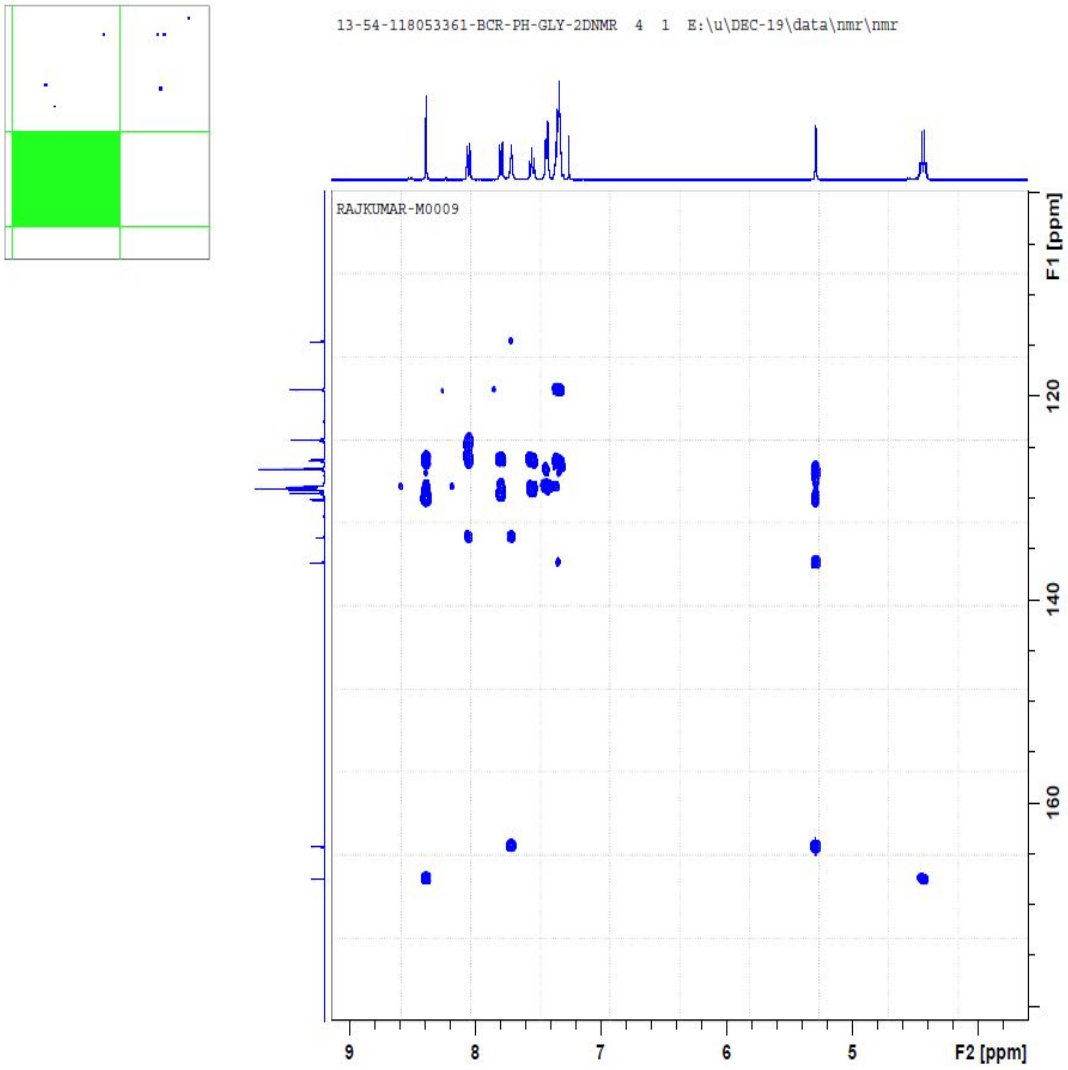
HSQC spectrum of compound 3ze



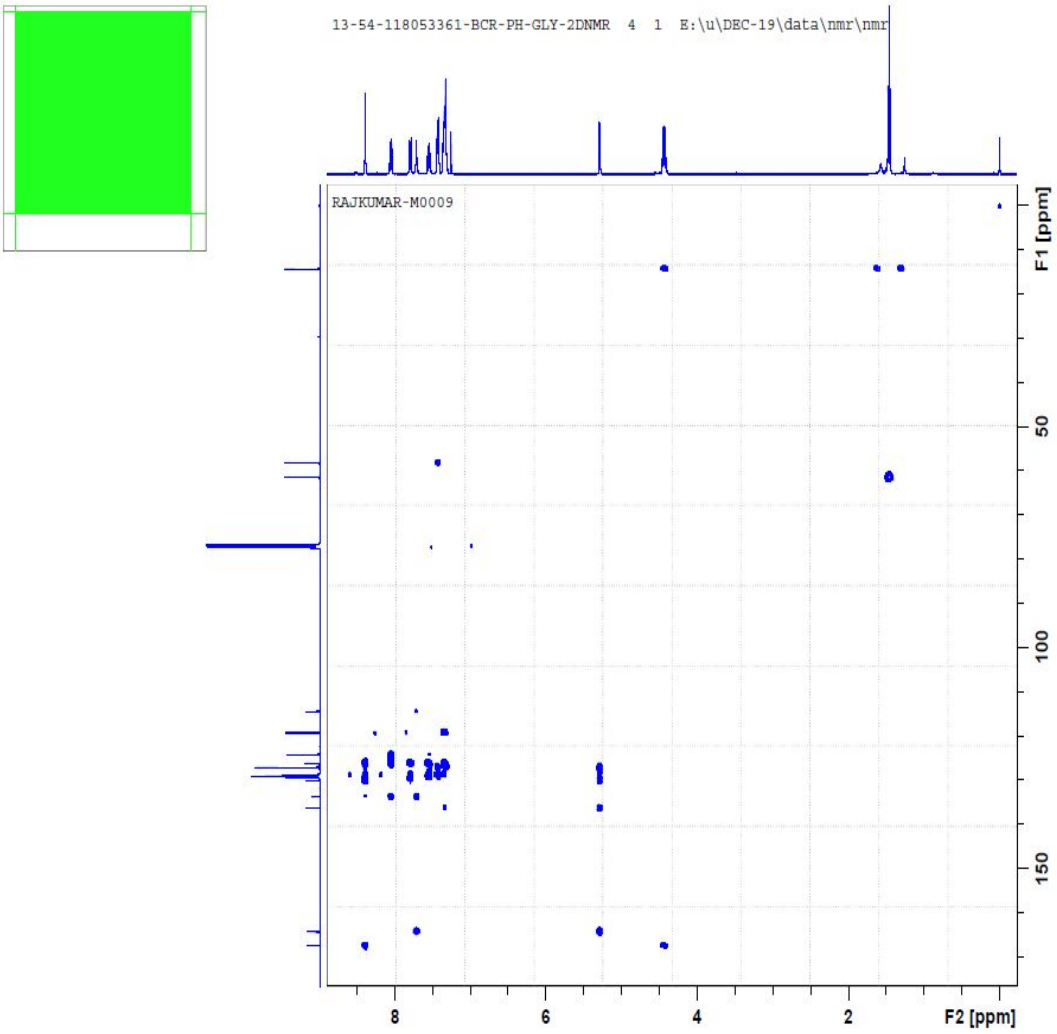
HSQC spectrum of compound 3ze



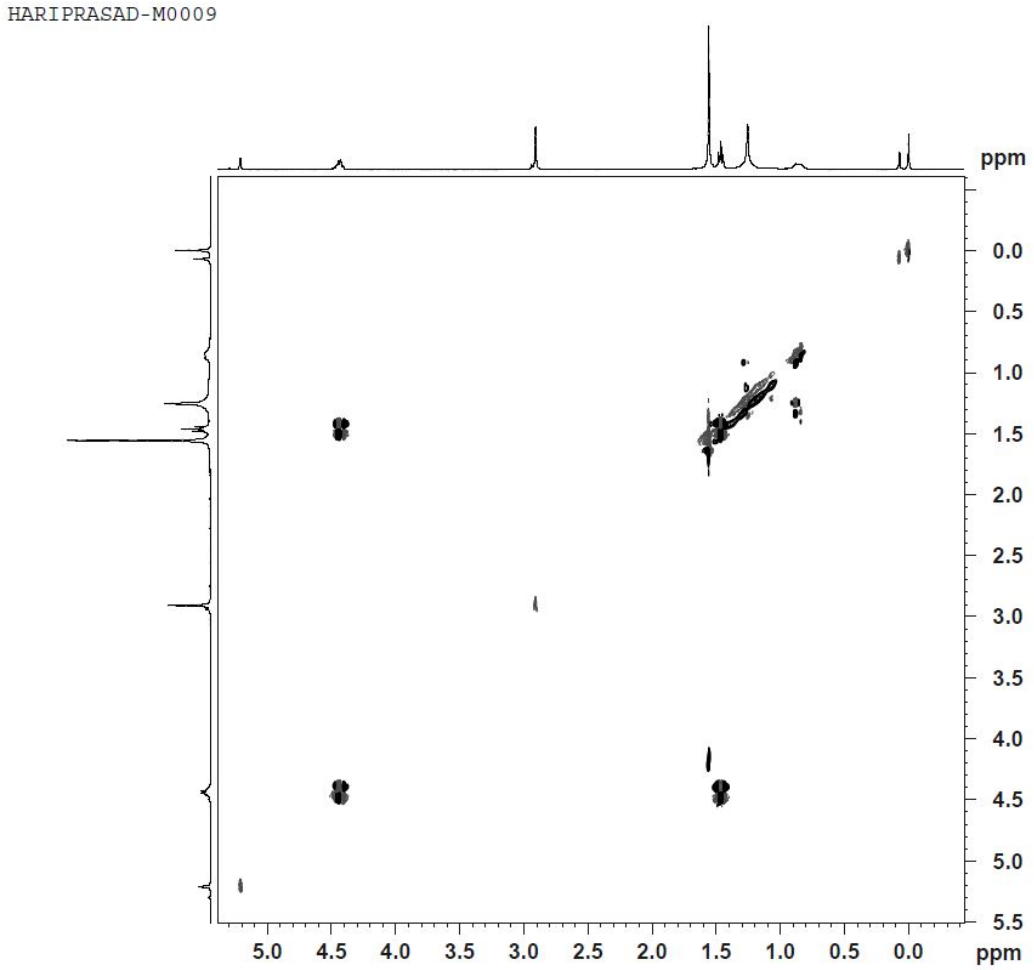
HMBC spectrum of compound 3ze



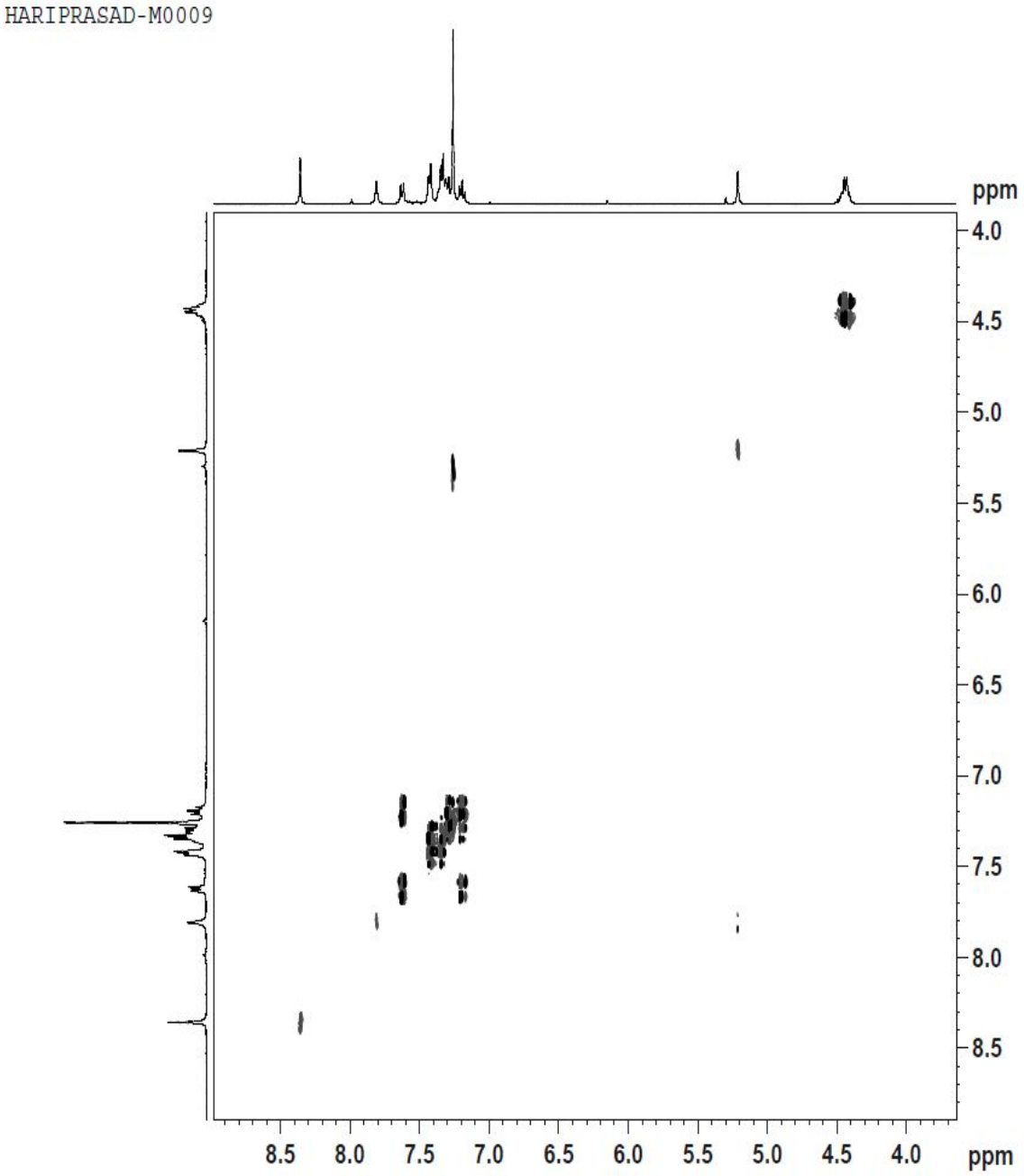
HMBC spectrum of compound 3ze



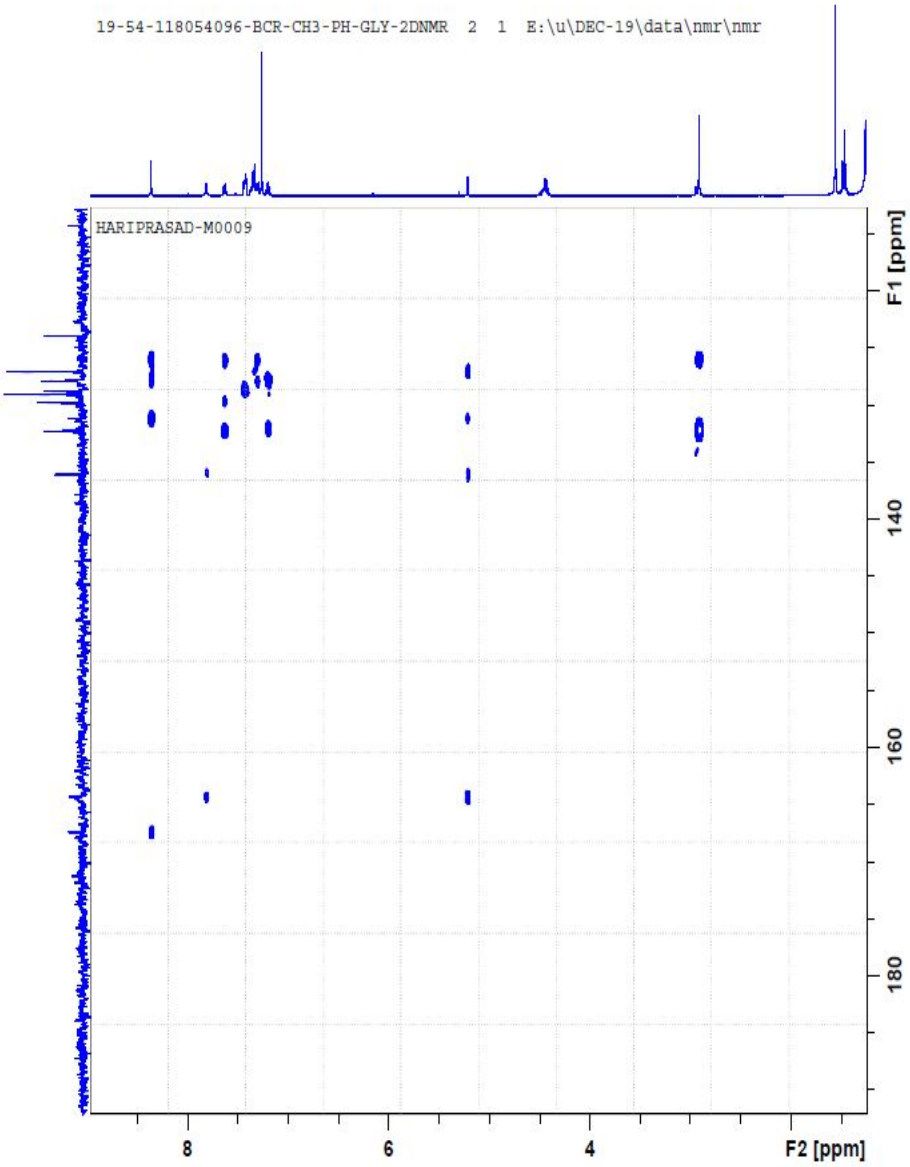
HMBC spectrum of compound 3ze



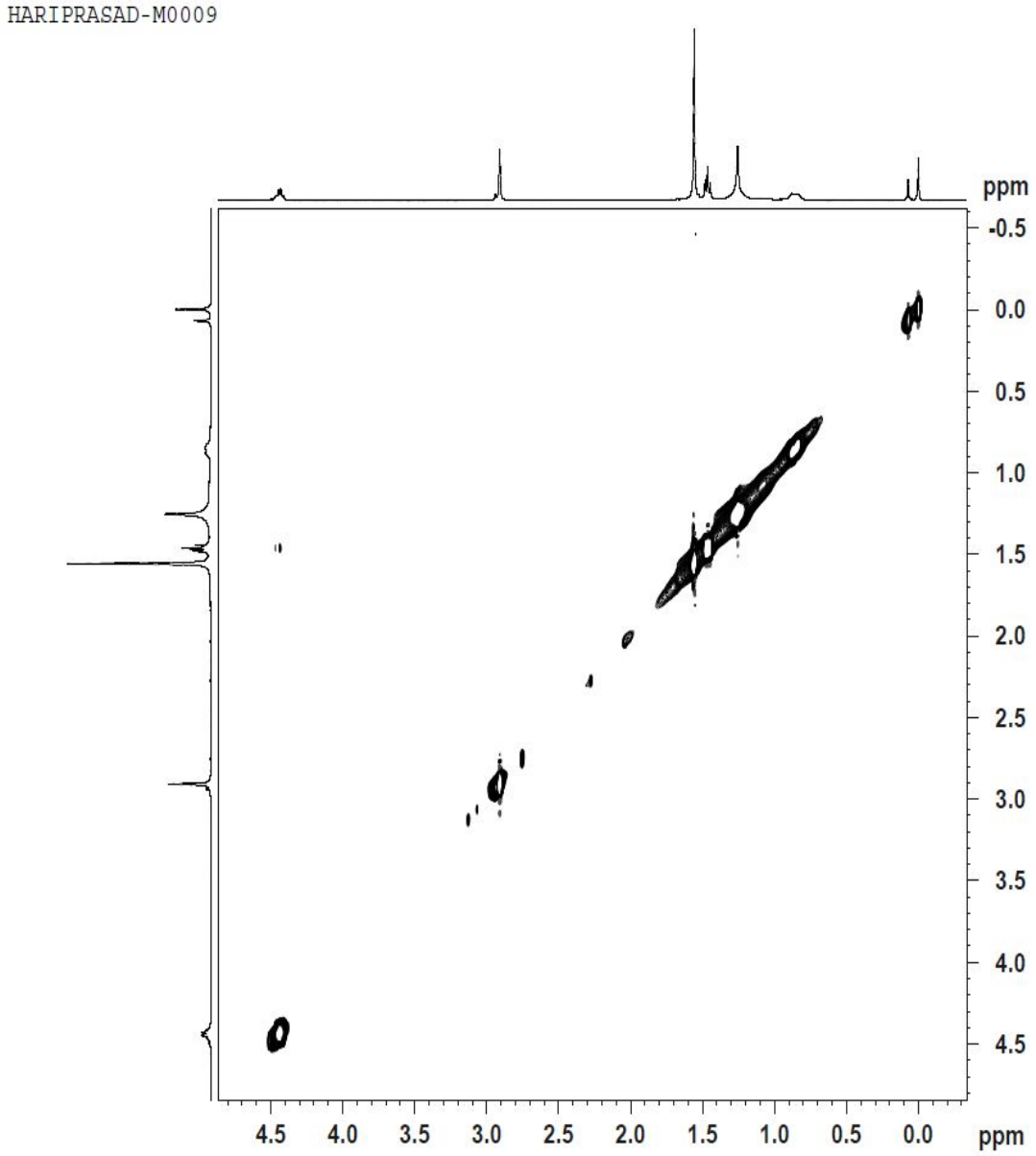
COSY spectrum of compound 3zg



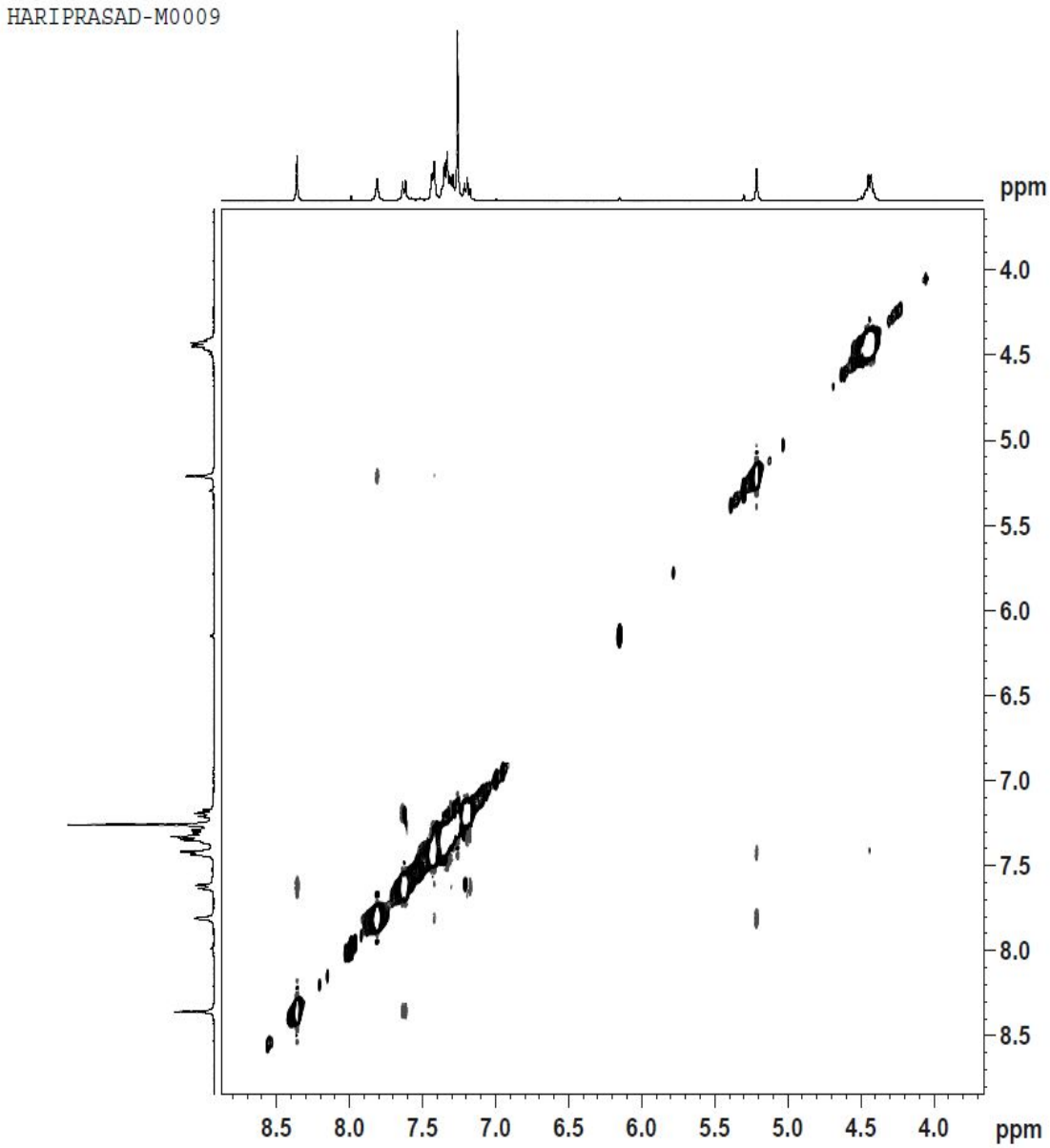
COSY spectrum of compound 3zg



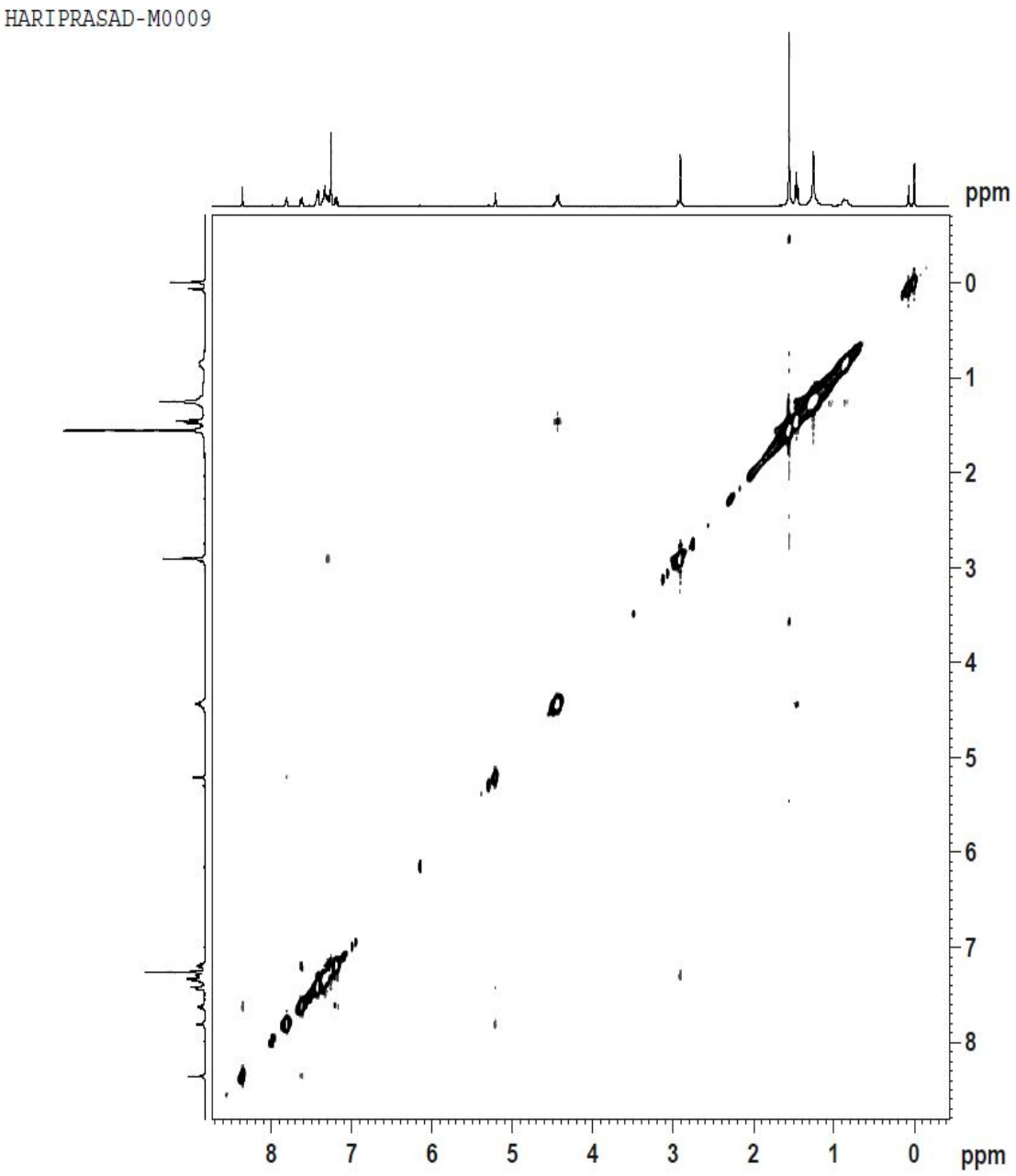
COSY spectrum of compound 3zg



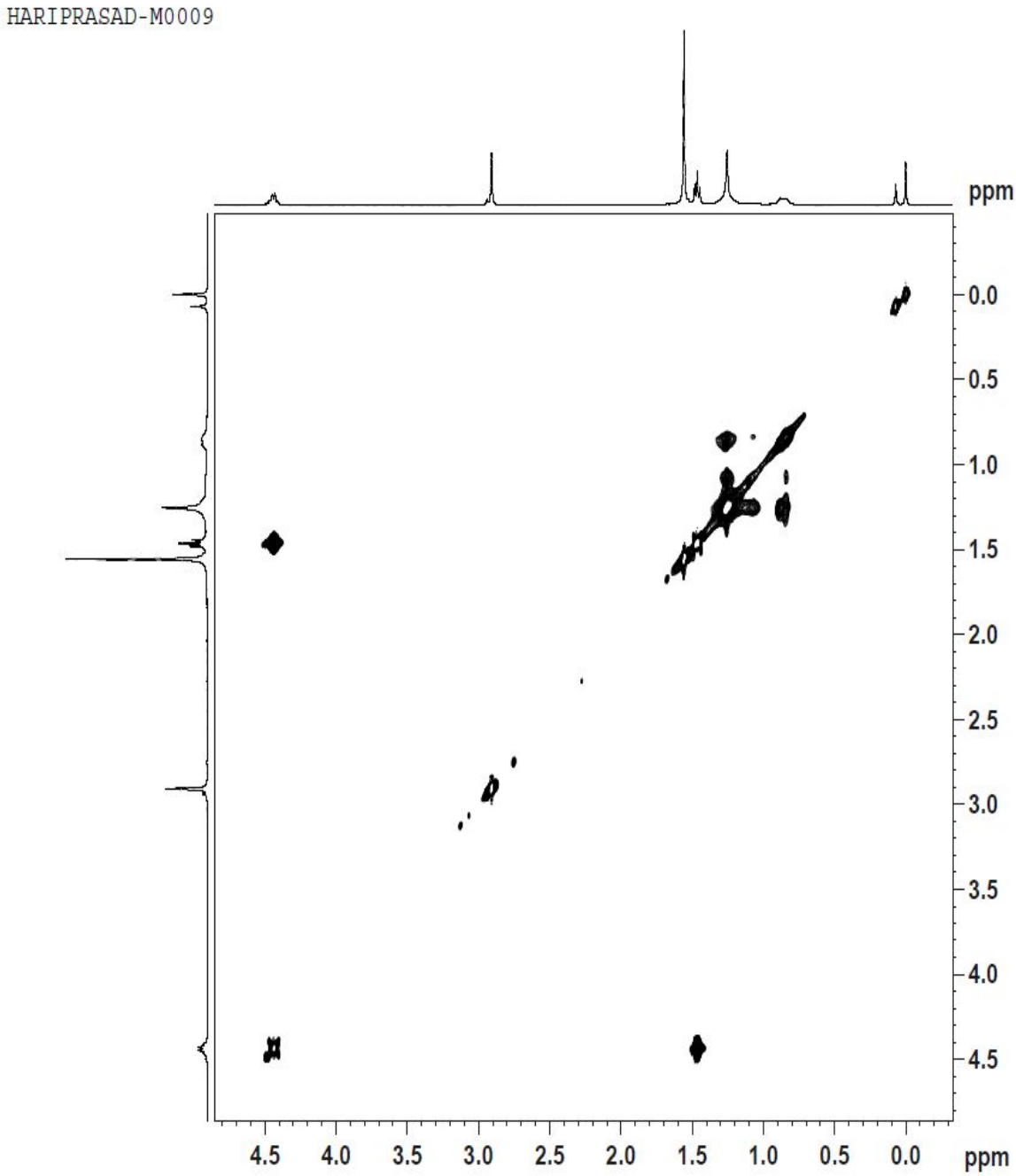
NOESY spectrum of compound 3zg



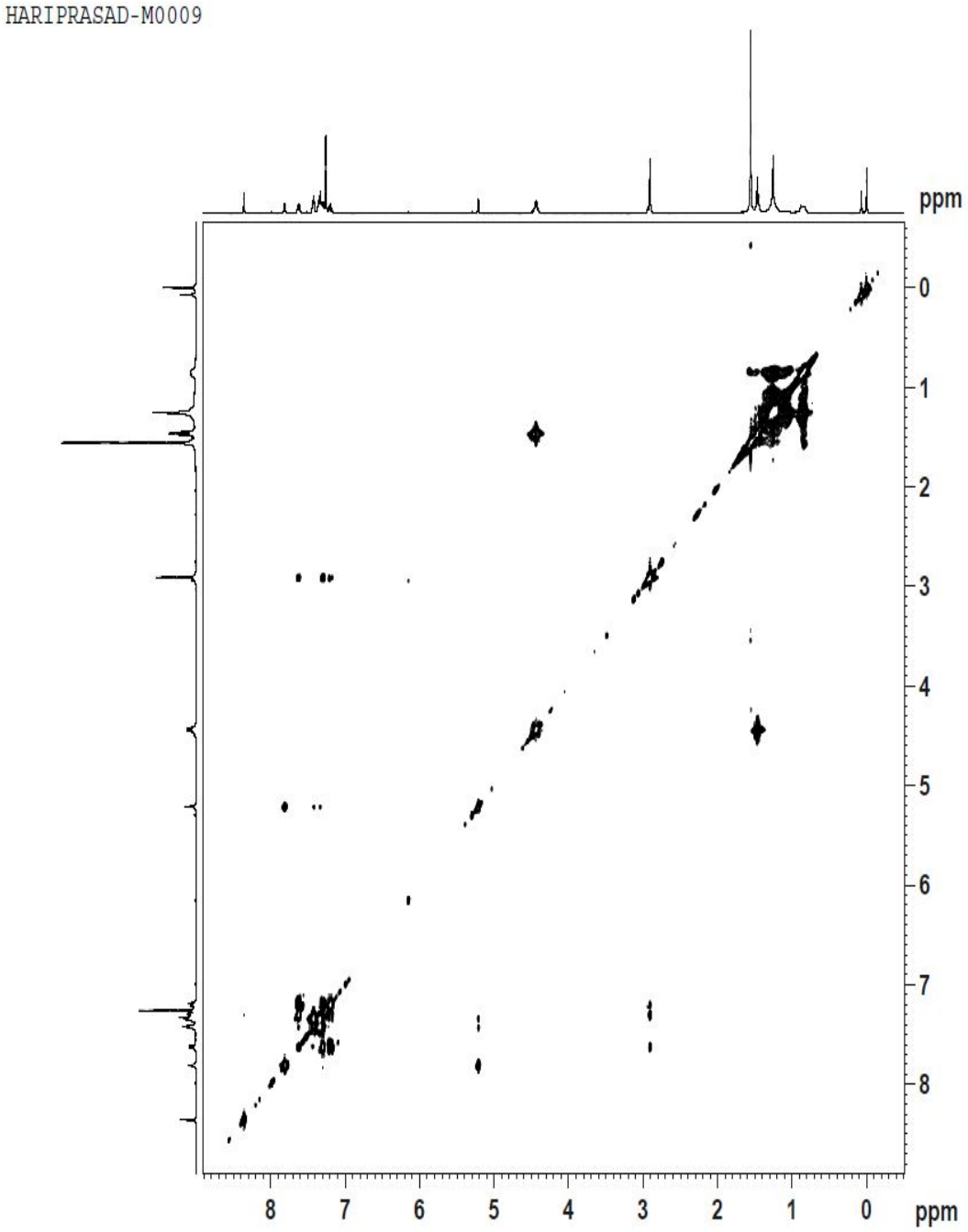
NOESY spectrum of compound 3zg



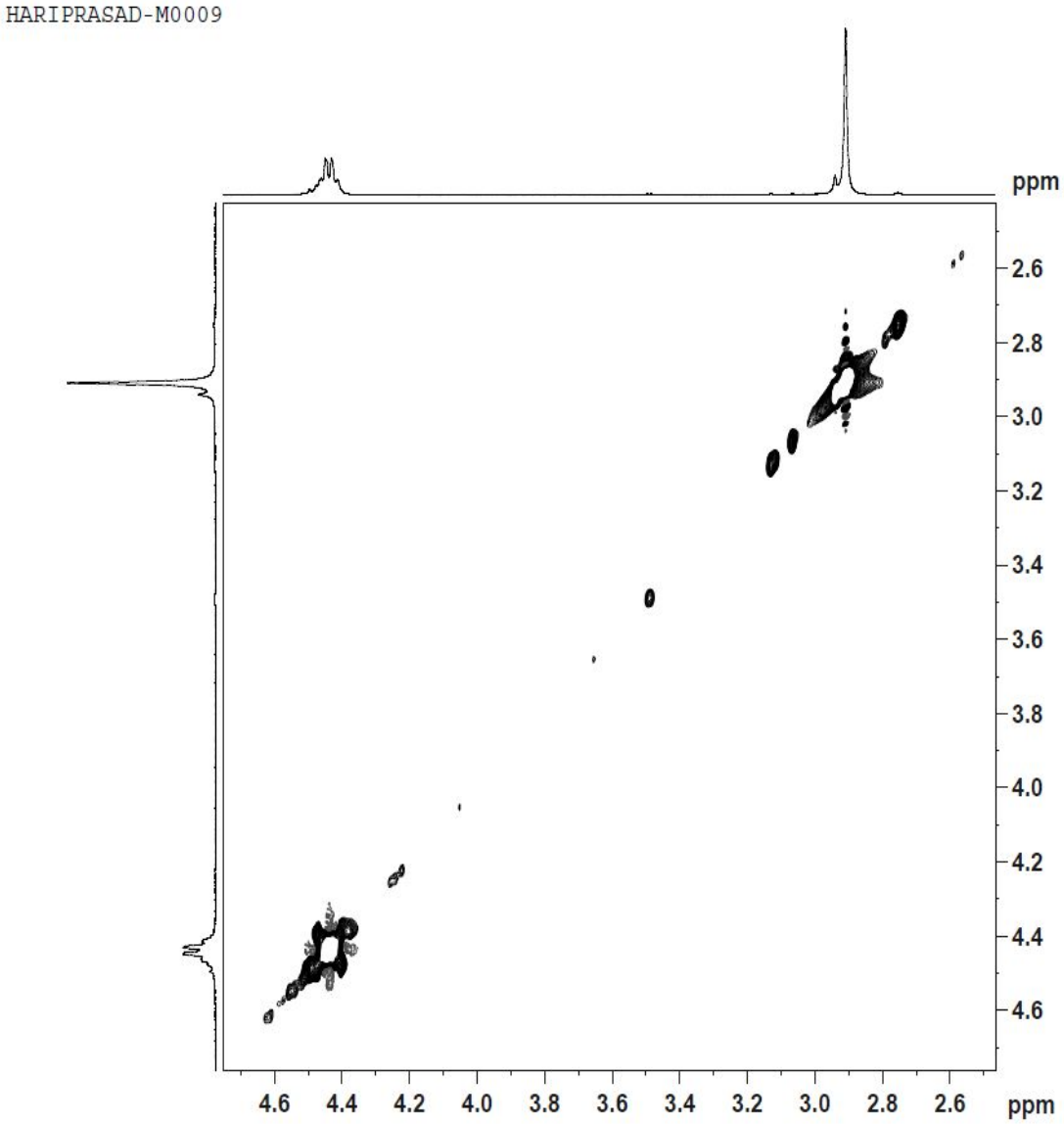
NOESY spectrum of compound 3zg



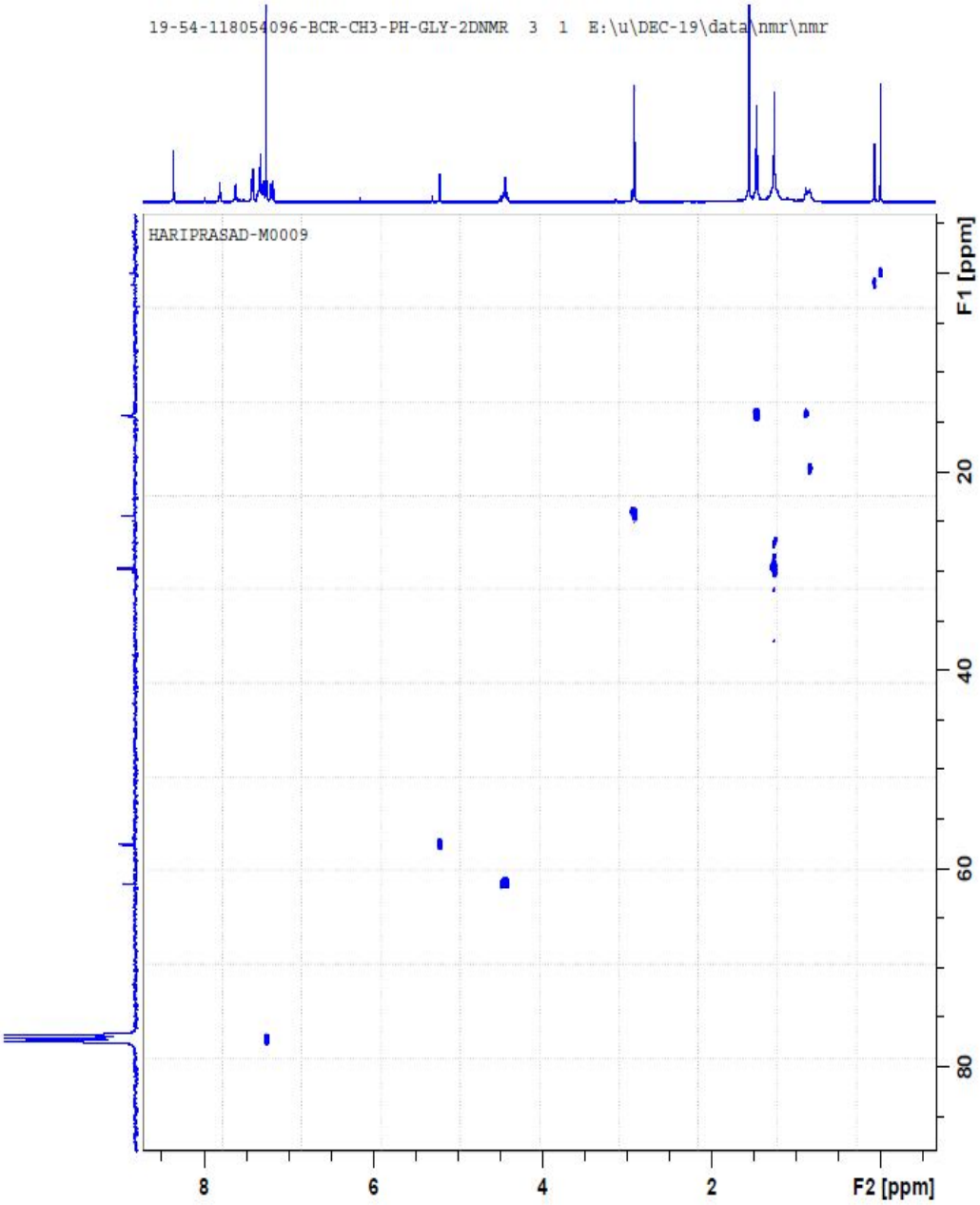
TOCSY spectrum of compound 3zg



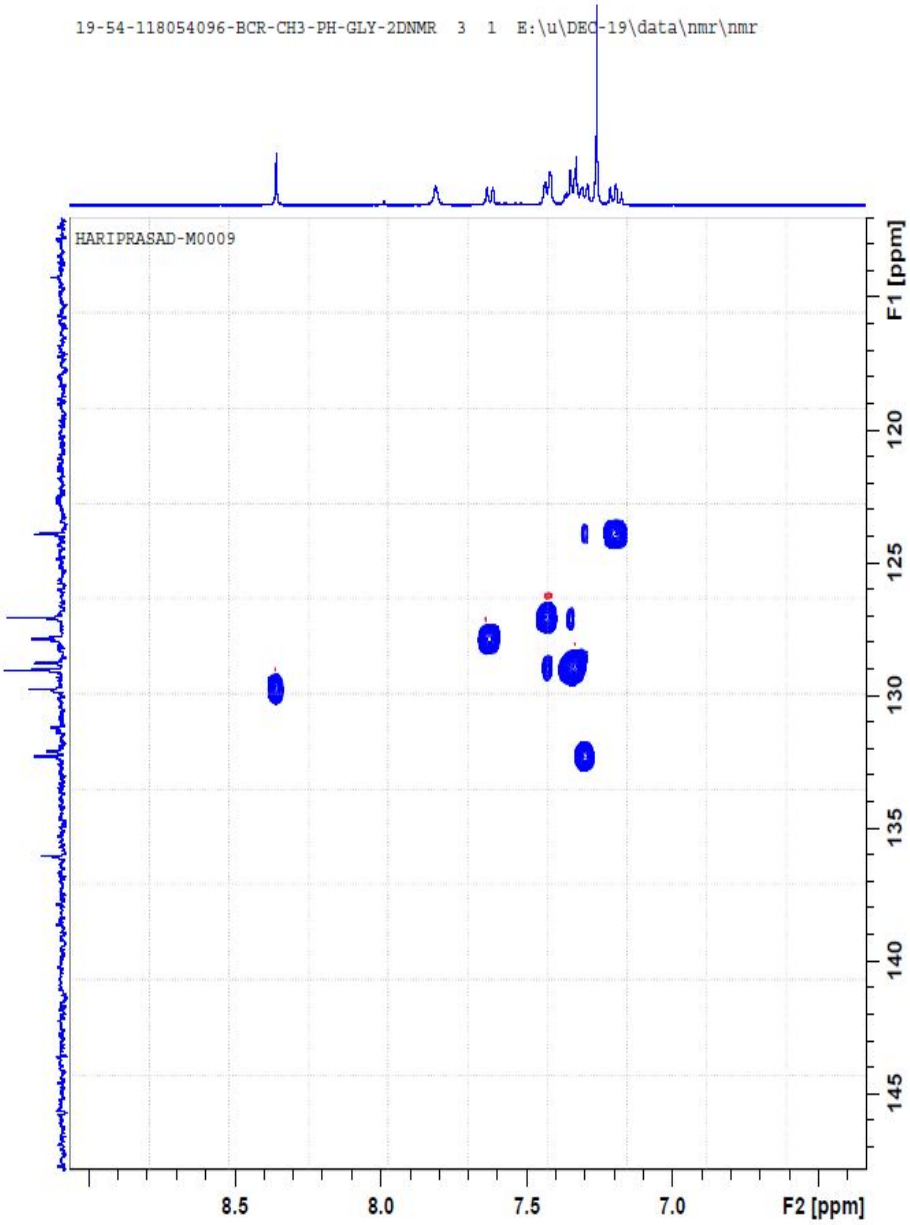
TOCSY spectrum of compound 3zg



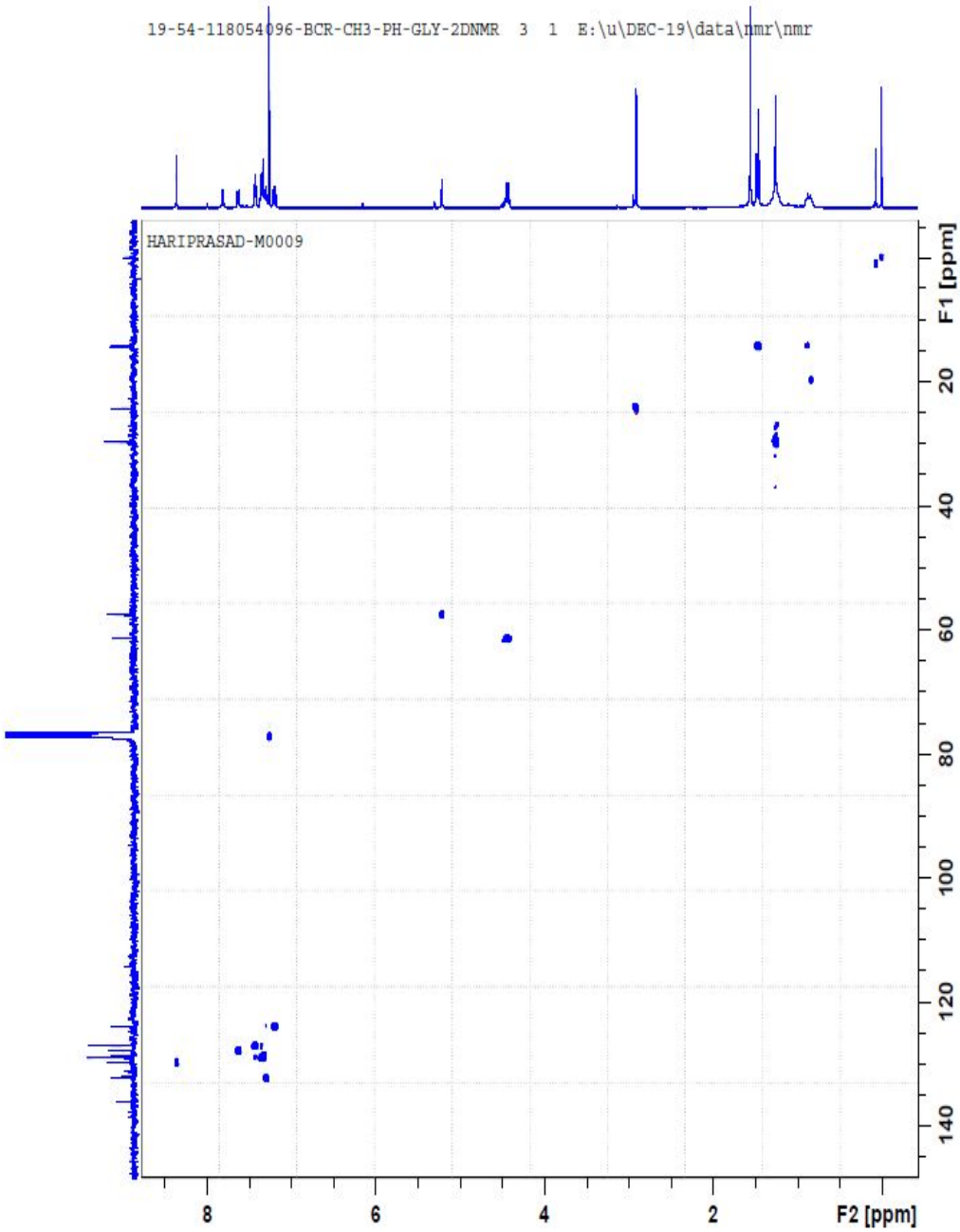
TOCSY spectrum of compound 3zg



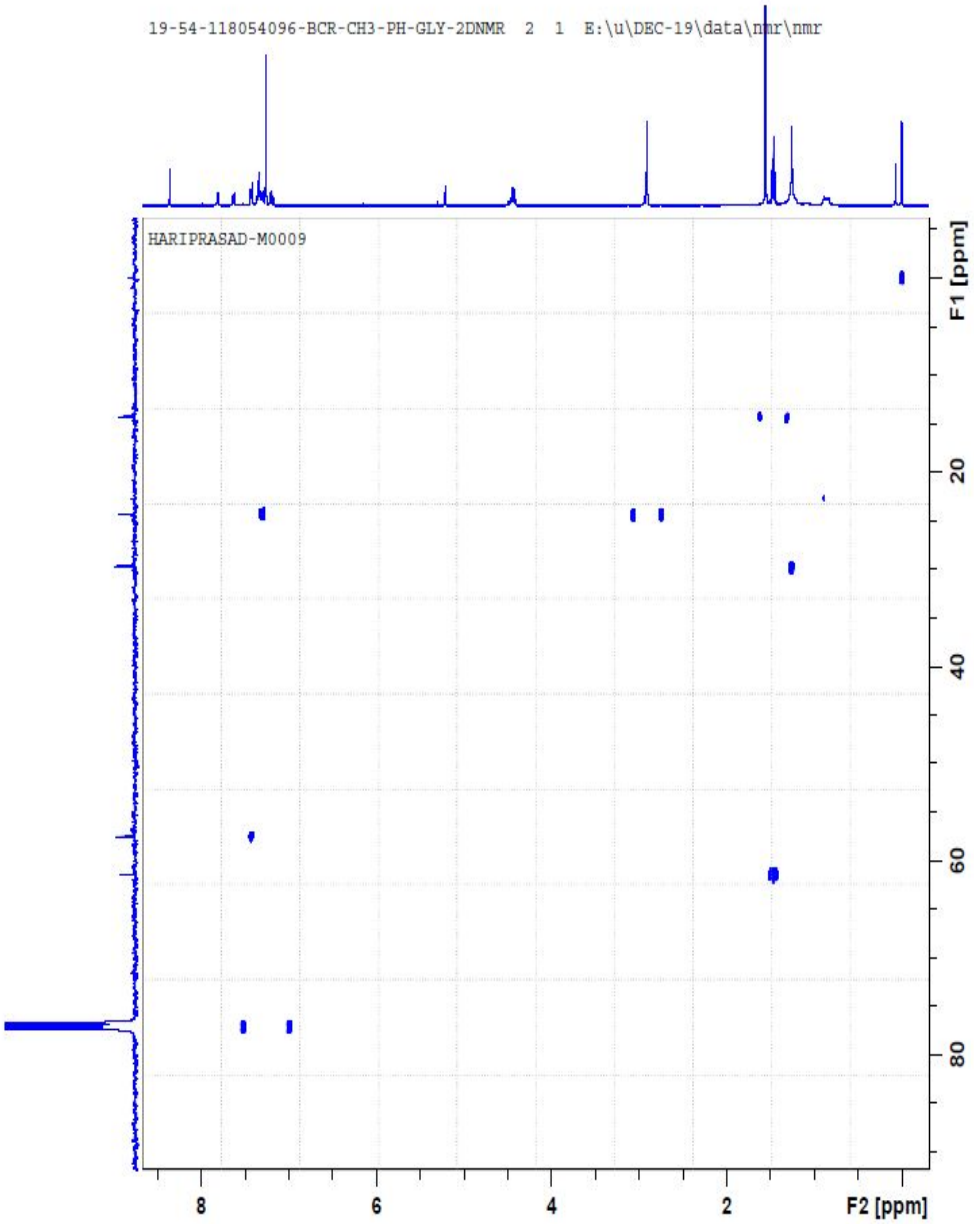
HSQC spectrum of compound 3zg



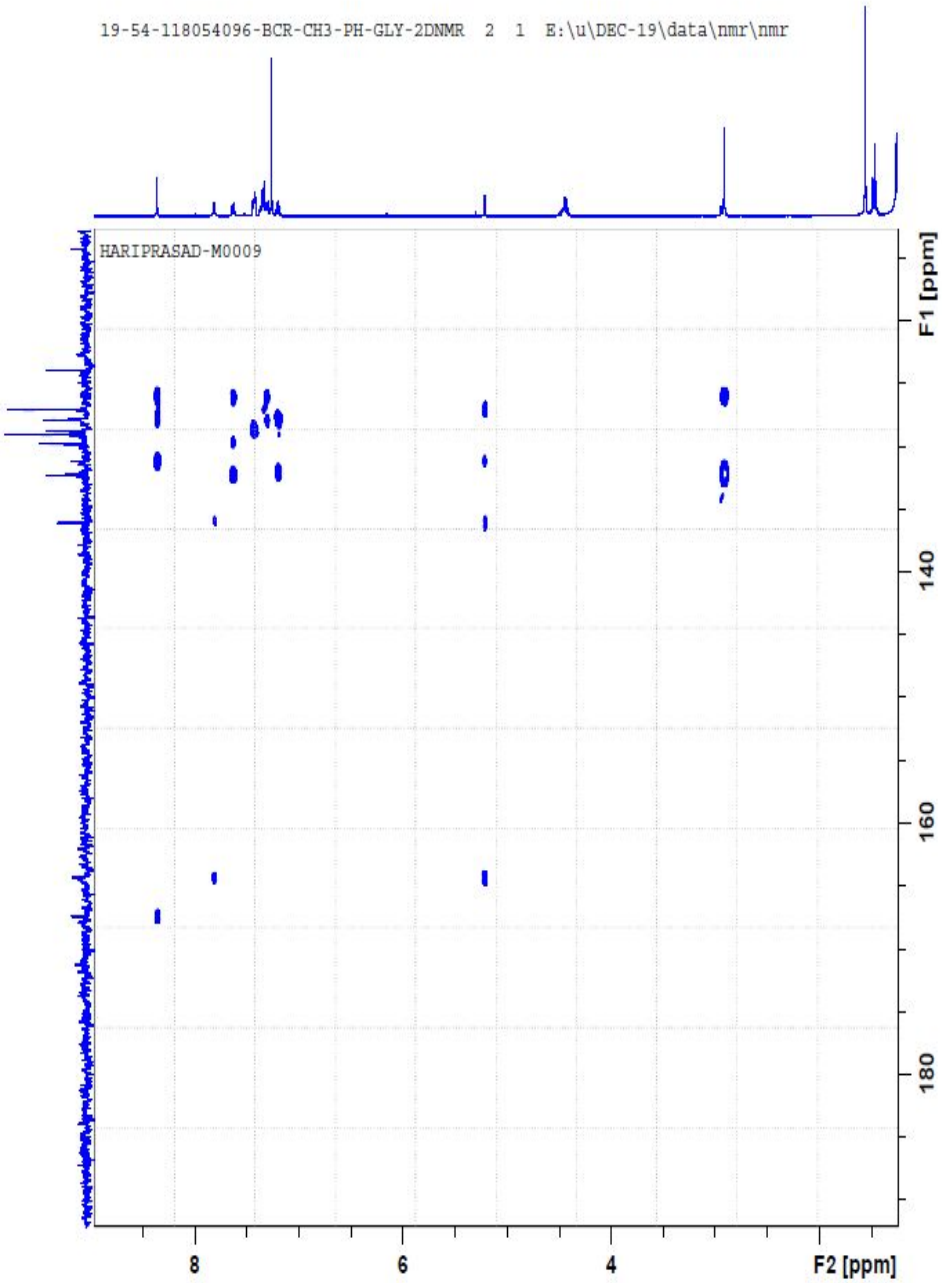
HSQC spectrum of compound 3zg



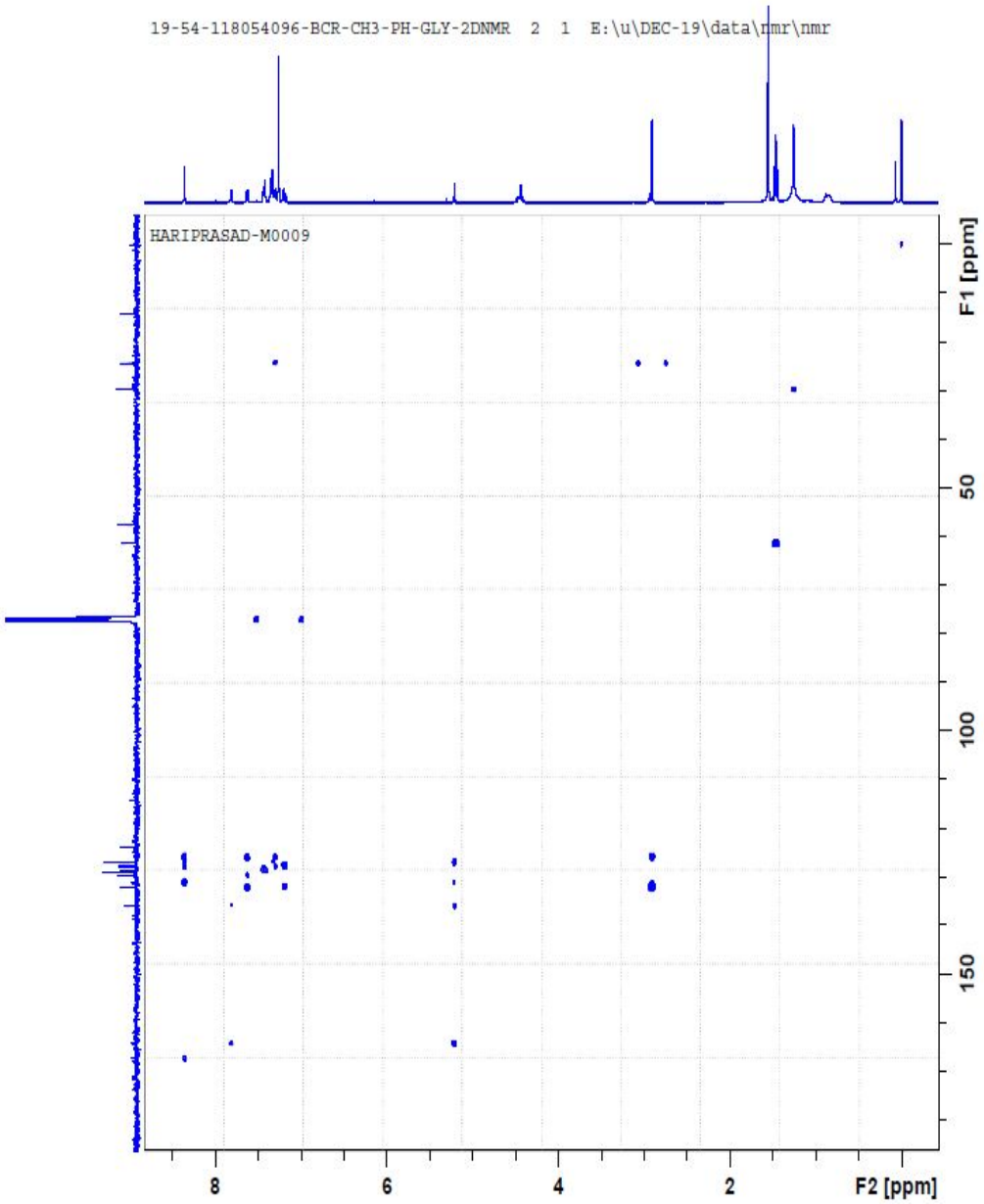
HSQC spectrum of compound 3zg



HMBC spectrum of compound 3zg



HMBC spectrum of compound 3zg



HMBC spectrum of compound 3zg