

Supplementary Information

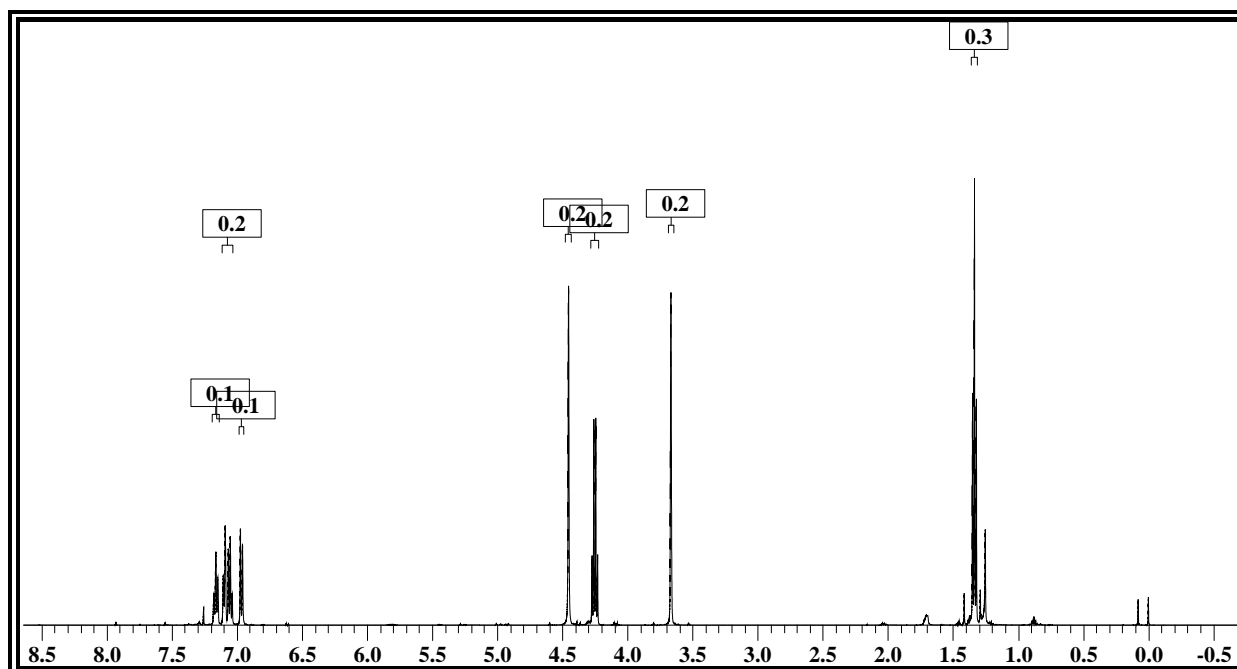
Synthesis of ethyl 2-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)-4*H*/2*H*-
chromene-
3-carboxylates by cycloaddition of ethyl 2-(azidomethyl)-4*H*-chromene-3-
carboxylates with alkynes

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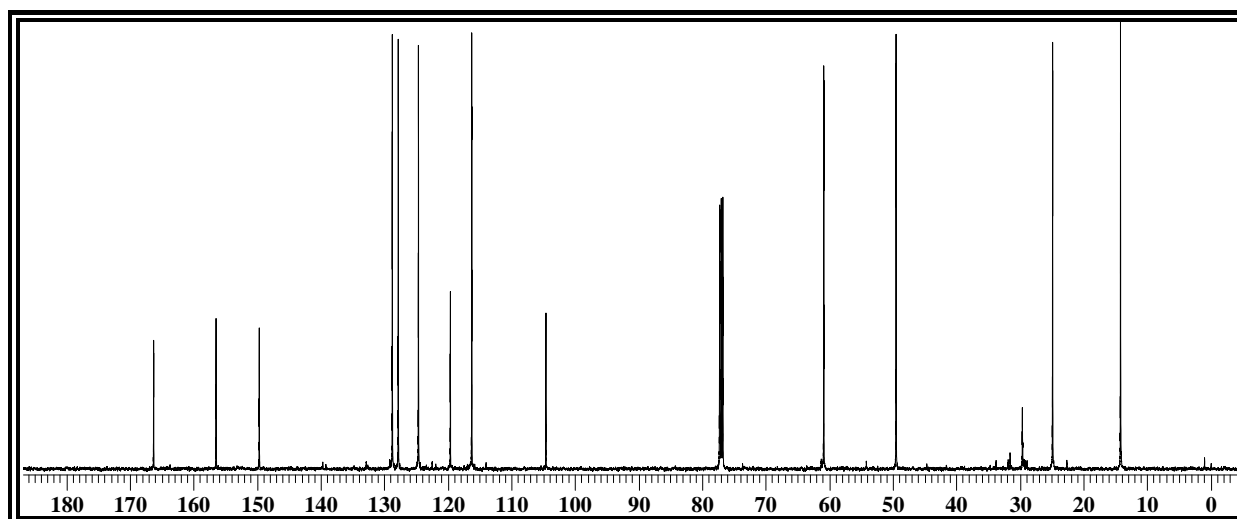
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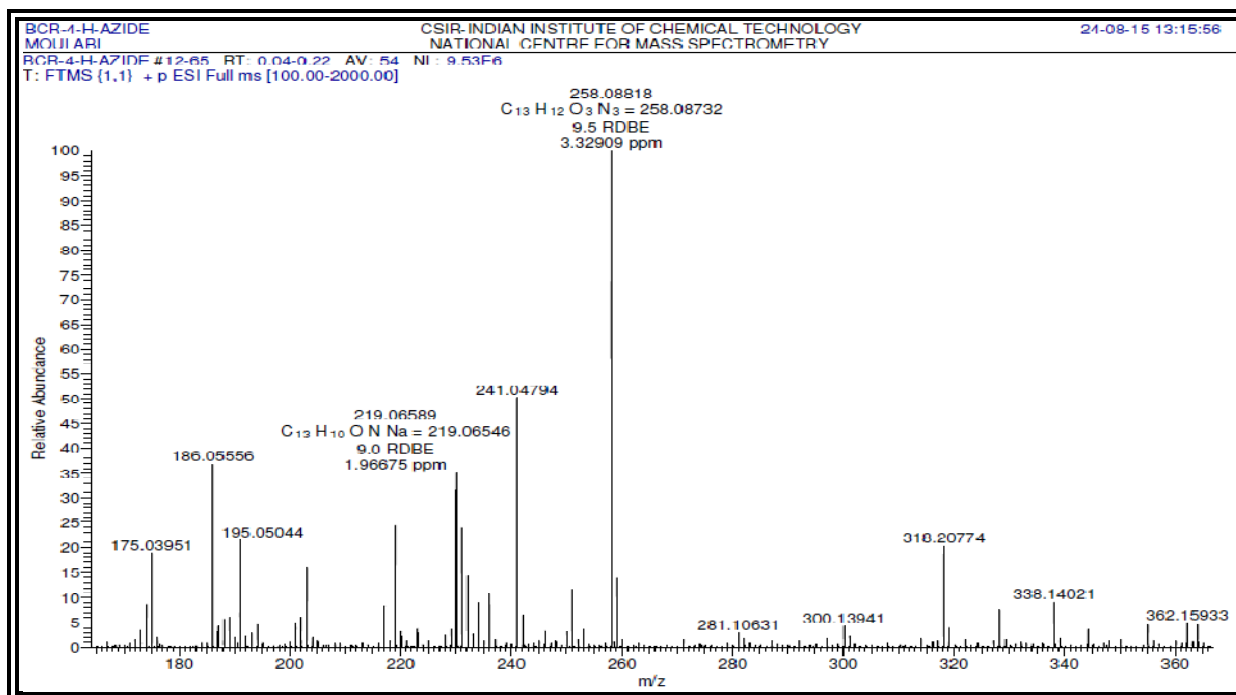
Copies of $^1\text{H-NMR}$, $^{13}\text{C-NMR}$, ESI-MS and HRMS of the compounds:



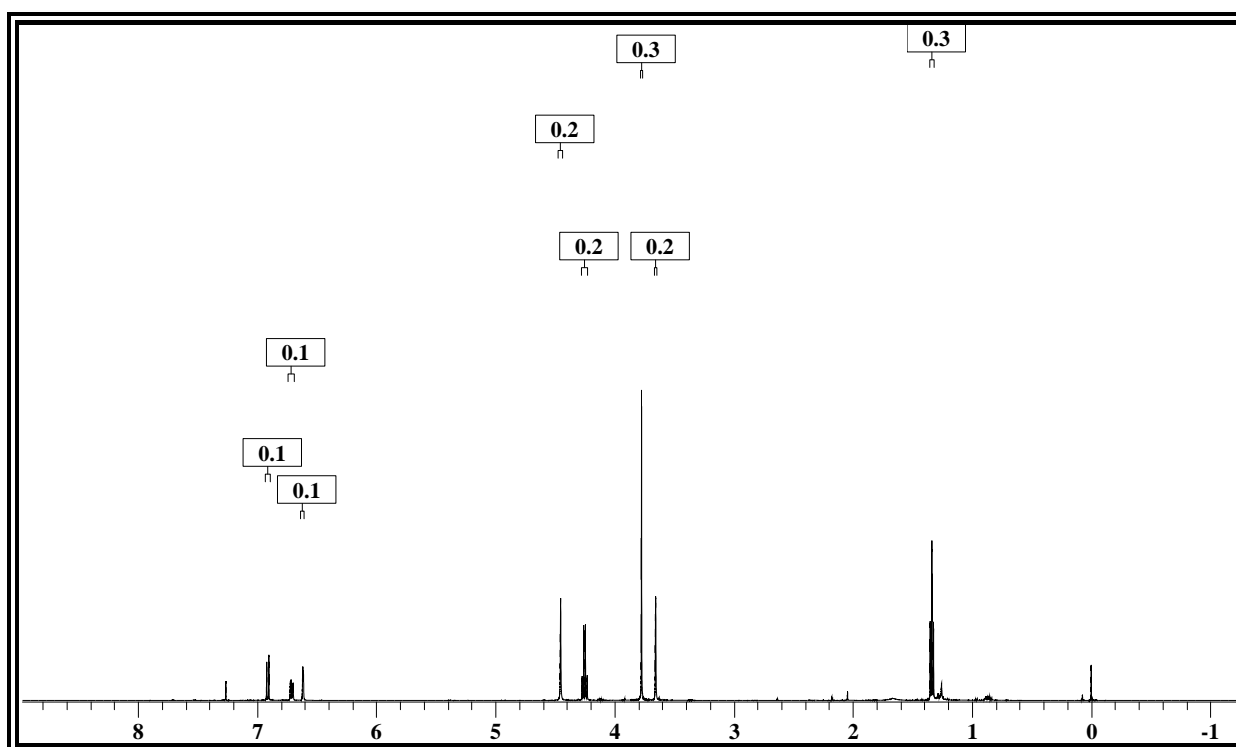
$^1\text{H-NMR}$ spectrum of compound 5a



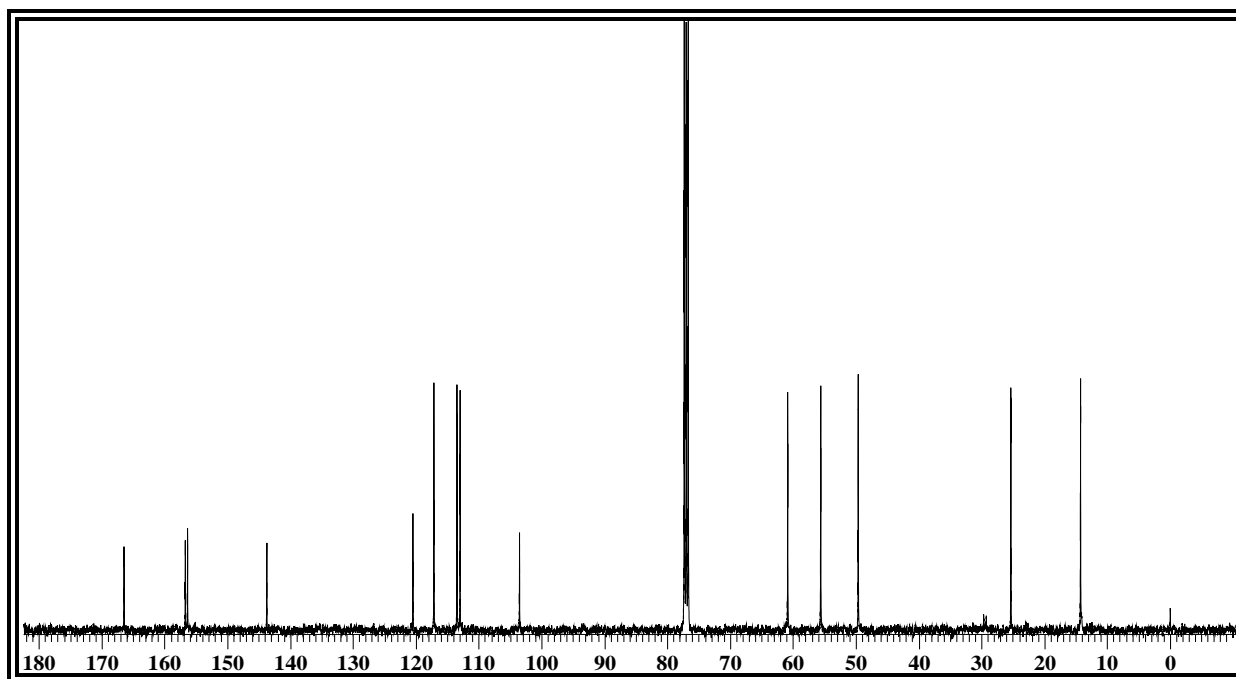
$^{13}\text{C-NMR}$ spectrum of compound 5a



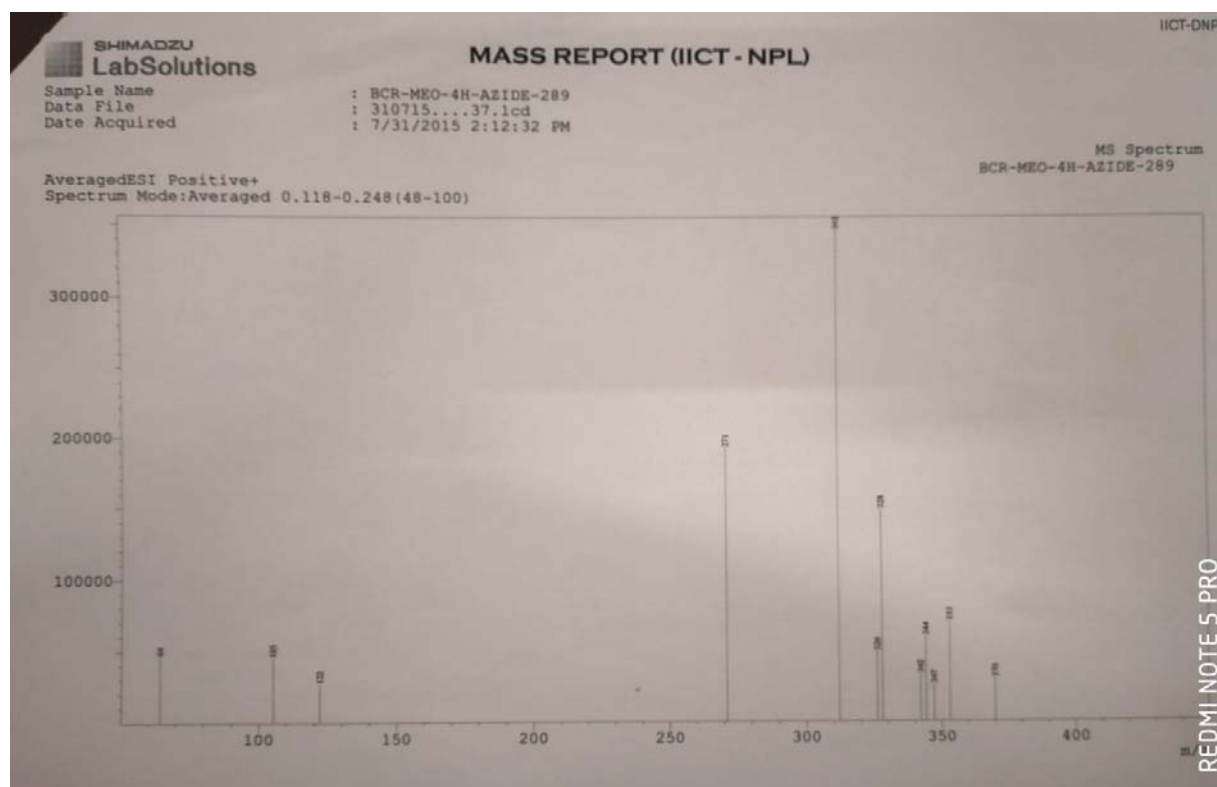
ESI-HRMS of compound **5a**



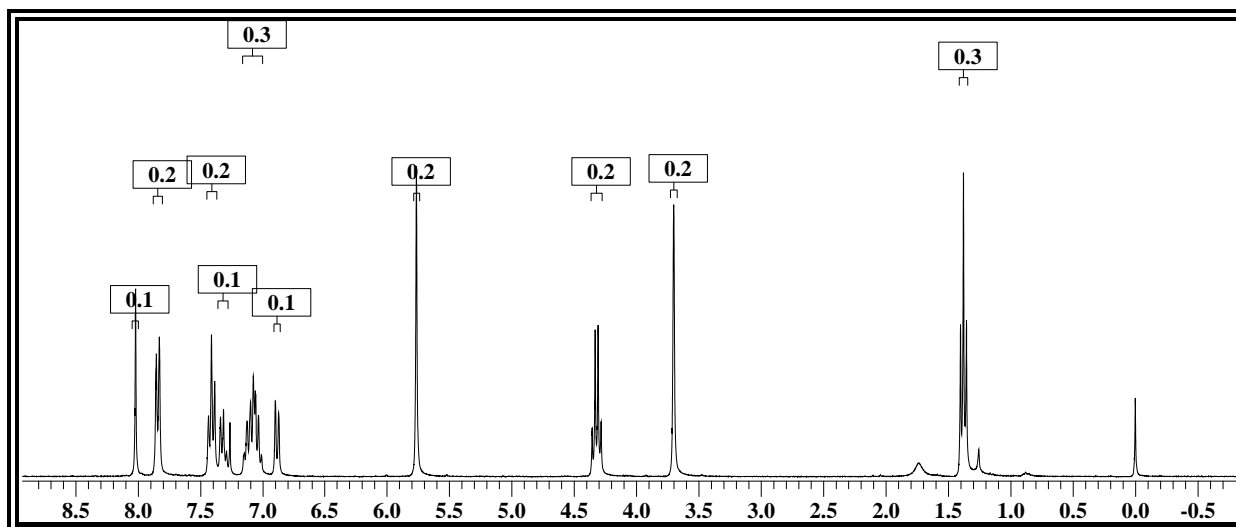
¹H-NMR spectrum of compound **5b**



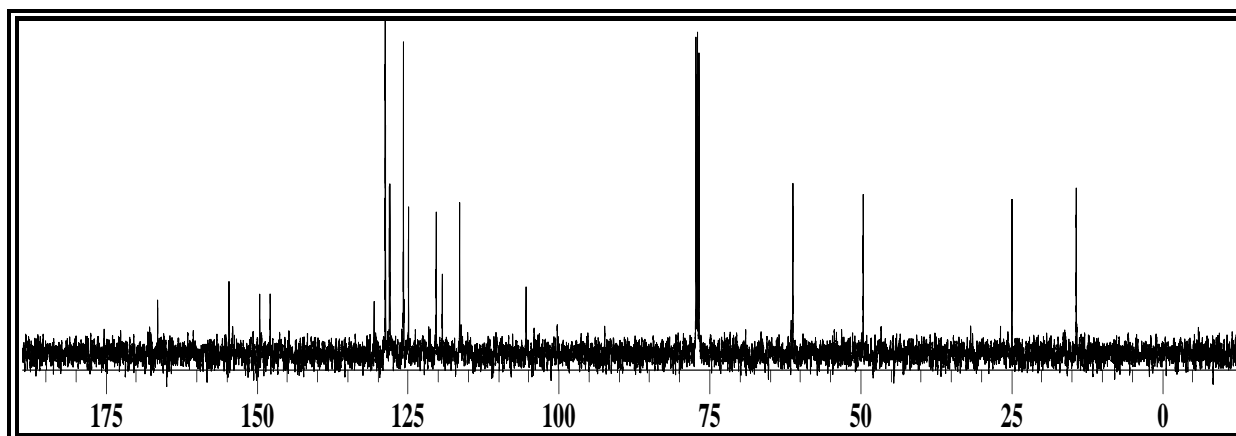
¹³C-NMR spectrum of compound **5b**



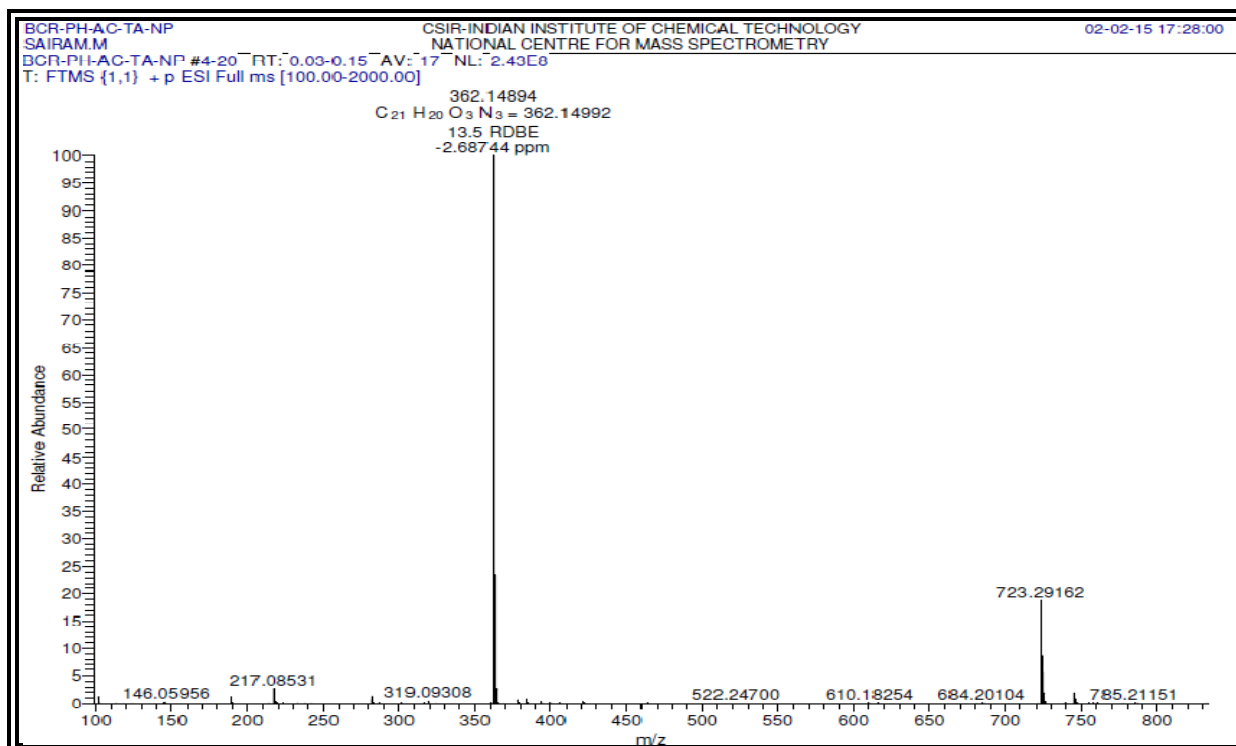
ESI-MS spectrum of compound **5b**



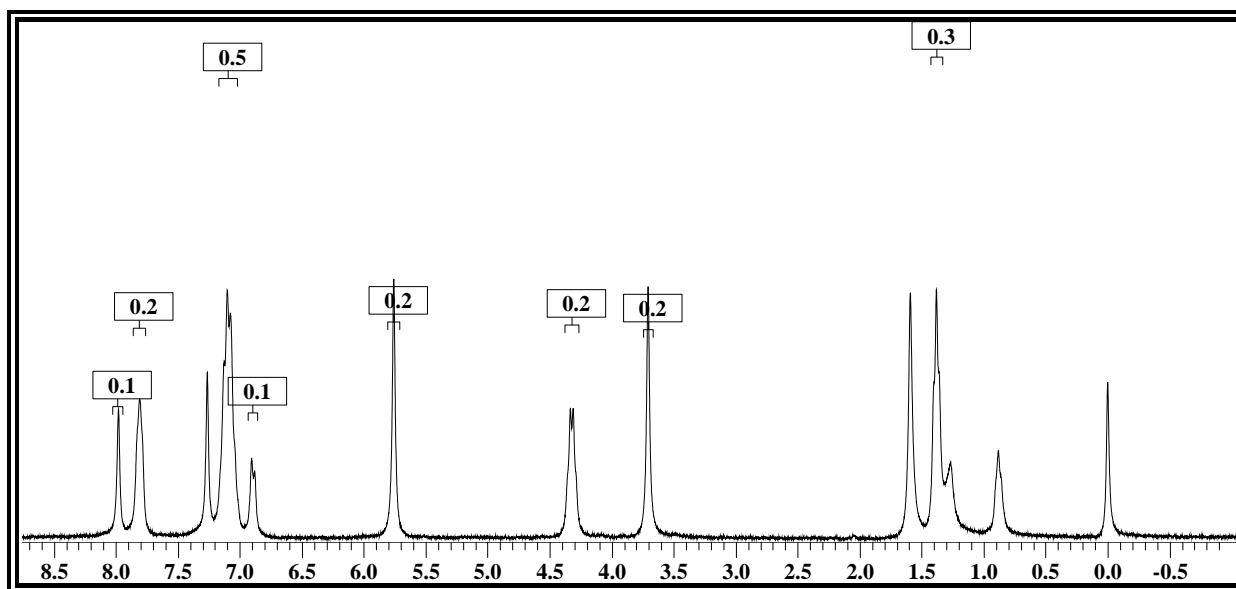
$^1\text{H-NMR}$ spectrum of compound 7a



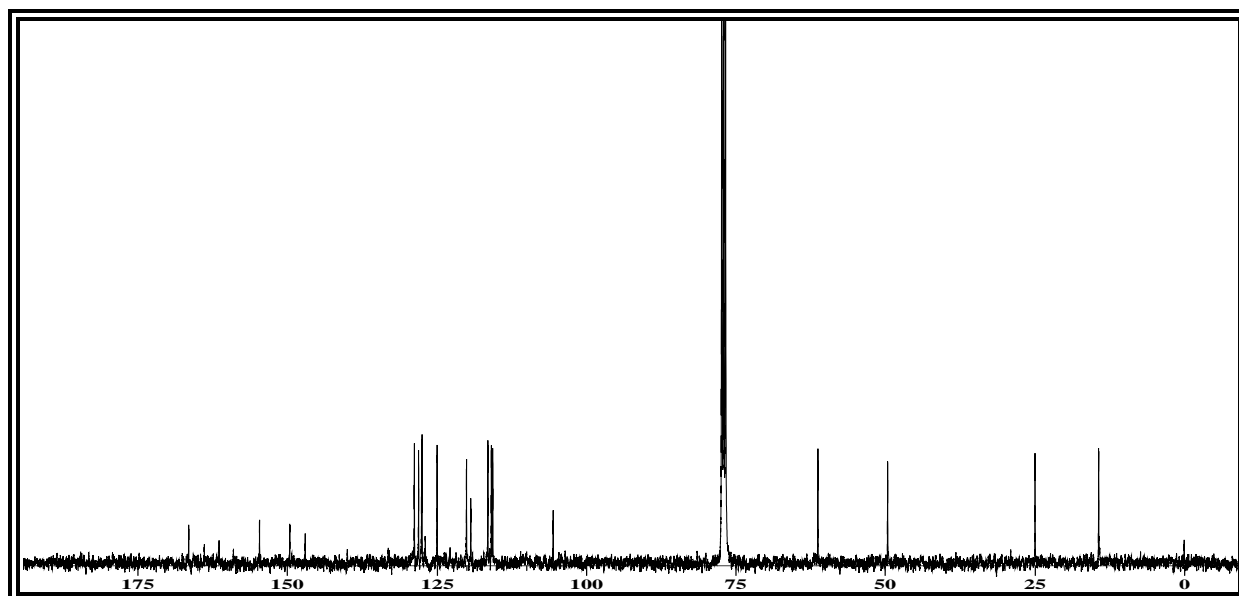
$^{13}\text{C-NMR}$ spectrum of compound 7a



ESI-HRMS of compound **7a**



¹H-NMR spectrum of compound **7b**

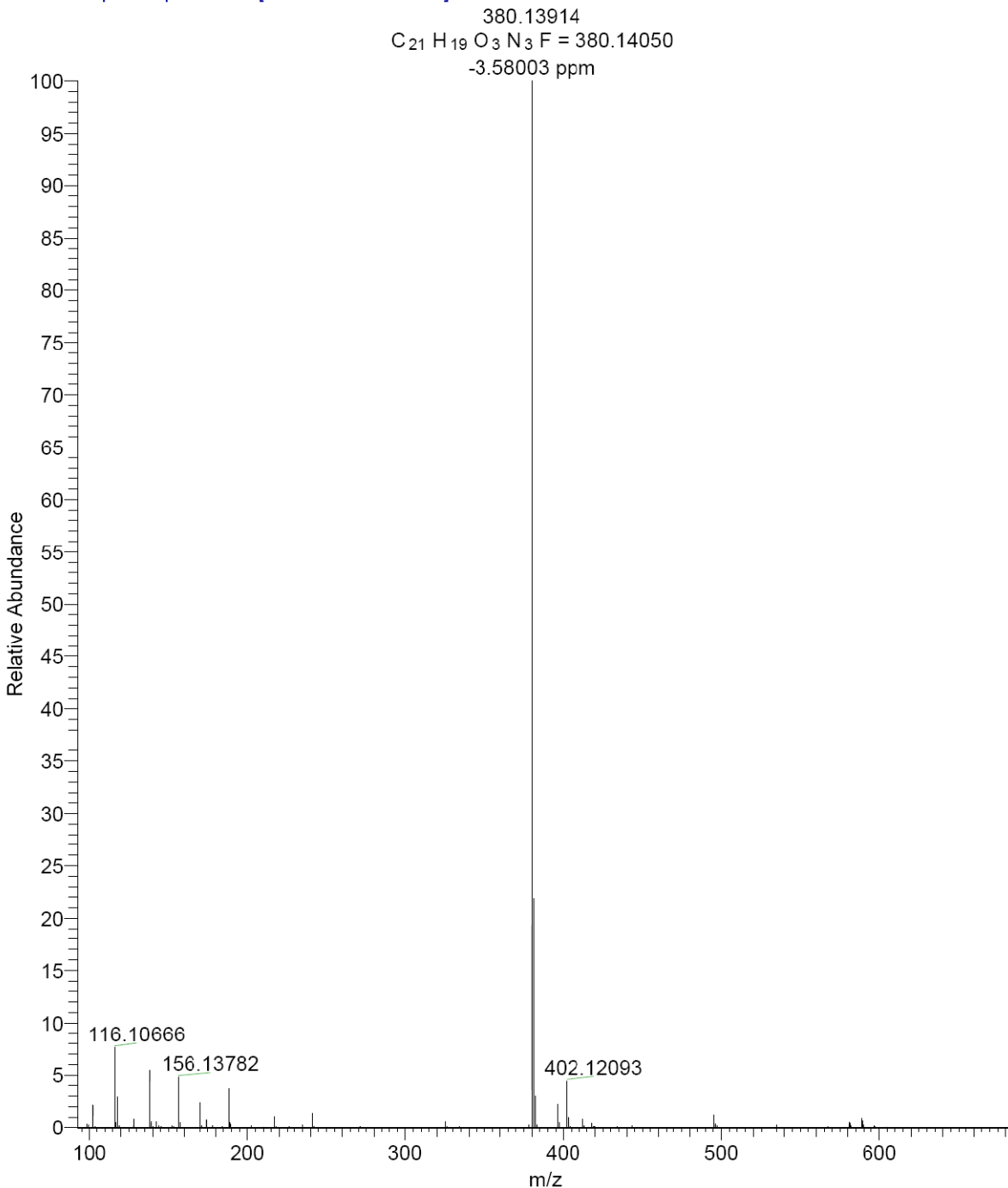


^{13}C -NMR spectrum of compound **7b**

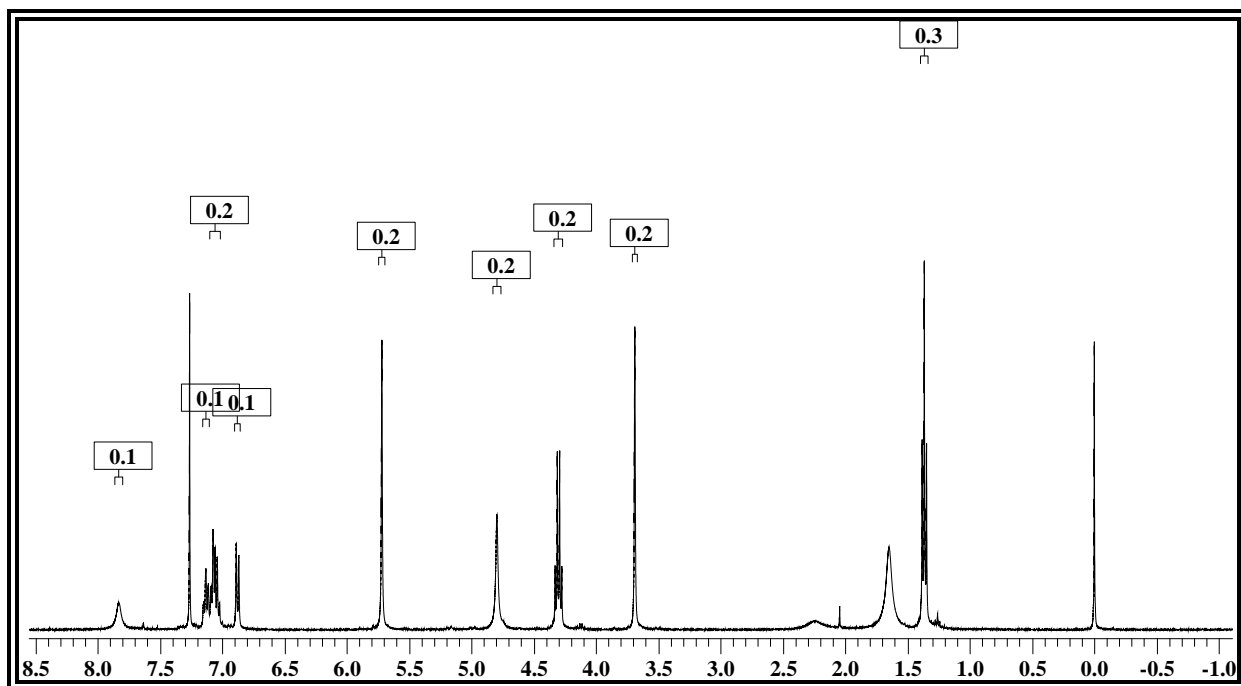
03/11/22 16:36:14
1180121423

Thermo Scientific Orbitrap Exploris 120
Analysed by G SAIKRISHNA

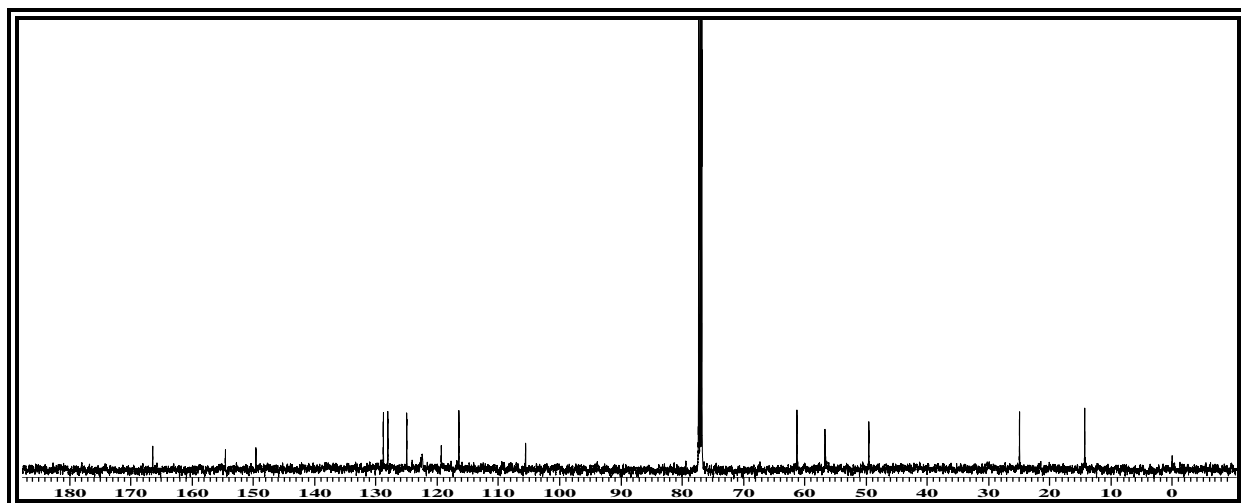
BCR-7B #10-32 RT: 0.03-0.08 AV: 23 SB: 373 0.32-1.20 NL: 1.94E7
T: FTMS + p ESI Ipi Full ms [50.0000-2000.0000]



HRMS Spectrum of compound **7b**

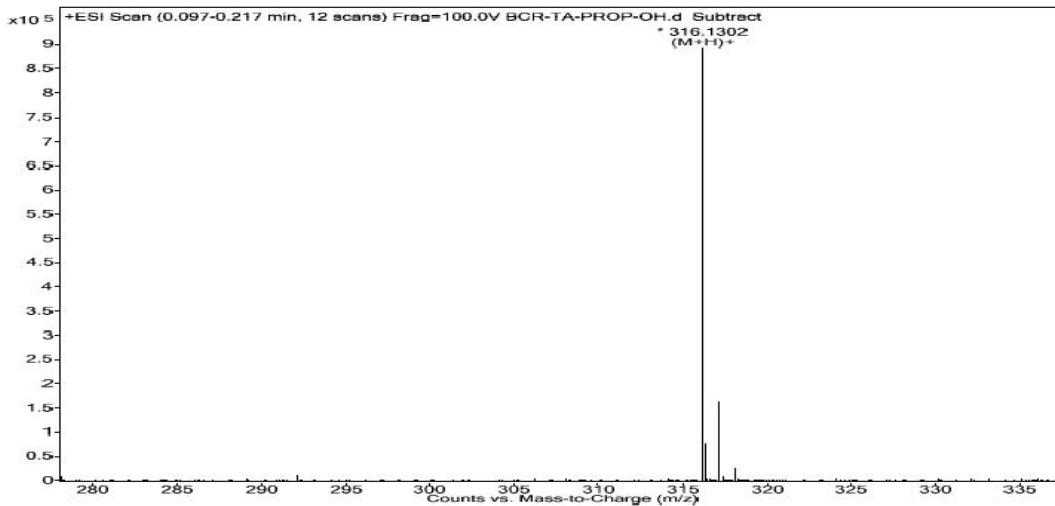


$^1\text{H-NMR}$ spectrum of compound **7e**



$^{13}\text{C-NMR}$ spectrum of compound **7e**

Sample Name BCR-TA-PROP-OH **Position** Vial 49 **Instrument Name** Instrument 1 **User Name**
Inj Vol -1 **InjPosition** **SampleType** Sample **IRM Calibration Status** Success
Data Filename BCR-TA-PROP-OH.d **ACQ Method** SCS.m **Comment** **Acquired Time** 6/1/2016 2:28:28 PM

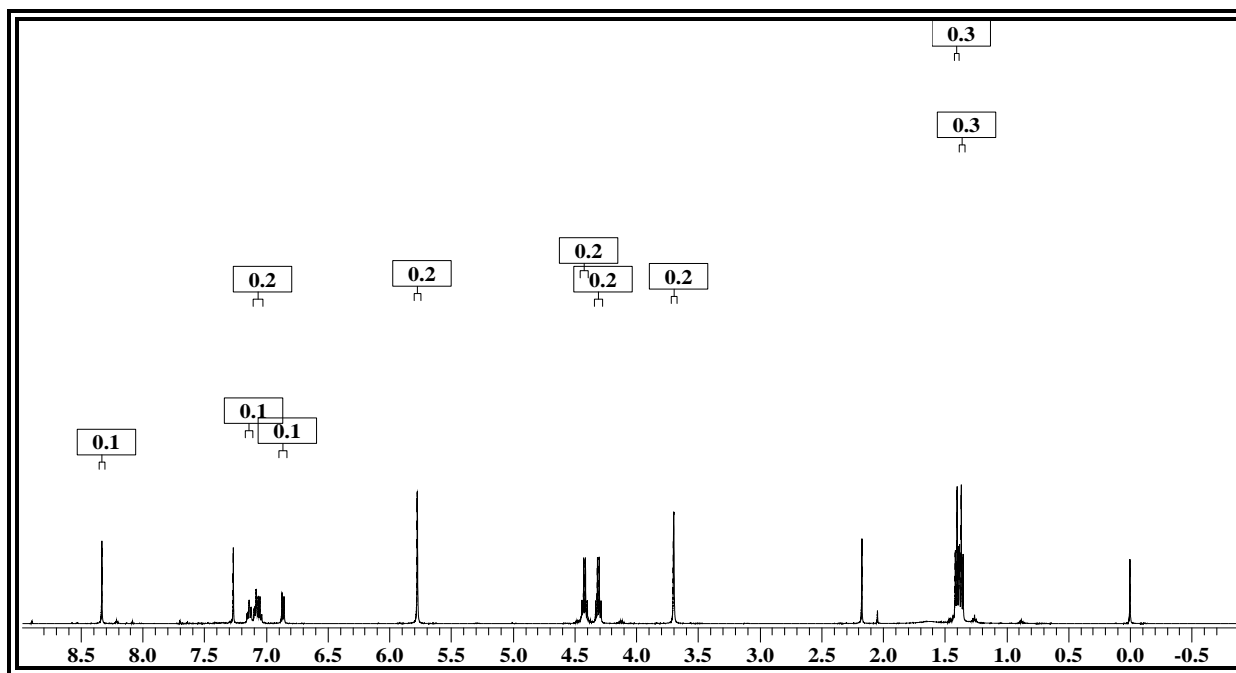


MS Formula Results: + Scan (0.097-0.217 min) Sub - BCR-TA-PROP-OH.d (BCR-TA-PROP-OH.d)

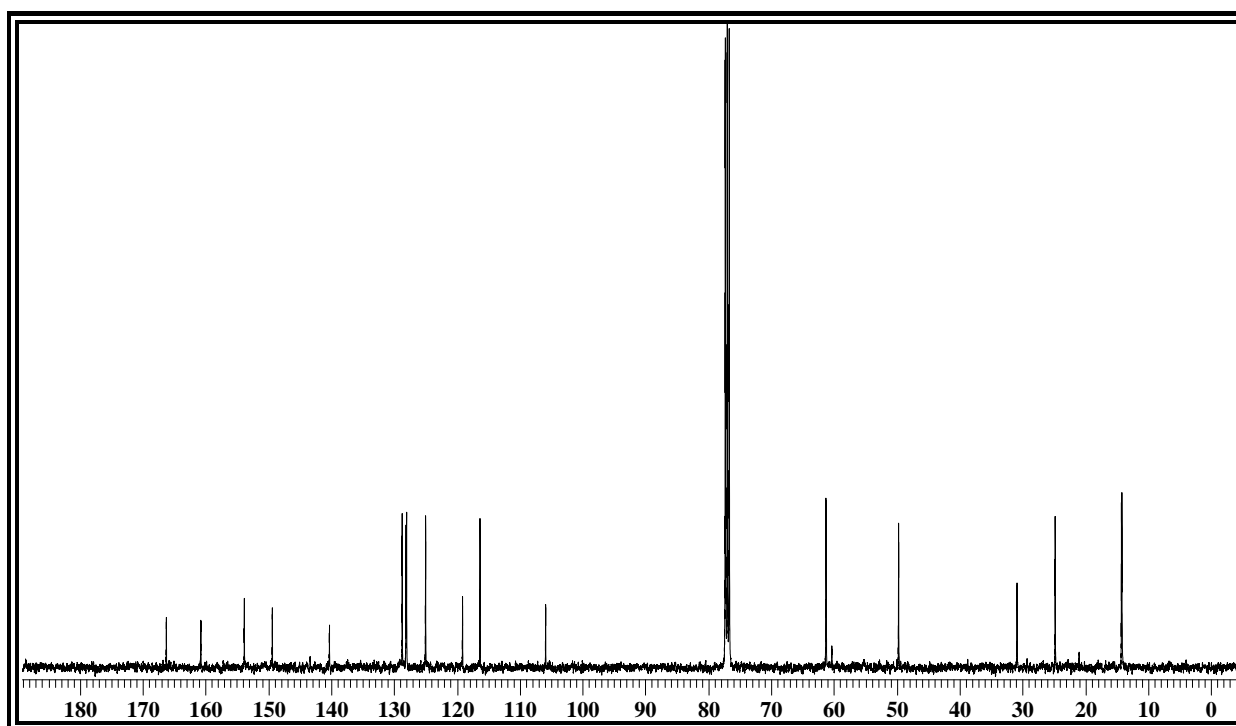
m/z	Ion	Formula	Abundance
316.1302	(M+H) ⁺	C ₁₆ H ₁₇ N ₃ O ₄	892426.1

Best	Formula (M)	Ion Formula	Calc m/z	Score	Close Score	Mass	Calc Mass	Diff (ppm)	Abn Diff (ppm)	Abund Match	Spacing Match	Mass Match	m/z	DBE
F2	C ₁₆ H ₁₇ N ₃ O ₄	C ₁₆ H ₁₇ N ₃ O ₄	316.1282	89.81		316.1228	316.1210	-3.22	3.22	99.93	76.22	93.01	316.1302	10

ESI-HRMS of compound **7e**



$^1\text{H-NMR}$ spectrum of compound **7f**

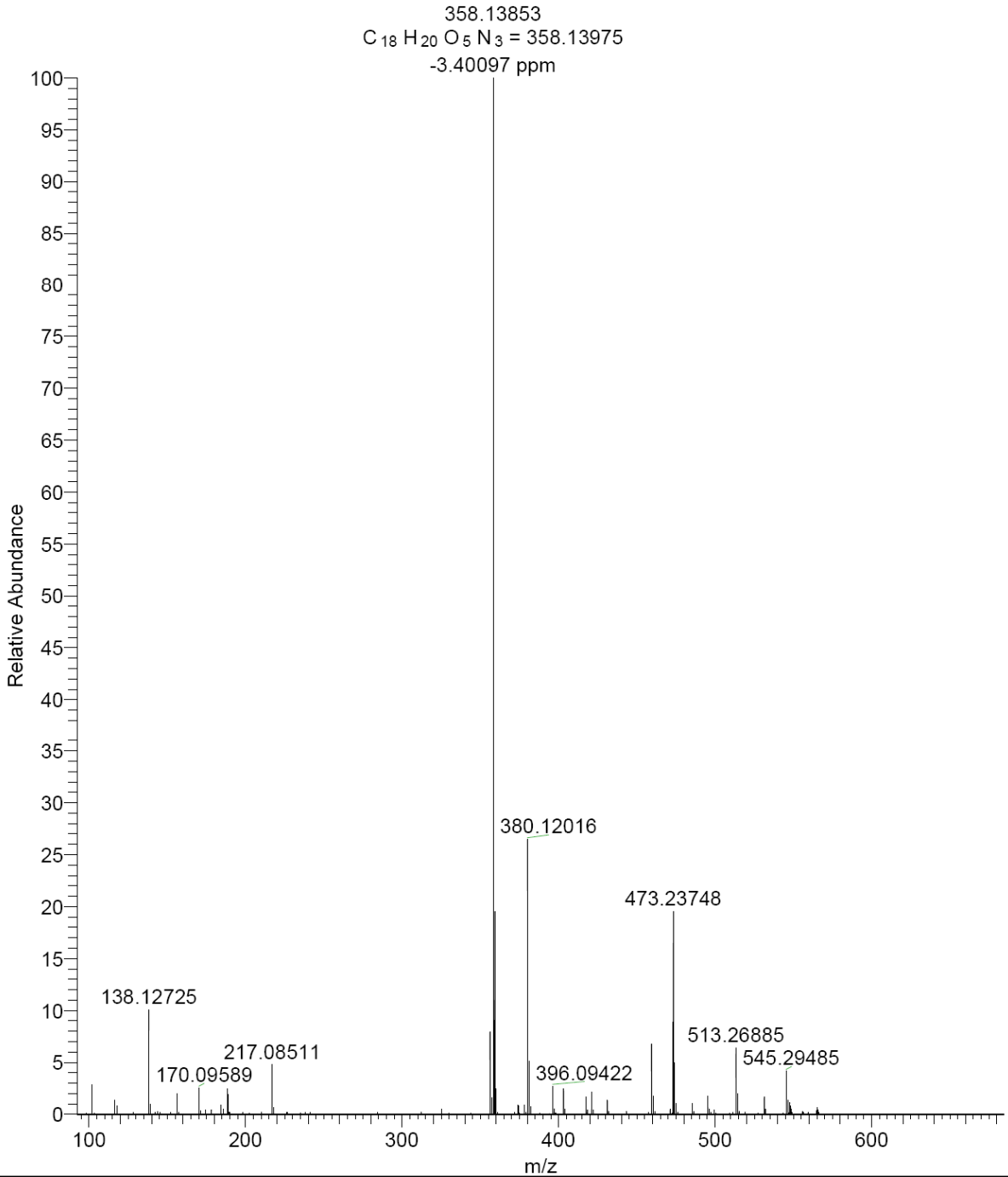


$^{13}\text{C-NMR}$ spectrum of compound **7f**

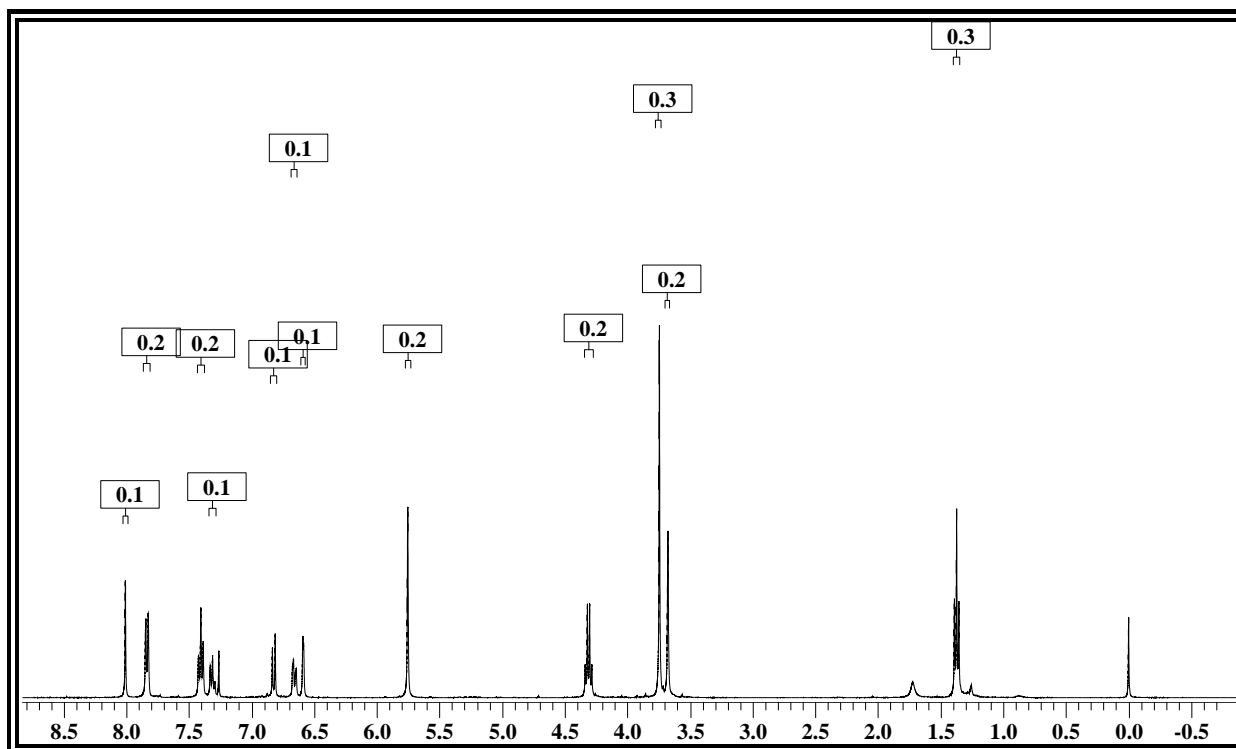
03/11/22 16:32:42
1180121424

Thermo Scientific Orbitrap Exploris 120
Analysed by G SAIKRISHNA

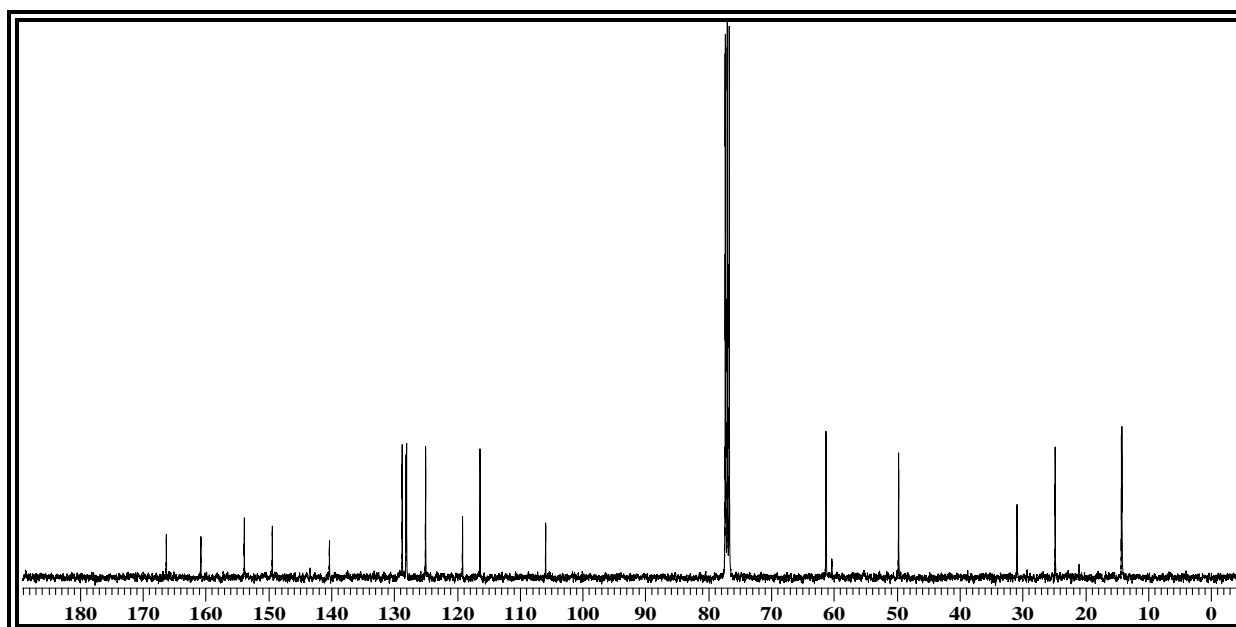
BCR-7F #11-27 RT: 0.03-0.06 AV: 17 SB: 373 0.32-1.20 NL: 1.68E7
T: FTMS + p ESI lpi Full ms [50.0000-2000.0000]



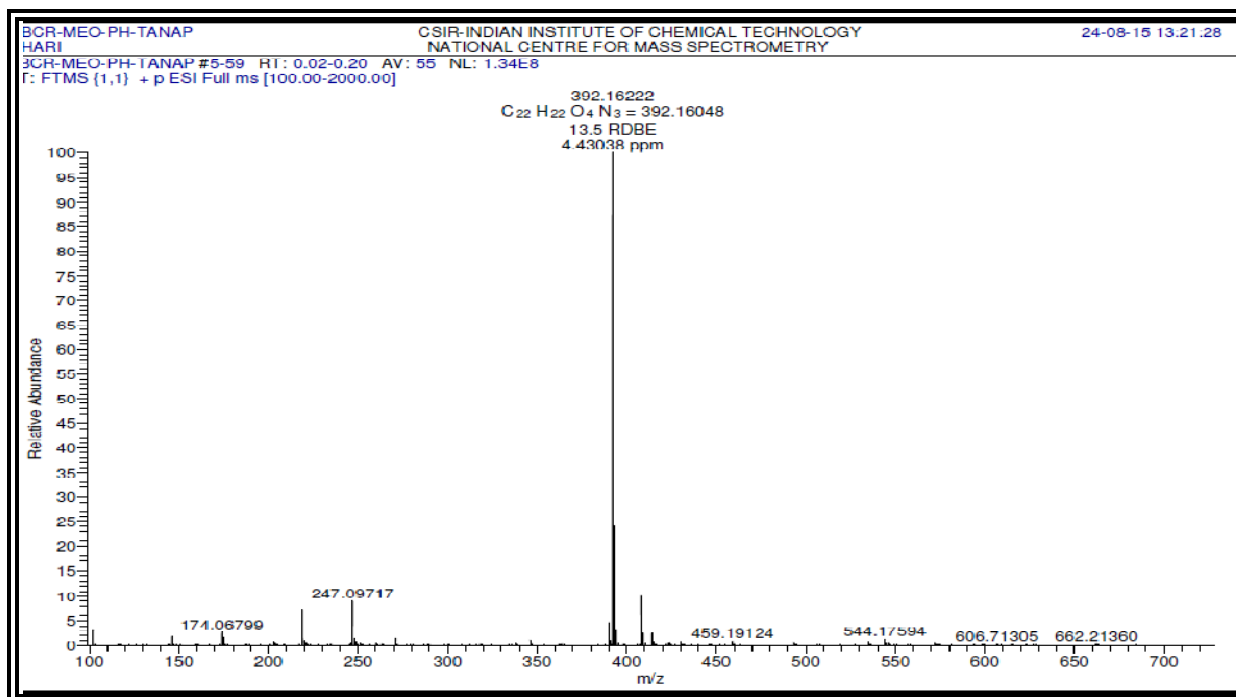
HRMS Spectrum of compound **7f**



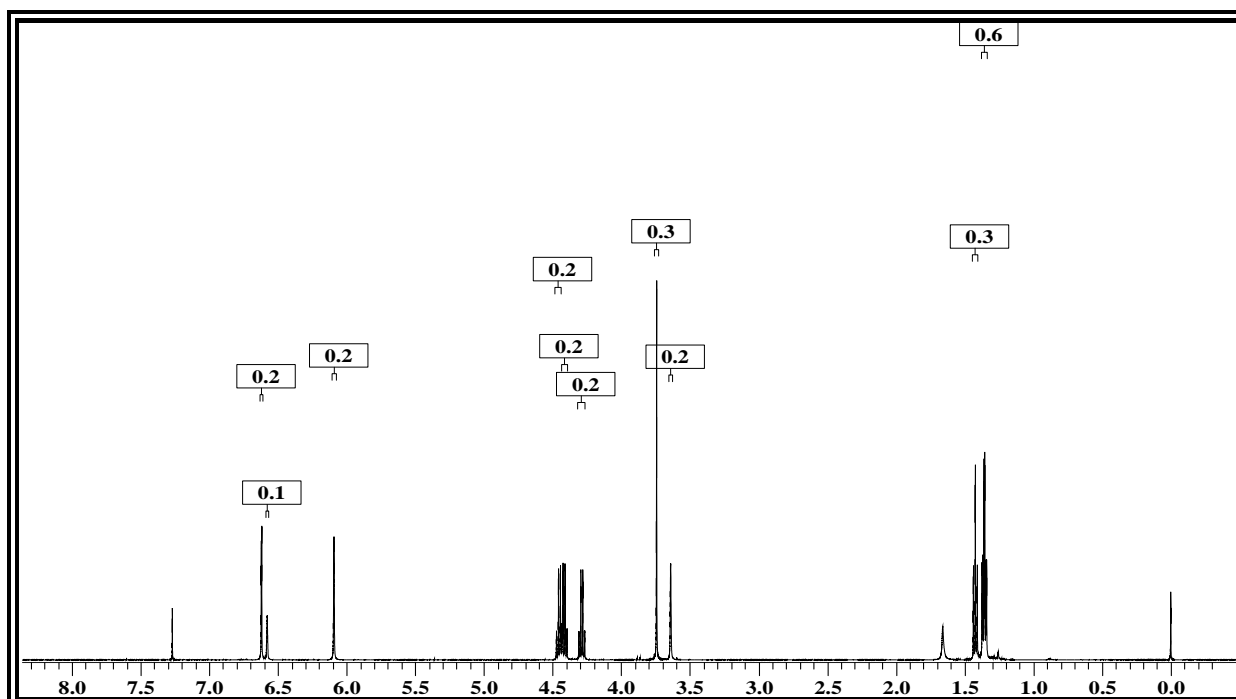
$^1\text{H-NMR}$ spectrum of compound **7g**



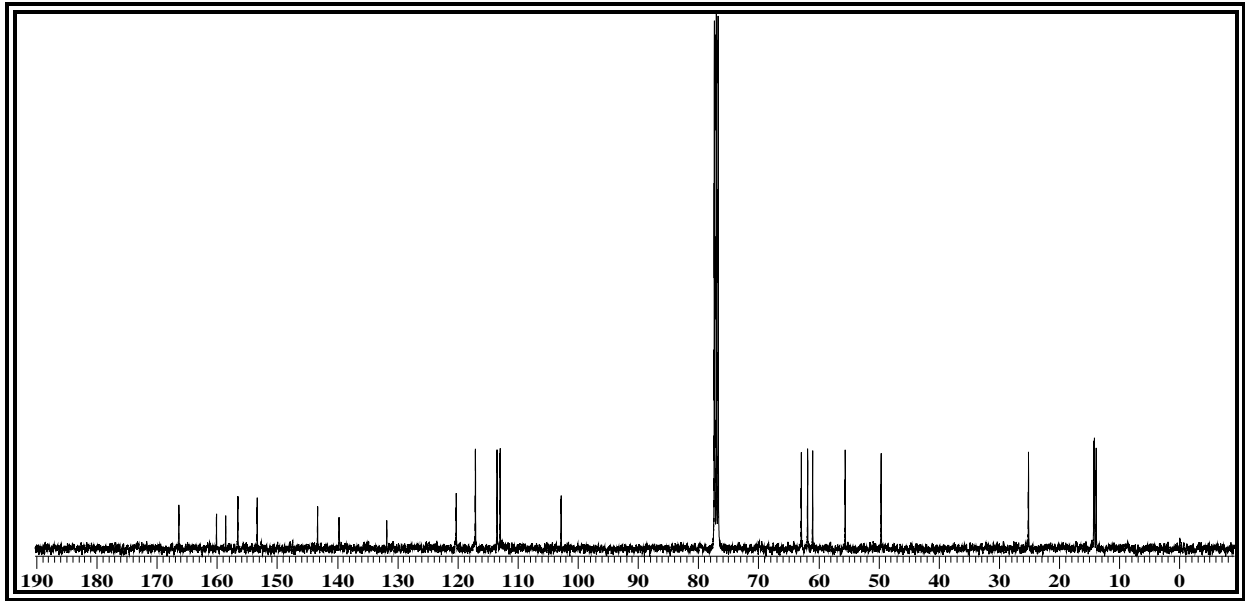
$^{13}\text{C-NMR}$ spectrum of compound **7g**



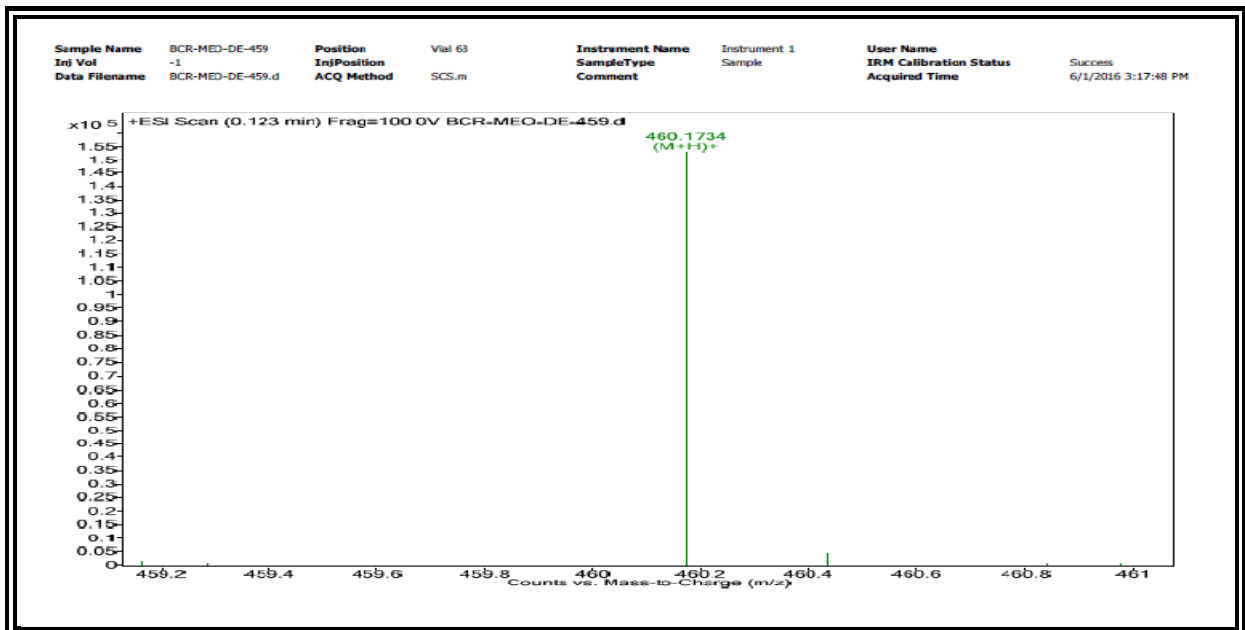
ESI-HRMS of compound **7g**



1H -NMR spectrum of compound **7j**



$^{13}\text{C-NMR}$ spectrum of compound **7j**

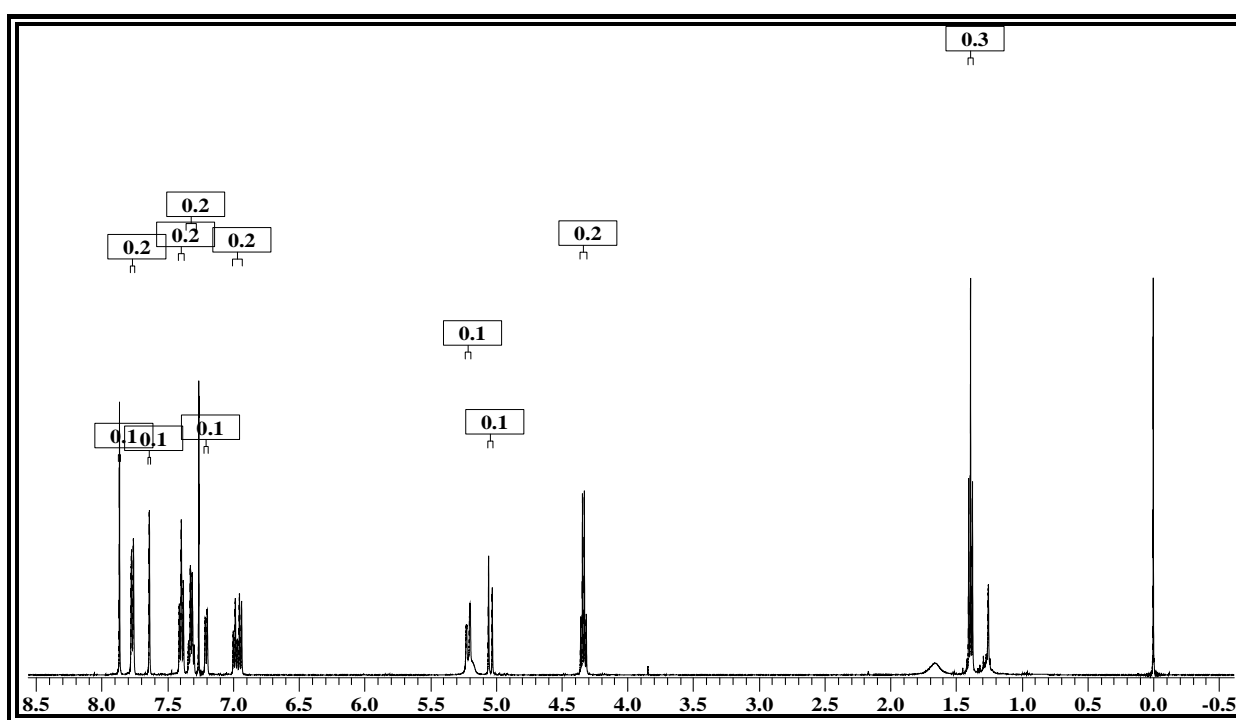


MS Formula Results: + Scan (0.123 min) - BCR-MEO-DE-459.d (BCR-MEO-DE-459.d)

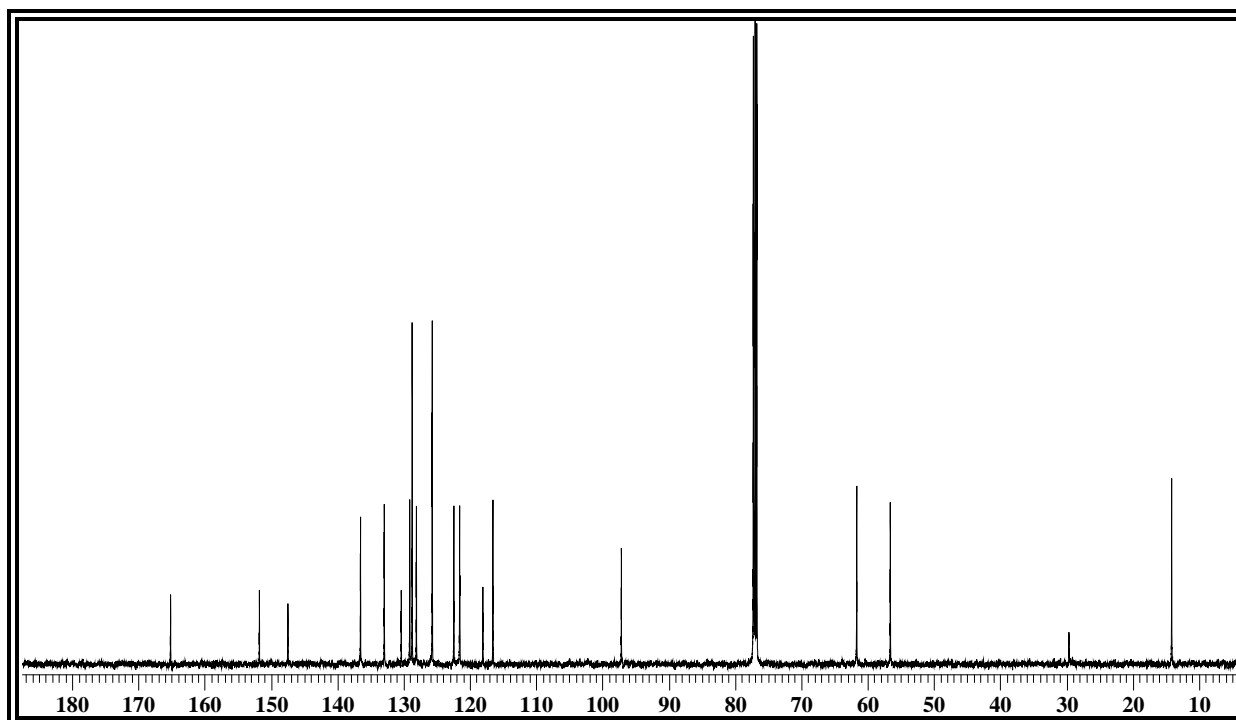
ms	Ion	Formula	Abundance
459.1734	[M+H] ⁺	C22 H26 N3 O8	152925.3

Sheet	Formula (M)	Ion Formula	Calc. m/z	Score	Crab Score	Mass	Calc. Mass	Diff (ppm)	Abn. Diff (ppm)	Abund. Match	Spec. Match	Mass Match	m/z	DBE
17	C22 H26 N3 O8	C22 H26 N3 O8	459.1714	90.91		459.1861	459.1642	-4.2	-4.2	99.34	95.16	83.72	459.1734	12

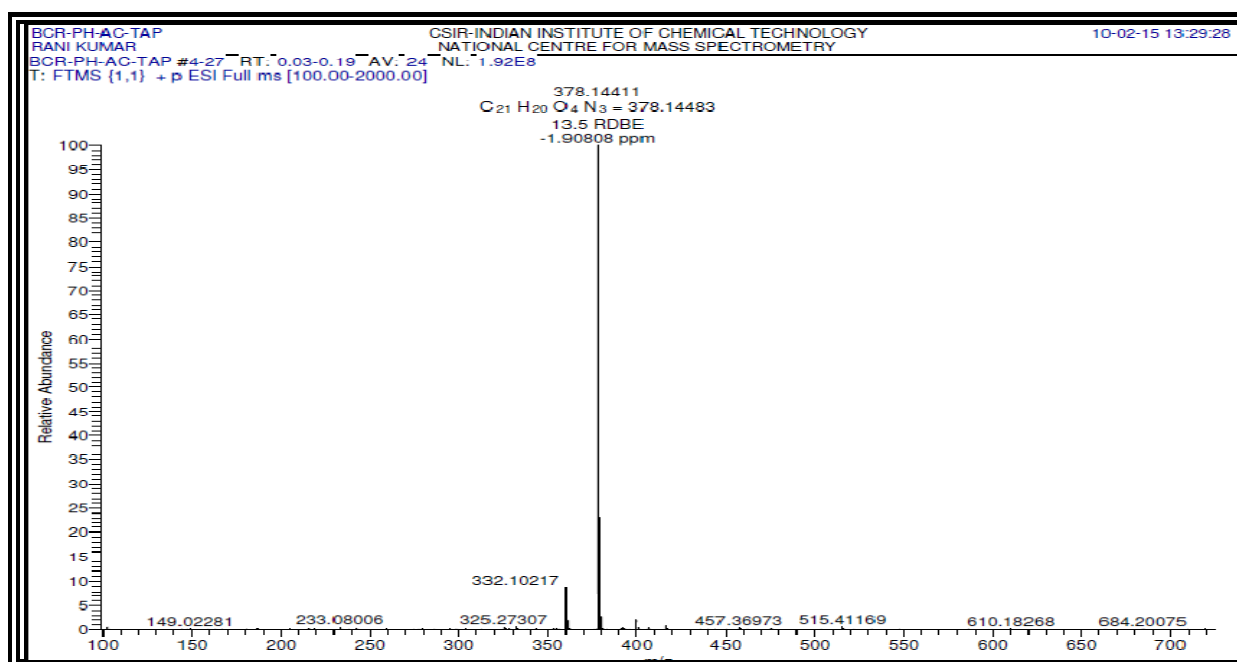
ESI-HRMS of compound **7j**



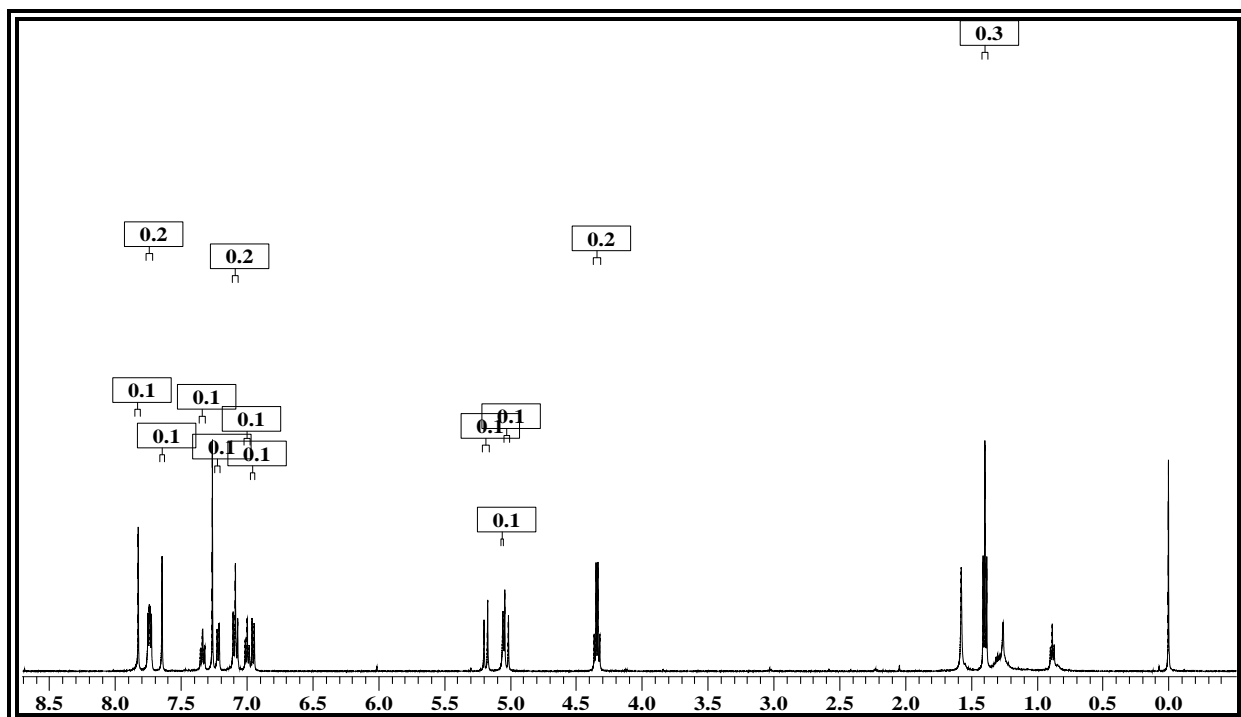
¹H-NMR spectrum of compound **8a**



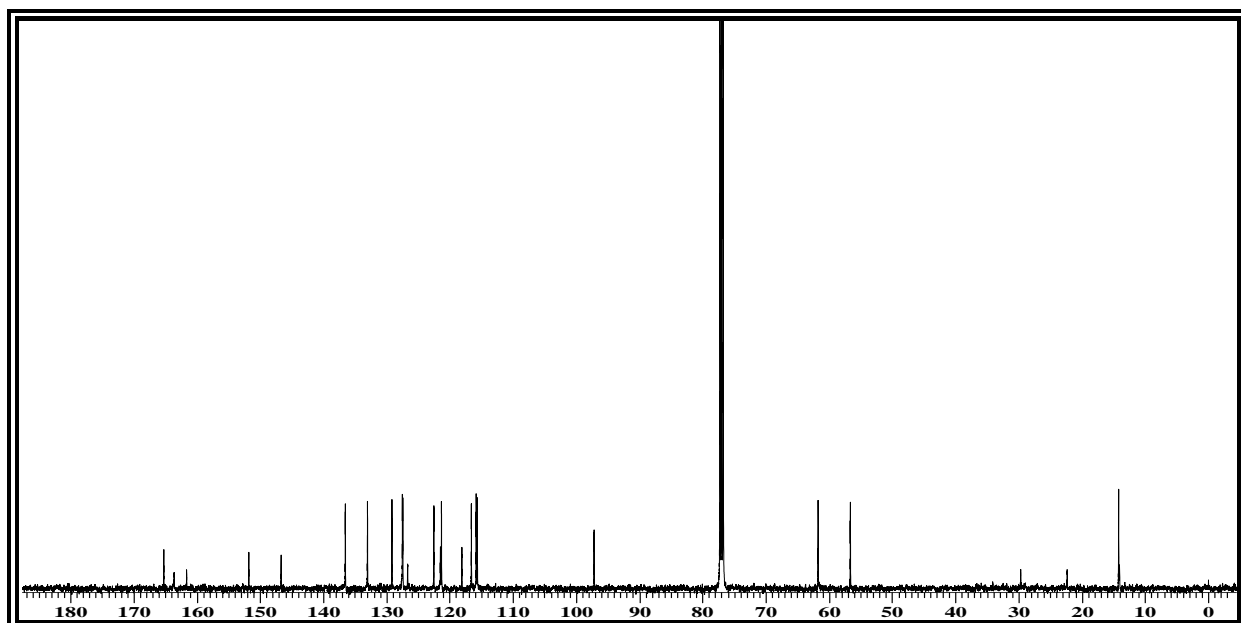
¹³C-NMR spectrum of compound **8a**



ESI-HRMS of compound **8a**



$^1\text{H-NMR}$ spectrum of compound **8b**



$^{13}\text{C-NMR}$ spectrum of compound **8b**

D:\HRMS\2022\MARCH\11-03-2022\BCR-8B

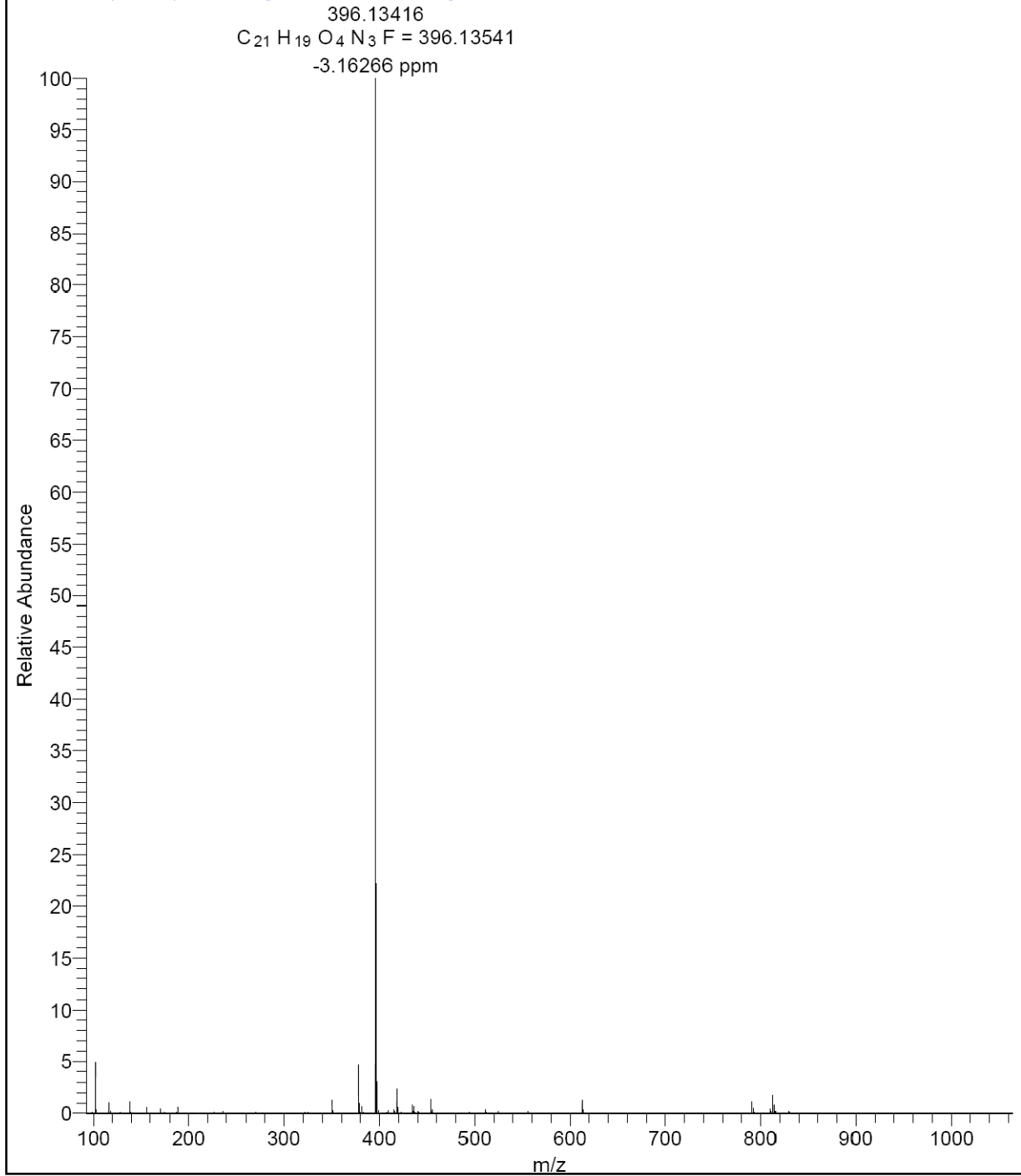
CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
DEPARTMENT OF ANALYTICAL & STRUCTURAL CHEMISTRY

03/11/22 16:29:09
1180121425

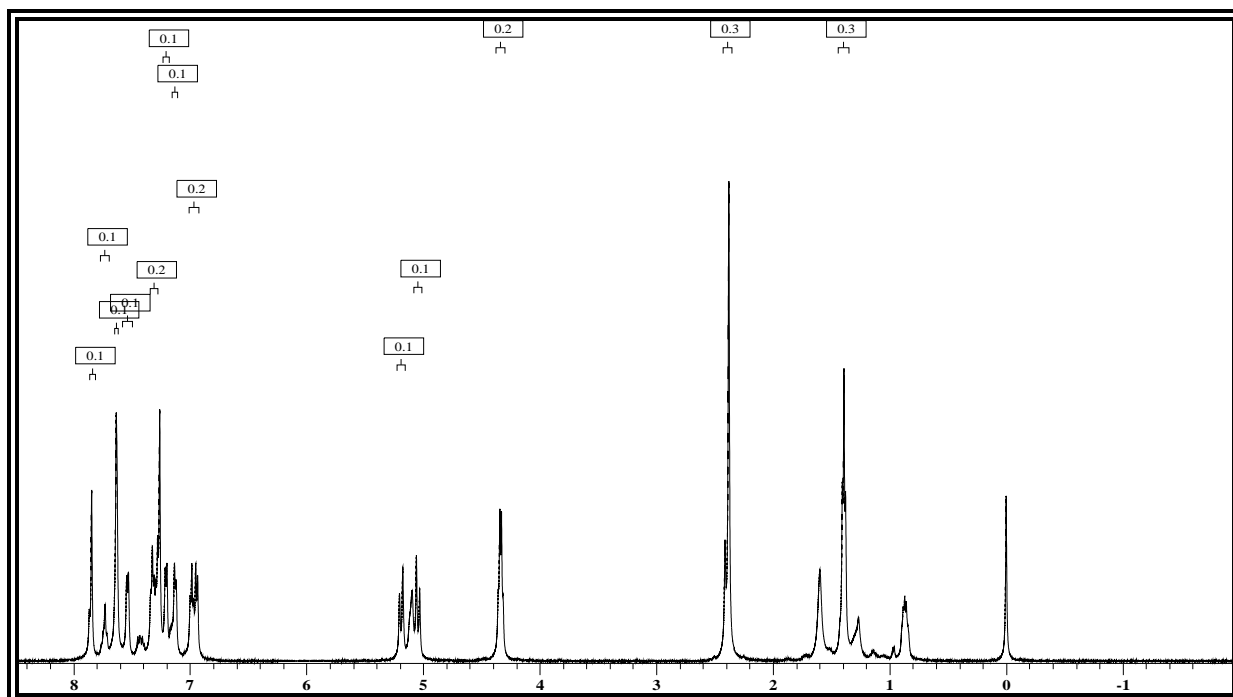
Thermo Scientific Orbitrap Exploris 120
Analysed by G SAIKRISHNA

BCR-8B #8-49 RT: 0.02-0.12 AV: 42 SB: 373 0.32-1.20 NL: 1.24E7

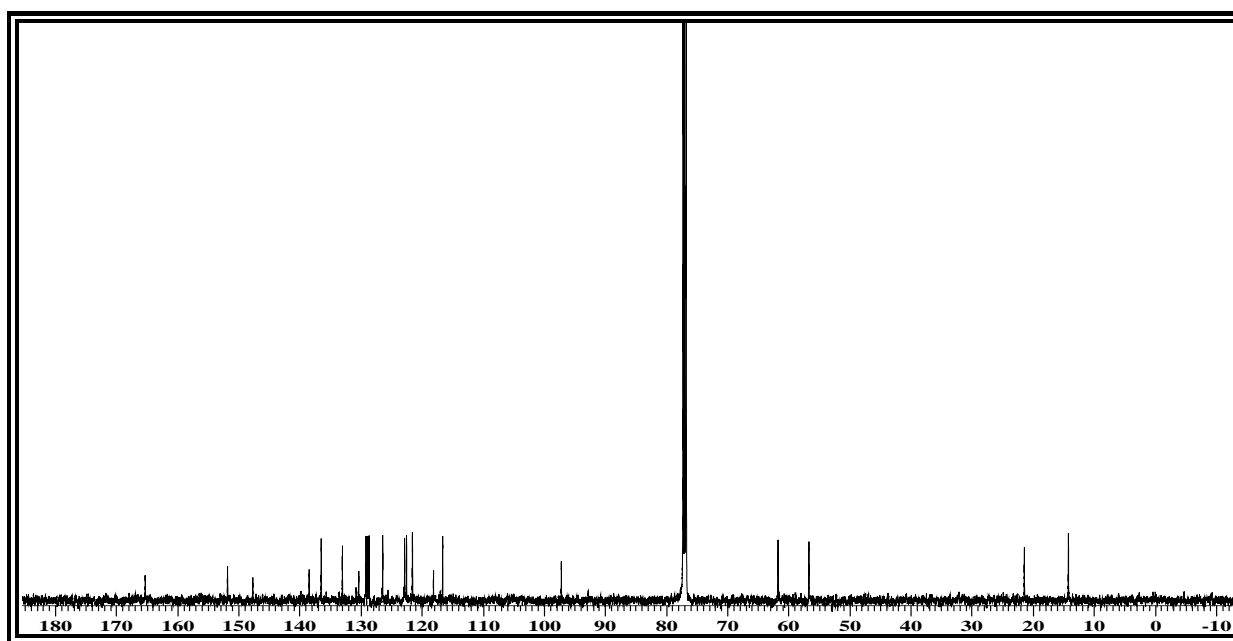
T: FTMS + p ESI Ipi Full ms [50.0000-2000.0000]



HRMS Spectrum of compound **8b**



¹H-NMR spectrum of compound **8c**



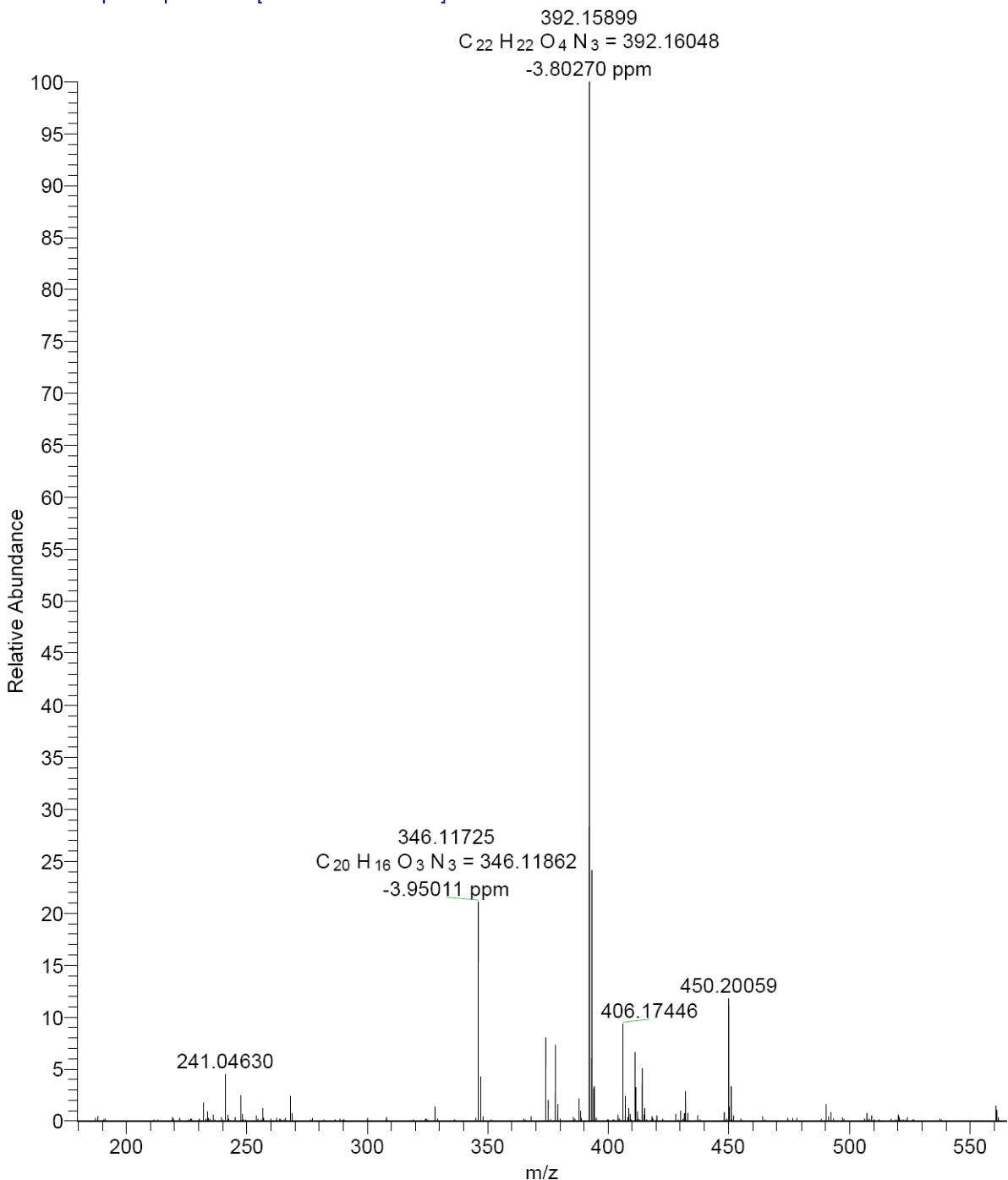
¹³C-NMR spectrum of compound **8c**

03/11/22 16:25:37
1180121426

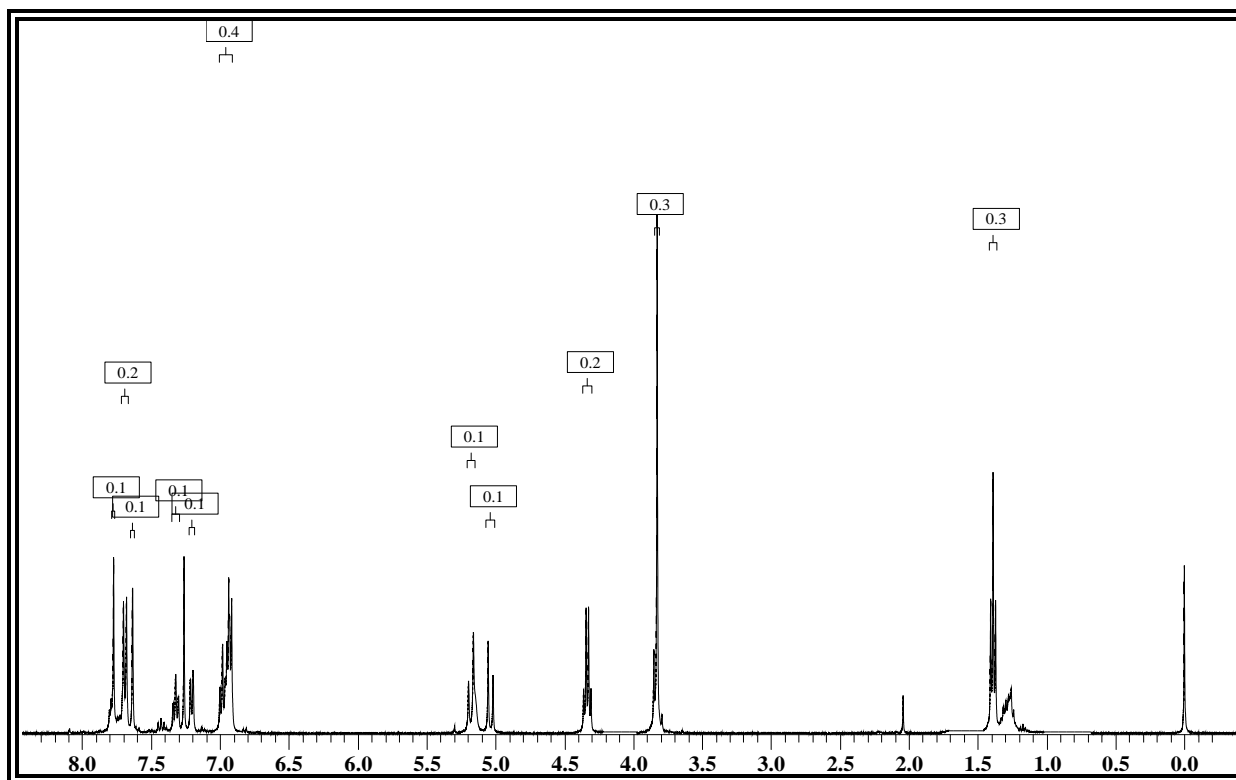
Thermo Scientific Orbitrap Exploris 120
Analysed by G SAIKRISHNA

BCR-8C #8-32 RT: 0.02-0.08 AV: 25 SB: 372 0.32-1.20 NL: 1.42E7

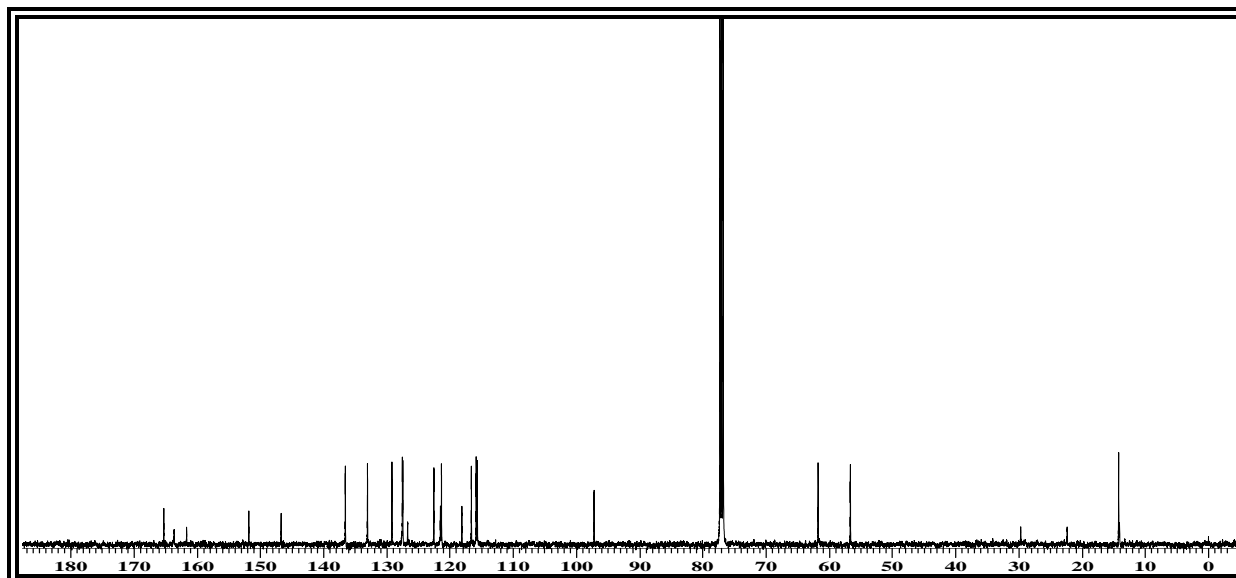
T: FTMS + p ESI Ipi Full ms [50.0000-2000.0000]



HRMS Spectrum of compound **8c**



$^1\text{H-NMR}$ spectrum of compound **8d**



$^{13}\text{C-NMR}$ spectrum of compound **8d**

03/11/22 16:22:03

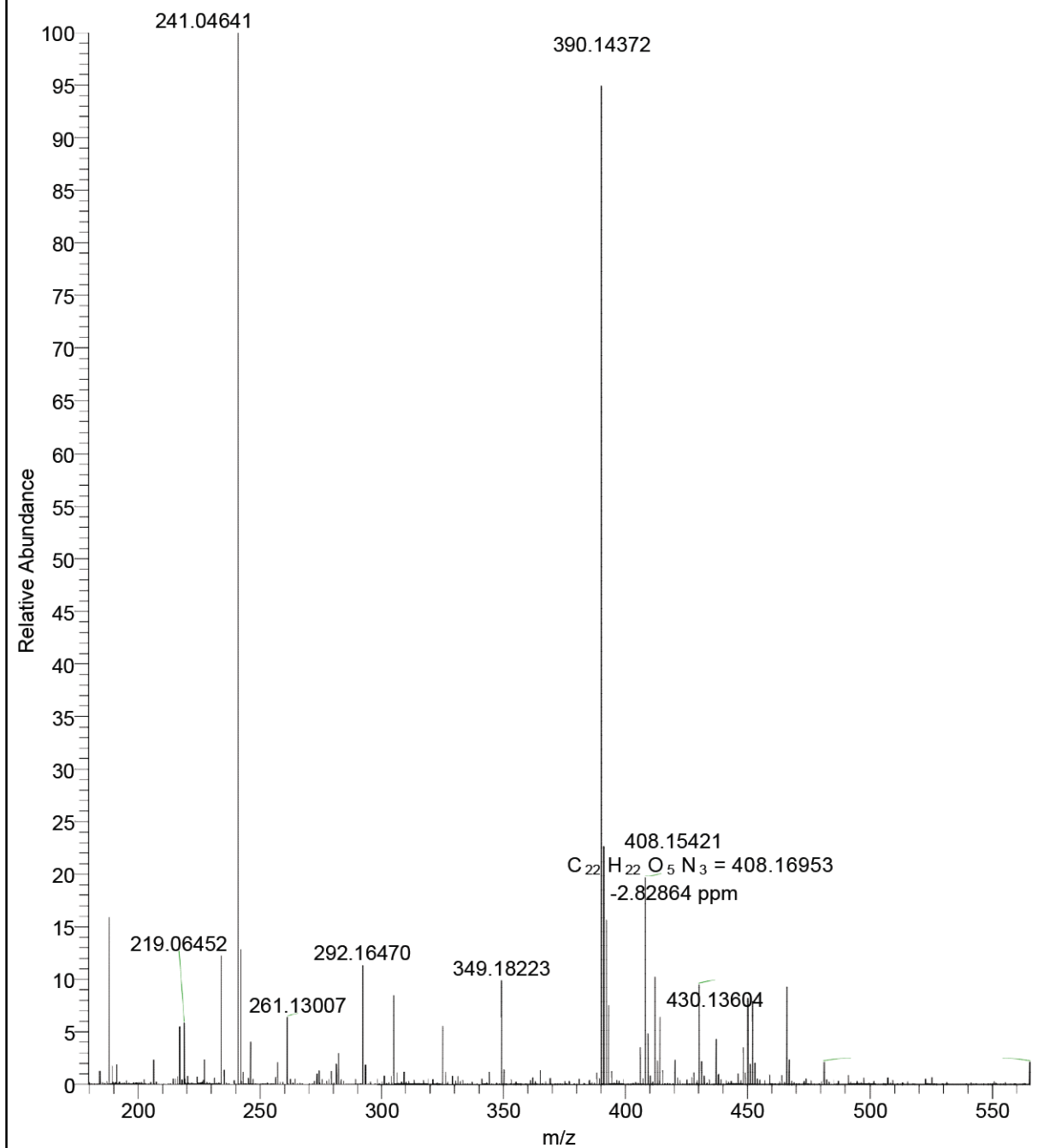
1180121427

Thermo Scientific Orbitrap Exploris 120

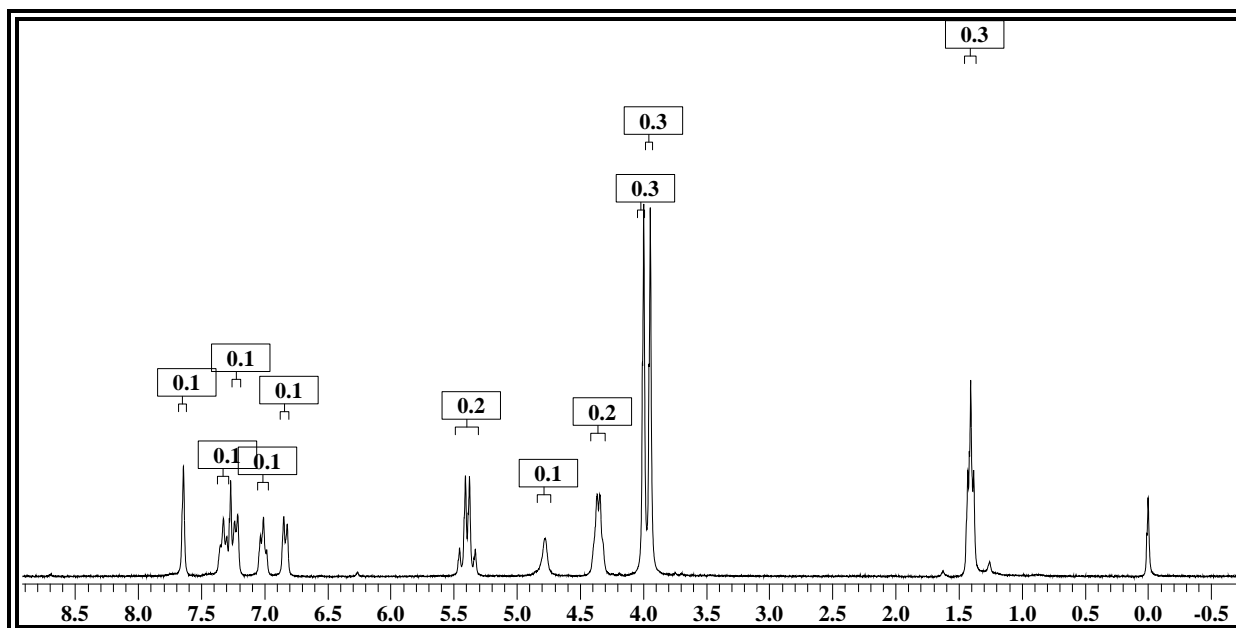
Analysed by G SAIKRISHNA

BCR-8D #5-34 RT: 0.01-0.08 AV: 30 SB: 373 0.32-1.20 NL: 2.17E6

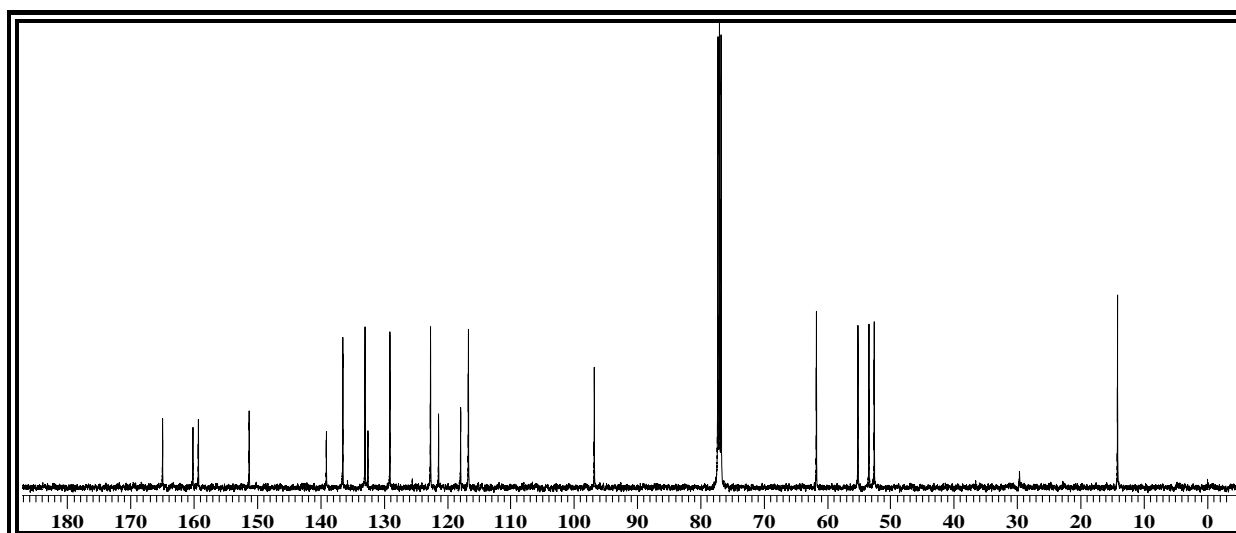
T: FTMS + p ESI Ipi Full ms [50.0000-2000.0000]



HRMS Spectrum of compound **8d**

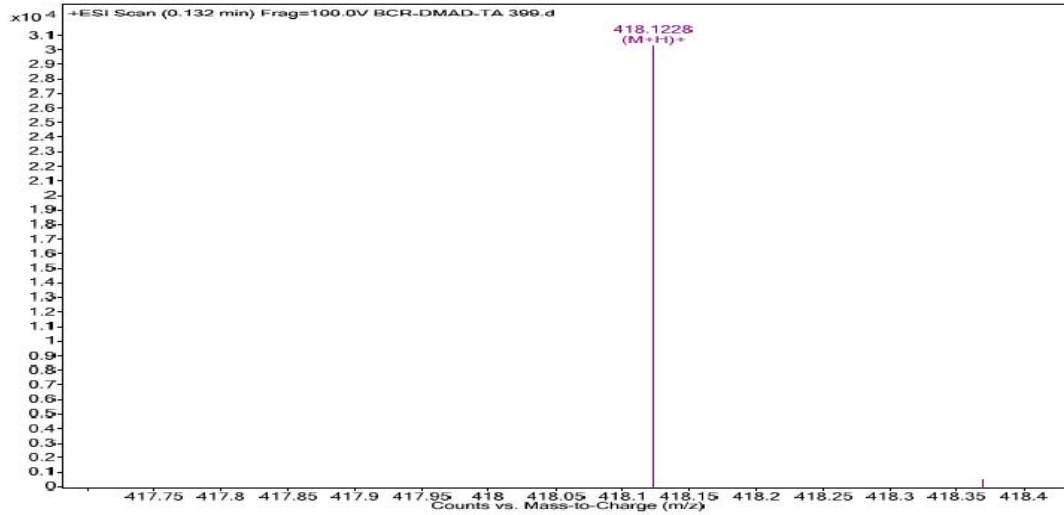


$^1\text{H-NMR}$ spectrum of compound **8h**



$^{13}\text{C-NMR}$ spectrum of compound **8h**

Sample Name BCR-DMAD-TA 399 **Position** Vial 39 **Instrument Name** Instrument 1 **User Name**
Inj Vol -1 **InjPosition** **SampleType** Sample **IRM Calibration Status** Success
Data Filename BCR-DMAD-TA 399.d **ACQ Method** SCS.m **Comment** **Acquired Time** 5/11/2016 12:21:08 PM

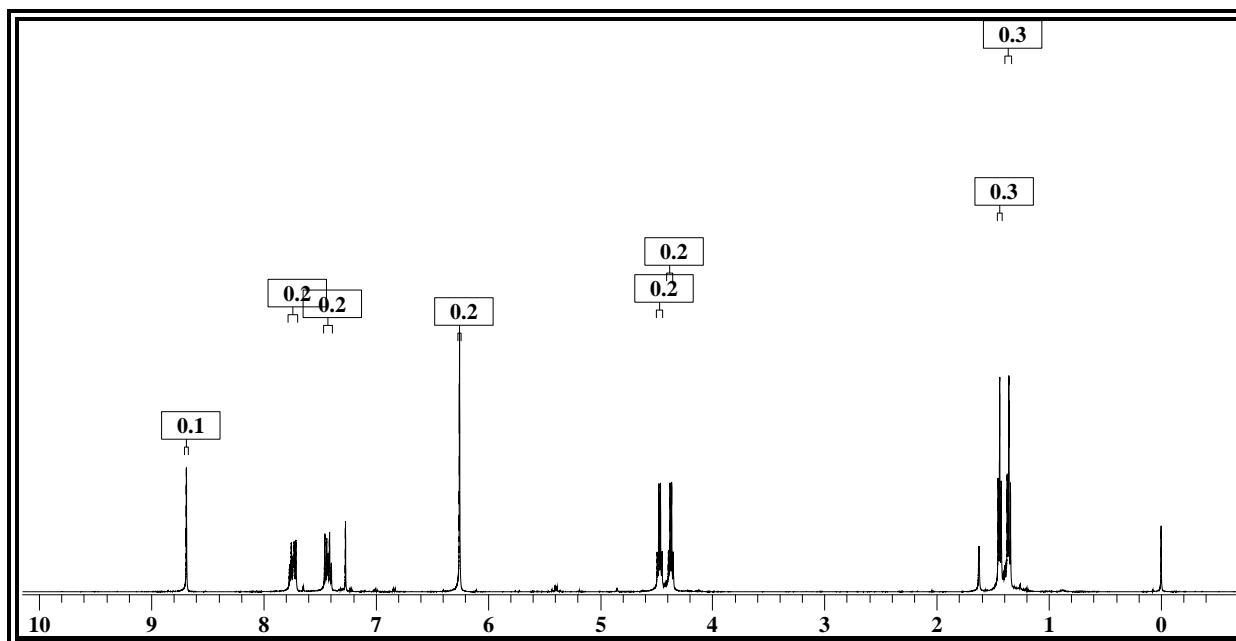


MS Formula Results: + Scan (0.132 min) - BCR-DMAD-TA 399.d (BCR-DMAD-TA 399.d)

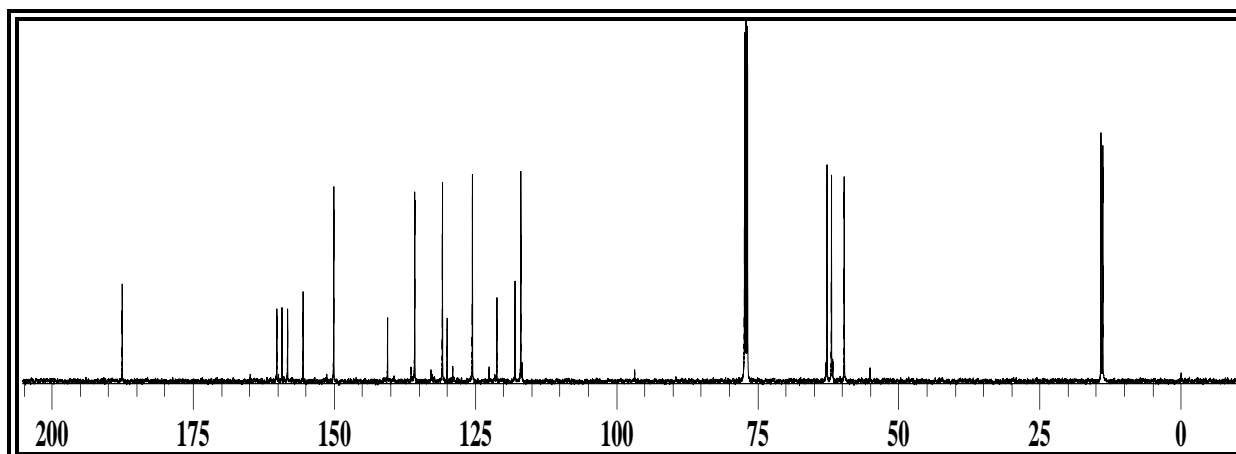
m/z	Ion	Formula	Abundance
418.1228	(M+H) ⁺	C ₁₉ H ₂₀ N ₃ O ₈	2021.63

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross Score	Mass	Calc Mass	Diff (ppm)	Abn Diff (ppm)	Abund Match	Spacing Match	Mass Match	m/z	DBE	
*	[C]	C ₁₉ H ₁₉ N ₃ O ₈	418.1245	98.38			417.1156	417.1172	3.89	3.89	91.26	87.66	86.99	418.1228	12

ESI-HRMS of compound **8h**



$^1\text{H-NMR}$ spectrum of compound **8i**

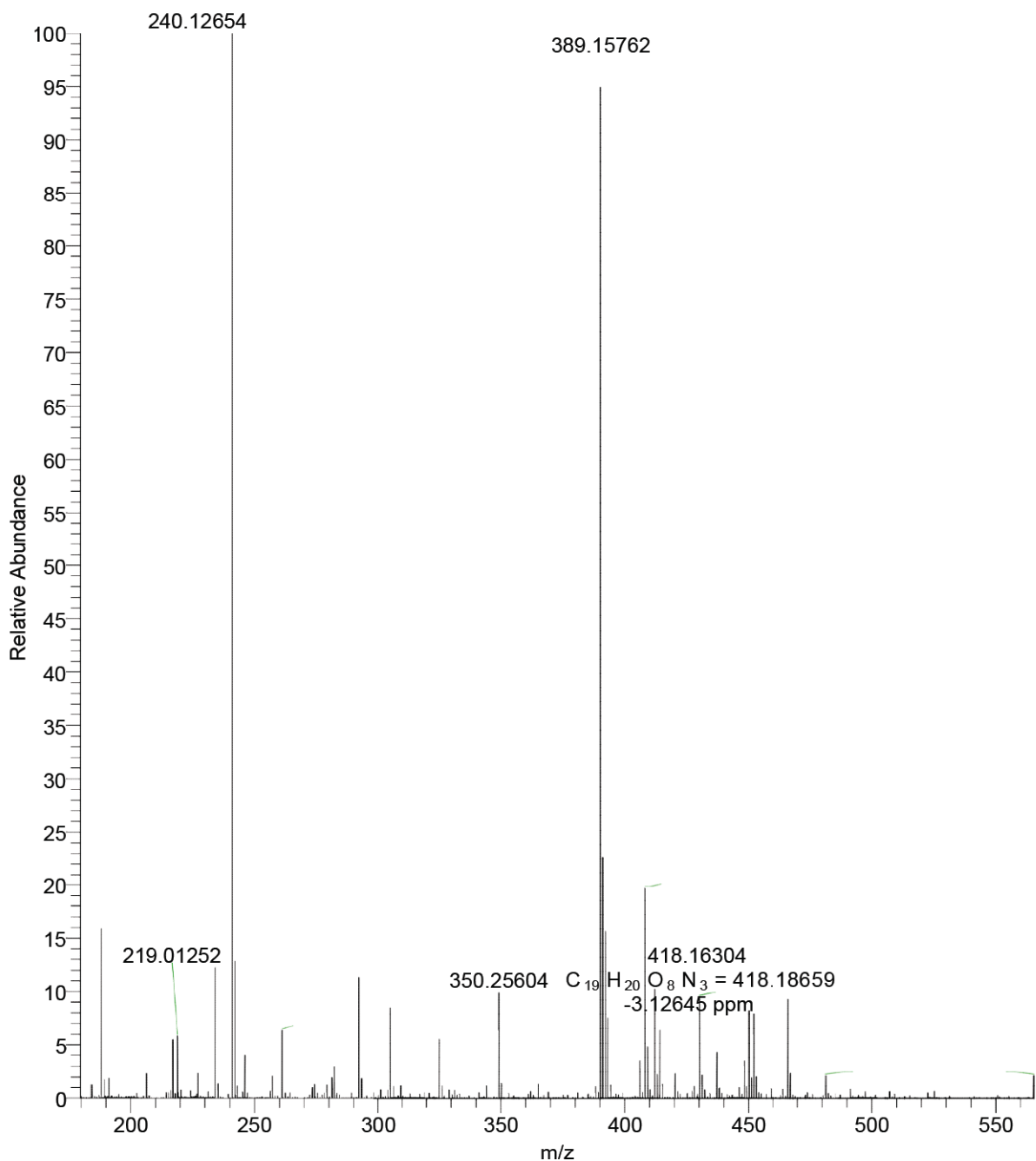


$^{13}\text{C-NMR}$ spectrum of compound **8i**

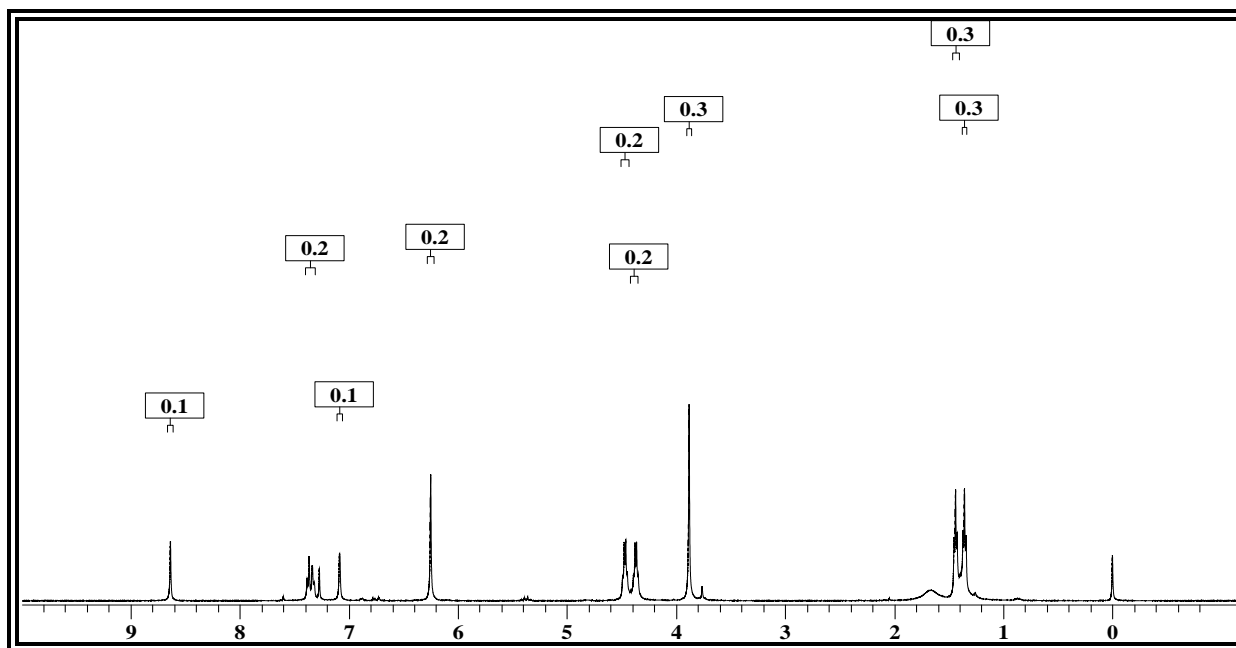
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Thermo Scientific Orbitrap Exploris 120
Analysed by G SAIKRISHNA

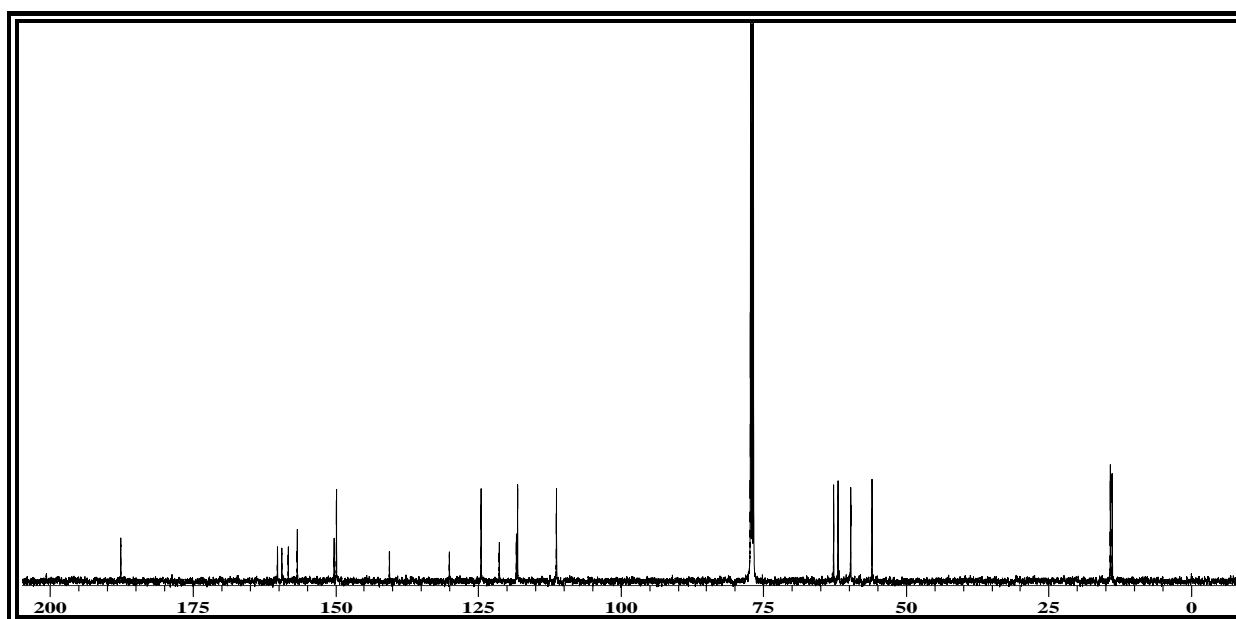
BCR-8I #5-34 RT: 0.01-0.08 AV: 30 SB: 373 0.32-1.20 NL: 2.17E6T:
FTMS + p ESI !pi Full ms [50.0000-2000.0000]



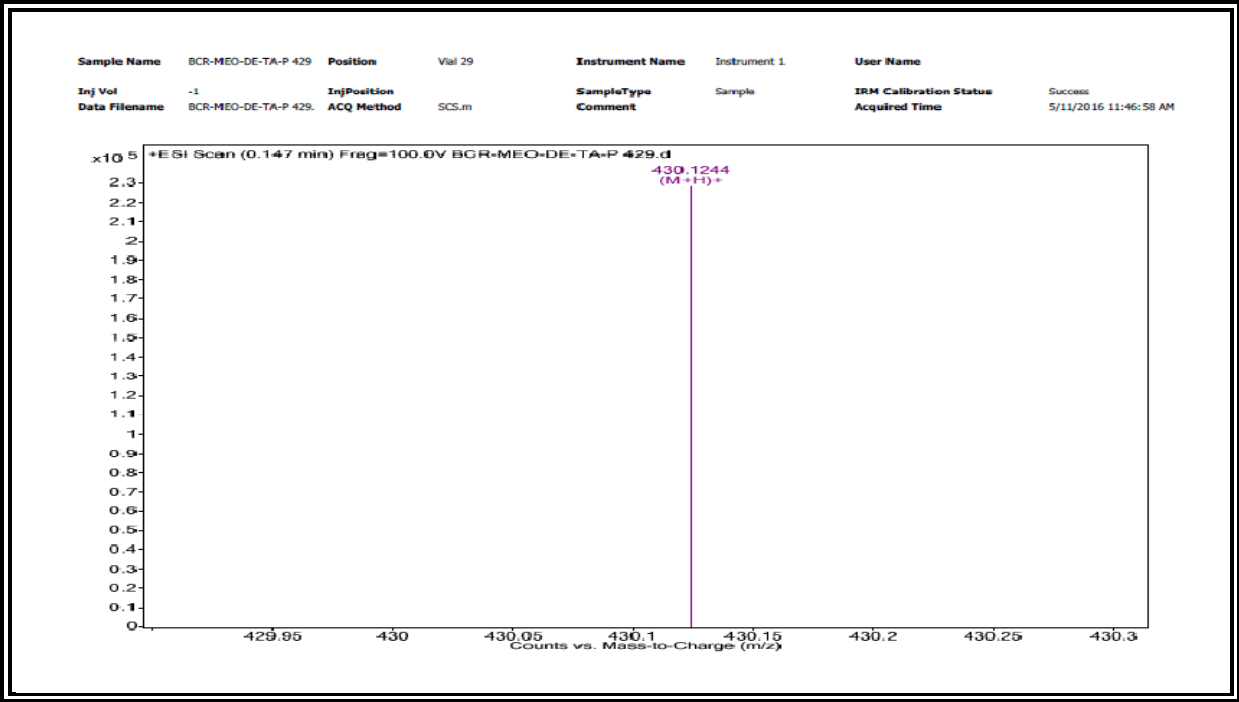
HRMS Spectrum of compound **8i**



$^1\text{H-NMR}$ spectrum of compound **8j**



$^{13}\text{C-NMR}$ spectrum of compound **8j**



MS Formula Results: + Scan (0.147 min) - BCR-MEO-DE-TA-P 429.d (BCR-MEO-DE-TA-P 429.d)

m/z	Ion	Formula	Abundance
430.1244	$[M+1]^+$	$C_{20}H_{20}N_3O_8$	228391.7

Best	Formula (M)	In Formula	Calc. m/z	Score	Crab. Score	Mass	Calc. Mass	Diff (ppm)	Alt. Diff (ppm)	Abund. Match	Spacing Match	Mass Match	m/z	DBE
1	$C_{20}H_{19}N_3O_8$	$C_{20}H_{20}N_3O_8$	430.1246	98.05		429.1172	429.1172	0.29	0.29	93.34	99.8	99.99	430.1244	13

ESI-HRMS of compound 8j