

Supplementary Material

Microwave induced synthesis of new class of pyrano isoxazoline and isoxazole annulated chromones - an intramolecular nitrile oxide cycloaddition with tethered olefins and alkynes

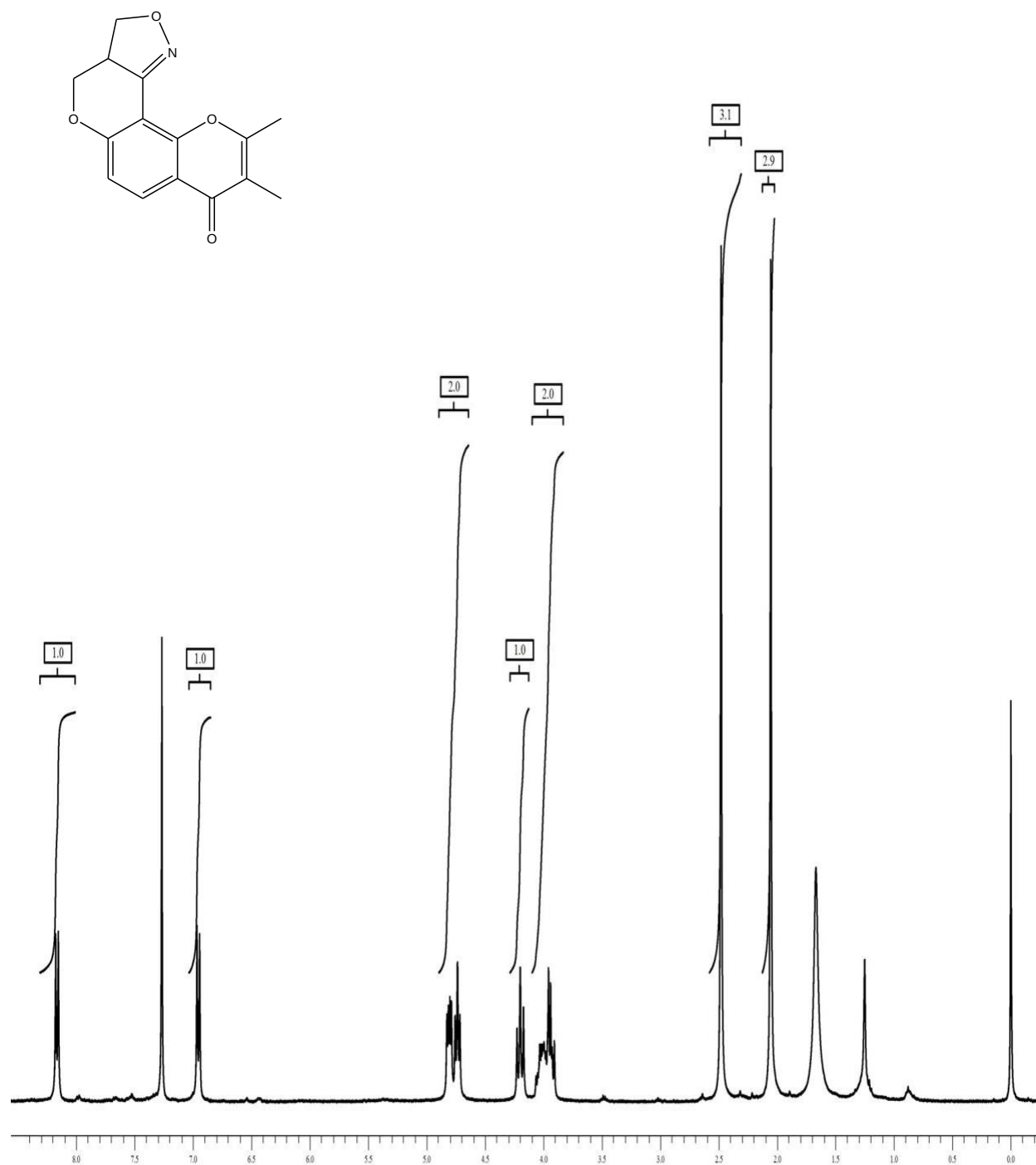
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^aNatural Products Laboratory, Department of Chemistry, Osmania University, Hyderabad-500007, Telangana, India

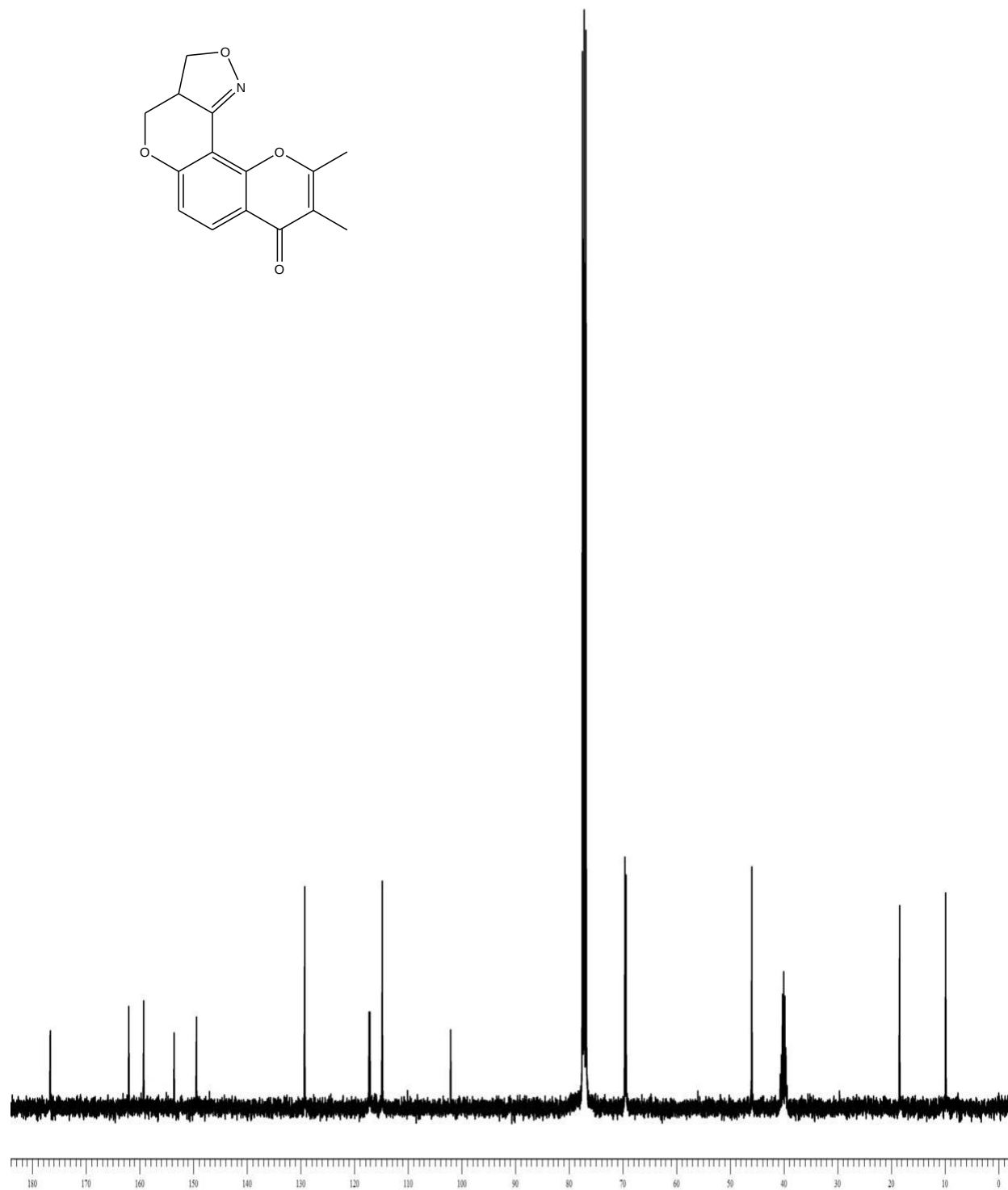
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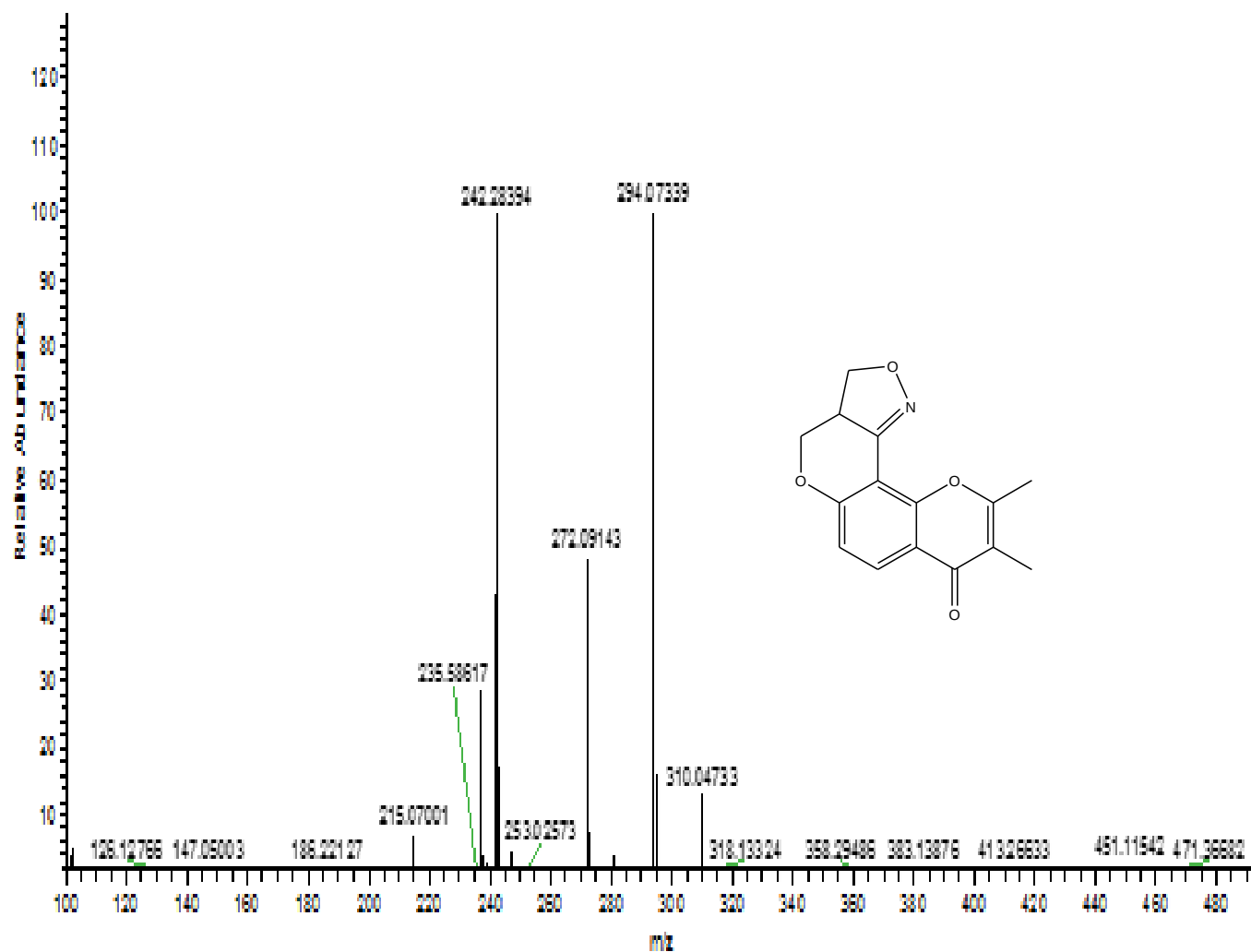
^1H -NMR of 9,10-dimethyl-3a,4-dihydropyran[2',3':5,6]chromeno[4,3-c]isoxazol-8(3H)-one (3a)

^{13}C -NMR of 9,10-dimethyl-3a,4-dihydropyran[2',3':5,6]chromeno[4,3-c]isoxazol-8(3H)-one (3a):

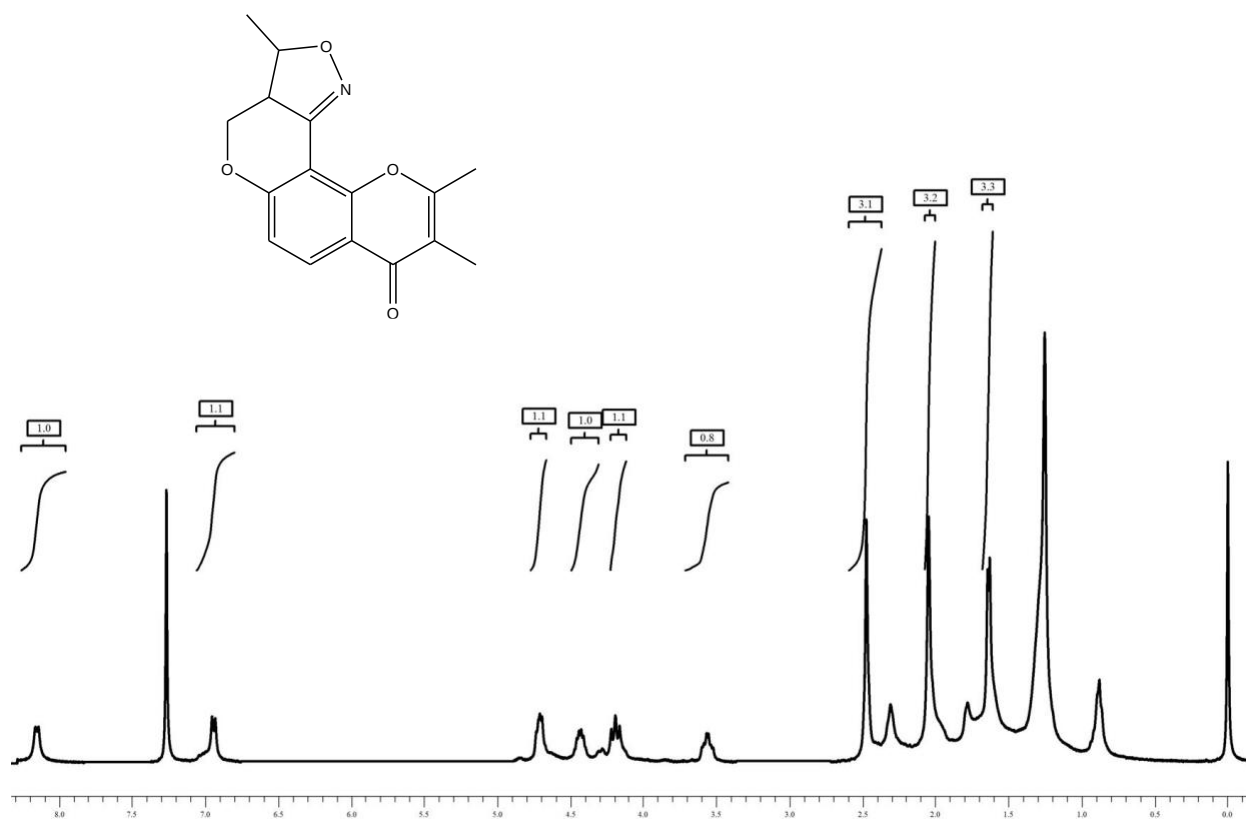


ESI-HRMS of 9,10-dimethyl-3a,4-dihydropyran[2',3':5,6]chromeno[4,3-c]isoxazol-8(3H)-one (3a)

271.1 RT: 0.01 AV: 1 NL: 3.78E7
T: FTMS +p ESIFullms (100.00-2000.00)



¹H-NMR spectra of 3,9,10-trimethyl-3a,4-dihydropyrano [2',3':5,6] chromeno [4,3-c] isoxazol-8(3H)-one (3b)



ESI-HRMS of 3,9,10-trimethyl-3a,4-dihydropyrano [2',3':5,6] chromeno [4,3-c] isoxazol-8(3H)-one (3b):

C:\ICT-HRMS\24.11.14\SURESH-1

CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY

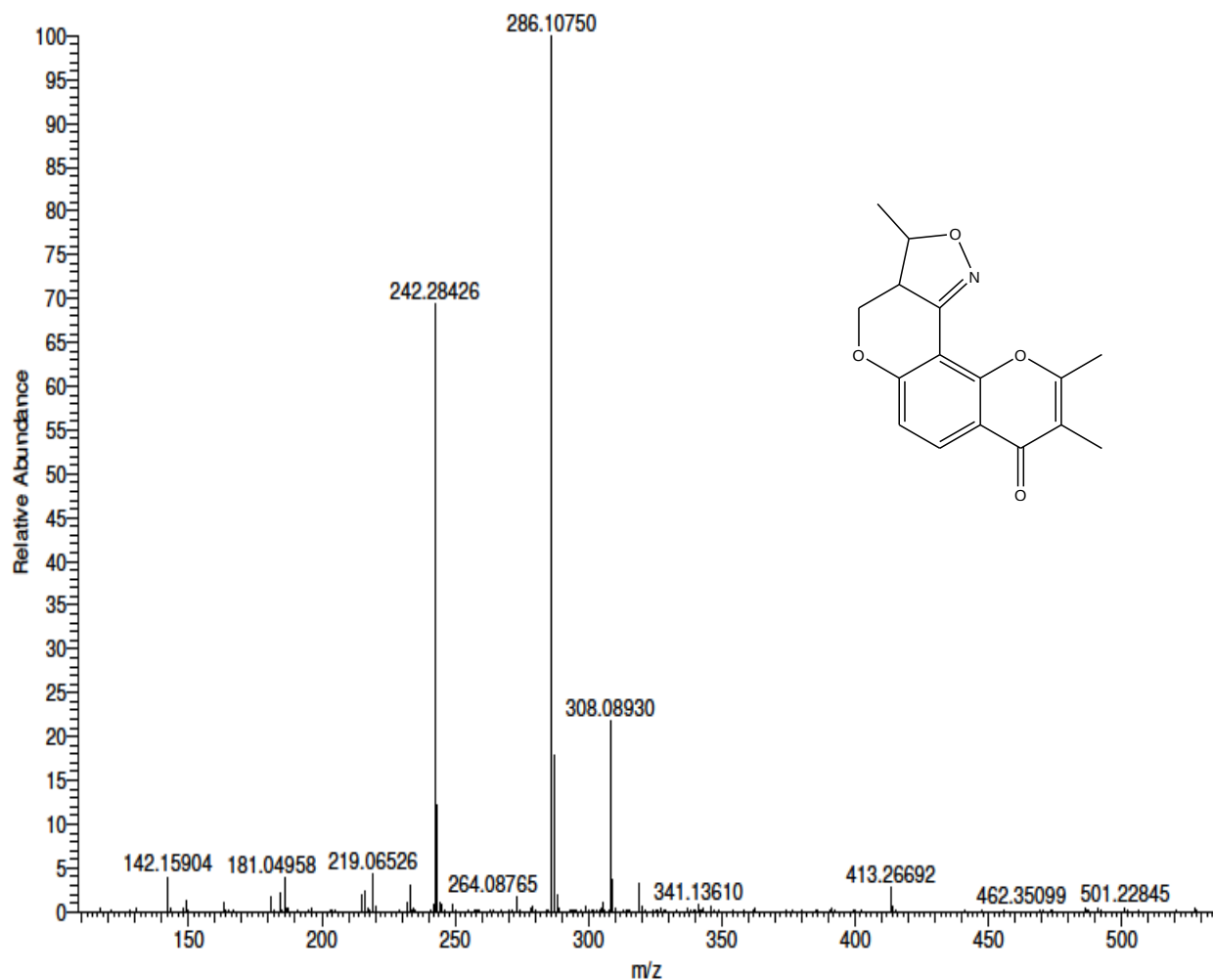
24-11-14 16:37:57

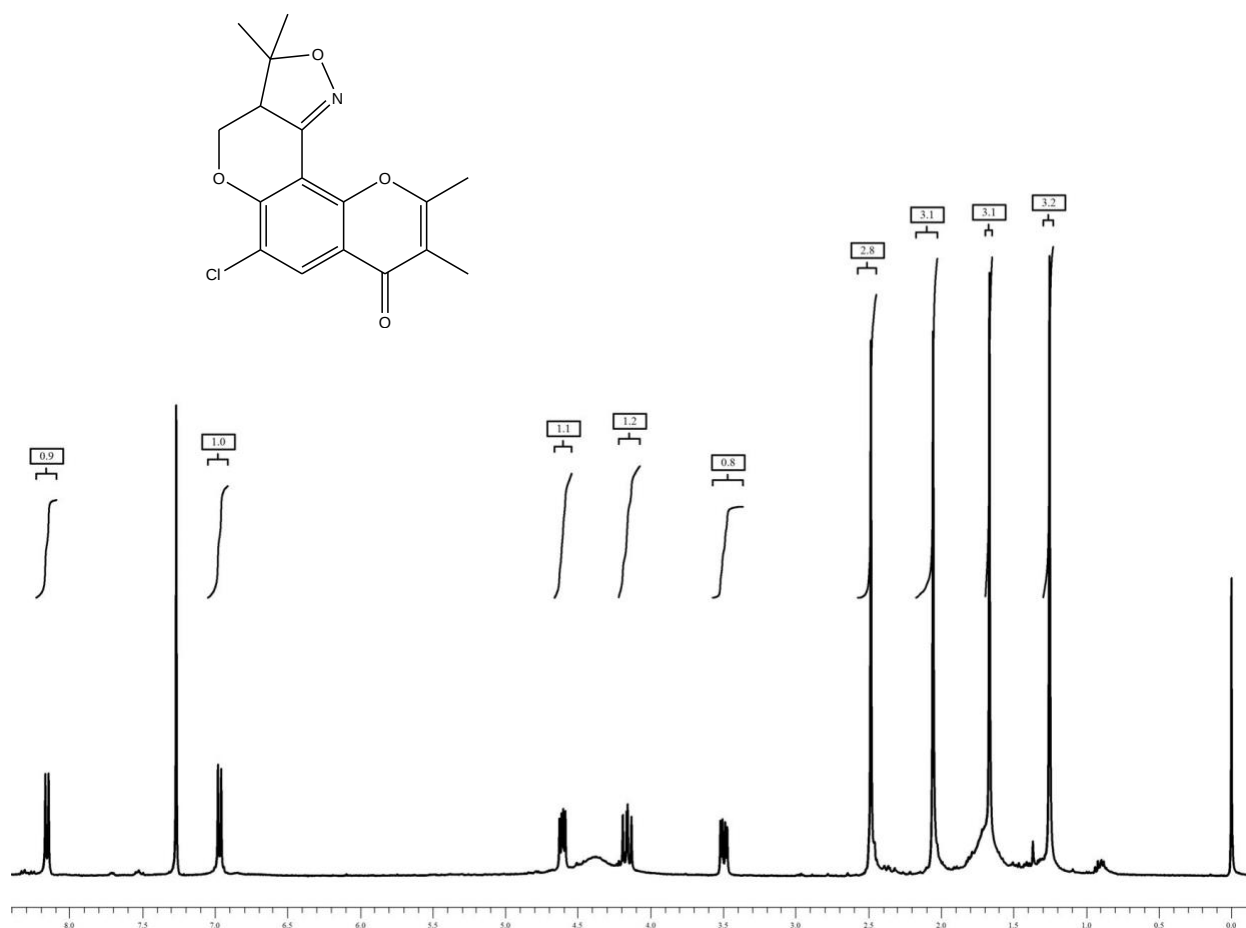
SURESH-NCMS

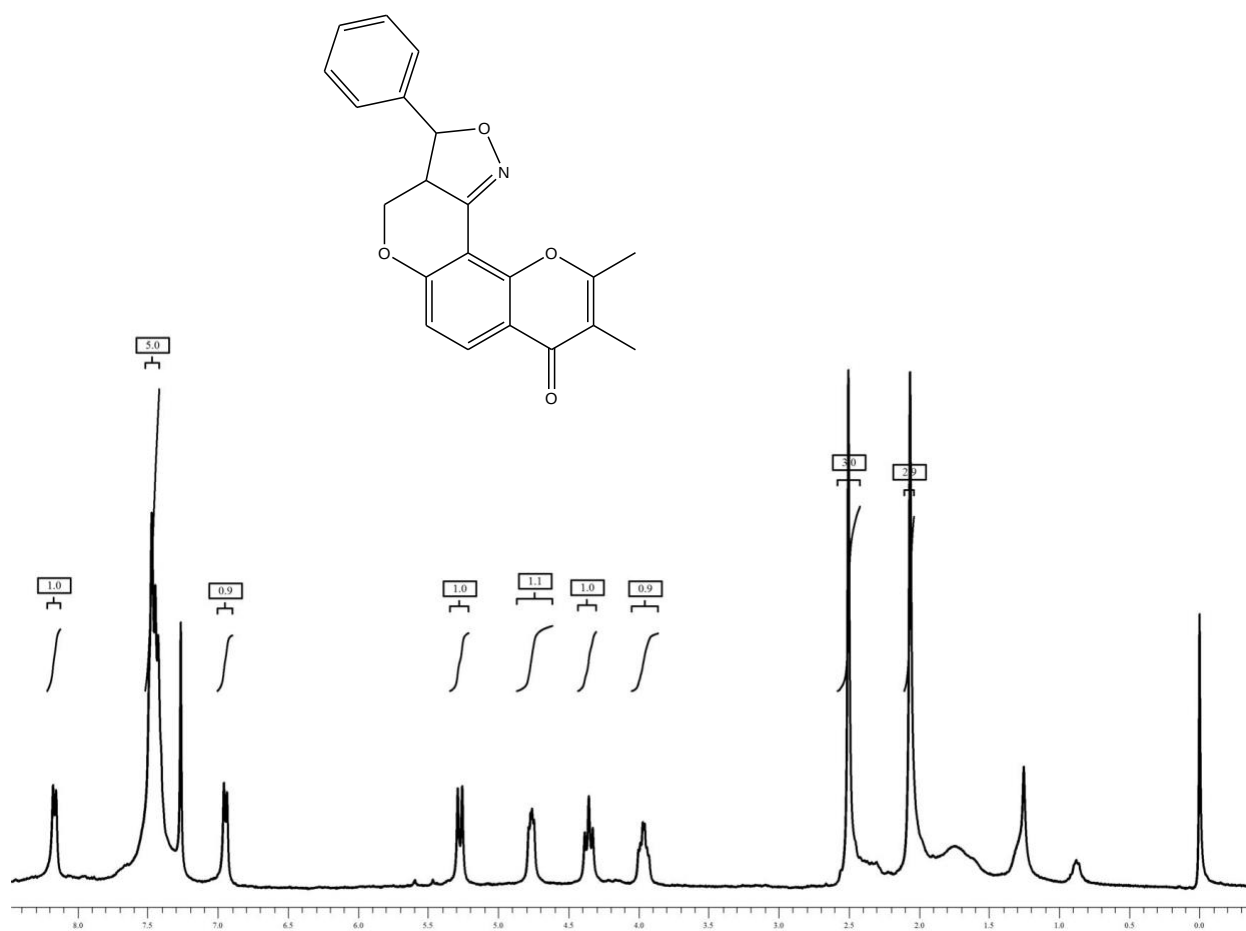
NATIONAL CENTRE FOR MASS SPECTROMETRY

SURESH-1 #8-46 RT: 0.04-0.17 AV: 39 NL: 4.57E7

T: FTMS (1,1) + p ESI Full ms [110.00-2000.00]



¹H-NMR Spectra of 3,3,9,10-tetramethyl-3a,4-dihydropyrano[2',3':5,6]chromeno[4,3-c]isoxazol-8(3H)-one (3c):

¹H-NMR Spectra of 9,10-dimethyl-3-phenyl-3a,4-dihydropyrano[2',3':5,6]chromeno[4,3-c]isoxazol-8(3H)-one (3d):

ESI-HRMS of 9,10-dimethyl-3-phenyl-3a,4-dihydropyrano[2',3':5,6]chromeno[4,3-c]isoxazol-8(3H)-one (3d)

C:\VICT-HRMS\24.11.14\SURESH-2

CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY

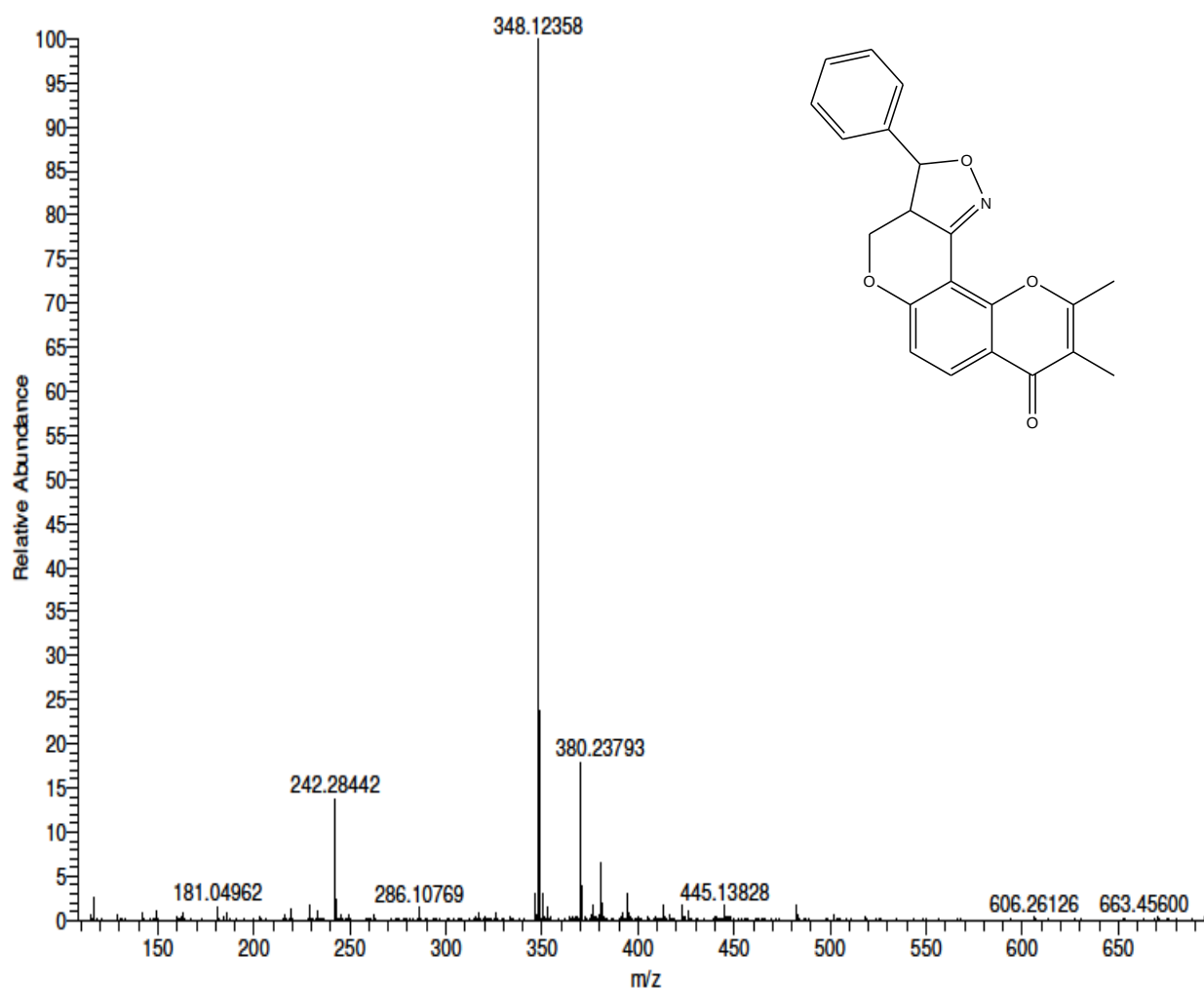
24-11-14 16:40:29

SURESH-NCMS

NATIONAL CENTRE FOR MASS SPECTROMETRY

SURESH-2 #5-50 RT: 0.02-0.17 AV: 46 NL: 3.51E7

T: FTMS (1,1) + p ESI Full ms [110.00-2000.00]



ESI-HRMS of 6-chloro-3,3,9,10-tetramethyl-3a,4-dihydropyrano[2',3':5,6]chromeno[4,3-c]isoxazol-8(3H)-one (3g)

C:\ICT-HRMS\24.11.14\SURESH-4

CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY

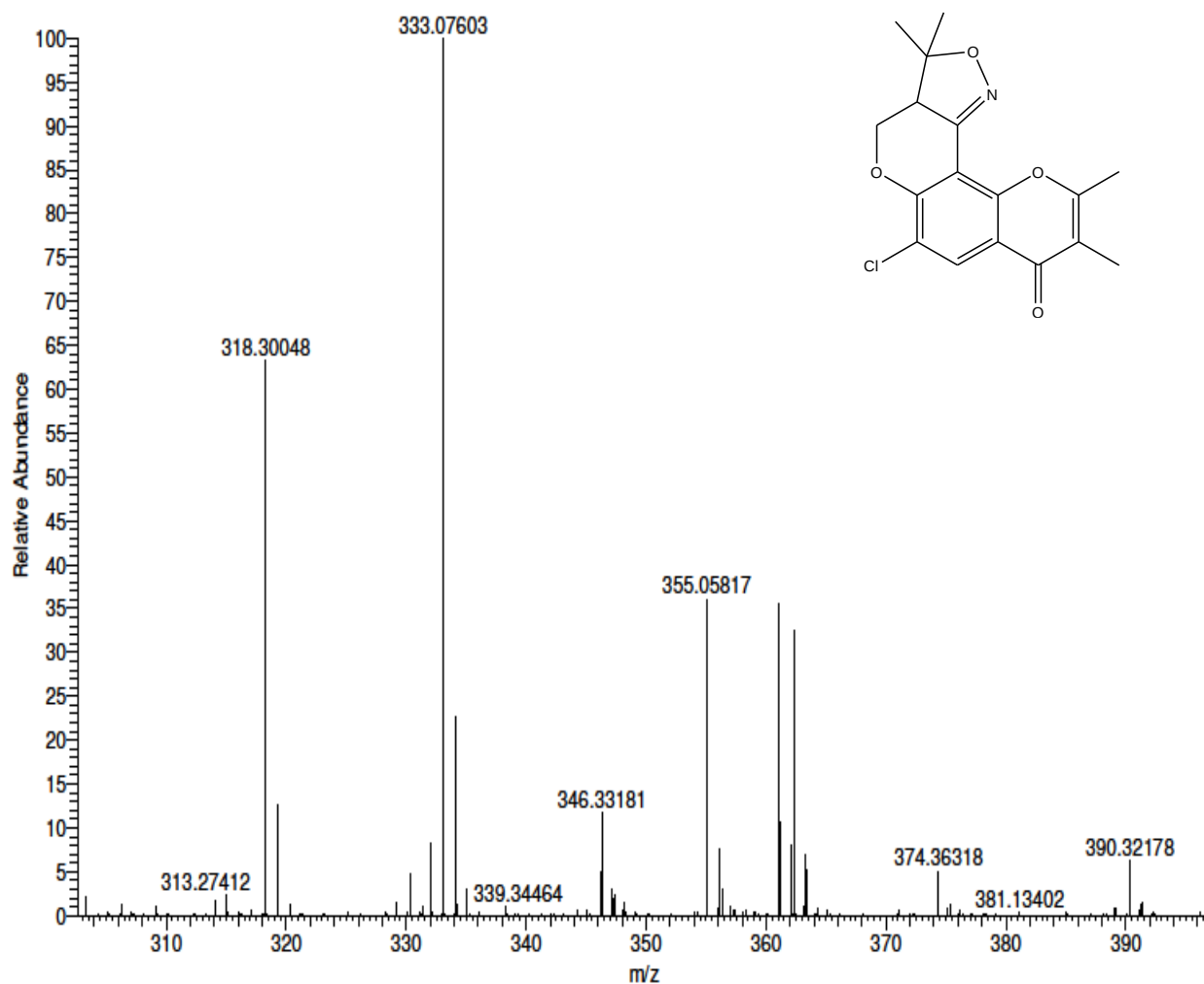
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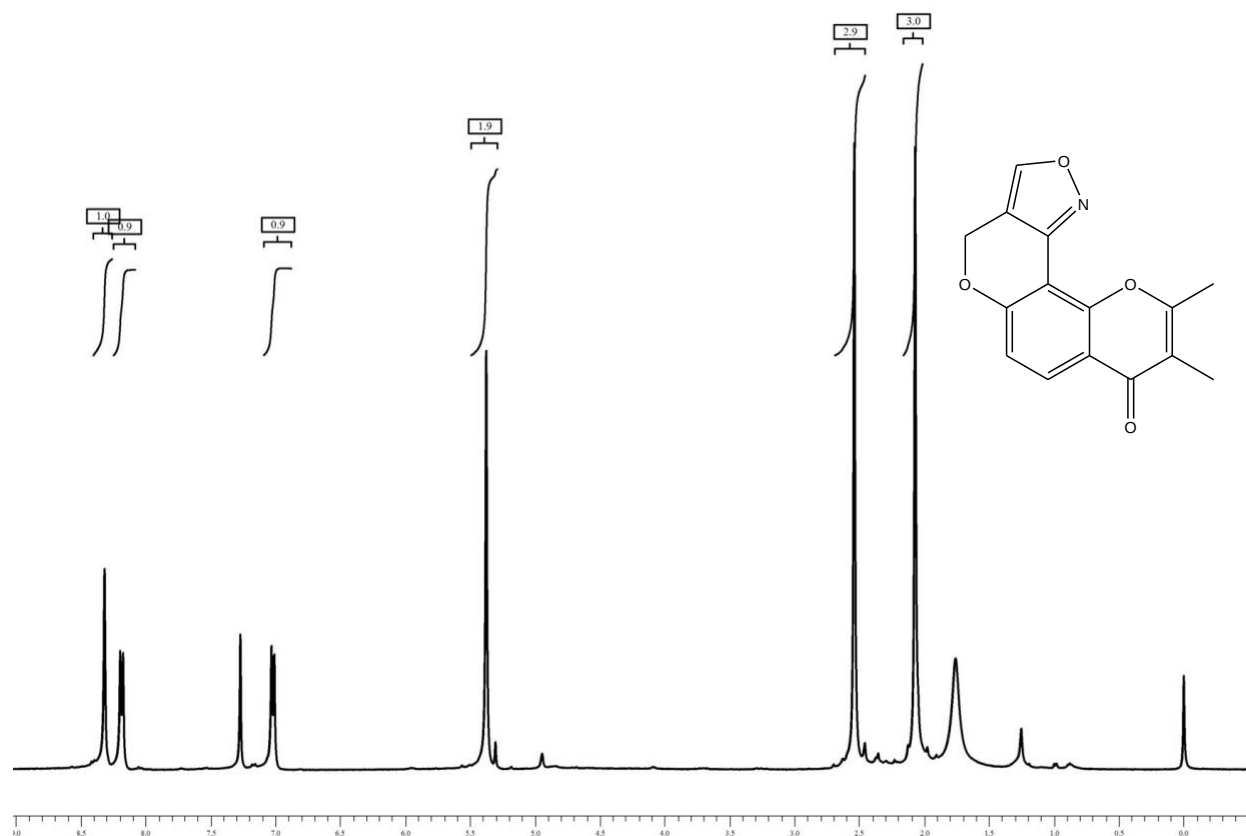
SURESH-NCMS

NATIONAL CENTRE FOR MASS SPECTROMETRY

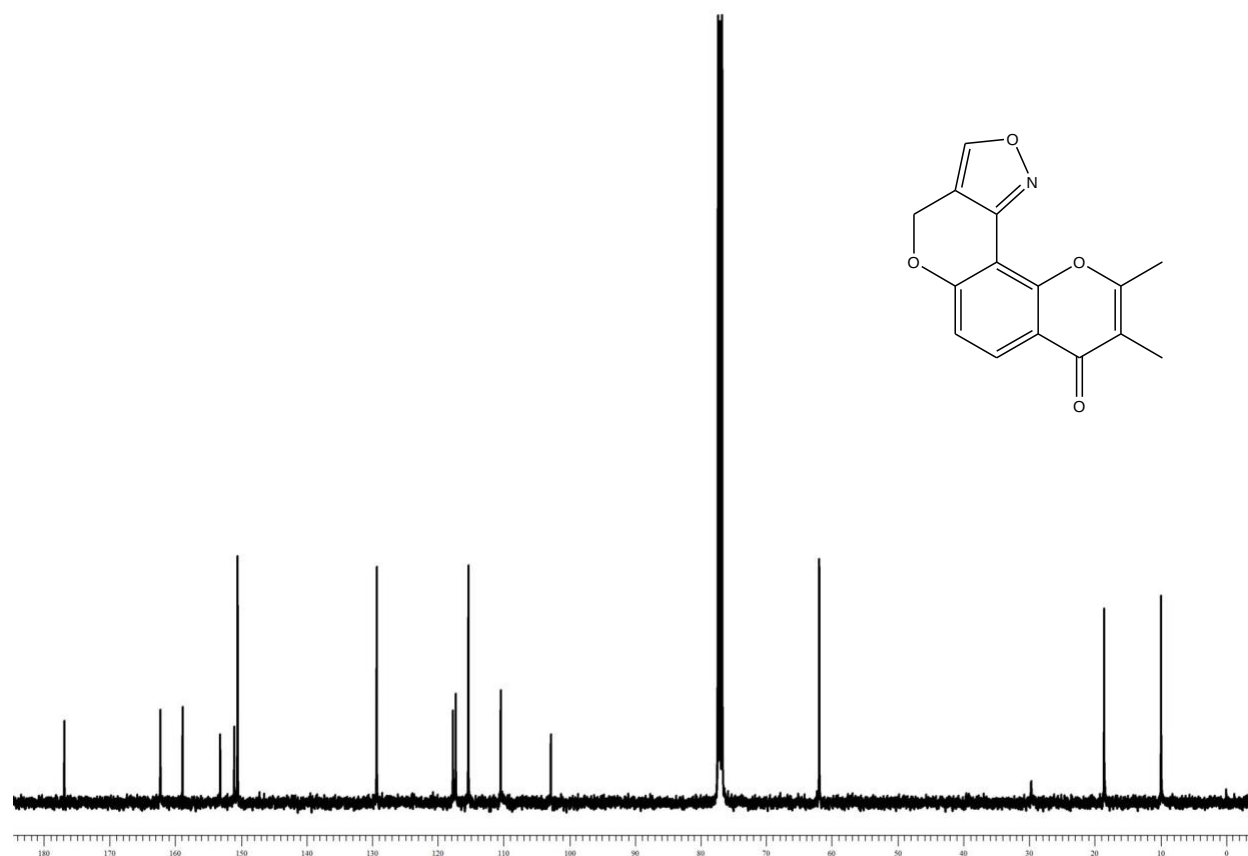
SURESH-4 #2-56 RT: 0.01-0.20 AV: 55 NL: 7.97E6

T: FTMS (1,1) + p ESI Full ms [110.00-2000.00]

**¹H-NMR Spectra of 9,10-dimethylpyrano[2',3':5,6]chromeno[4,3-c]isoxazol-8(4H)-one (5a)**



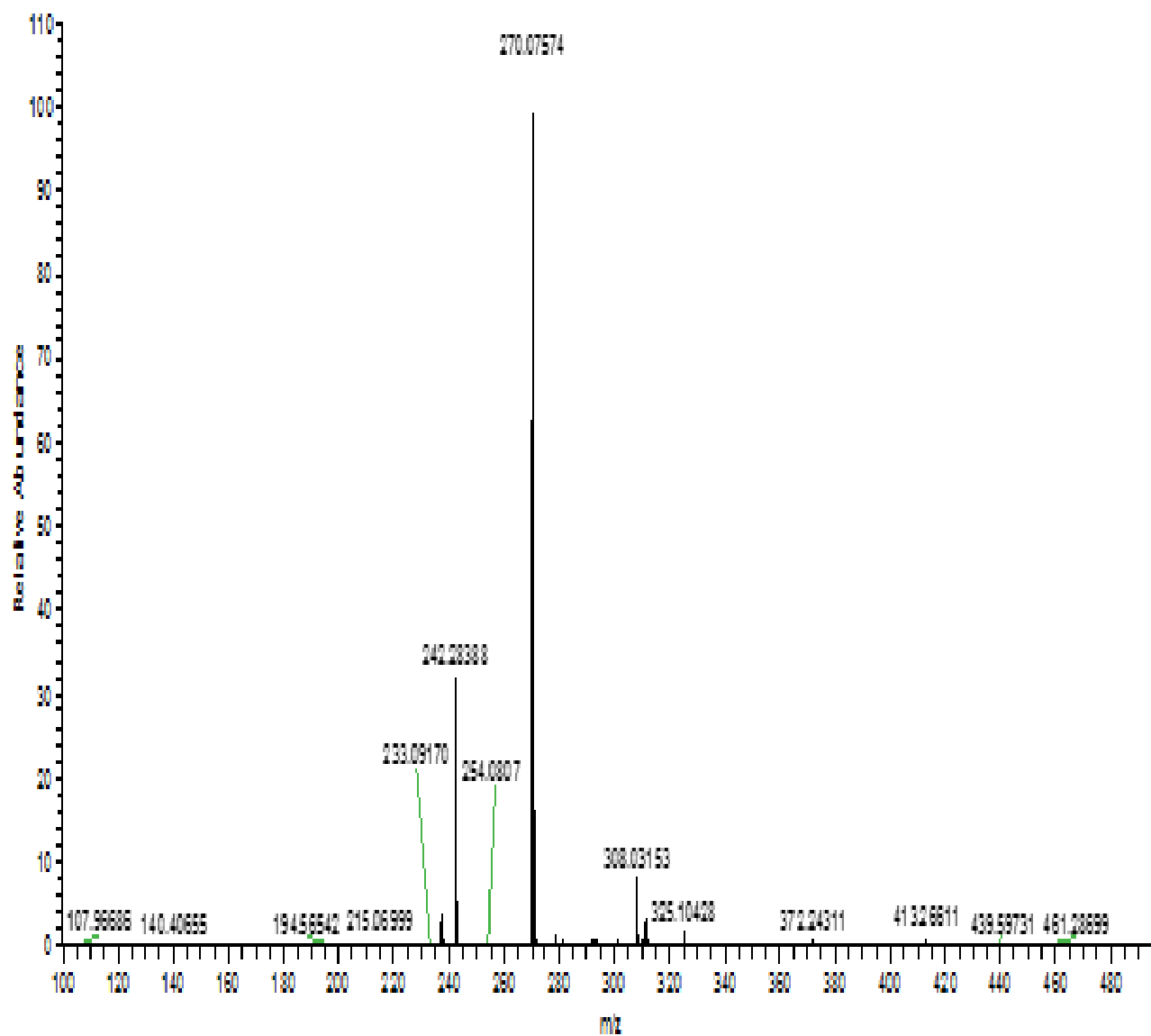
^{13}C -NMR Spectra of 9,10-dimethylpyrano[2',3':5,6]chromeno[4,3-c]isoxazol-8(4H)-one (5a):



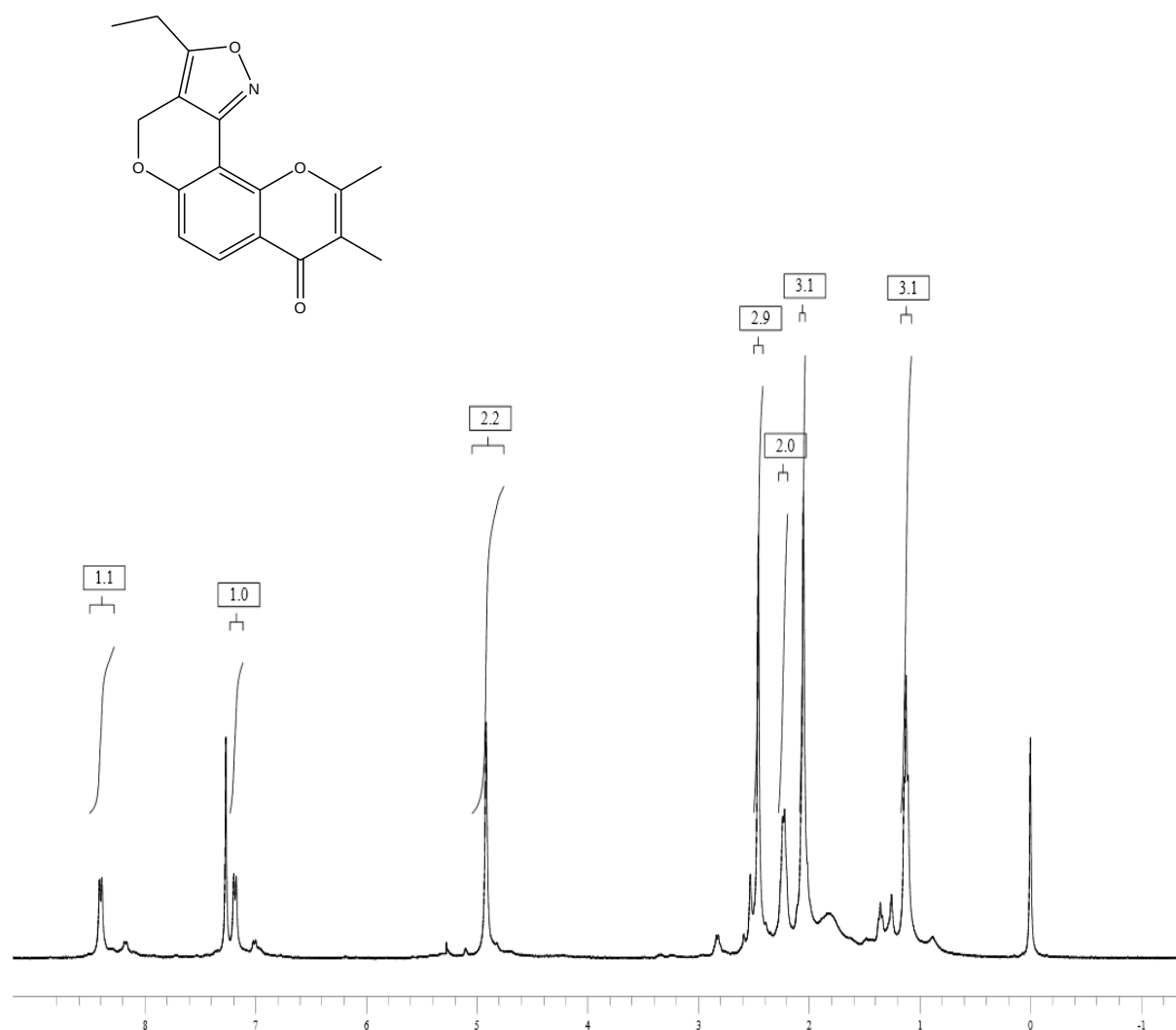
ESI-HRMS of 9,10-dimethylpyrano[2',3':5,6]chromeno[4,3-c]isoxazol-8(4H)-one (5a):

269 #5-108 RT: 0.04-0.79 AV: 104 NL: 558E7

T: FTMS + p ESI/Fulms (00.00-2000.00)



¹H-NMR Spectra of 3-ethyl-9,10-dimethylpyrano[2',3':5,6]chromeno[4,3-c]isoxazol-8(4H)-one (5c)



ESI-HRMS of 3-ethyl-9,10-dimethylpyrano[2',3':5,6]chromeno[4,3-c]isoxazol-8(4H)-one (5c)

3297 #7-11 RT: 0.08-0.09 AV: 5 BB: 36 0.27-0.59, 0.01-0.03 NL: 2.57E7
T: FTMS (1.1) + p ESI Fullms (110.00-1000.00)

