

# **Rational design of 9-vinyl-phenyl noscapine as potent tubulin binding anticancer agent and evaluation of the effects of its combination on Docetaxel**

**Shruti Gamy Dash<sup>1</sup>, Charu Suri<sup>2</sup>, Praveen Kumar Reddy Nagireddy<sup>3</sup>, Srinivas Kantevari<sup>3</sup> and Pradeep Kumar Naik<sup>1\*</sup>**

<sup>1</sup>Centre of Excellence in Natural Products and Therapeutics, Department of Biotechnology and Bioinformatics, Sambalpur University, Jyoti Vihar, Burla, Sambalpur-768 019, Odisha, India

<sup>2</sup>Drug Discovery Research Centre, Translational Health Science and Technology Institute, 3<sup>rd</sup> Milestone, Faridabad-Gurgaon Expressway, Pali, Haryana 121 004, India

<sup>3</sup>Fluoro and agrochemicals Division, CSIR-Indian Institute of Chemical Technology, Hyderabad 500 007, India

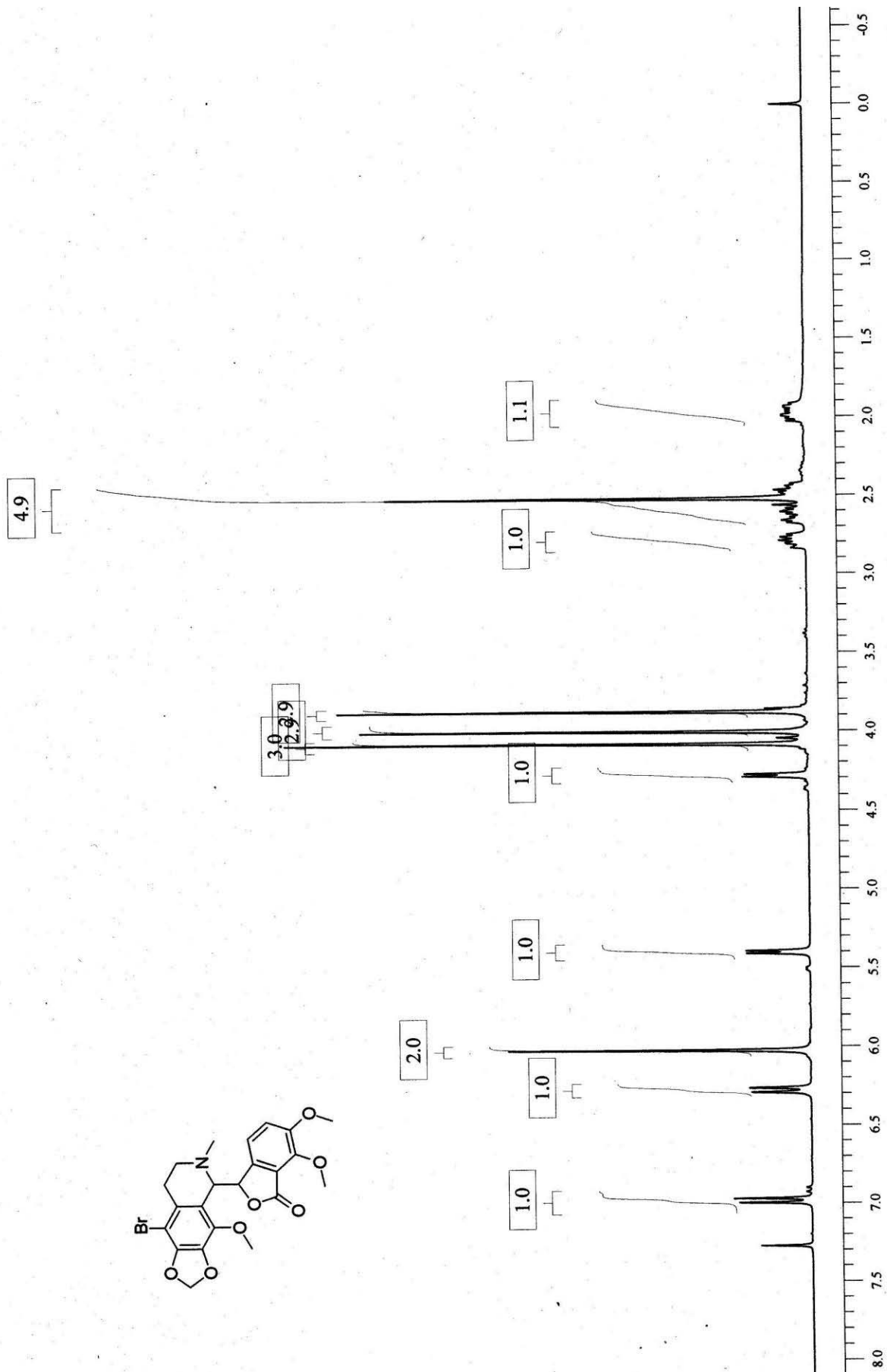
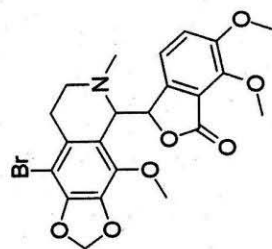
\* Corresponding author: Phone No.: +91-9479268802; E-mail: pknaik1973@gmail.com

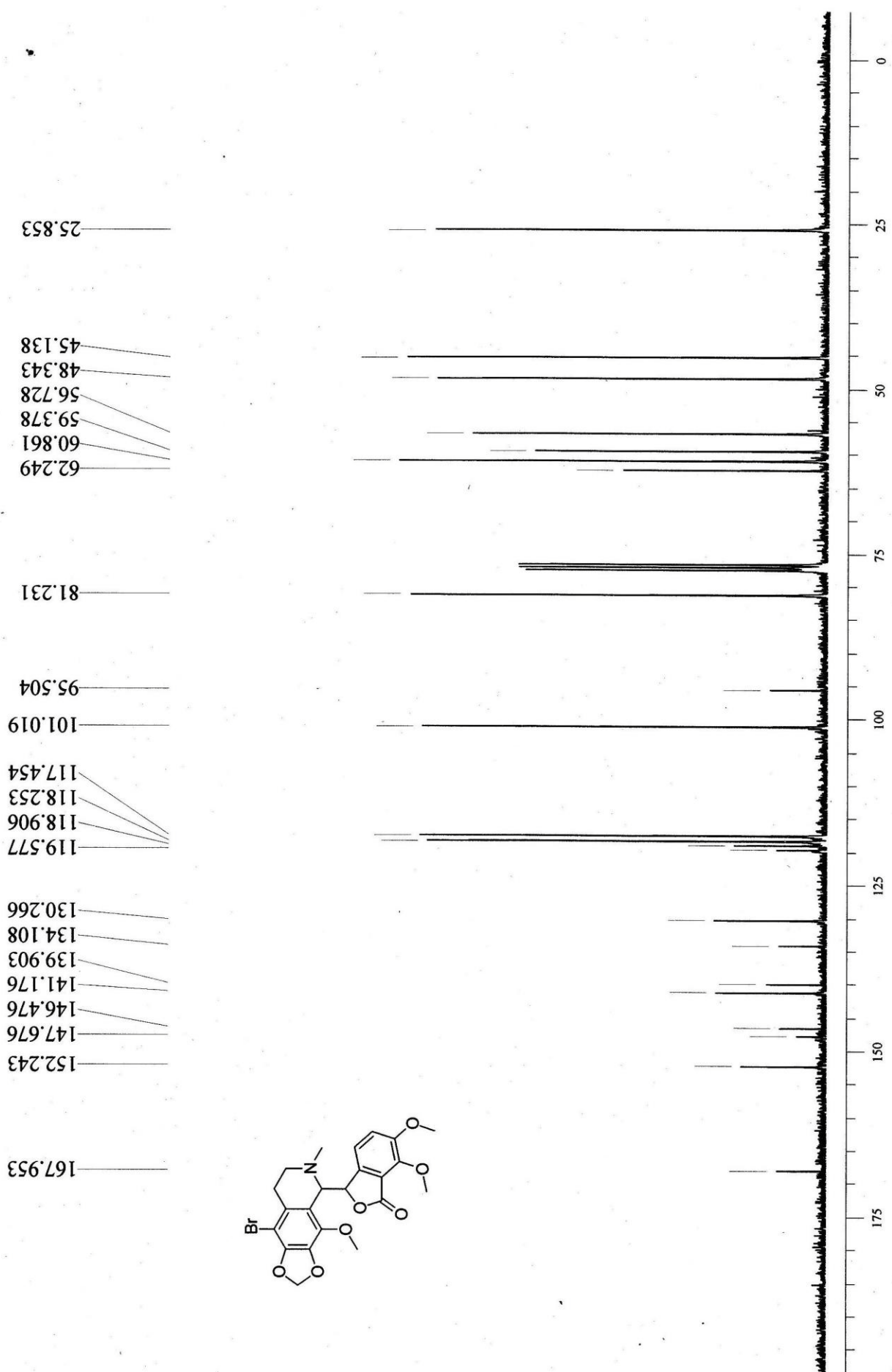
## **Supporting Information**

**Copies of <sup>1</sup>H, <sup>13</sup>C NMR and mass spectra (ESI and HR-MS) of**

**9-Bromo- $\alpha$ -noscapine (9-Br-nos) ..... S1-S5**

**9-Vinyl phenyl noscapine (VPN).....S6-S9**





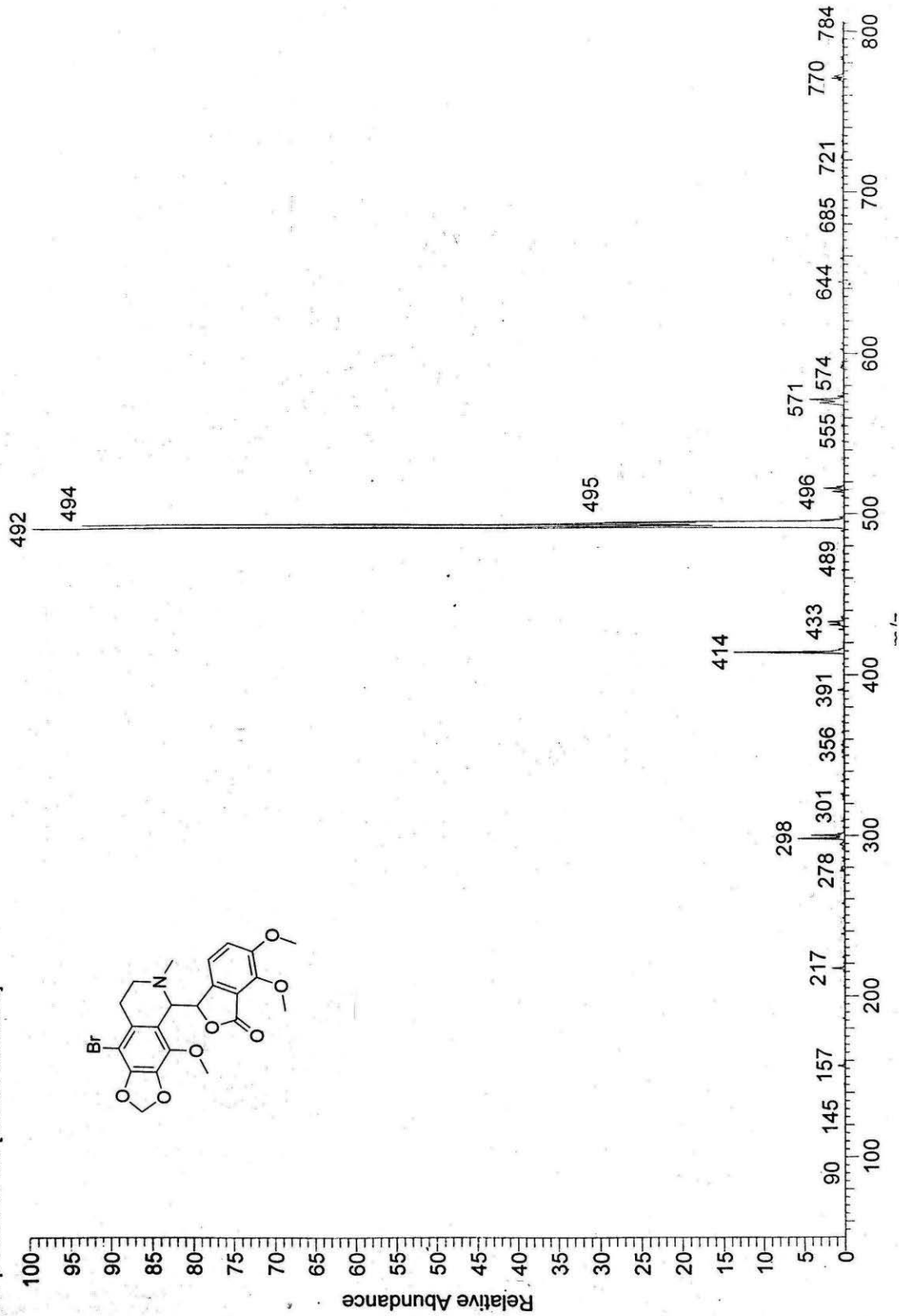
C:\Xcalibur\methods\NOSBROI  
ESI LABSAMPLES

7/16/2010 5:24:12 PM

NARESH K M,MLP-0002

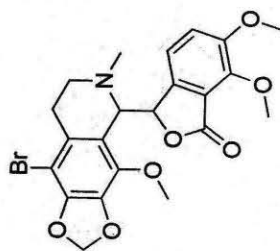
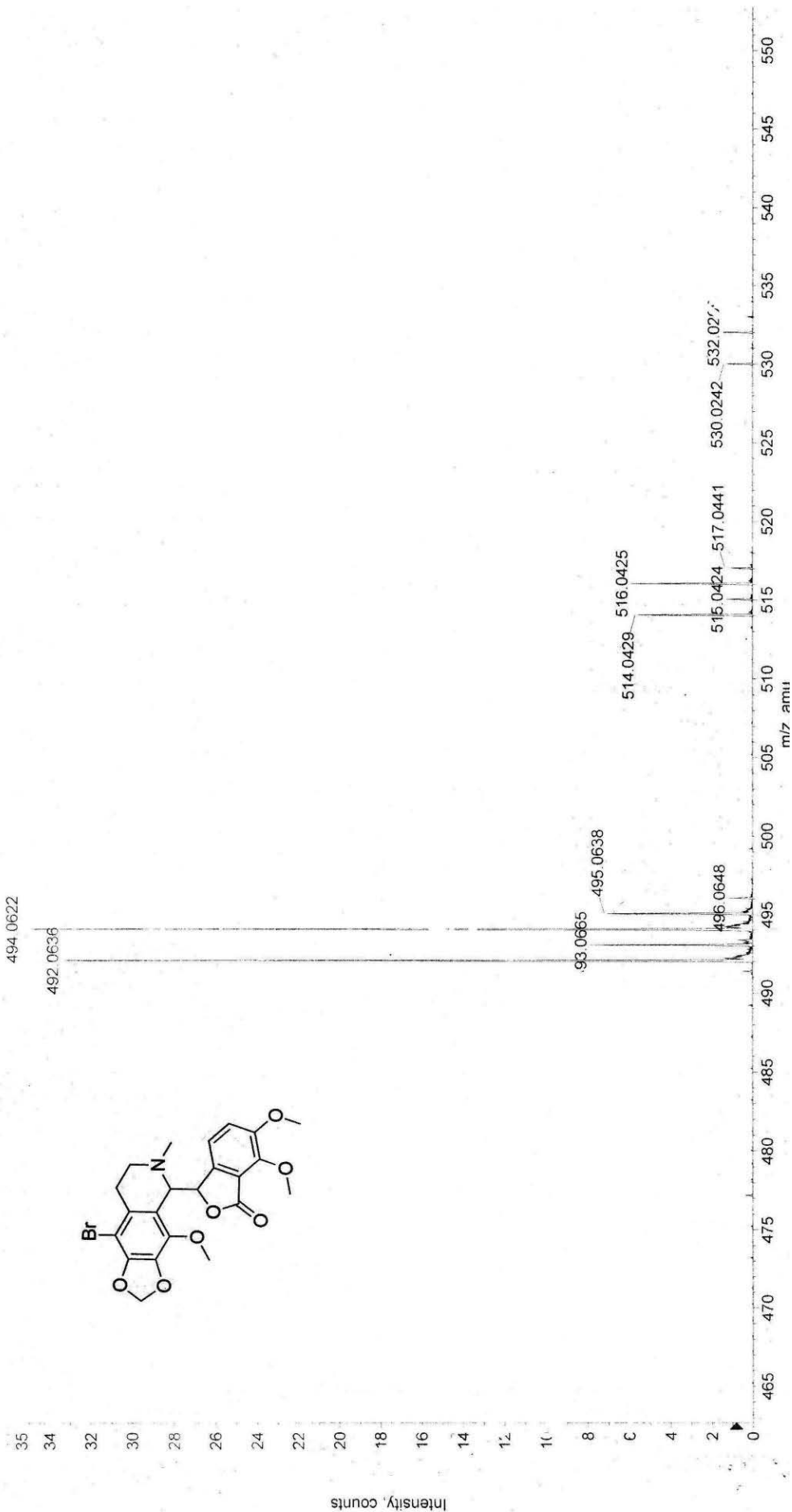
NOSBROI #14-20 RT: 0.39-0.55 AV: 7 SM: 15G NL: 4.58E7

T: + p ESI Full ms [ 50.00-2000.00]



4.0F MS 2.084 to 3.084 min from 07JUNE2011.wiff  
a=3.54797354226072420e-004, t0=-1.39882085296994770e+001

NARESH KUMAR, KS-BR-NDS, ESIHRMS, +VE



File: n/a

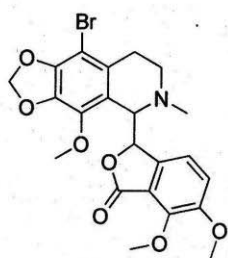
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Reference: n/a

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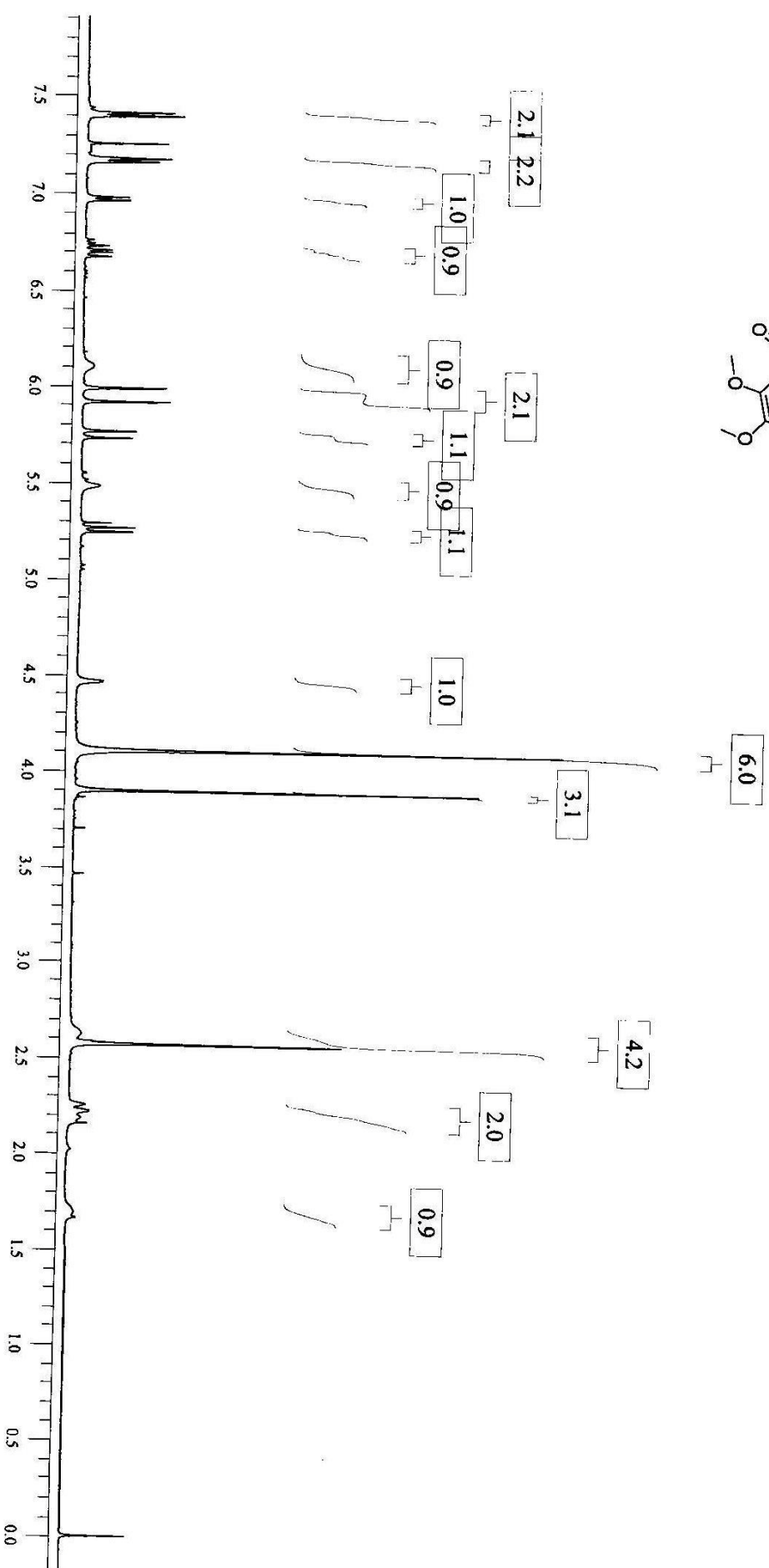
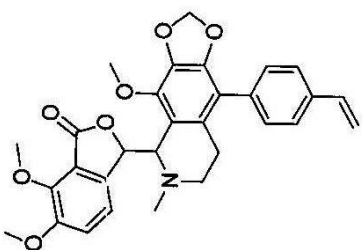
## Elemental composition calculator

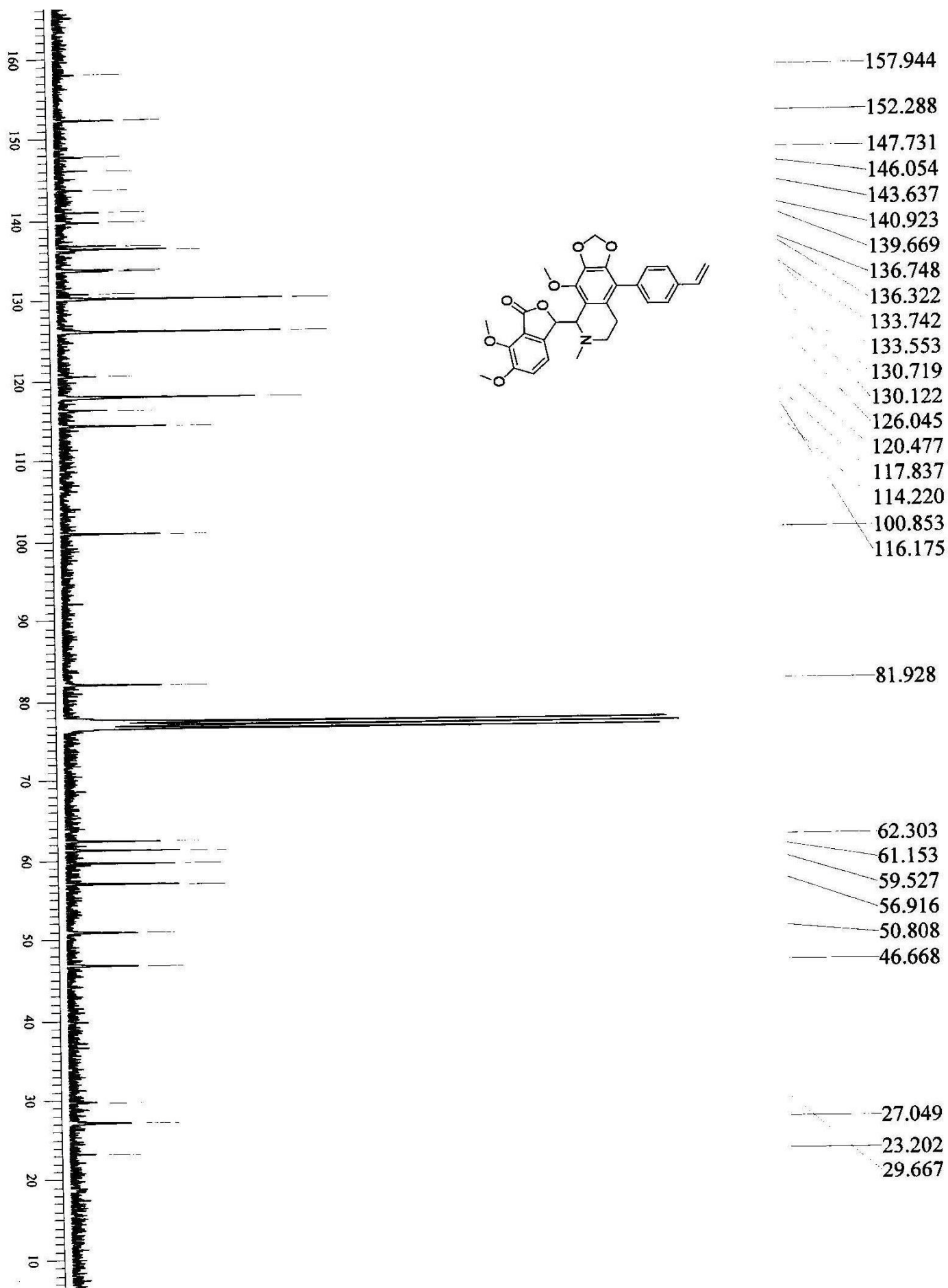


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Tolerance: +5.0000 ppm  
Result type: Elemental  
Max num of results: 100  
Min DBE: -0.5000 Max DBE: +50.0000  
Electron state: OddAndEven  
Num of charges: 0  
Add water: N/A  
Add proton: N/A  
File Name: 07JUNE2011.wiff

	Elements	Min Number	Max Number
1	Br	0	1
2	C	0	22
3	H	0	23
4	N	0	1
5	Na	0	1
6	O	0	7

	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C22 H23 N O7 Br	492.0657	-2.1885	-4.4476	11.5







Acq. File: 26JULY2011.wiff

Sample ID: TuneSample1.D

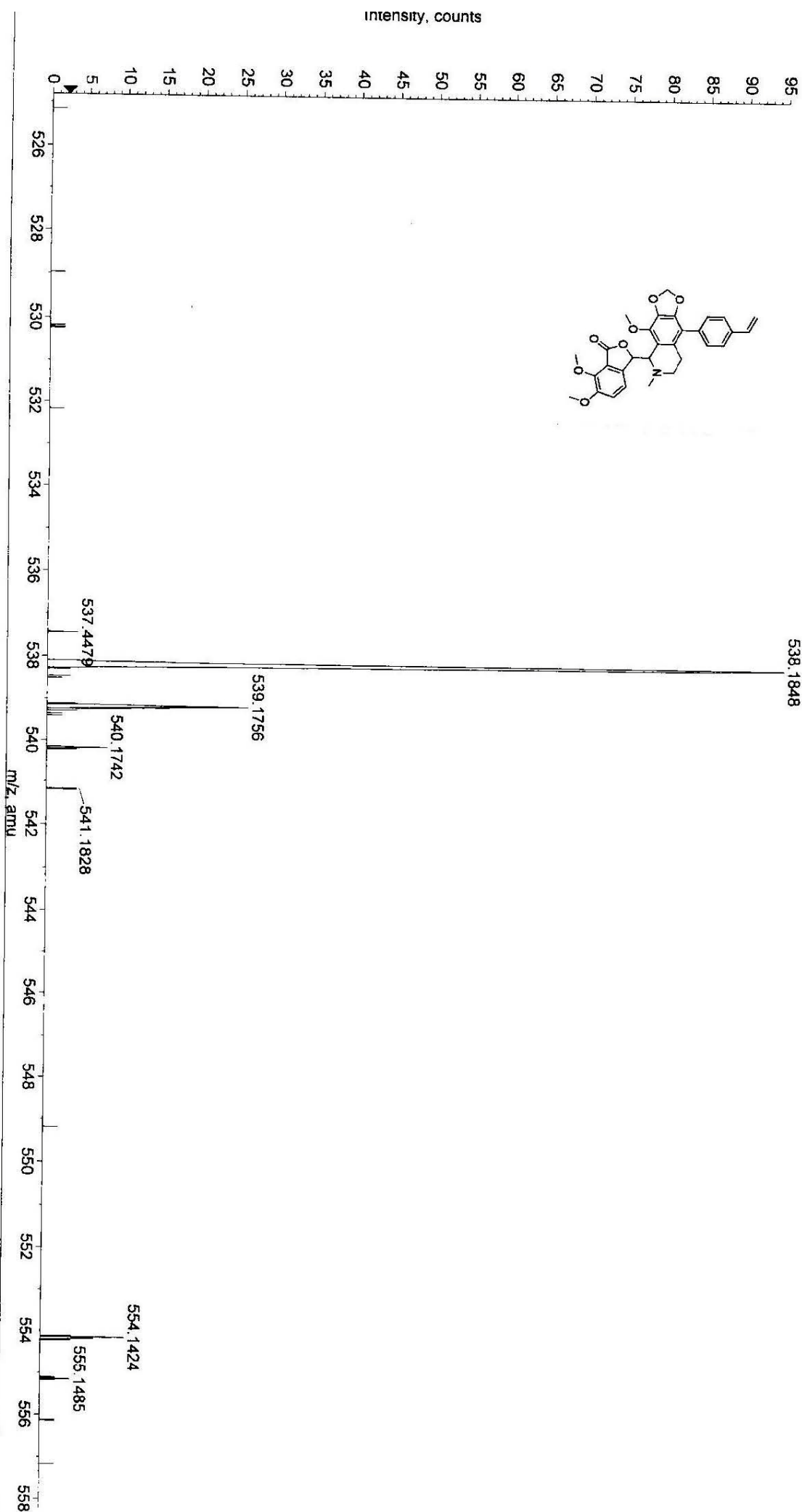
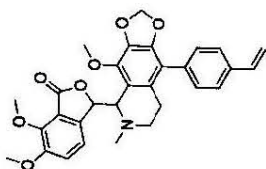
Acq. Date: Tuesday, July 26, 2011

Sample Comment: NARESH KUMAR.M., KS-SUZ-4-VINYLPHENYL, ESIHRMS, ESI-VE

Acq. Time: 11:24

+TOF MS: 0.134 min from Sample 4 (KSSUZ4VINYLPHENYL) of 26JULY2011.wiff  
a=3.54783692272171560e-004, f0=-1.41615385689947290e+001

Max. 95.0 coun



Acq. File: n/a

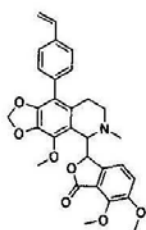
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Sample Comment: r/a

Acq. Time: n/a

## Elemental composition calculator



Target m/z: +538.1848 amu  
Tolerance: +5.0000 ppm  
Result type: Elemental  
Max num of results: 100  
Min DBE: -0.5000 Max DBE: +50.0000  
Electron state: OddAndEven  
Num of charges: 0  
Add water: N/A  
Add proton: N/A  
File Name: 26JULY2011.wiff

	Elements	Min Number	Max Number
1	C	0	31
2	H	0	32
3	N	0	2
4	Na	0	1
5	O	0	9

	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C30 H29 N O7 Na	538.1841	0.6276	1.1662	16.5