

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

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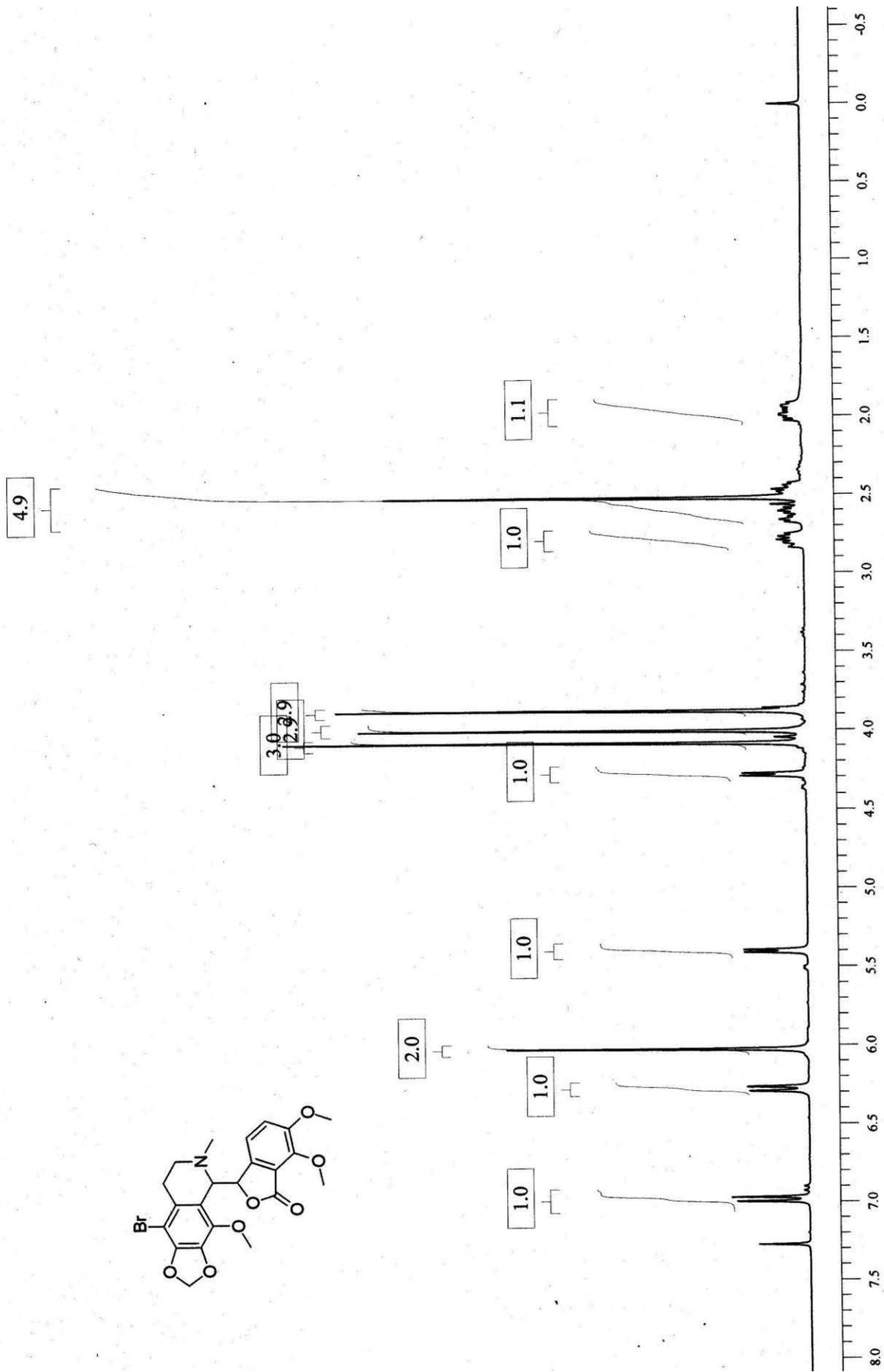
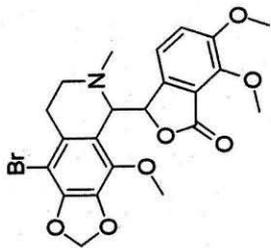
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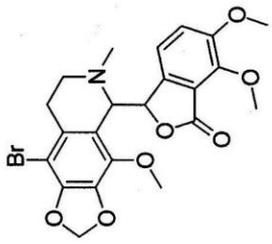
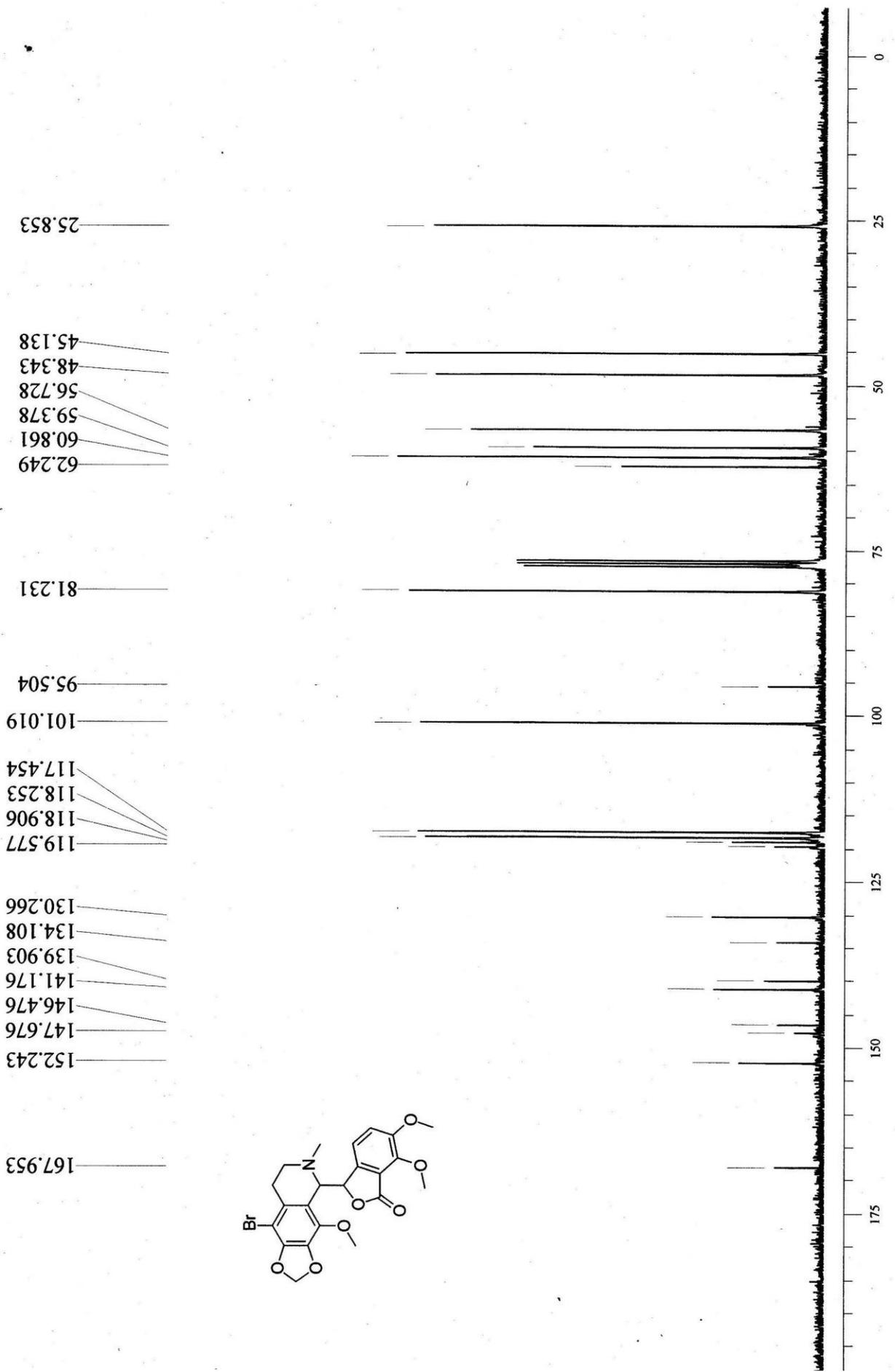
Supporting Information

Copies of ¹H, ¹³C NMR and mass spectra (ESI and HR-MS) of

9-Bromo- α -noscapine (9-Br-nos) S1-S5

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





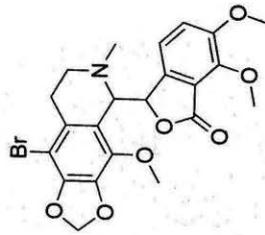
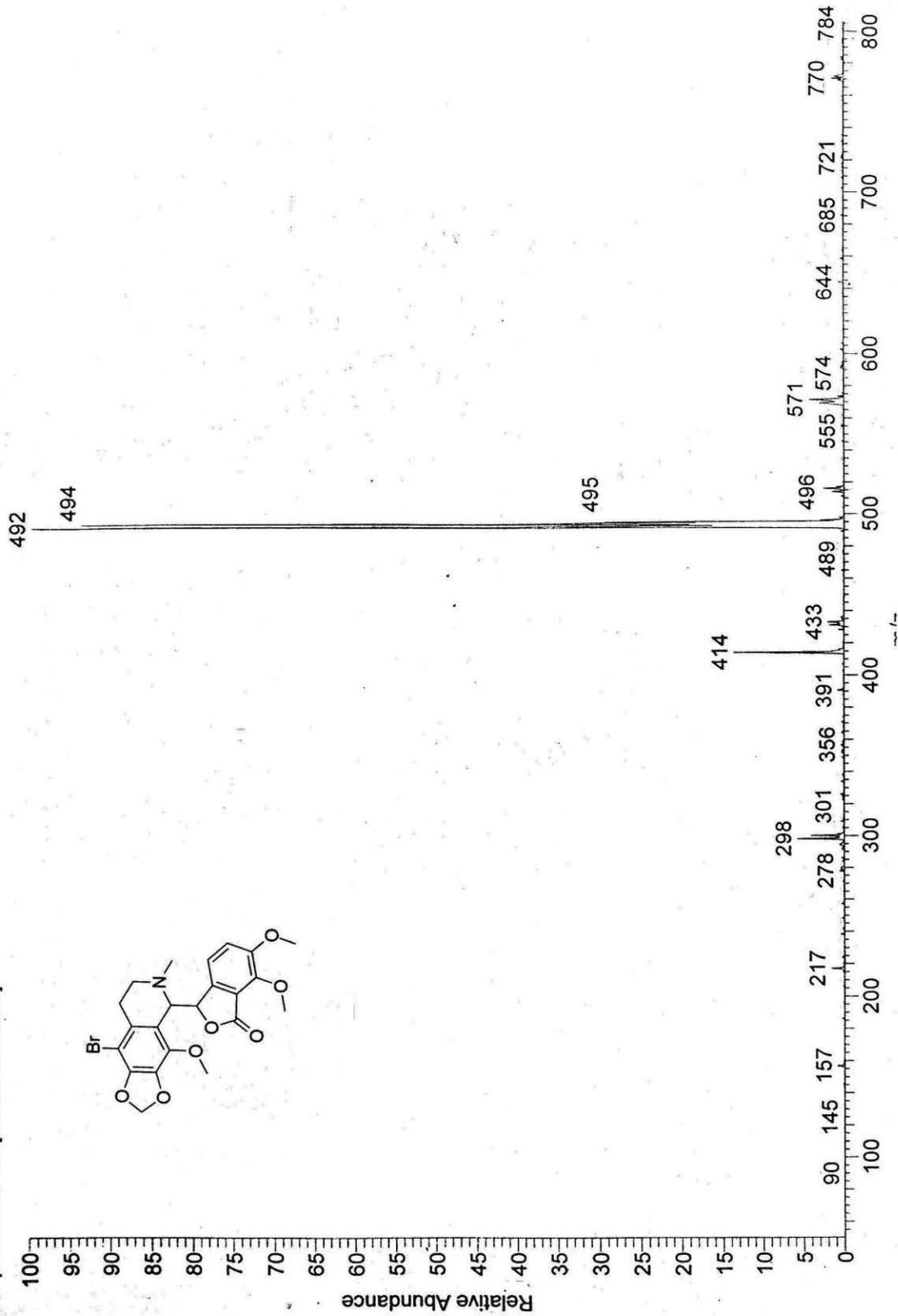
C:\Xcalibur\methods\NOSBROI
ESI LABSAMPLES

7/16/2010 5:24:12 PM

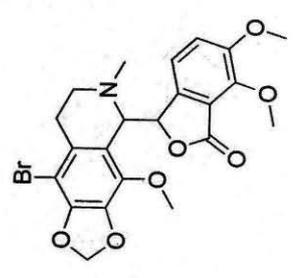
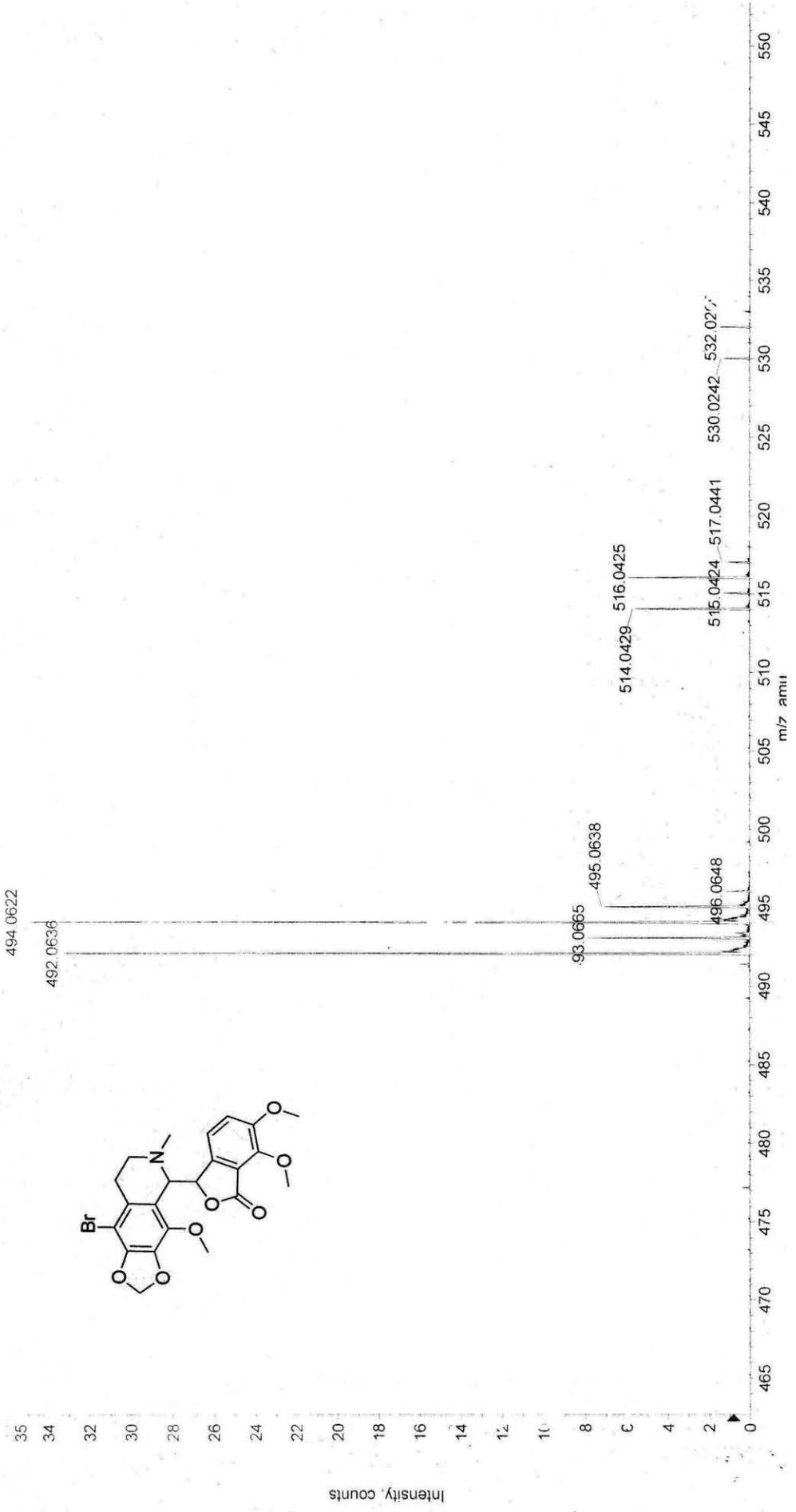
NARESH K M_MLP-0002

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

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



1.01F MS 2.084 to 3.084 min from 07JUNE2011.wiff
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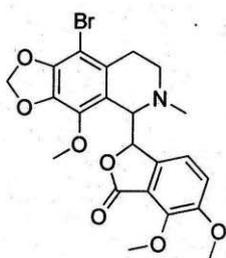
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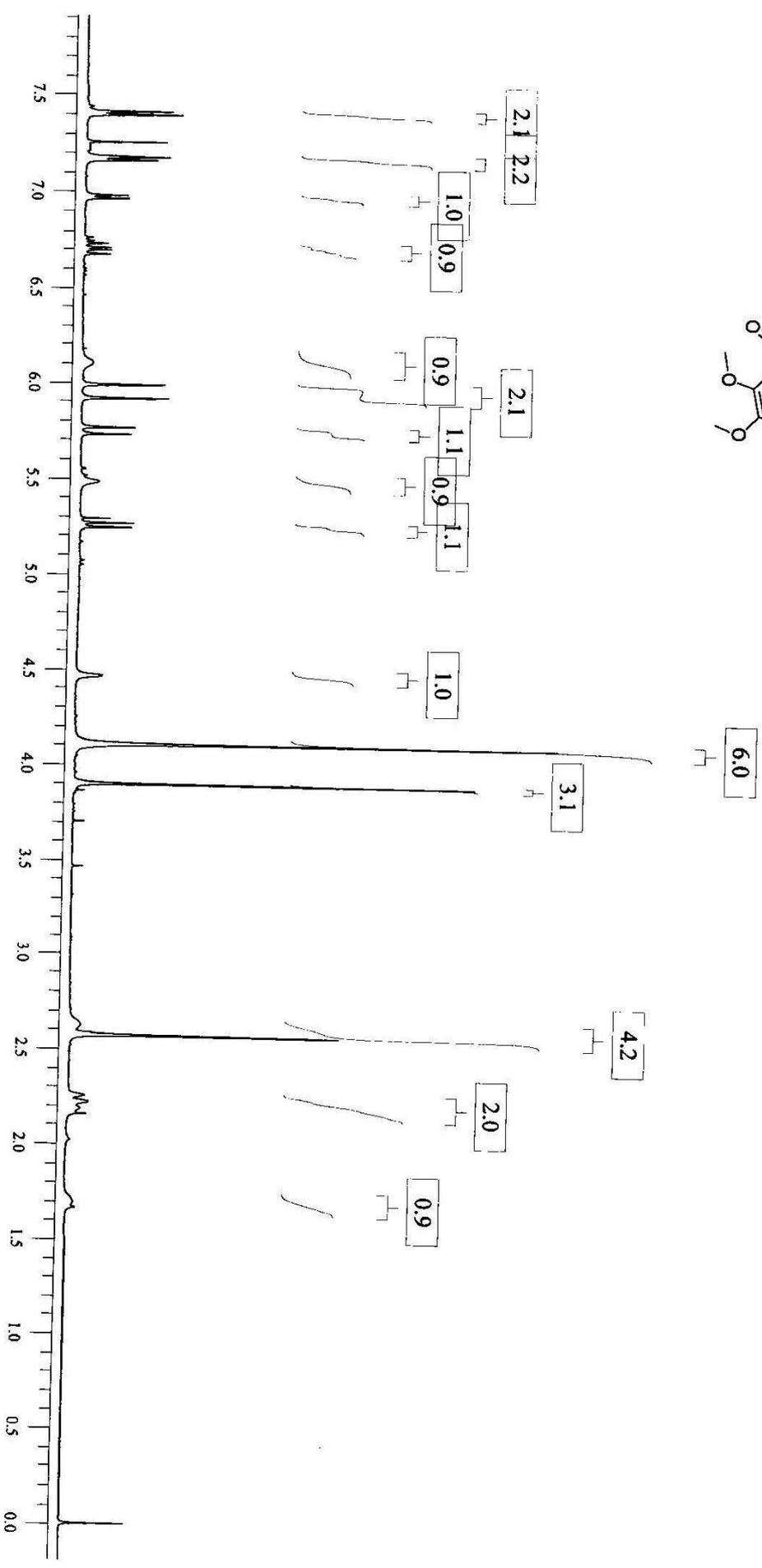
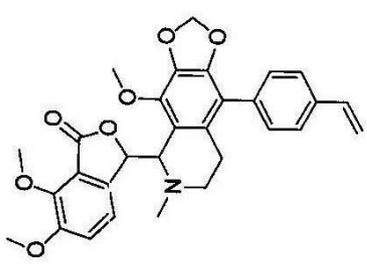
Elemental composition calculator

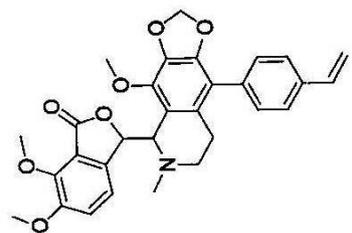
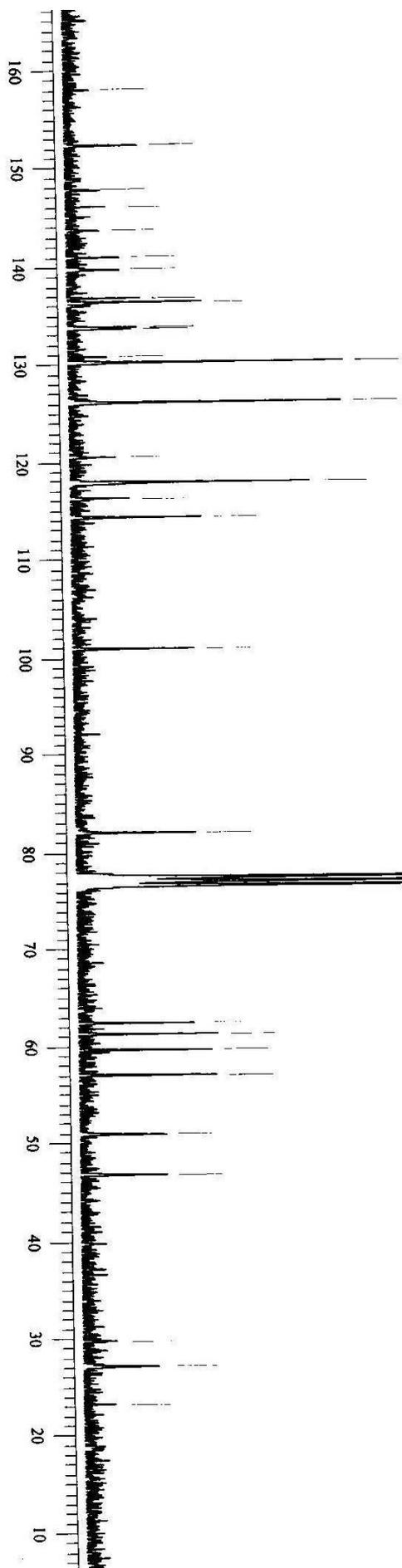


Target m/z: +492.0636 amu
 Tolerance: +5.0000 ppm
 Result type: Elemental
 Max num of results: 100
 Min DBE: -0.5000 Max DBE: +50.0000
 Electron state: OddAndEven
 Num of charges: 0
 Add water: N/A
 Add proton: N/A
 File Name: 07JUNE2011.wiff

	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





- 157.944
- 152.288
- 147.731
- 146.054
- 143.637
- 140.923
- 139.669
- 136.748
- 136.322
- 133.742
- 133.553
- 130.719
- 130.122
- 126.045
- 120.477
- 117.837
- 114.220
- 100.853
- 116.175

- 81.928

- 62.303
- 61.153
- 59.527
- 56.916
- 50.808
- 46.668

- 27.049
- 23.202
- 29.667

Acq. File: n/a

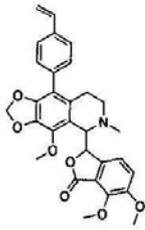
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Acq. Time: n/a

Elemental composition calculator



Target m/z: +538.1848 amu
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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