

# “Diversity Oriented Synthesis of a Vinblastine-Templated Library of 7-Aryl Octahydroazonino[5,4-*b*]indoles via a Three-Component Reaction”

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## **LC/MS chromatograms of post-purification samples**

Pages S3-S4: LS/MS chromatogram of sample **2**{3}

Pages S5-S6: LS/MS chromatogram of sample **2**{11}

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Pages S39-S40: LS/MS chromatogram of sample **15**{13}

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Pages S43-S44: LS/MS chromatogram of sample **16**{1}

Pages S45-S46: LS/MS chromatogram of sample **16**{12}

Pages S47-S49: LS/MS chromatogram of sample **17**{15}

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Pages S53-S54: LS/MS chromatogram of sample **19**{12}

Pages S55-S56: LS/MS chromatogram of sample **19**{20}

Pages S57-S58: LS/MS chromatogram of sample **20**{10}

2{3}

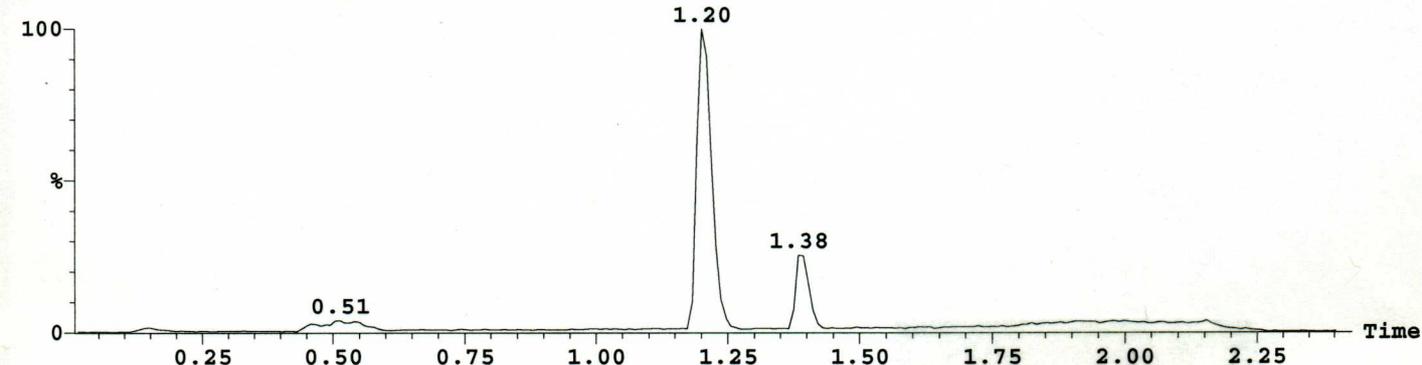
Printed: Mon Nov 07 09:35:49 2005

Sample Report:

Sample 5 Vial 4:4 ID A38570101A03-2281128 File N38570203 Date 08-Jul-2004 Time 00:16:45 Description 3440906

MS ES+ :BPI

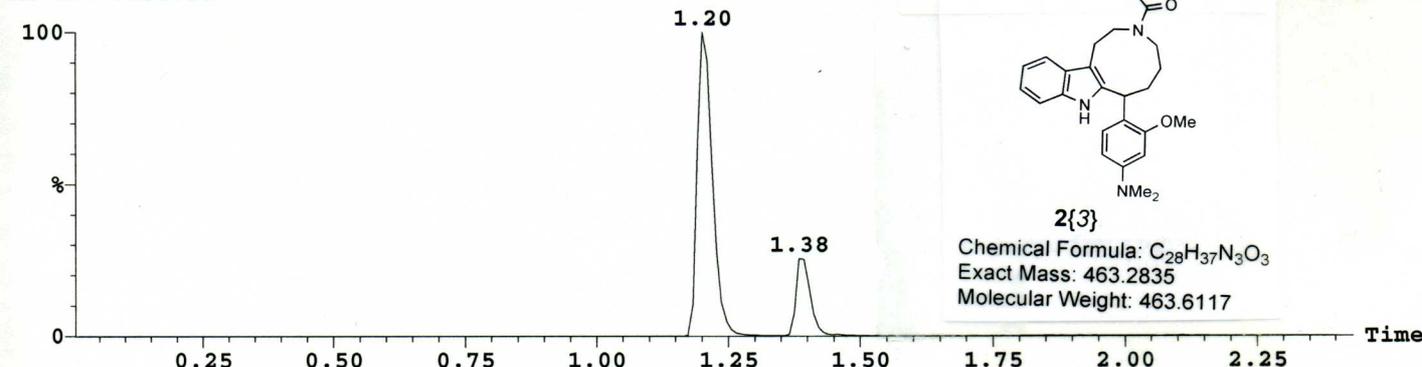
6.2e+007



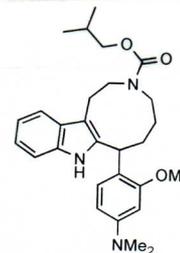
Peak Number	Compound	Time	AreaAbs	Area%Total	Width	Height	Mass Found
-------------	----------	------	---------	------------	-------	--------	------------

MS ES+ :464.28

6.2e+007



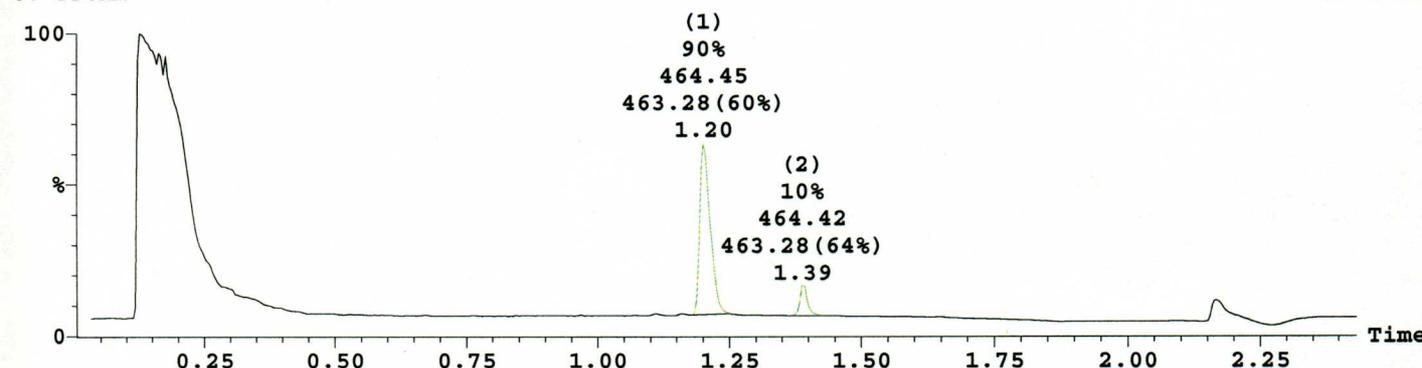
Peak Number	Compound	Time	AreaAbs	Area%Total	Width	Height	Mass Found
-------------	----------	------	---------	------------	-------	--------	------------



2{3}  
 Chemical Formula: C<sub>28</sub>H<sub>37</sub>N<sub>3</sub>O<sub>3</sub>  
 Exact Mass: 463.2835  
 Molecular Weight: 463.6117

UV 214nm

3.7e+005

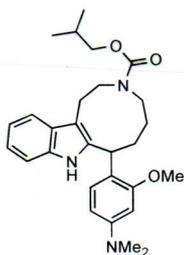
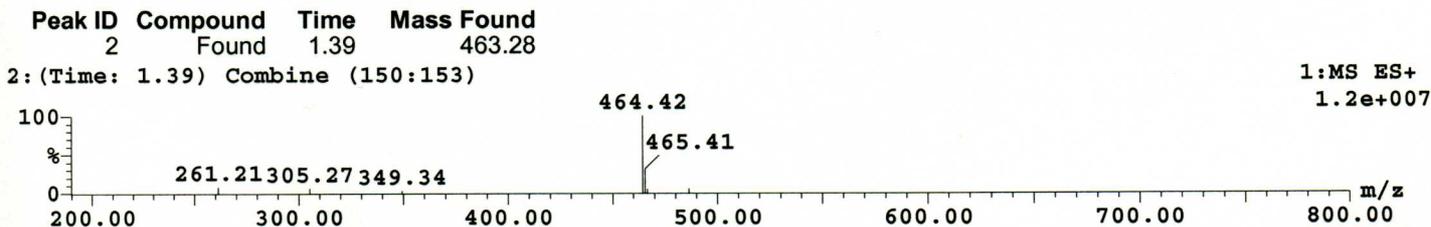
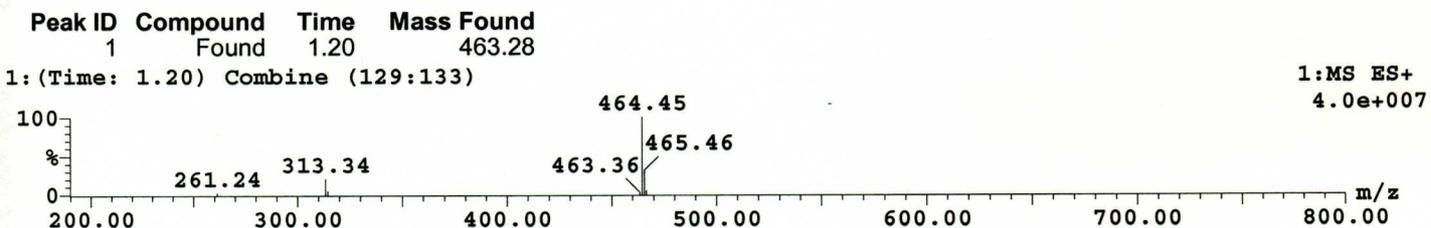
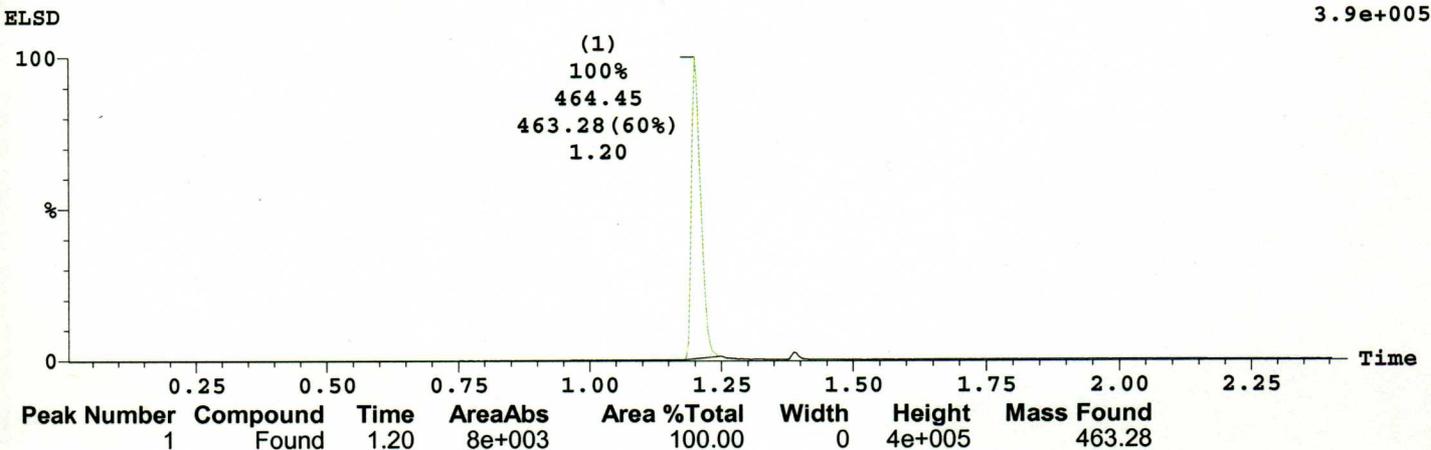


Peak Number	Compound	Time	AreaAbs	Area%Total	Width	Height	Mass Found
1	Found	1.20	5e+003	89.68	0	2e+005	463.28
2	Found	1.39	5e+002	10.32	0	3e+004	463.28

2{3}

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Sample Report (continued):



2{3}

Chemical Formula: C<sub>28</sub>H<sub>37</sub>N<sub>3</sub>O<sub>3</sub>  
Exact Mass: 463.2835  
Molecular Weight: 463.6117

Openlynx Report -  
Sample: 13  
File:N38570211  
Description:3440914

Vial:4:14  
Date:08-Jul-2004

ID:A38570101C01-2281136  
Time:00:37:23

Printed: Wed Nov 02 14:23:47 2005

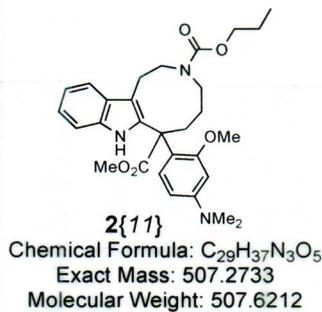
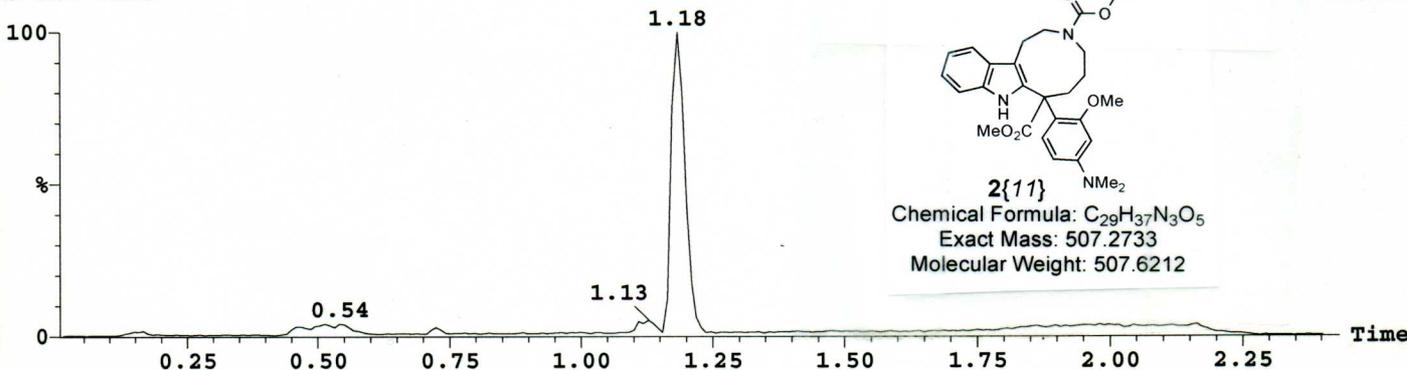
25113

Sample Report:

Sample 13 Vial 4:14 ID A38570101C01-2281136 File N38570211 Date 08-Jul-2004 Time 00:37:23 Description 3440914

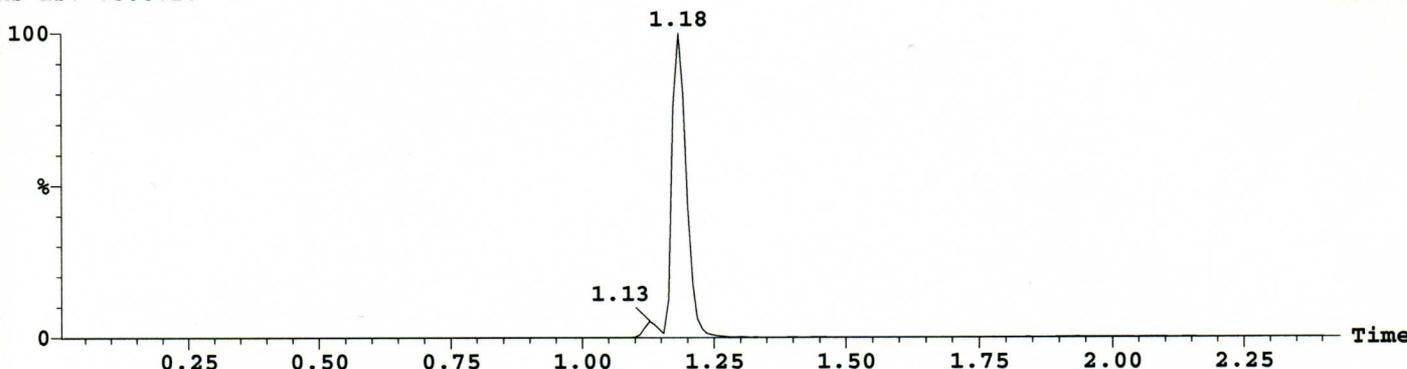
MS ES+ :BPI

6.4e+007



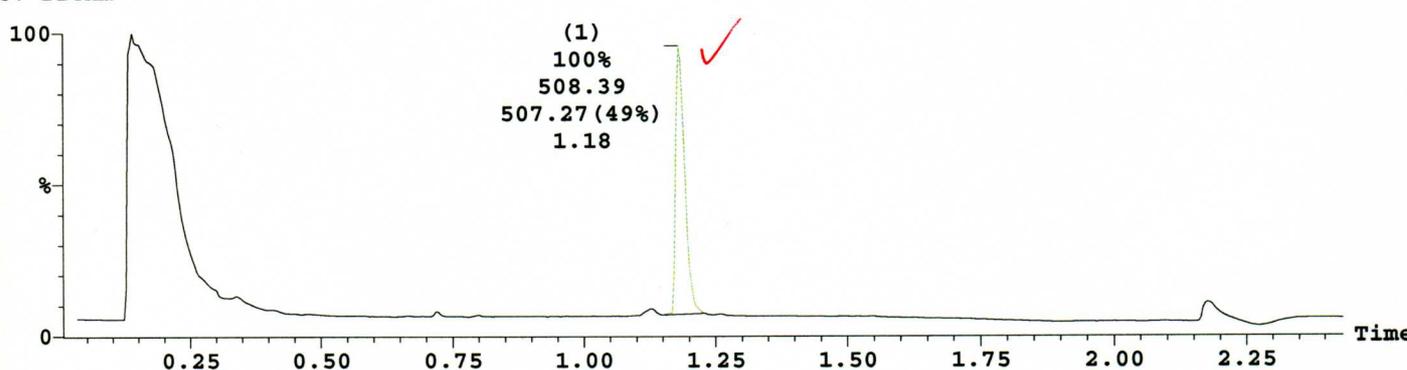
MS ES+ :508.27

6.4e+007



UV 214nm

3.7e+005



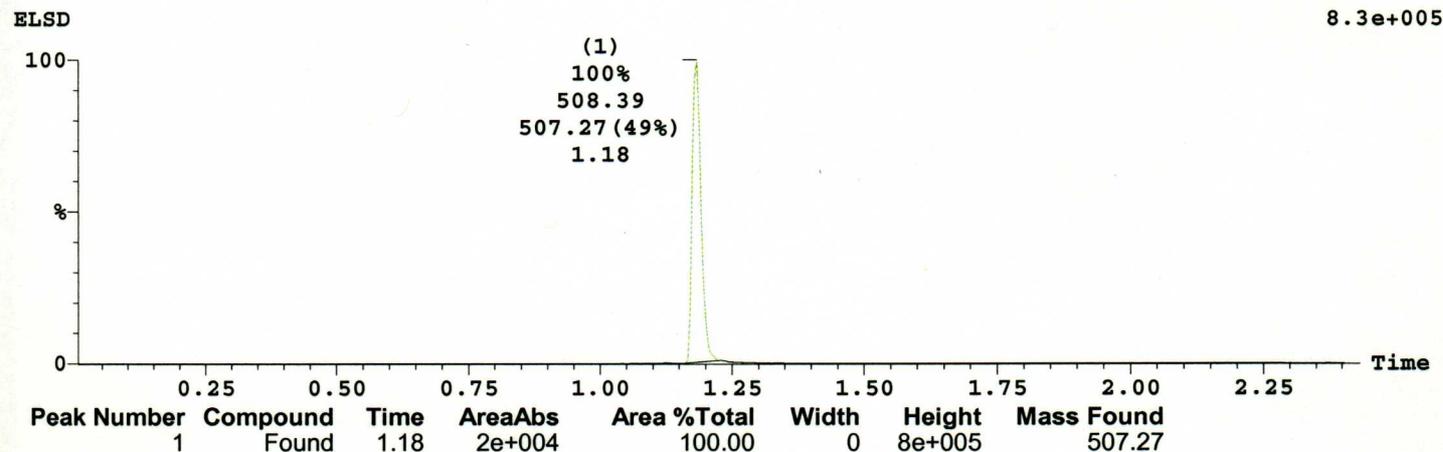
(1)  
100%  
508.39  
507.27 (49%)  
1.18

Peak Number	Compound Found	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1	Found	1.18	7e+003	100.00	0	3e+005	507.27

25113

Printed: Wed Nov 02 14:23:47 2005

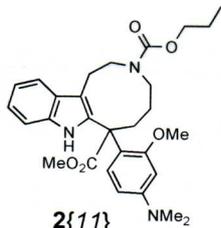
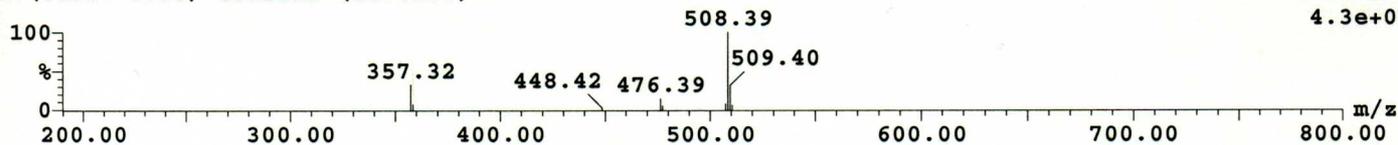
Sample Report (continued):



Peak ID	Compound	Time	Mass Found
1	Found	1.18	507.27

1:(Time: 1.18) Combine (127:130)

1:MS ES+  
4.3e+007



Chemical Formula: C<sub>29</sub>H<sub>37</sub>N<sub>3</sub>O<sub>5</sub>  
Exact Mass: 507.2733  
Molecular Weight: 507.6212

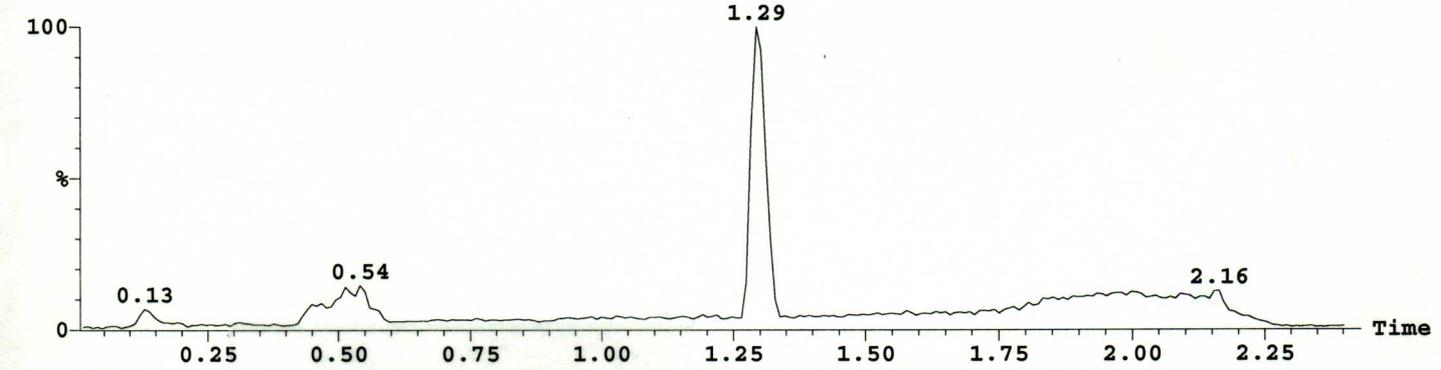
Printed: Wed Nov 02 14:24:52 2005

25163

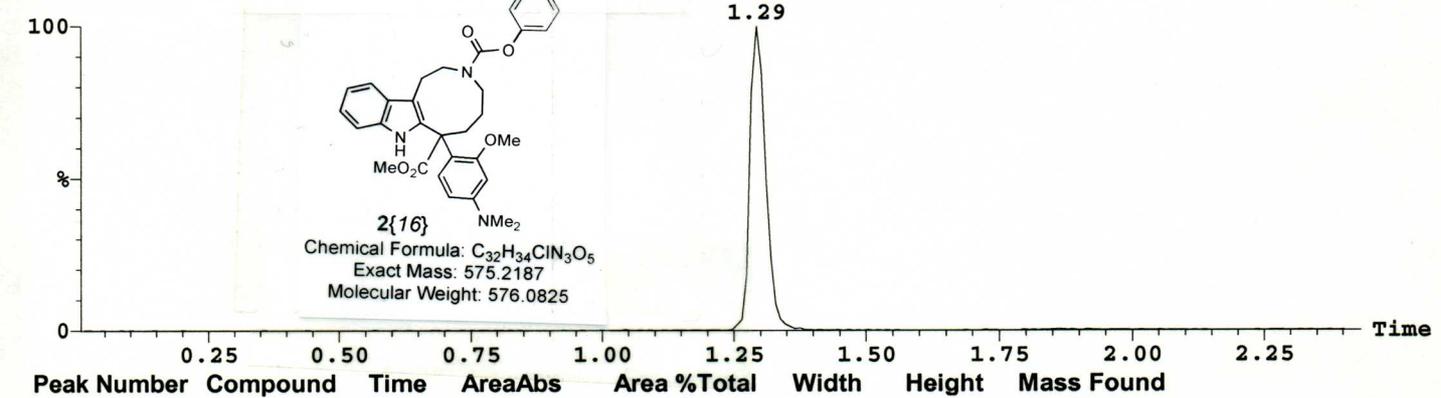
Sample Report:

Sample 18 Vial 4:19 ID A38570101D01-2281141 File N38570216 Date 08-Jul-2004 Time 00:50:15 Description 3440919

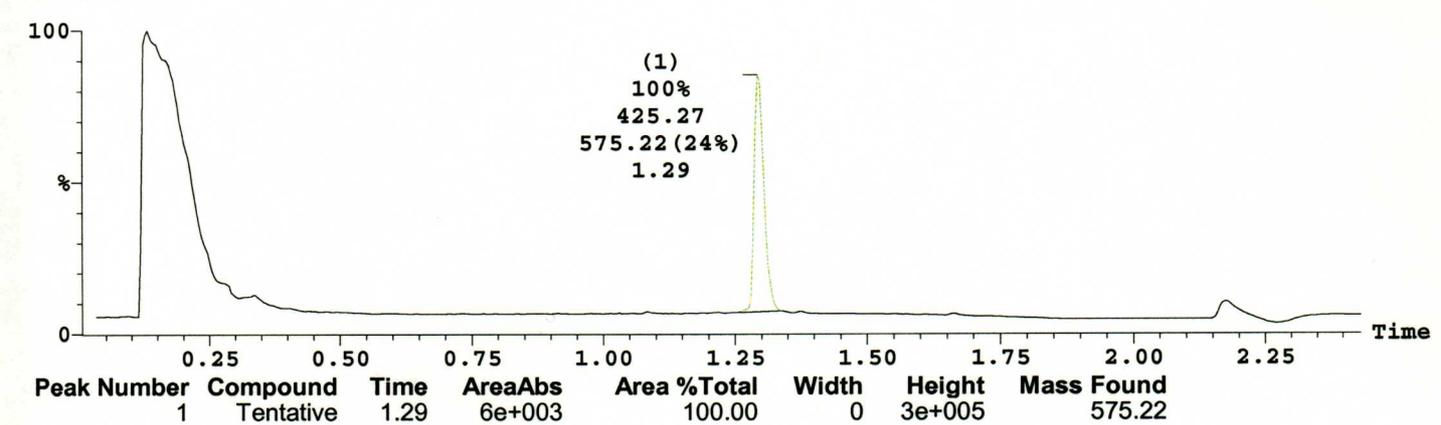
MS ES+ :BPI 1.9e+007



MS ES+ : 576.22 1.6e+007

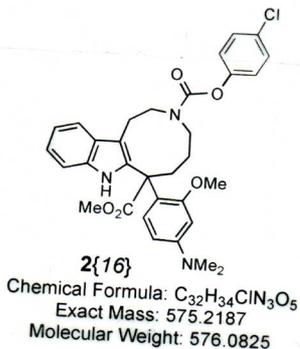
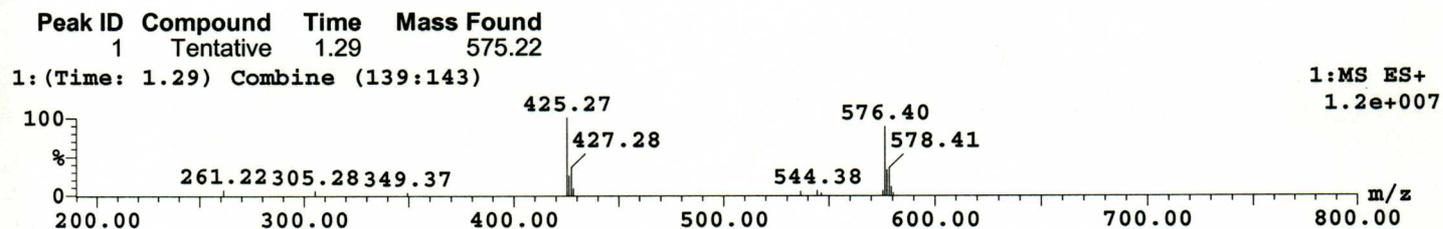
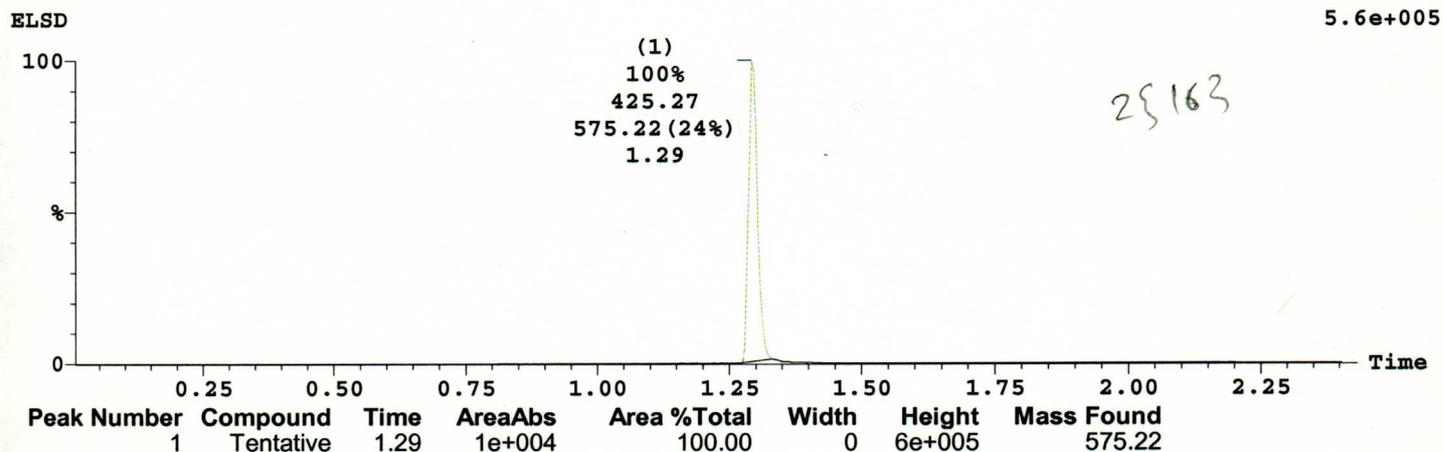


UV 214nm 3.7e+005



Printed: Wed Nov 02 14:24:52 2005

Sample Report (continued):



Printed: Wed Nov 02 14:25:30 2005

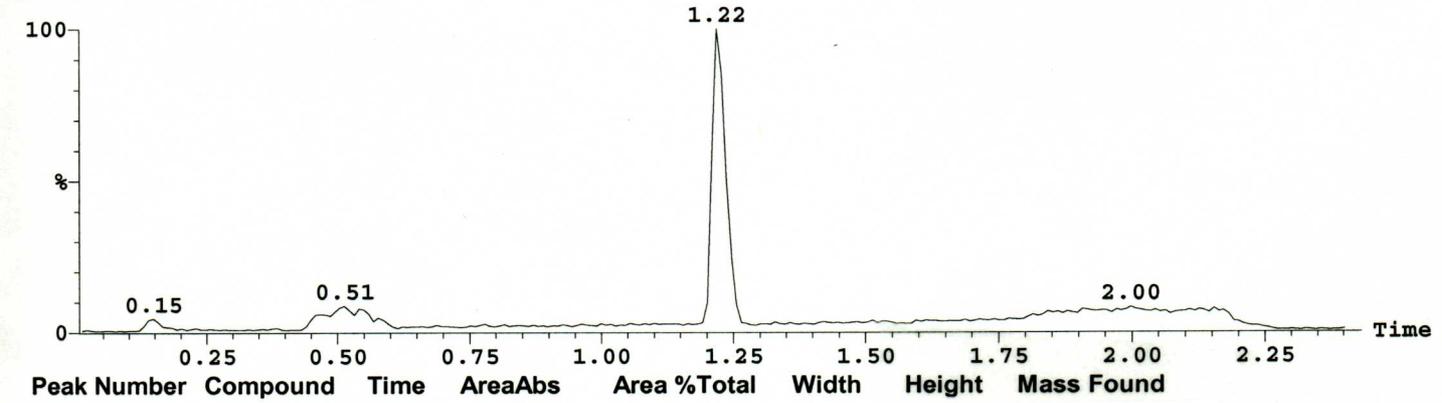
25183

Sample Report:

Sample 20 Vial 4:21 ID A38570101D03-2281143 File N38570218 Date 08-Jul-2004 Time 00:55:27 Description 3440921

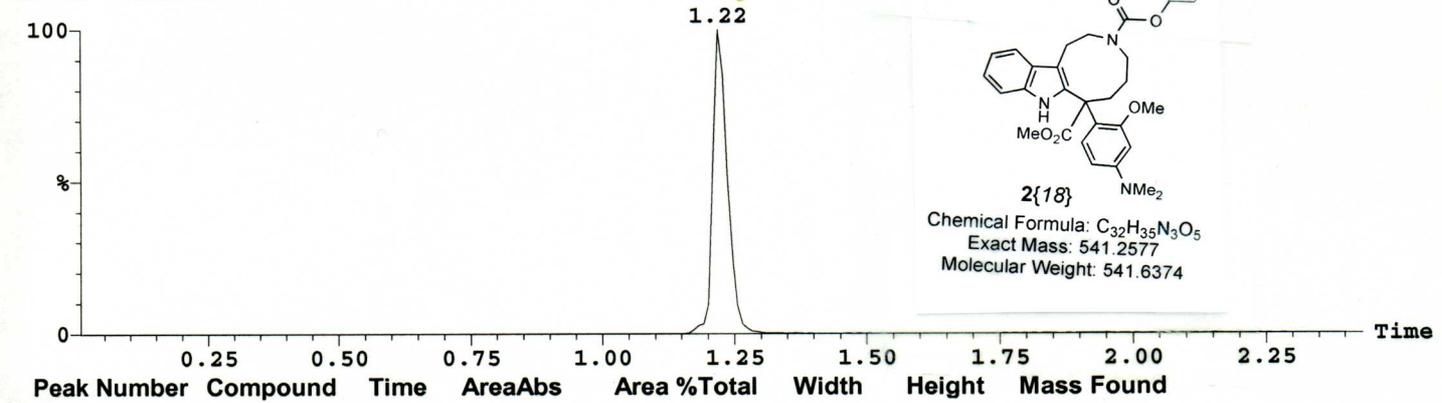
MS ES+ :BPI

3.0e+007



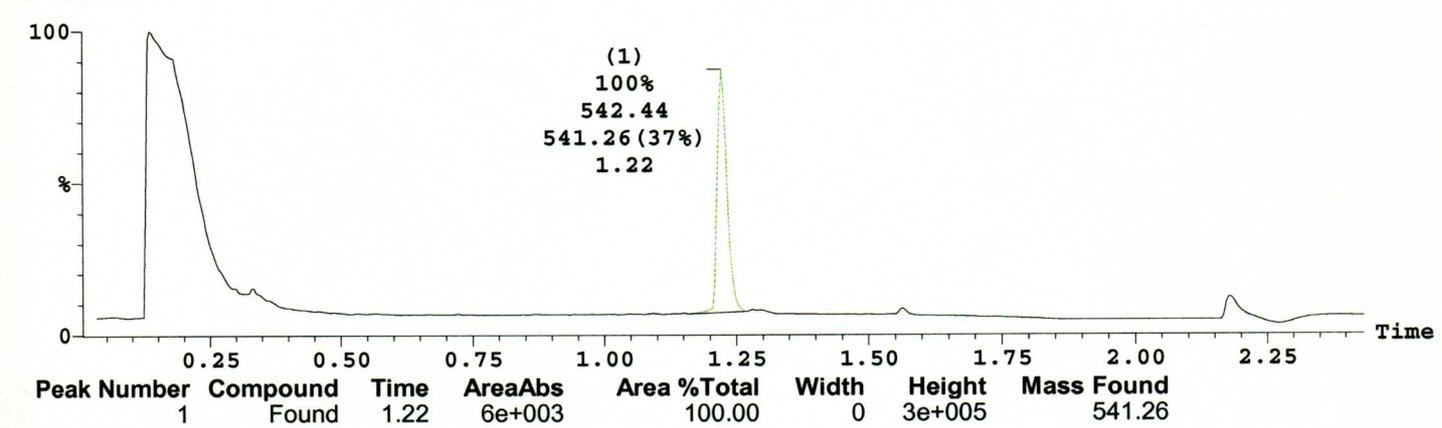
MS ES+ :542.26

3.0e+007



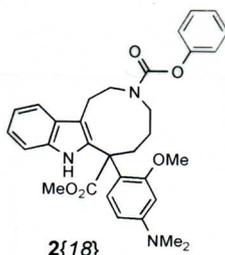
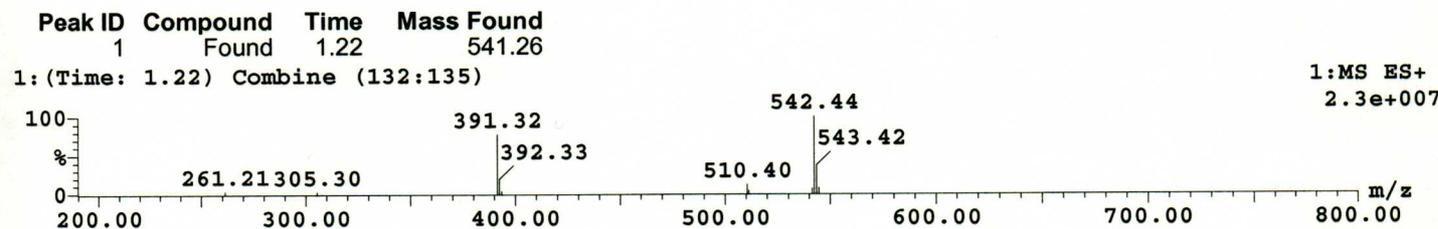
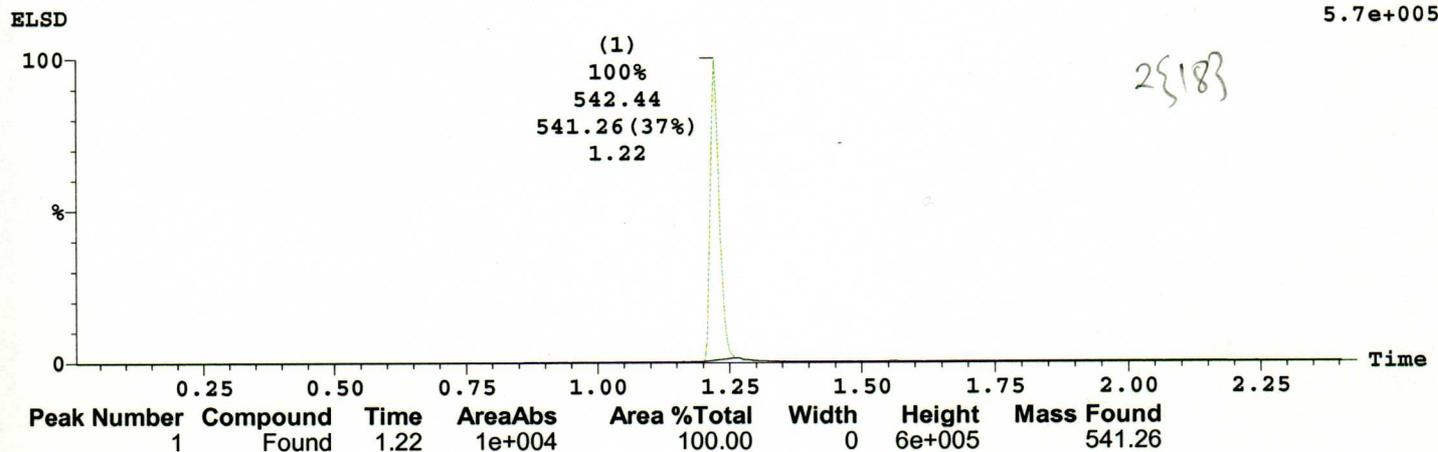
UV 214nm

3.7e+005



Printed: Wed Nov 02 14:25:30 2005

Sample Report (continued):



2{18}  
Chemical Formula: C<sub>32</sub>H<sub>35</sub>N<sub>3</sub>O<sub>5</sub>  
Exact Mass: 541.2577  
Molecular Weight: 541.6374

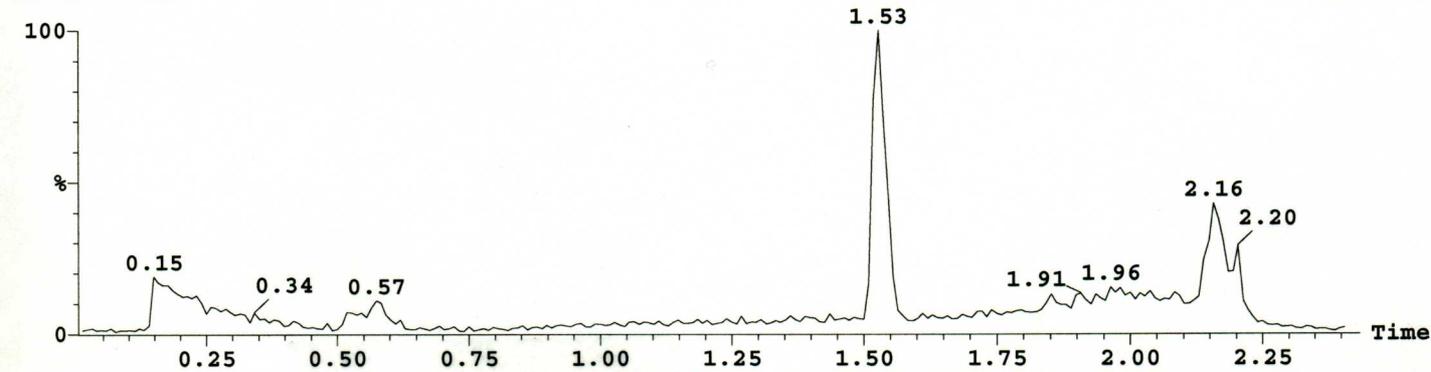
Printed: Wed Nov 02 15:23:02 2005

353

Sample Report:

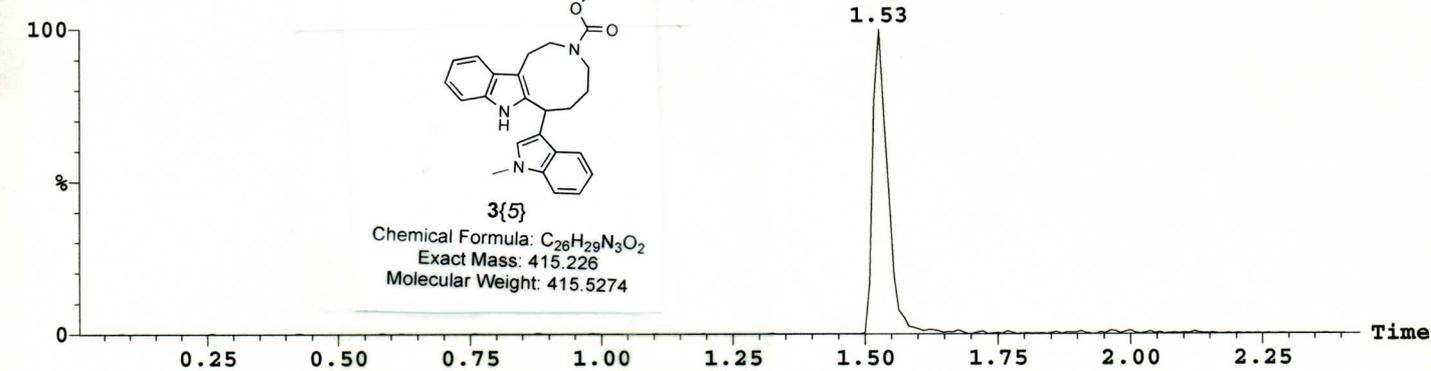
Sample 7 Vial 6:6 ID A38540101A05-2281150 File J38540205 Date 09-Jul-2004 Time 09:52:10 Description 3462439

MS ES+ : BPI 4.4e+006



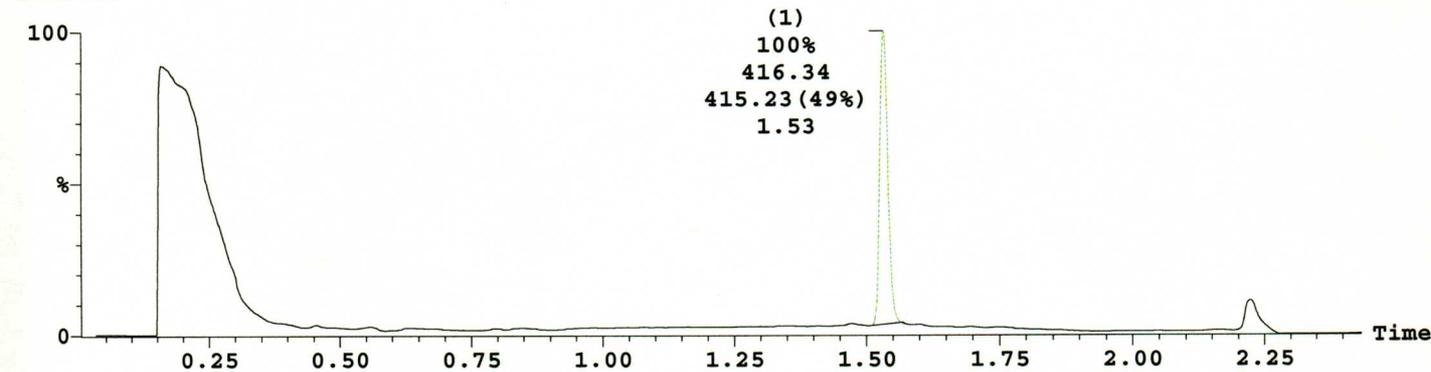
Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
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MS ES+ : 416.23 4.4e+006



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
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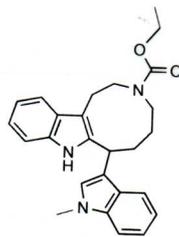
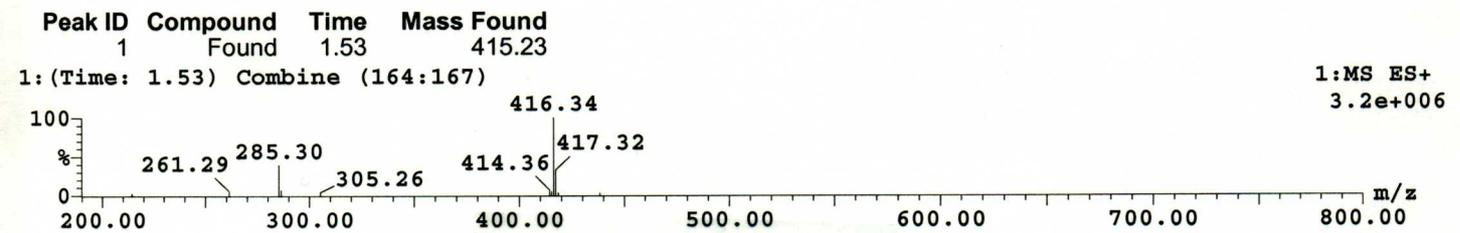
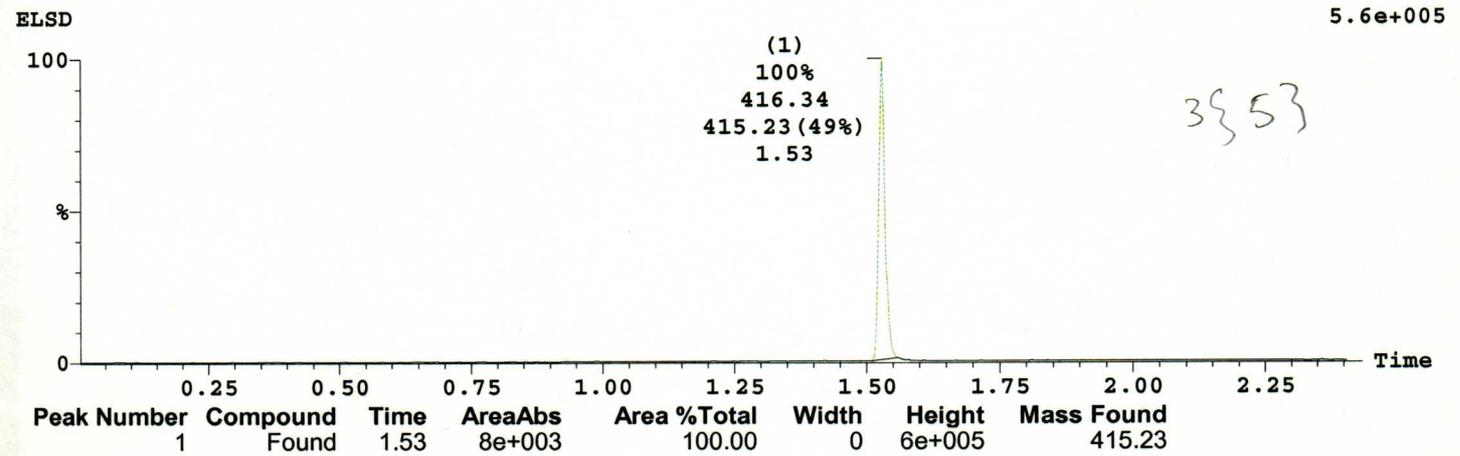
UV214nm 3.0e+005



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1	Found	1.53	5e+003	100.00	0	3e+005	415.23

Printed: Wed Nov 02 15:23:02 2005

Sample Report (continued):



3{5}

Chemical Formula: C<sub>26</sub>H<sub>29</sub>N<sub>3</sub>O<sub>2</sub>  
Exact Mass: 415.226  
Molecular Weight: 415.5274

Printed: Wed Nov 02 15:23:32 2005

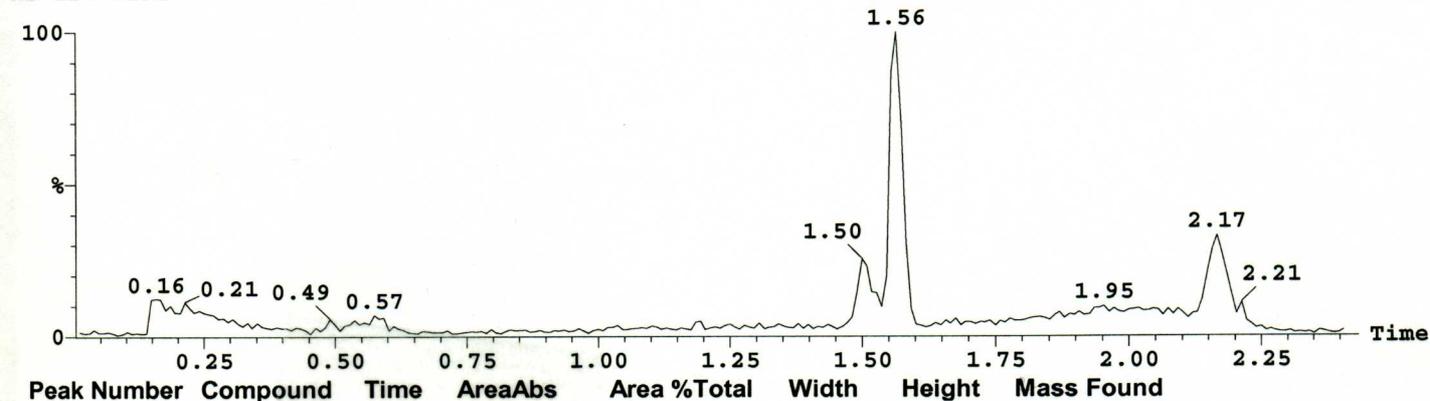
3{17}

Sample Report:

Sample 19 Vial 6:20 ID A38540101C05-2281162 File J38540217 Date 09-Jul-2004 Time 10:27:25 Description 3462451

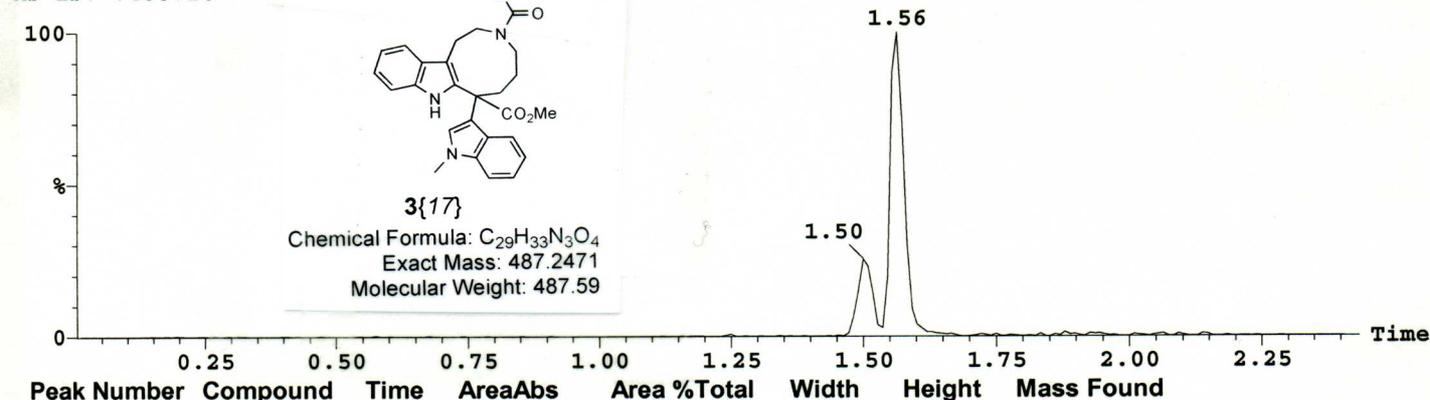
MS ES+ : BPI

6.3e+006



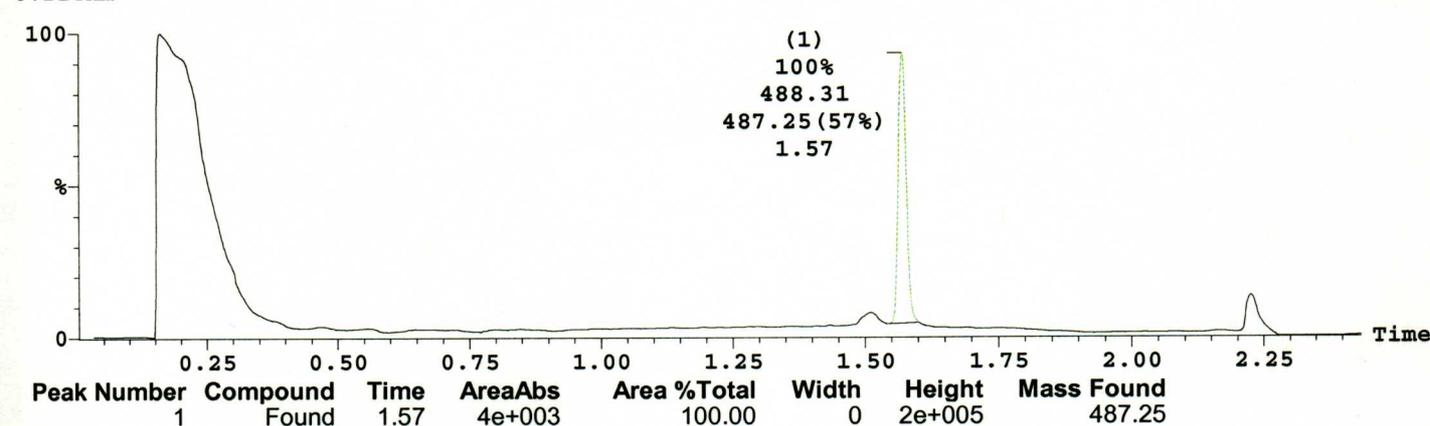
MS ES+ : 488.25

6.3e+006



UV214nm

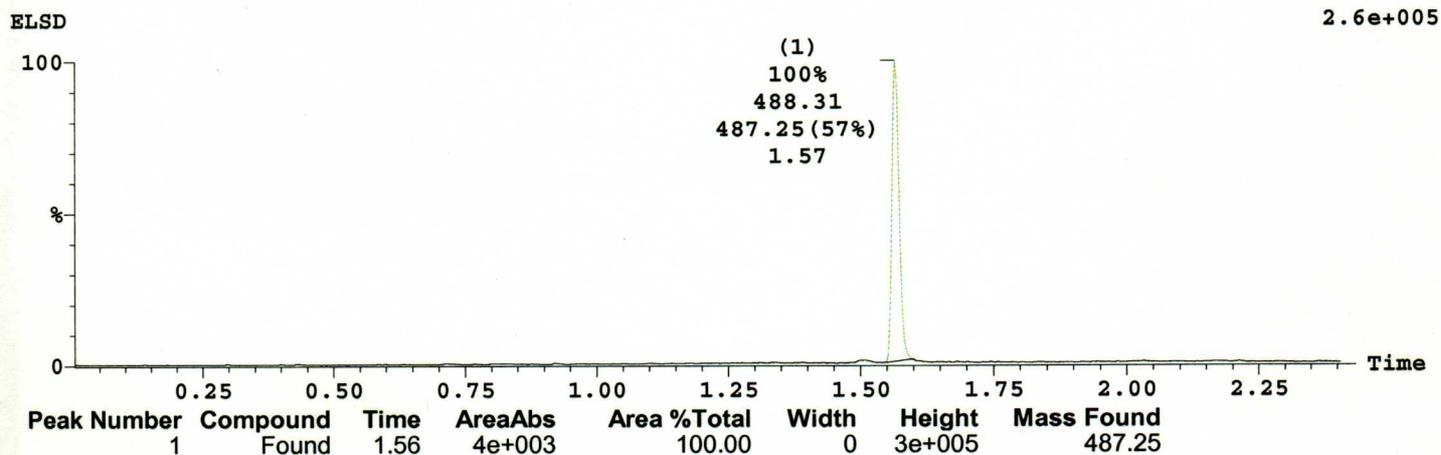
2.7e+005



Printed: Wed Nov 02 15:23:32 2005

38173

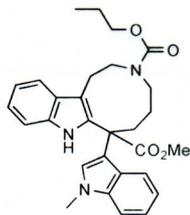
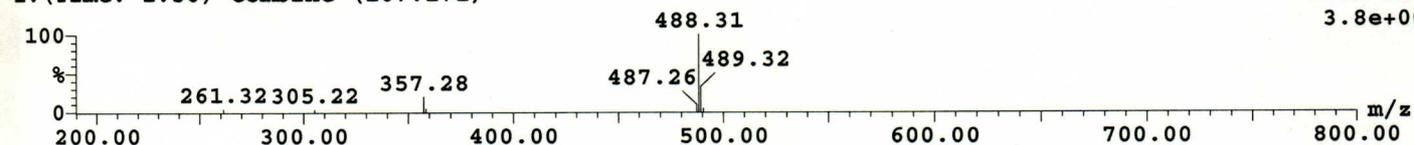
Sample Report (continued):



Peak ID	Compound	Time	Mass Found
1	Found	1.57	487.25

1: (Time: 1.56) Combine (167:171)

1: MS ES+  
3.8e+006



3{17}

Chemical Formula: C<sub>29</sub>H<sub>33</sub>N<sub>3</sub>O<sub>4</sub>  
Exact Mass: 487.2471  
Molecular Weight: 487.59

4513

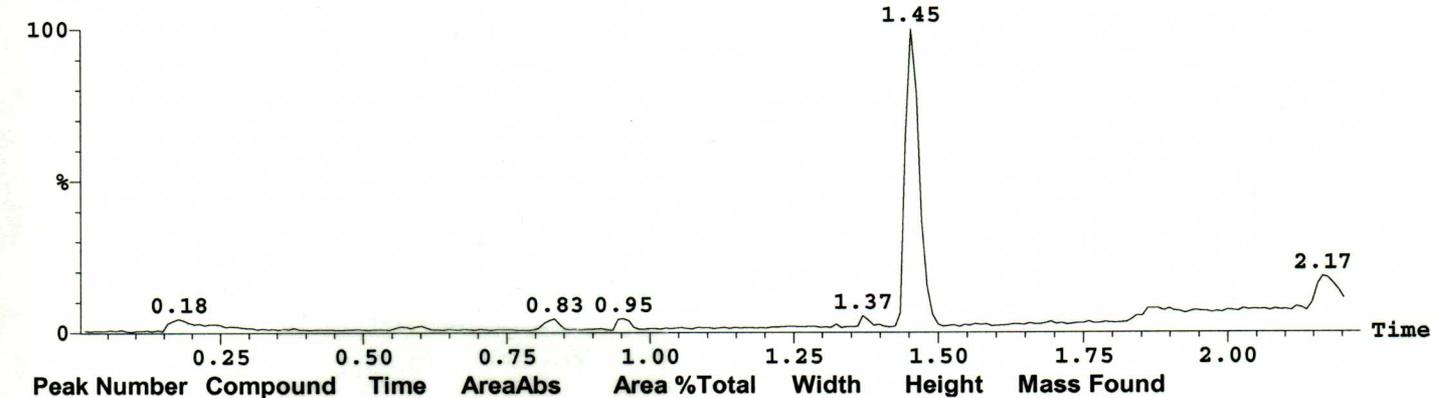
Printed: Wed Nov 02 14:21:27 2005

Sample Report:

Sample 3 Vial 6:2 ID A38550101A01-2278536 File J38550201 Date 03-Jul-2004 Time 06:04:50 Description 3441914

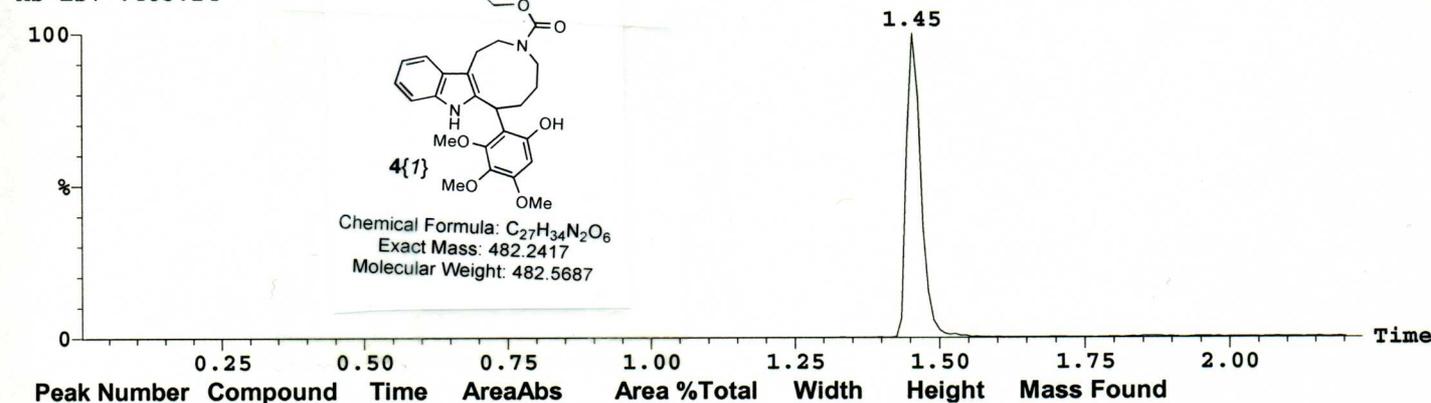
MS ES+ : BPI

3.2e+007



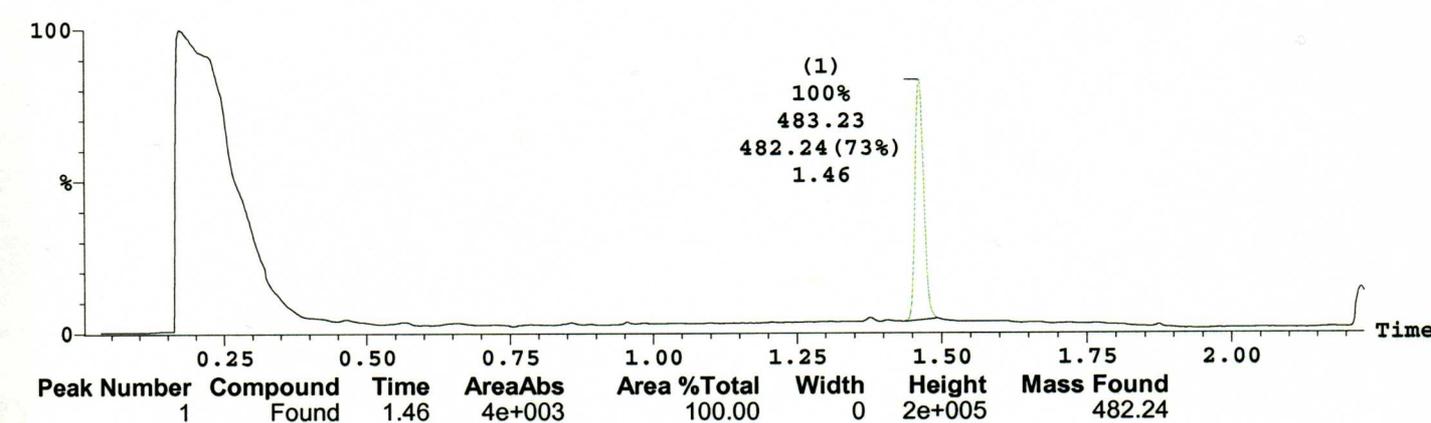
MS ES+ : 483.24

3.2e+007



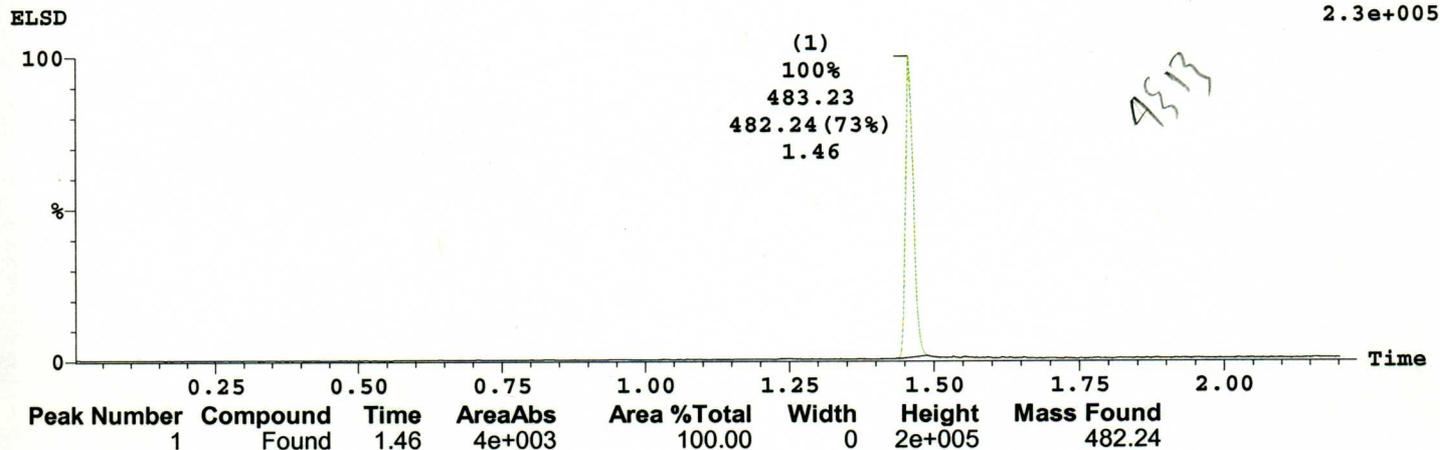
UV214nm

2.7e+005



Printed: Wed Nov 02 14:21:27 2005

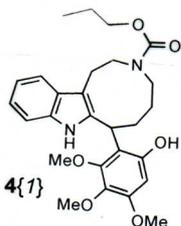
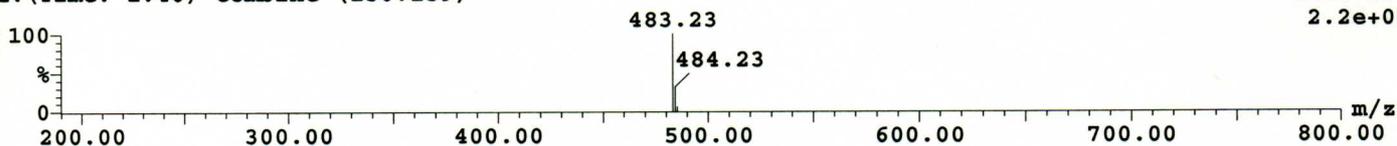
Sample Report (continued):



Peak ID	Compound	Time	Mass Found
1	Found	1.46	482.24

1: (Time: 1.46) Combine (156:159)

1: MS ES+  
2.2e+007



Chemical Formula: C<sub>27</sub>H<sub>34</sub>N<sub>2</sub>O<sub>6</sub>  
Exact Mass: 482.2417  
Molecular Weight: 482.5687

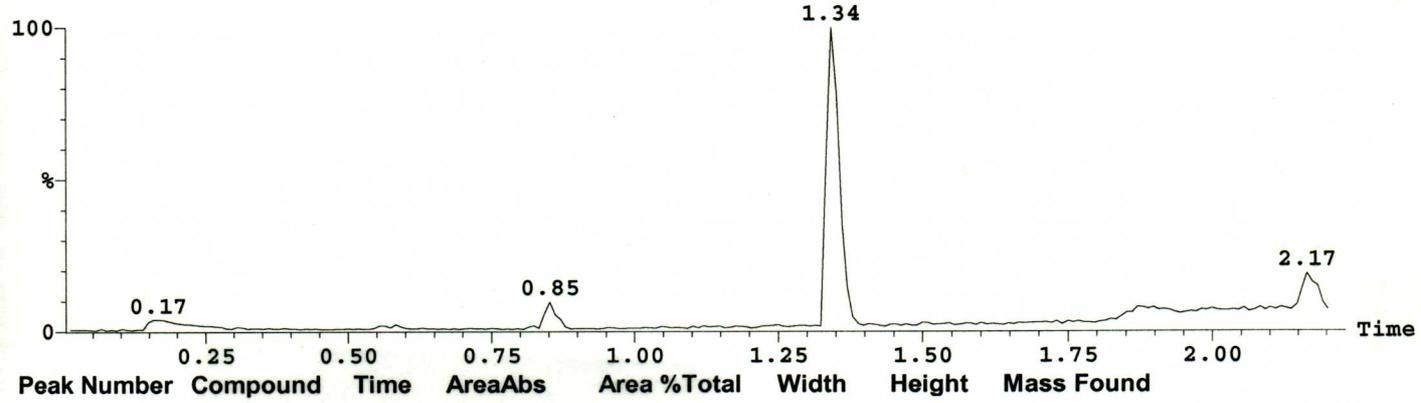
Printed: Wed Nov 02 14:21:49 2005

Sample Report:

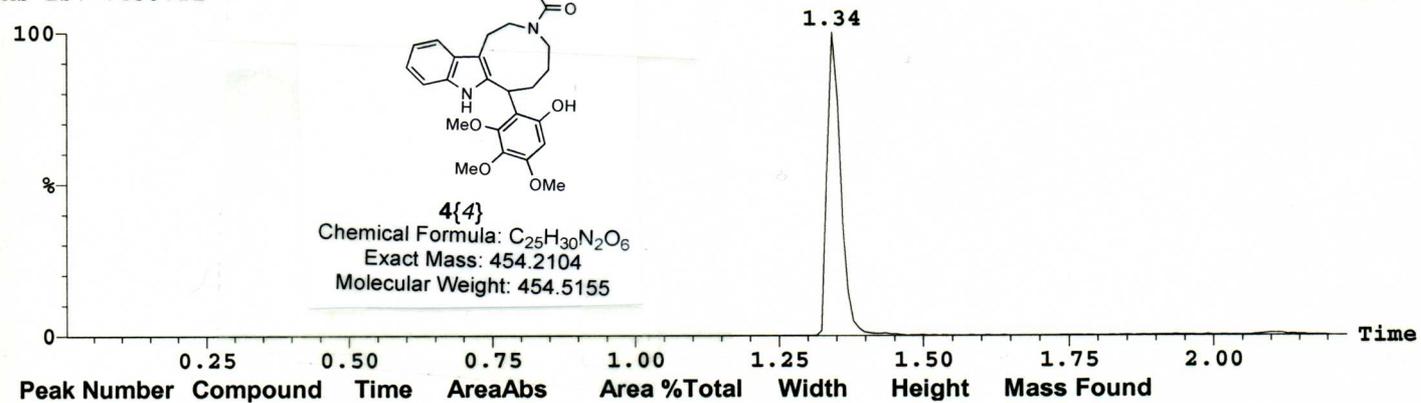
4543

Sample 6 Vial 6:5 ID A38550101A04-2278539 File J38550204 Date 03-Jul-2004 Time 06:13:02 Description 3441917

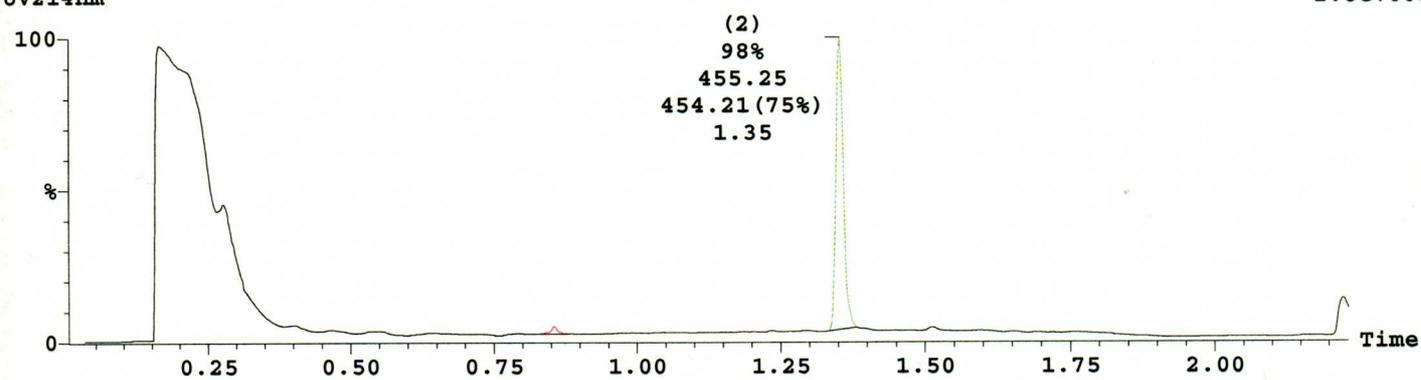
MS ES+ : BPI 3.4e+007



MS ES+ : 455.21 3.4e+007



UV214nm 2.8e+005

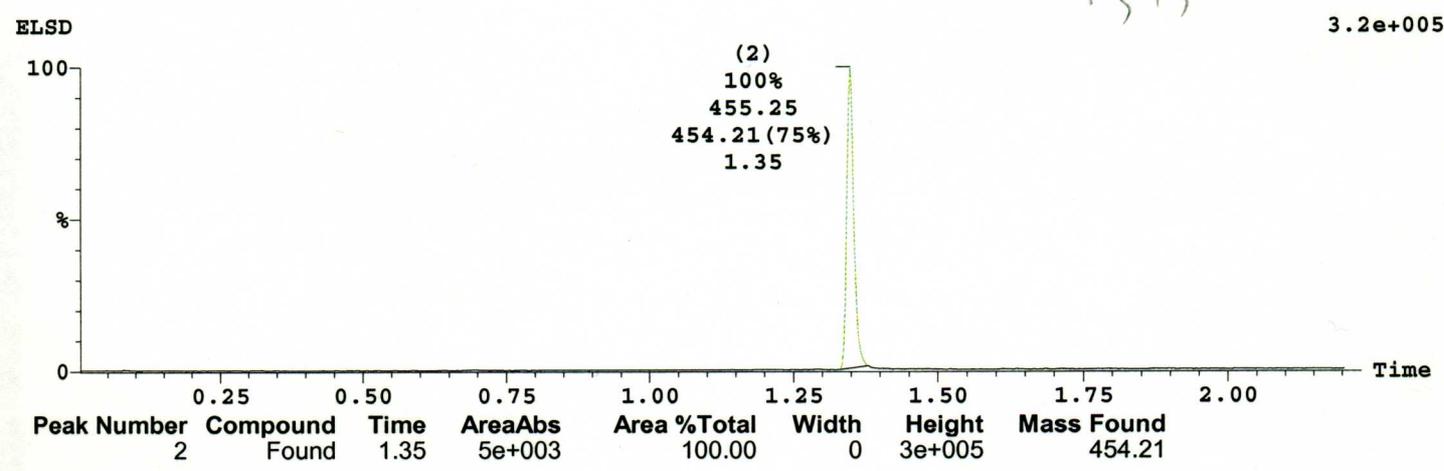


Printed: Wed Nov 02 14:21:49 2005

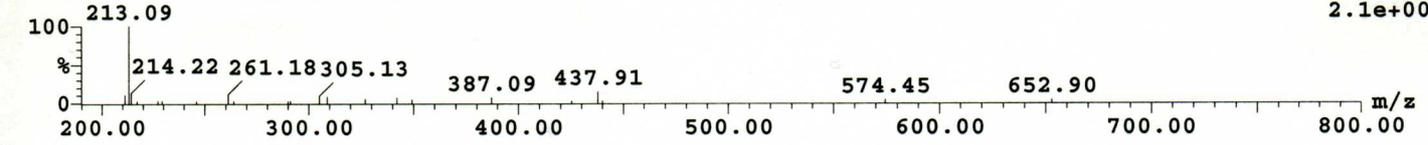
Sample Report (continued):

4{4}

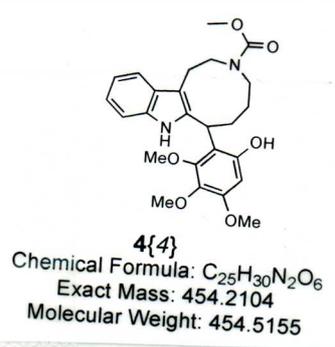
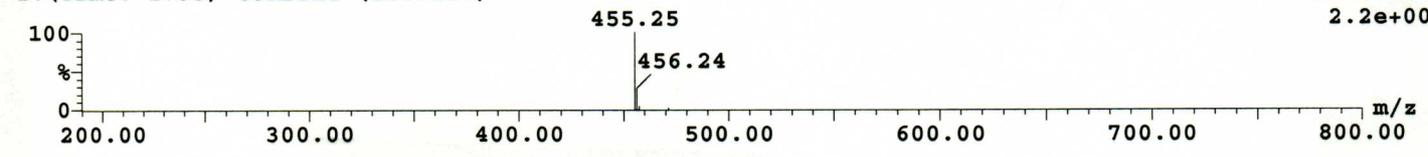
3.2e+005



Peak ID Compound Time Mass Found  
1 0.85  
1: (Time: 0.85) Combine (91:94) 1:MS ES+  
2.1e+006



Peak ID Compound Time Mass Found  
2 Found 1.35 454.21  
2: (Time: 1.35) Combine (144:147) 1:MS ES+  
2.2e+007

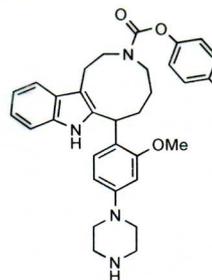


Printed: Mon Nov 07 09:37:52 2005

Sample Report:

557

Sample 17 Vial 3:62 ID A38500101B02-2278872 File N38500315 Date 02-Jul-200



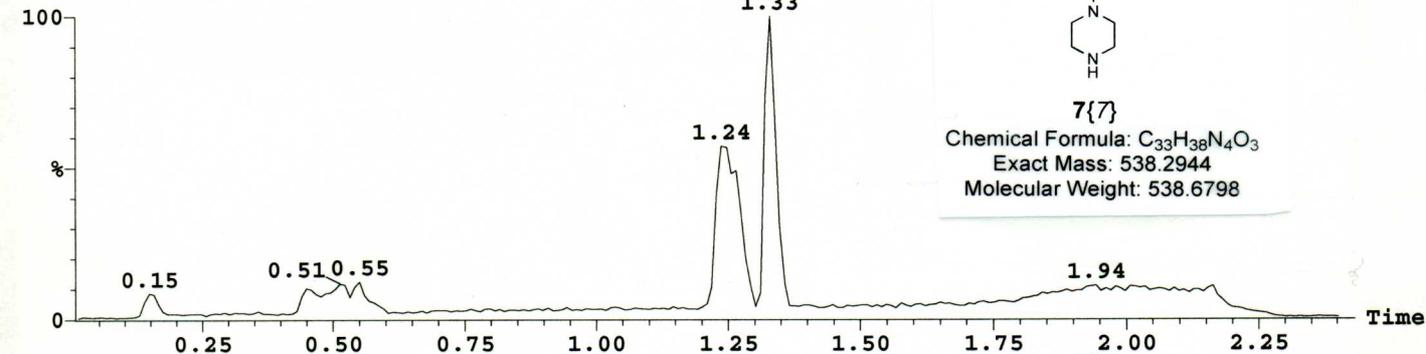
7{7}

Chemical Formula: C<sub>33</sub>H<sub>38</sub>N<sub>4</sub>O<sub>3</sub>  
 Exact Mass: 538.2944  
 Molecular Weight: 538.6798

41900

2.1e+007

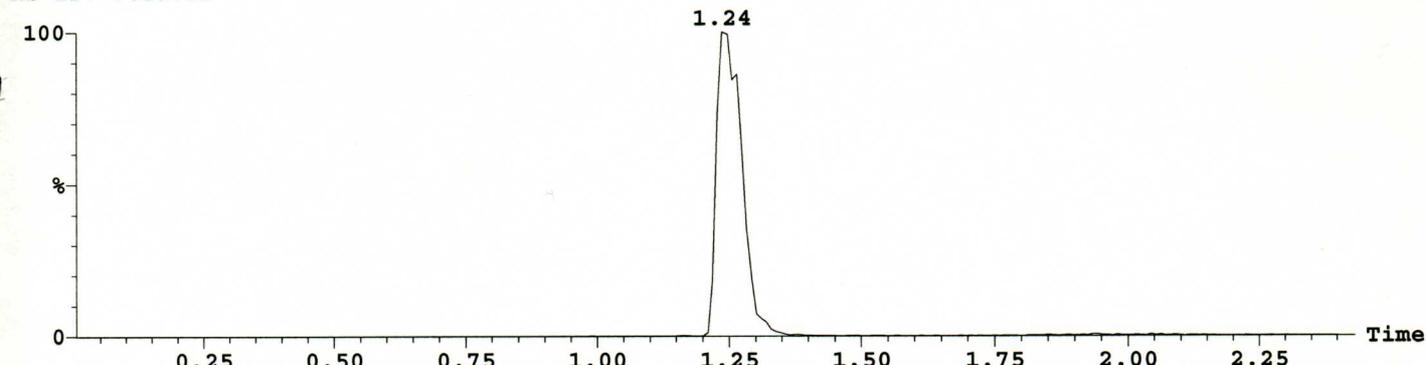
MS ES+ :BPI



Peak Number	Compound	Time	AreaAbs	Area%Total	Width	Height	Mass Found
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MS ES+ :539.29

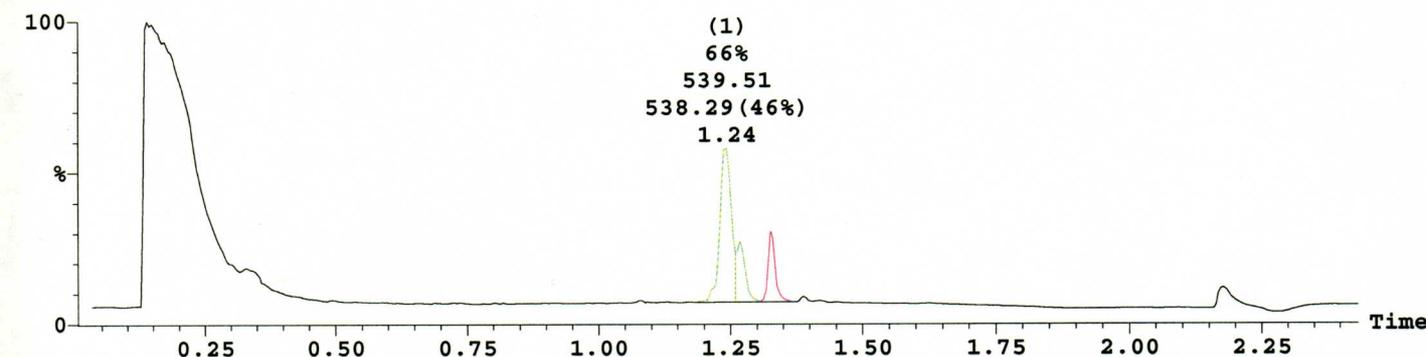
1.2e+007



Peak Number	Compound	Time	AreaAbs	Area%Total	Width	Height	Mass Found
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UV 214nm

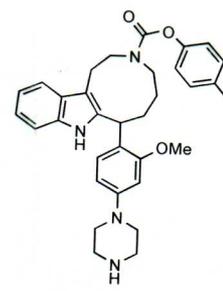
3.7e+005



Peak Number	Compound	Time	AreaAbs	Area%Total	Width	Height	Mass Found
1	Found	1.24	5e+003	66.31	0	2e+005	538.29
2	Found	1.27	1e+003	15.65	0	7e+004	538.29
3		1.33	1e+003	18.04	0	9e+004	

Printed: Mon Nov 07 09:37:52 2005

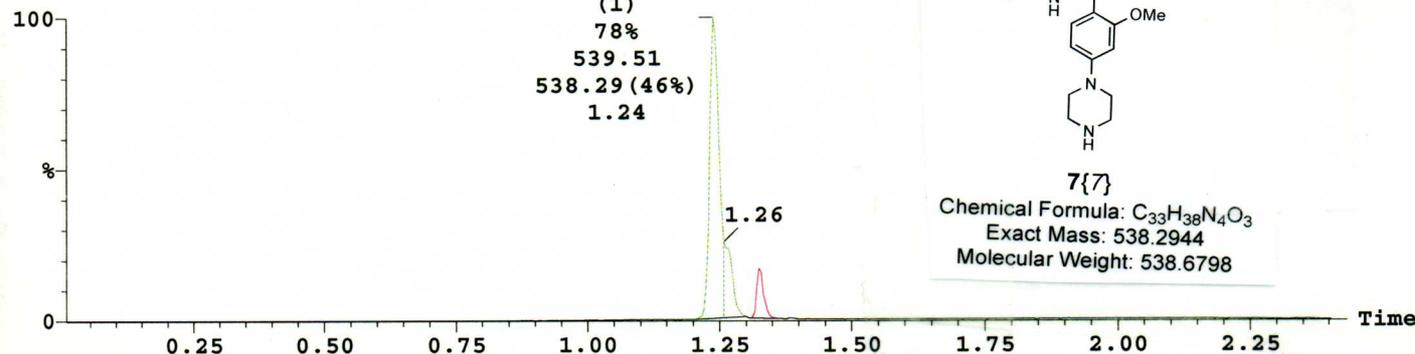
Sample Report (continued):



7{7}  
 Chemical Formula: C<sub>33</sub>H<sub>36</sub>N<sub>4</sub>O<sub>3</sub>  
 Exact Mass: 538.2944  
 Molecular Weight: 538.6798

1.7e+005

ELSD

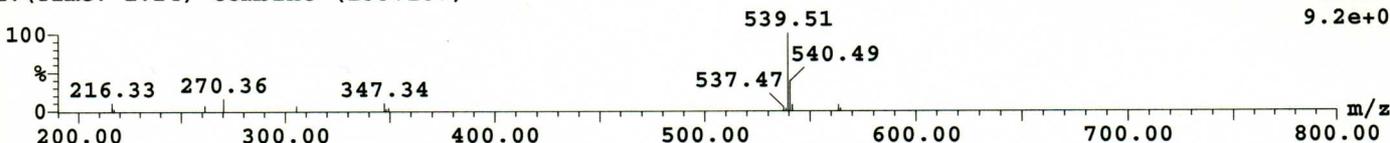


Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1	Found	1.24	4e+003	78.31	0	2e+005	538.29
2	Found	1.27	6e+002	12.41	0	4e+004	538.29
3		1.33	4e+002	9.27	0	3e+004	

Peak ID Compound Time Mass Found  
 1 Found 1.24 538.29

1: (Time: 1.24) Combine (133:137)

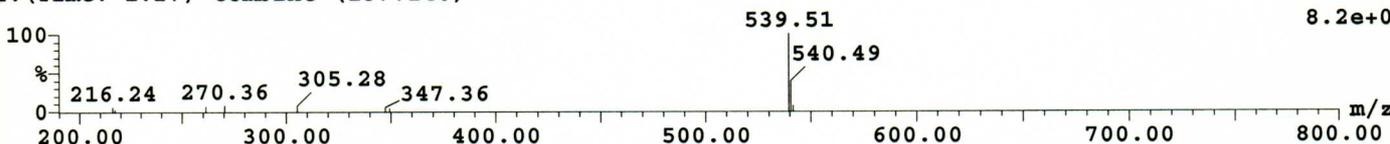
1:MS ES+  
 9.2e+006



Peak ID Compound Time Mass Found  
 2 Found 1.27 538.29

2: (Time: 1.27) Combine (137:140)

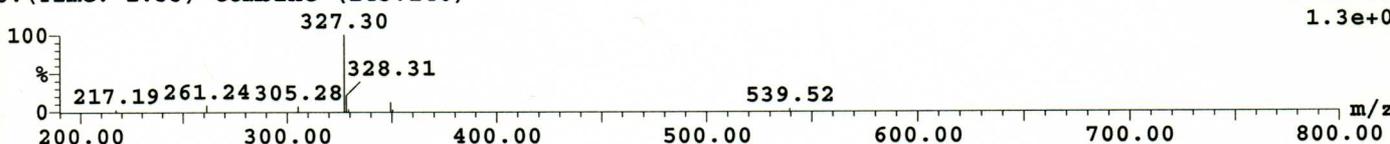
1:MS ES+  
 8.2e+006



Peak ID Compound Time Mass Found  
 3 1.33

3: (Time: 1.33) Combine (143:146)

1:MS ES+  
 1.3e+007

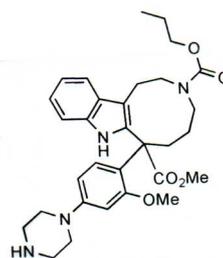


Printed: Wed Nov 02 14:42:09 2005

Sample Report:

Sample 9 Vial 3:26 ID A38500101C01-2278869 File N38500307 Date 02-Jul-2004

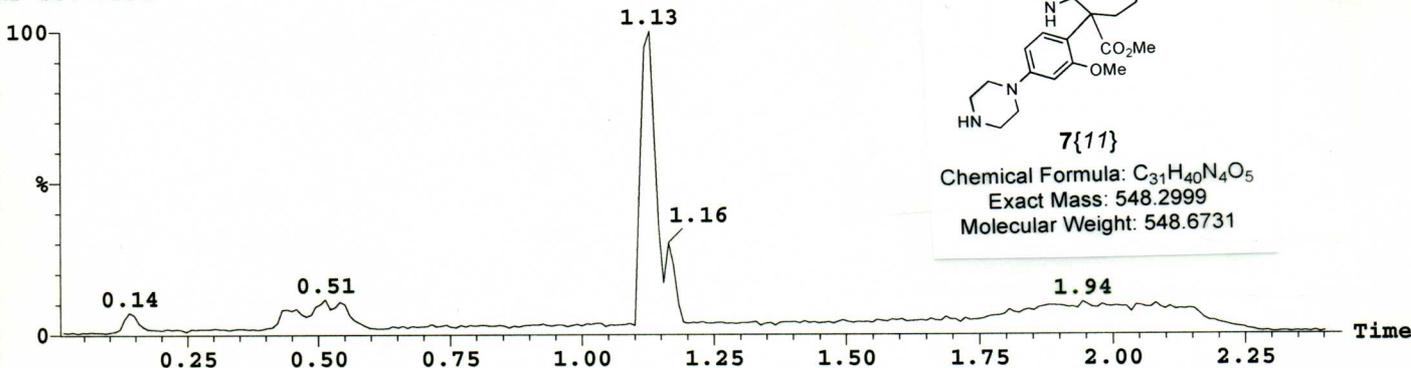
7{11}



41904

2.4e+007

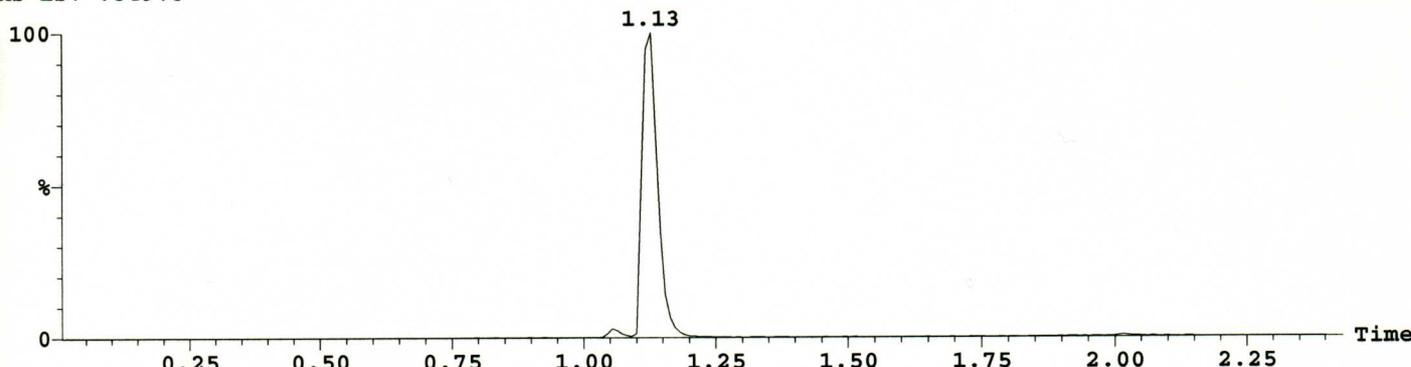
MS ES+ :BPI



7{11}  
Chemical Formula: C<sub>31</sub>H<sub>40</sub>N<sub>4</sub>O<sub>5</sub>  
Exact Mass: 548.2999  
Molecular Weight: 548.6731

MS ES+ :549.3

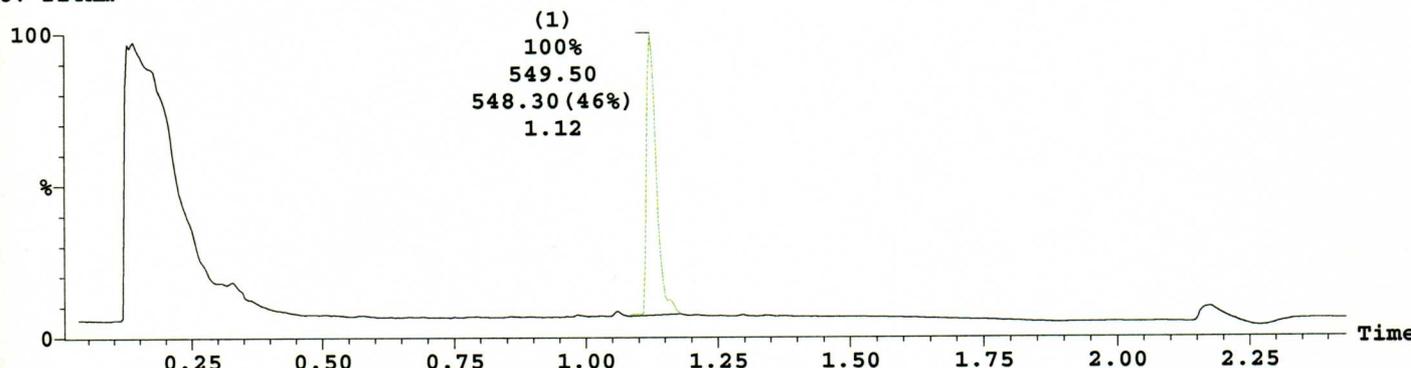
2.4e+007



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
-------------	----------	------	---------	-------------	-------	--------	------------

UV 214nm

3.8e+005

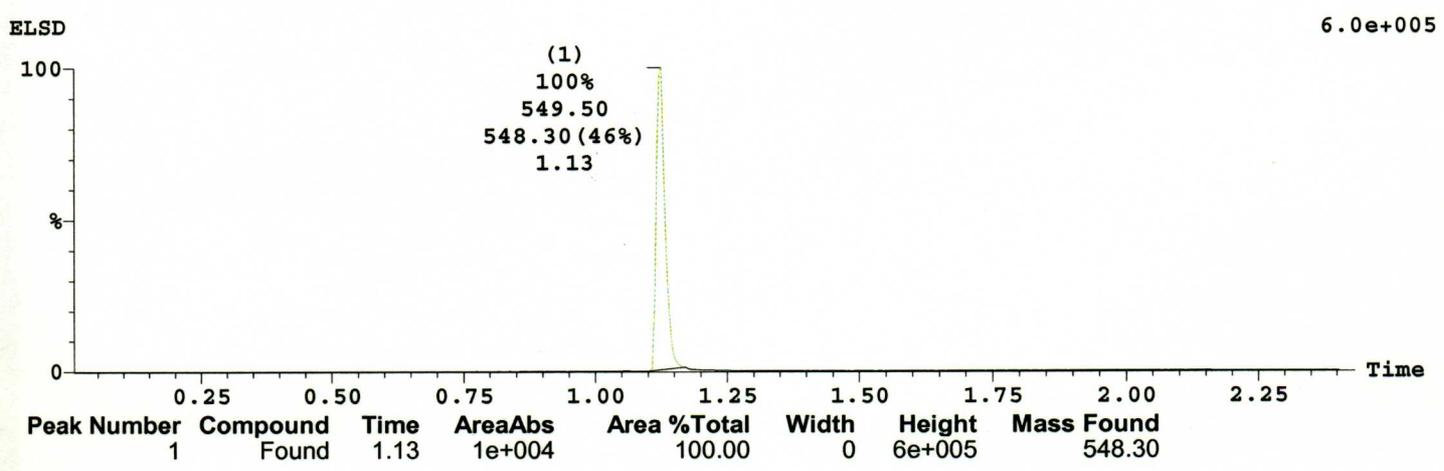


(1)							
100%							
549.50							
548.30 (46%)							
1.12							
Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1	Found	1.12	8e+003	100.00	0	4e+005	548.30

7{11}

Printed: Wed Nov 02 14:42:09 2005

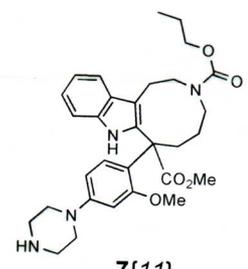
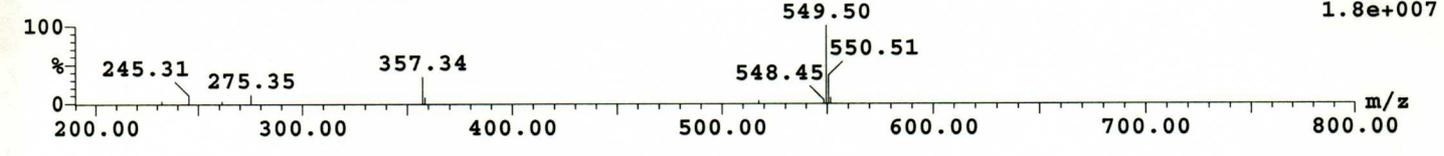
Sample Report (continued):



Peak ID	Compound	Time	Mass Found
1	Found	1.12	548.30

1: (Time: 1.12) Combine (121:124)

1:MS ES+  
1.8e+007



7{11}

Chemical Formula: C<sub>31</sub>H<sub>40</sub>N<sub>4</sub>O<sub>5</sub>  
Exact Mass: 548.2999  
Molecular Weight: 548.6731

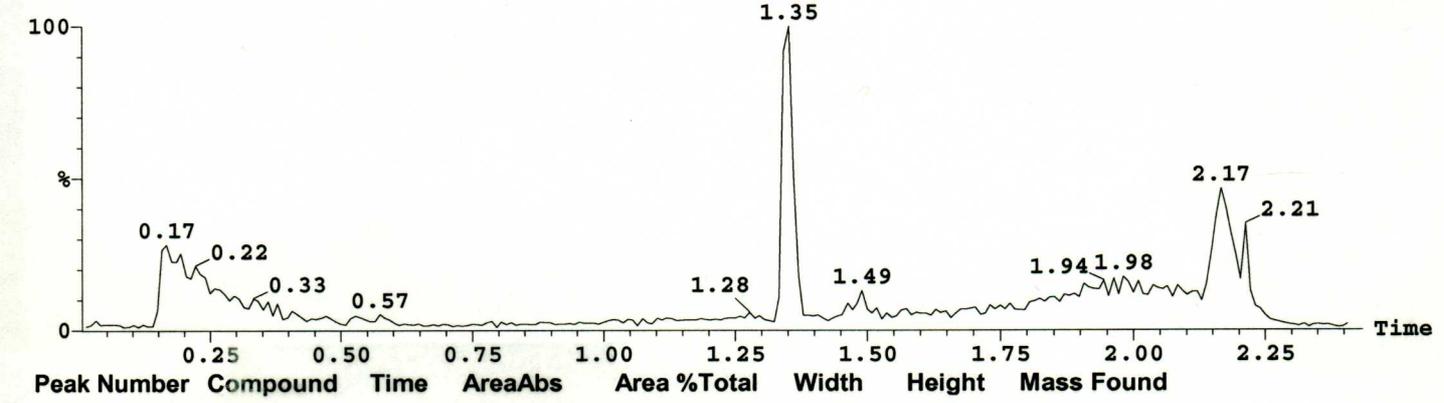
Printed: Wed Nov 02 14:07:19 2005

8{12}

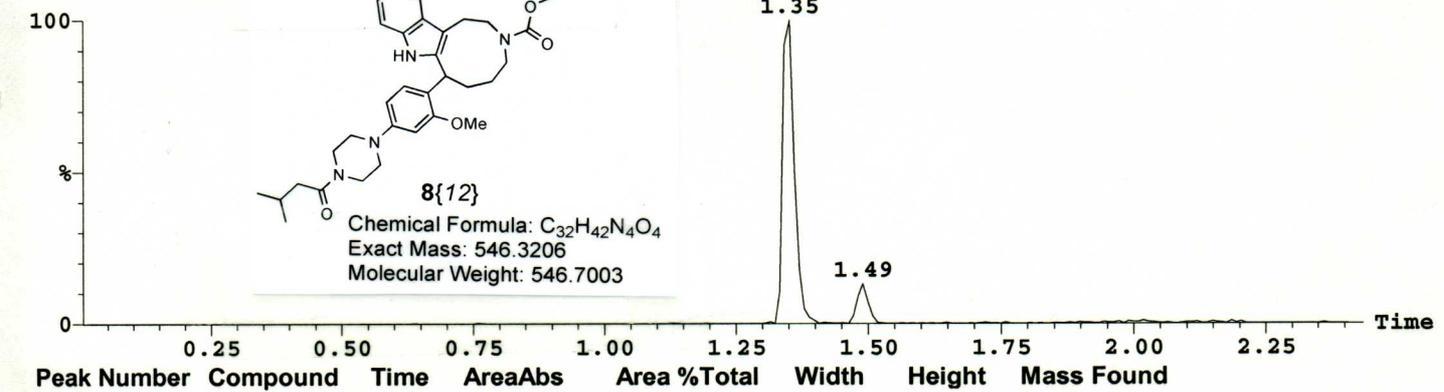
Sample Report:

Sample 14 Vial 6:15 ID A38390101B06-2275018 File J38390212 Date 01-Jul-2004 Time 05:58:40 Description 3438141

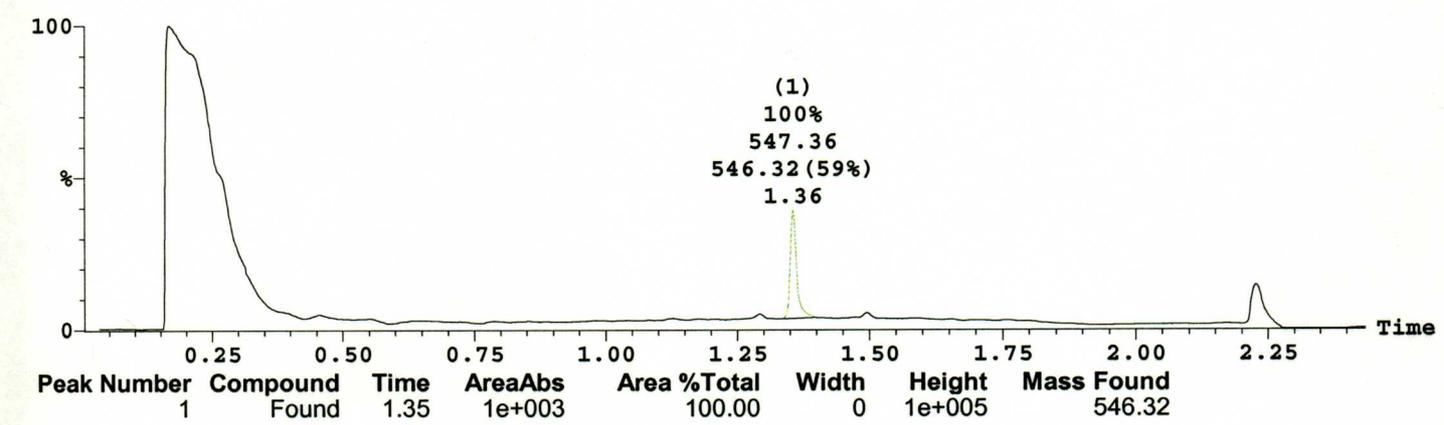
MS ES+ : BPI 4.1e+006



MS ES+ : 547.32 4.1e+006



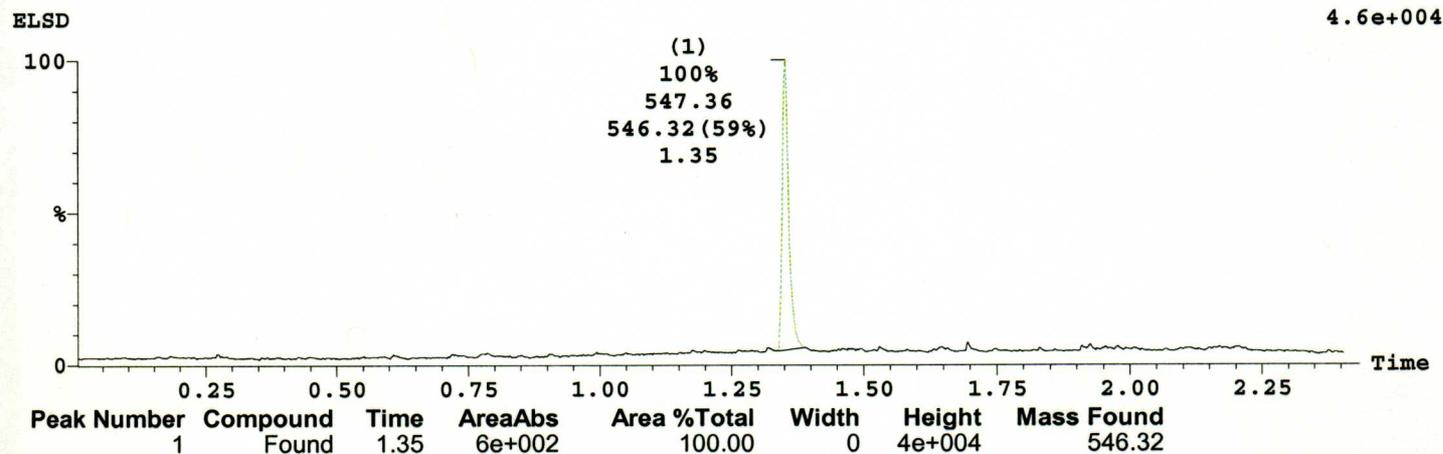
UV214nm 2.7e+005



85123

Printed: Wed Nov 02 14:07:19 2005

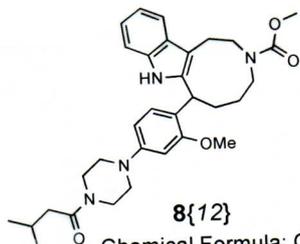
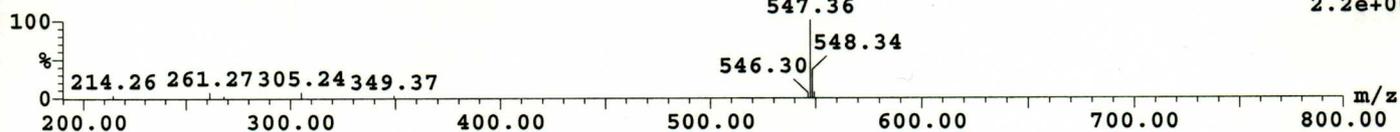
Sample Report (continued):



Peak ID	Compound	Time	Mass Found
1	Found	1.35	546.32

1:(Time: 1.35) Combine (144:148)

1:MS ES+  
2.2e+006



8{12}

Chemical Formula: C<sub>32</sub>H<sub>42</sub>N<sub>4</sub>O<sub>4</sub>  
Exact Mass: 546.3206  
Molecular Weight: 546.7003

85323

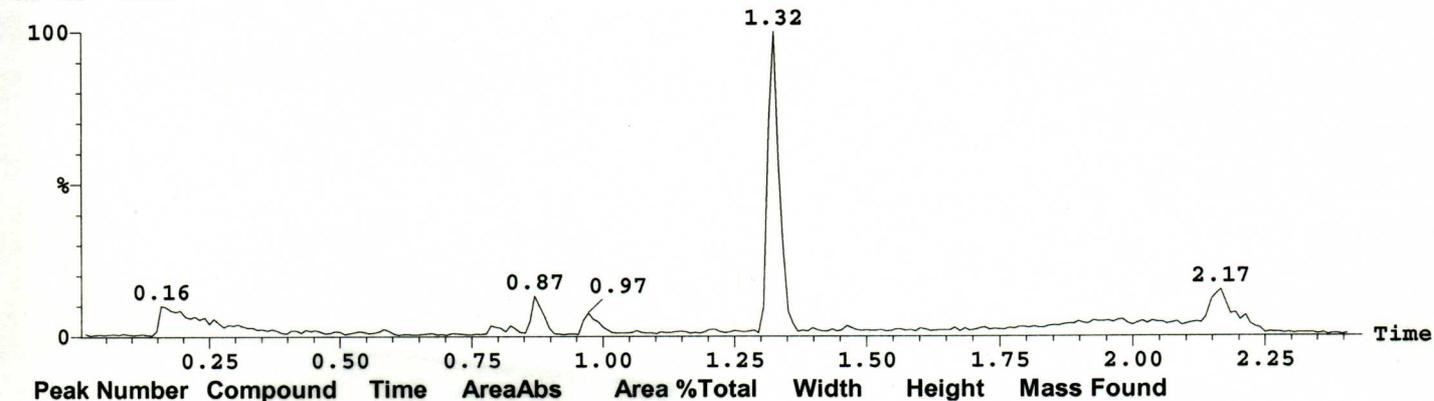
Printed: Wed Nov 02 14:07:47 2005

Sample Report:

Sample 31 Vial 6:34 ID A38390102A05-2275035 File J38390229 Date 01-Jul-2004 Time 06:48:29 Description 3438160

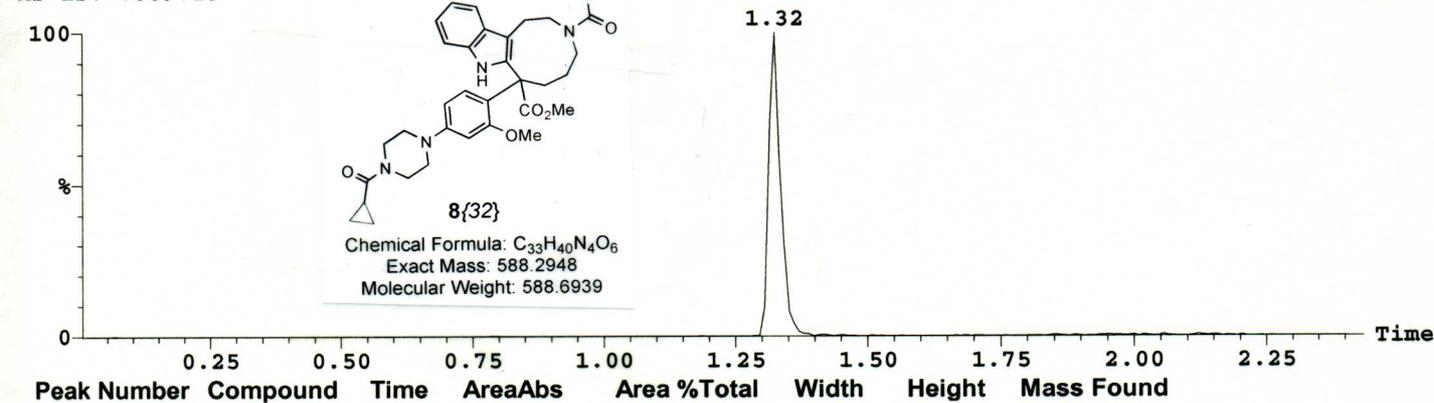
MS ES+ : BPI

1.2e+007



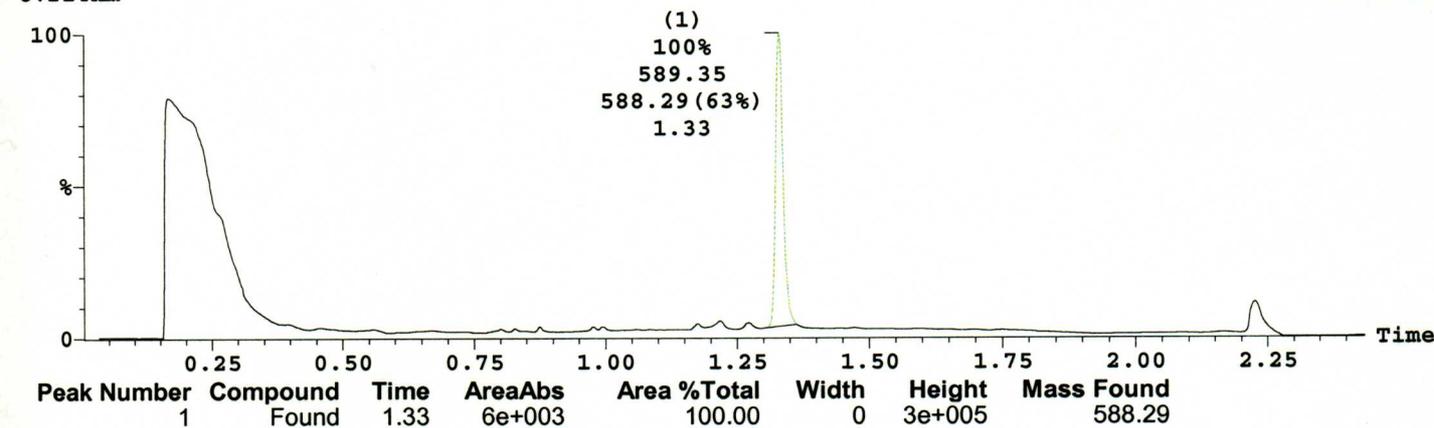
MS ES+ : 589.29

1.2e+007



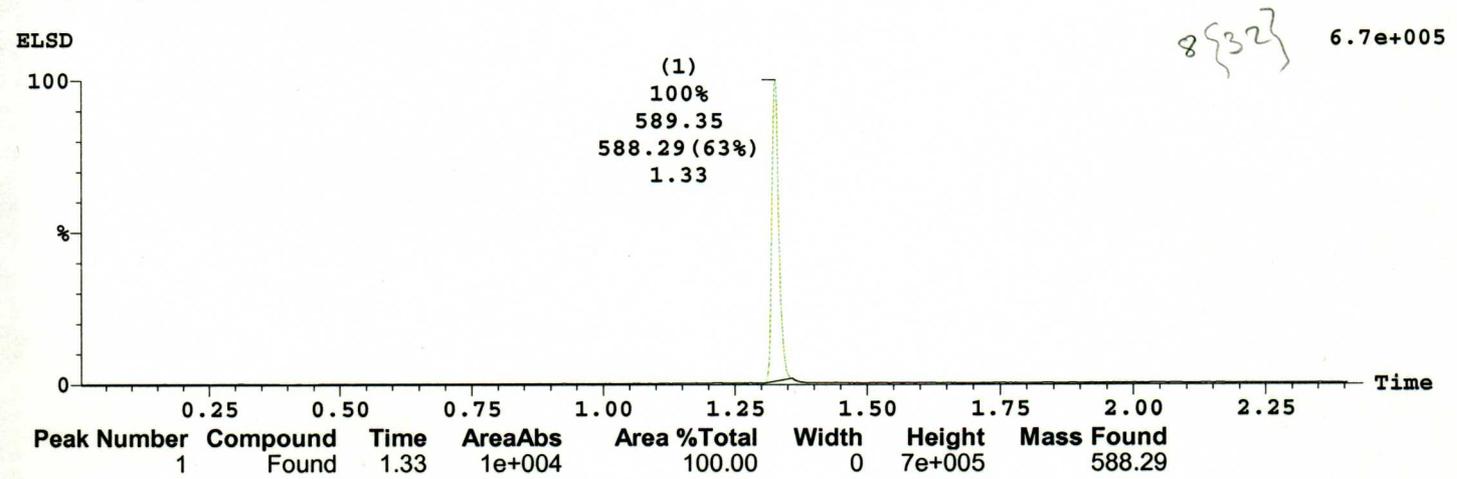
UV214nm

3.4e+005



Printed: Wed Nov 02 14:07:47 2005

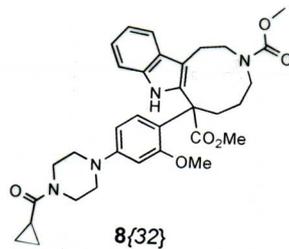
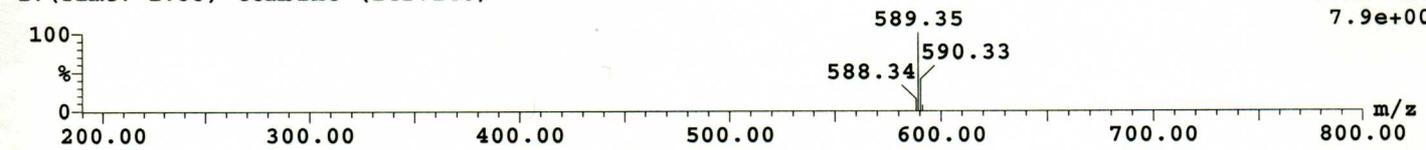
Sample Report (continued):



Peak ID	Compound	Time	Mass Found
1	Found	1.33	588.29

1: (Time: 1.33) Combine (142:145)

1: MS ES+  
7.9e+006



Chemical Formula: C<sub>33</sub>H<sub>40</sub>N<sub>4</sub>O<sub>6</sub>  
Exact Mass: 588.2948  
Molecular Weight: 588.6939

Sample: 33  
 File: J38390231  
 Description: 3438149

Vial: 6:38  
 Date: 01-Jul-2004

ID: A38390102B02-2275037  
 Time: 06:54:20

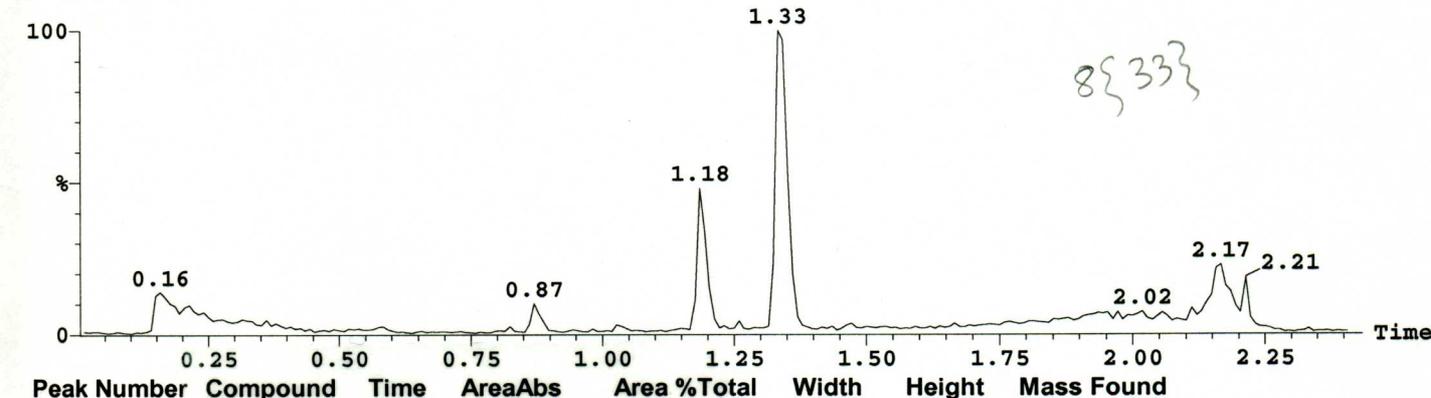
Printed: Wed Nov 02 14:08:07 2005

Sample Report:

Sample 33 Vial 6:38 ID A38390102B02-2275037 File J38390231 Date 01-Jul-2004 Time 06:54:20 Description 3438149

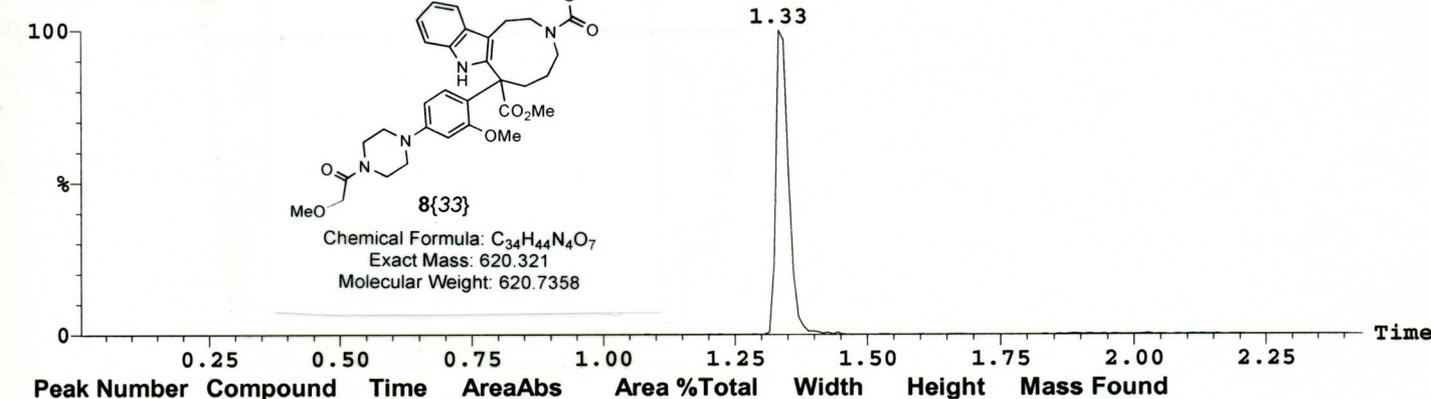
MS ES+ : BPI

9.3e+006



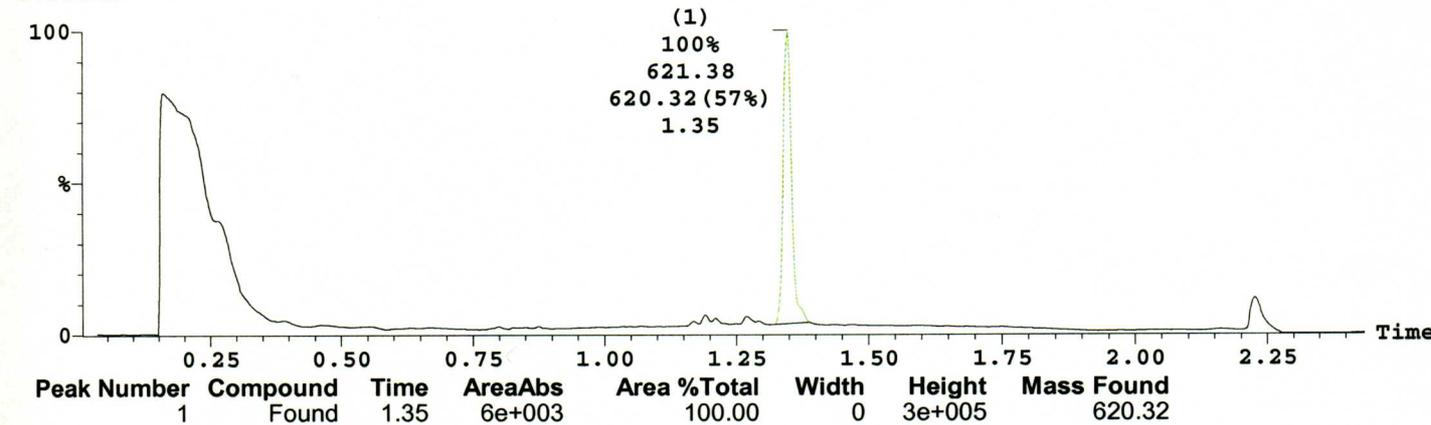
MS ES+ : 621.32

9.3e+006



UV214nm

3.4e+005



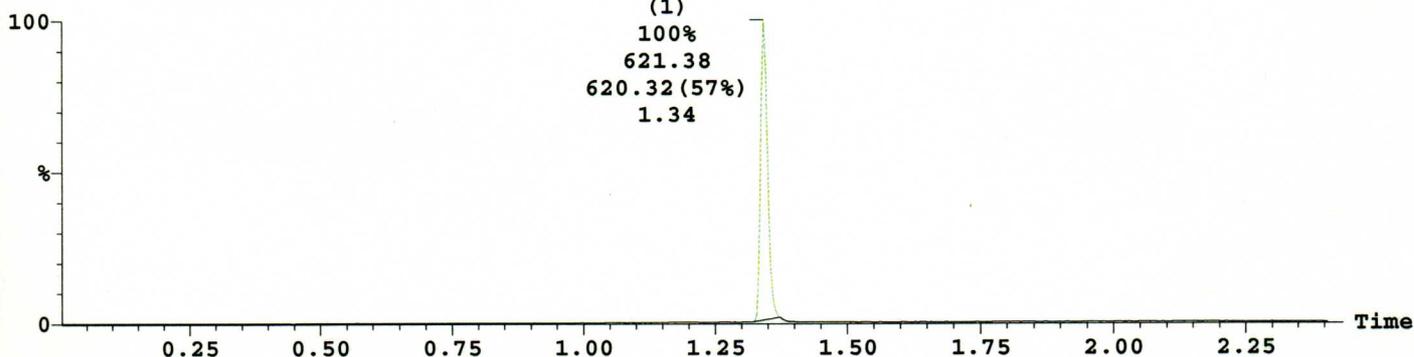
Printed: Wed Nov 02 14:08:07 2005

Sample Report (continued):

8{33}

6.9e+005

ELSD



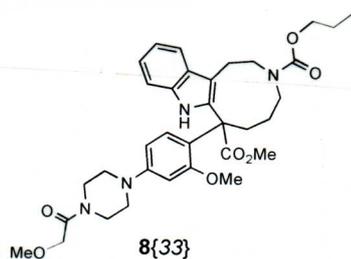
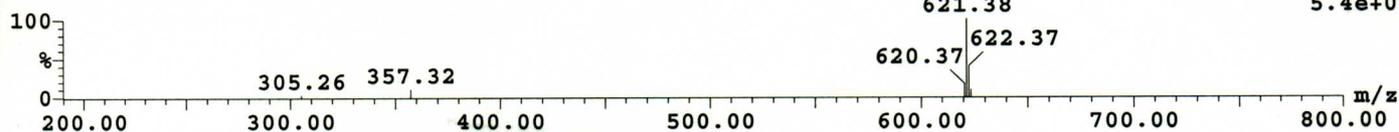
(1)  
100%  
621.38  
620.32 (57%)  
1.34

Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1	Found	1.34	1e+004	100.00	0	7e+005	620.32

Peak ID	Compound	Time	Mass Found
1	Found	1.35	620.32

1: (Time: 1.34) Combine (143:147)

1: MS ES+  
5.4e+006



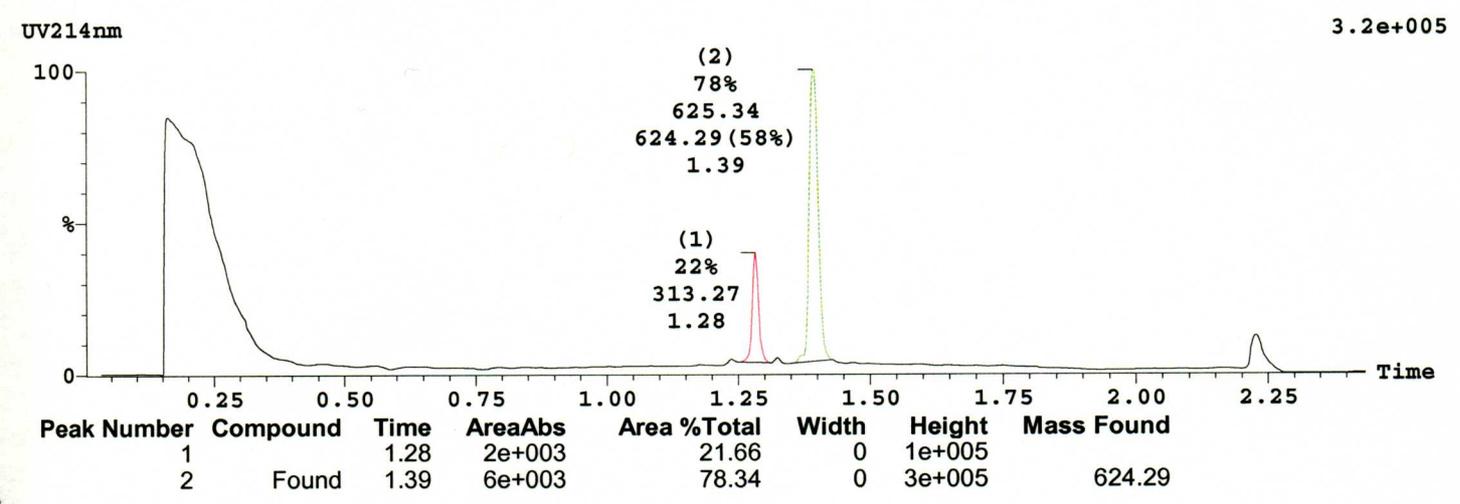
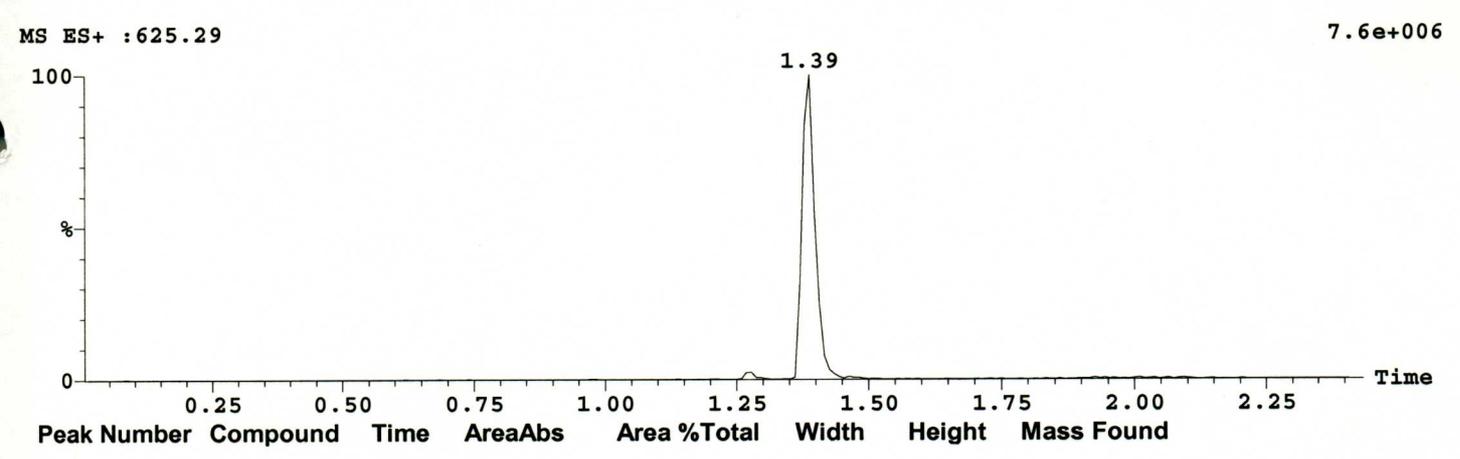
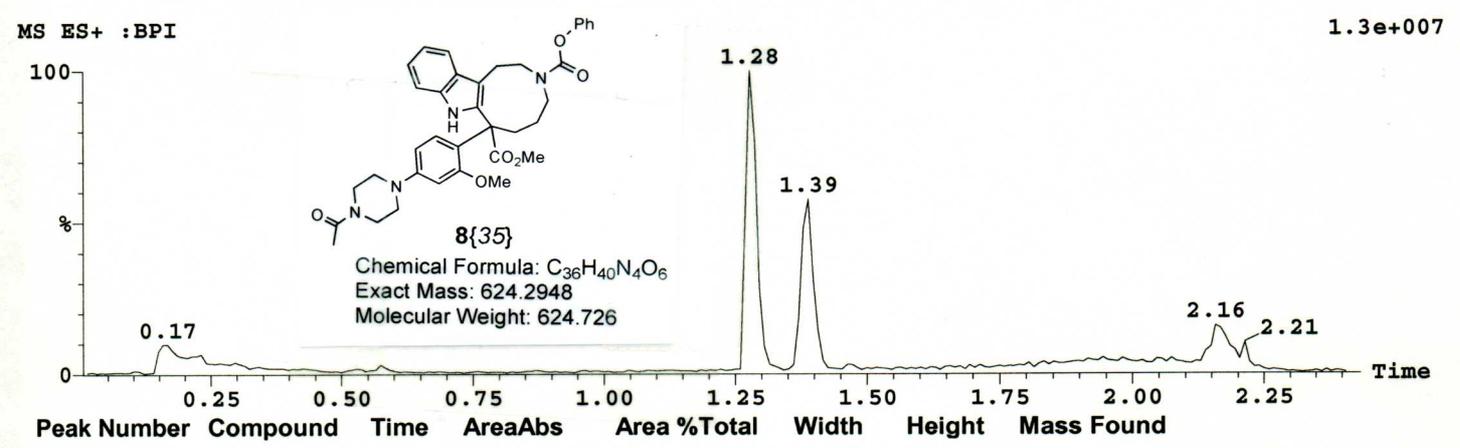
Chemical Formula: C<sub>34</sub>H<sub>44</sub>N<sub>4</sub>O<sub>7</sub>  
Exact Mass: 620.321  
Molecular Weight: 620.7358

8{35}

Printed: Mon Nov 07 09:39:18 2005

Sample Report:

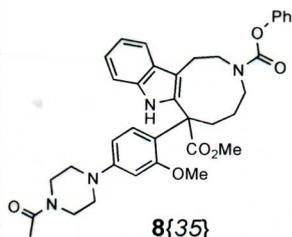
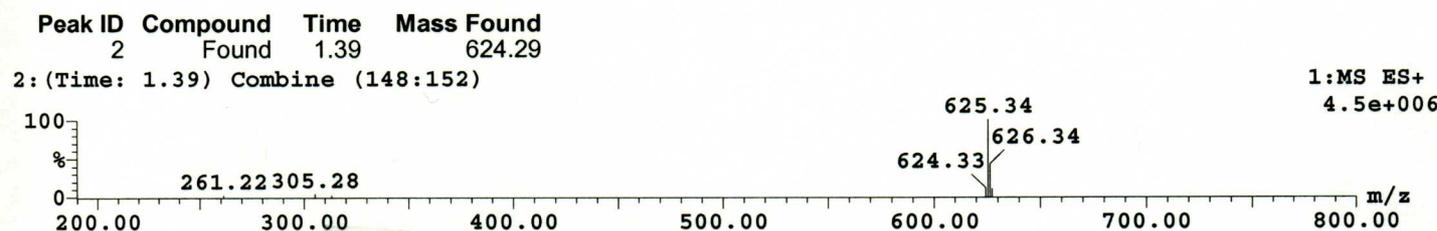
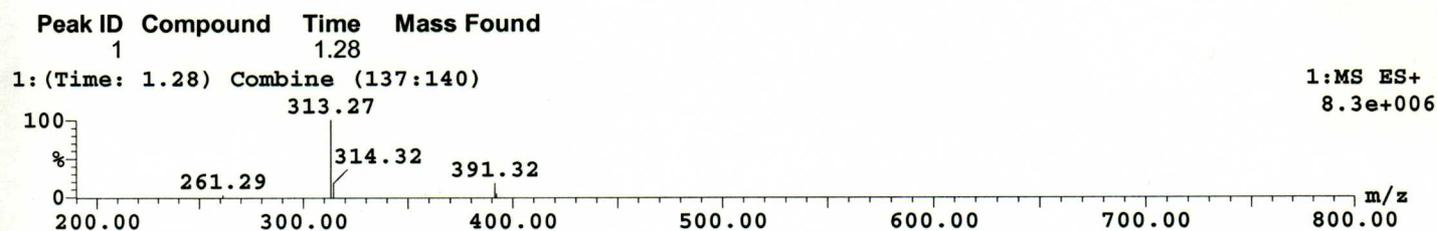
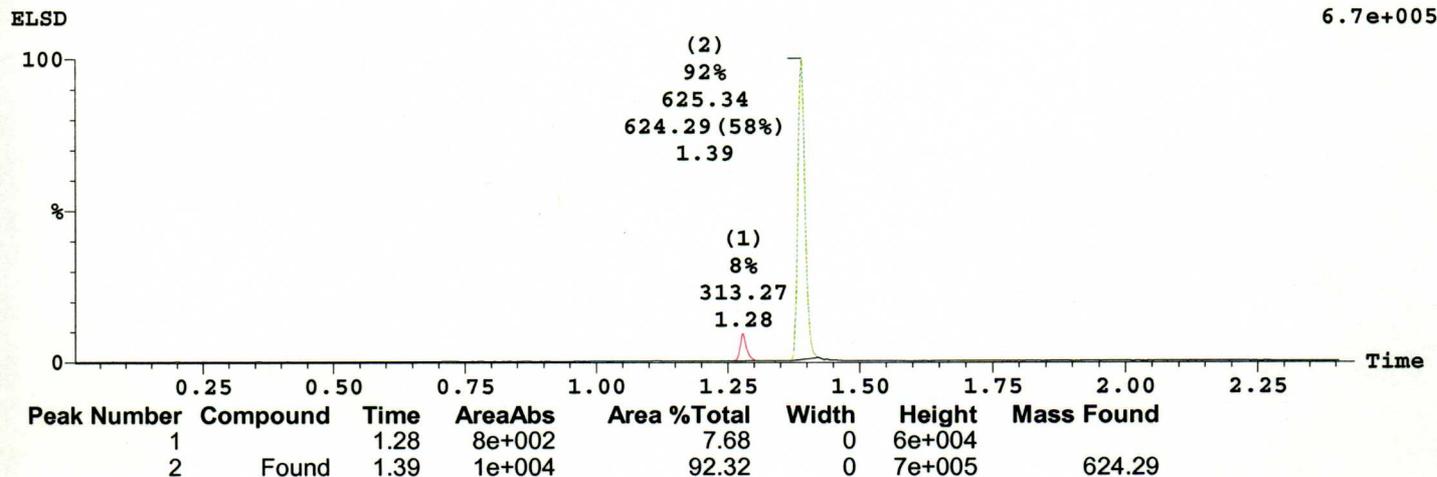
Sample 35 Vial 6:40 ID A38390102B04-2275039 File J38390233 Date 01-Jul-2004 Time 07:00:14 Description 3438157



8{35}

Printed: Mon Nov 07 09:39:18 2005

Sample Report (continued):



Chemical Formula: C<sub>36</sub>H<sub>40</sub>N<sub>4</sub>O<sub>6</sub>  
Exact Mass: 624.2948  
Molecular Weight: 624.726

Openlynx Report -  
Sample: 40  
File: J38390238  
Description: 3438158

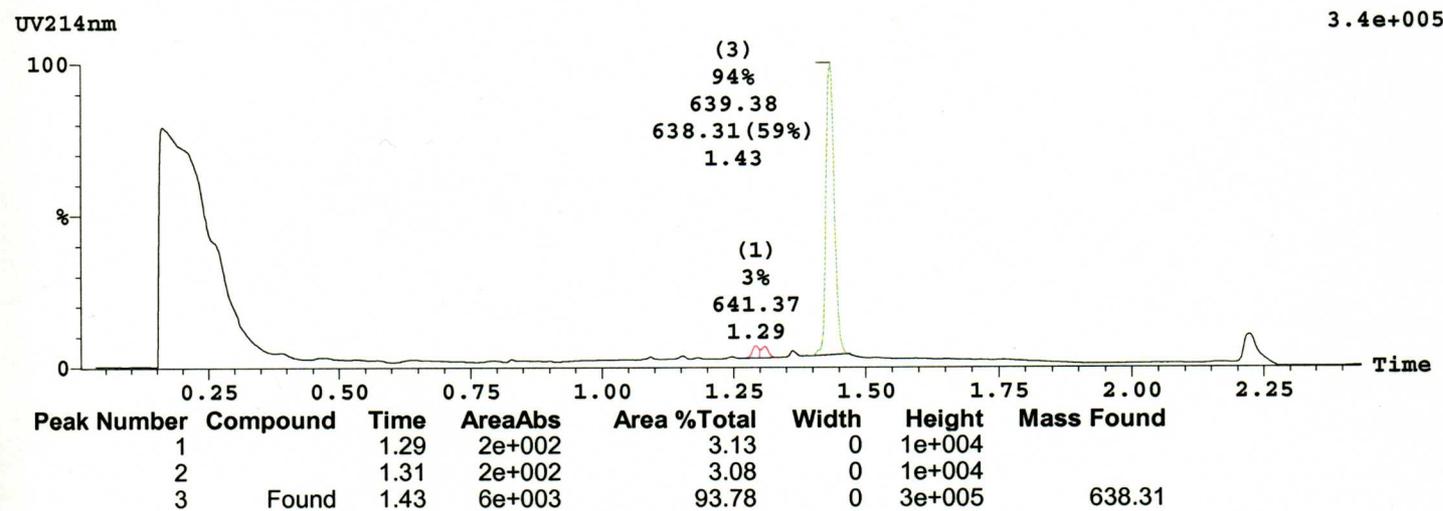
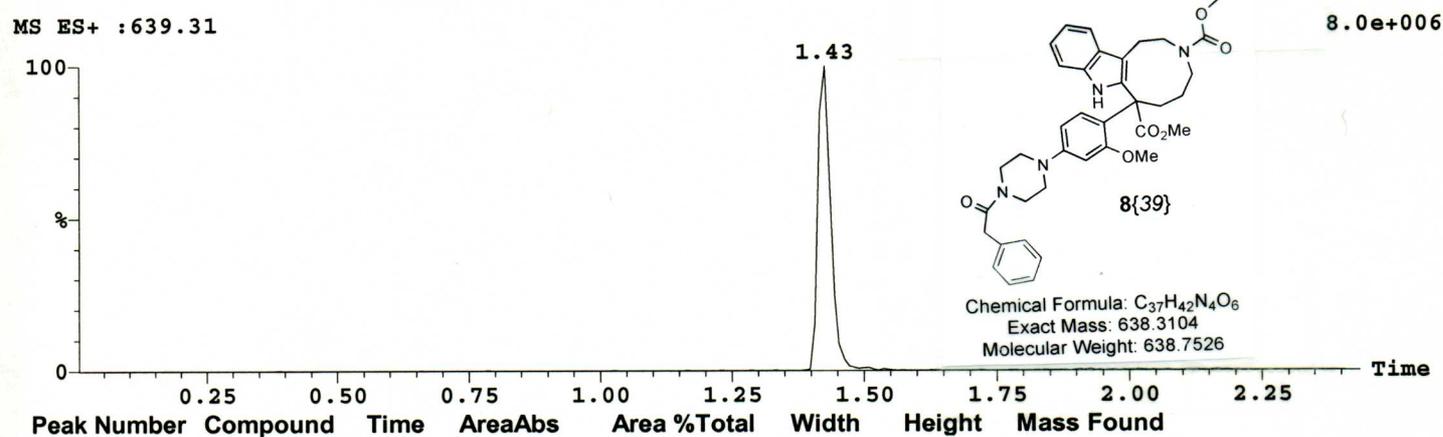
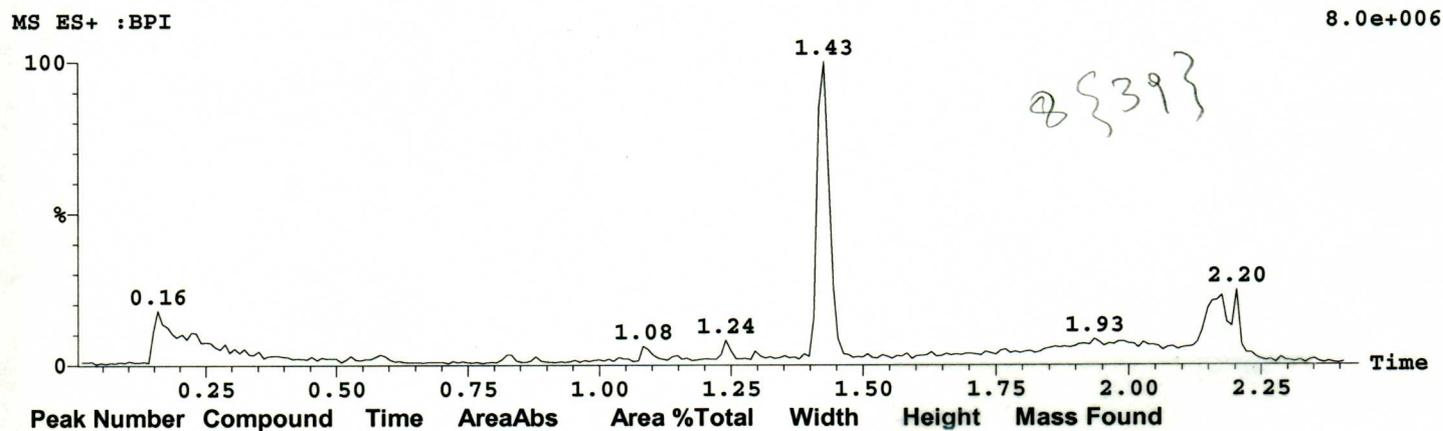
Vial: 6:45  
Date: 01-Jul-2004

ID: A38390102C04-2275044  
Time: 07:14:54

Printed: Wed Nov 02 14:10:36 2005

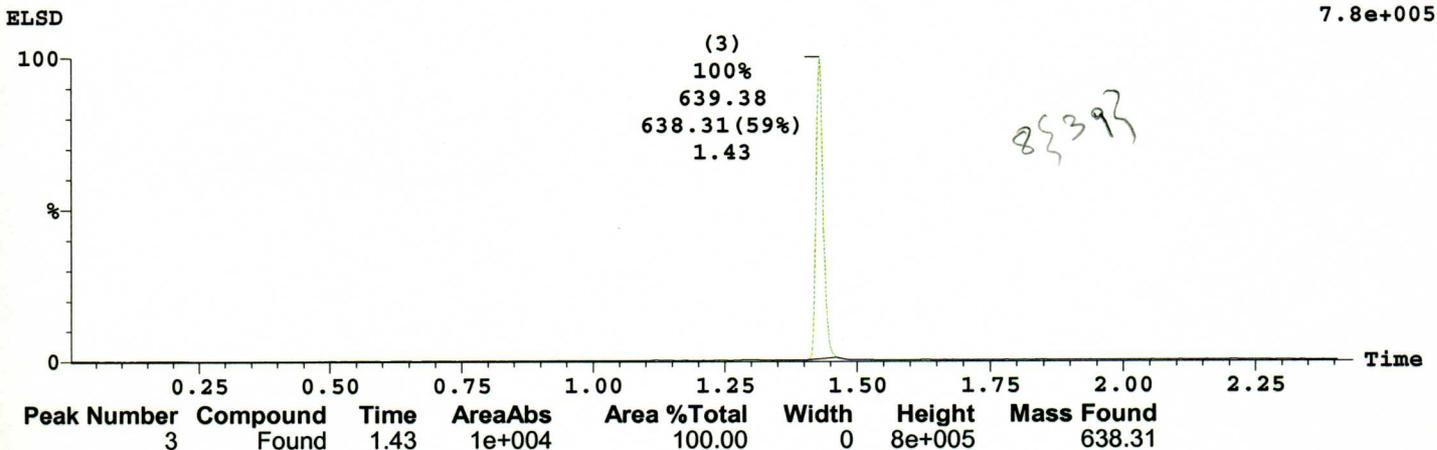
Sample Report:

Sample 40 Vial 6:45 ID A38390102C04-2275044 File J38390238 Date 01-Jul-2004 Time 07:14:54 Description 3438158



Printed: Wed Nov 02 14:10:36 2005

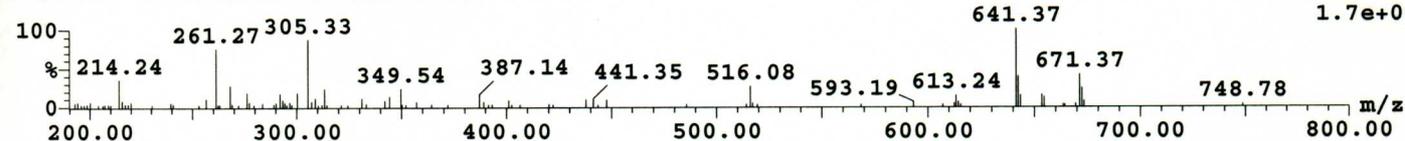
Sample Report (continued):



Peak ID Compound Time Mass Found  
1 1.29

1: (Time: 1.29) Combine (138:141)

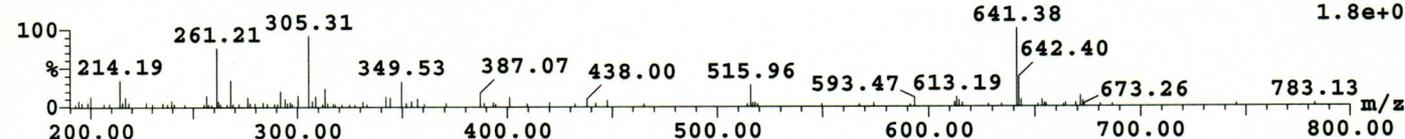
1: MS ES+  
1.7e+005



Peak ID Compound Time Mass Found  
2 1.31

2: (Time: 1.31) Combine (140:143)

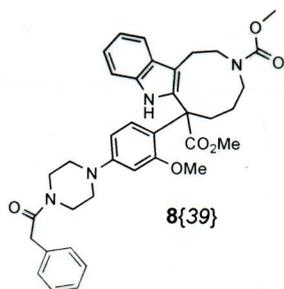
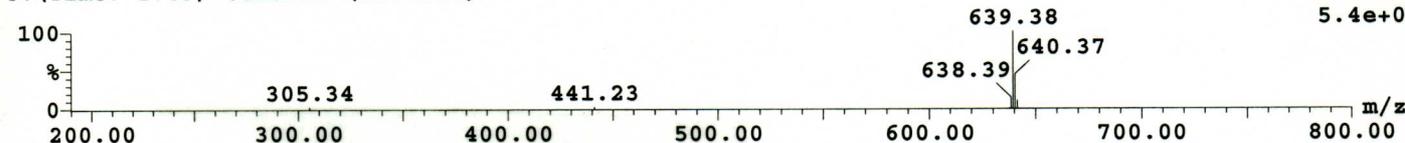
1: MS ES+  
1.8e+005



Peak ID Compound Time Mass Found  
3 Found 1.43 638.31

3: (Time: 1.43) Combine (153:156)

1: MS ES+  
5.4e+006



Chemical Formula: C<sub>37</sub>H<sub>42</sub>N<sub>4</sub>O<sub>6</sub>  
Exact Mass: 638.3104  
Molecular Weight: 638.7526

9{3}

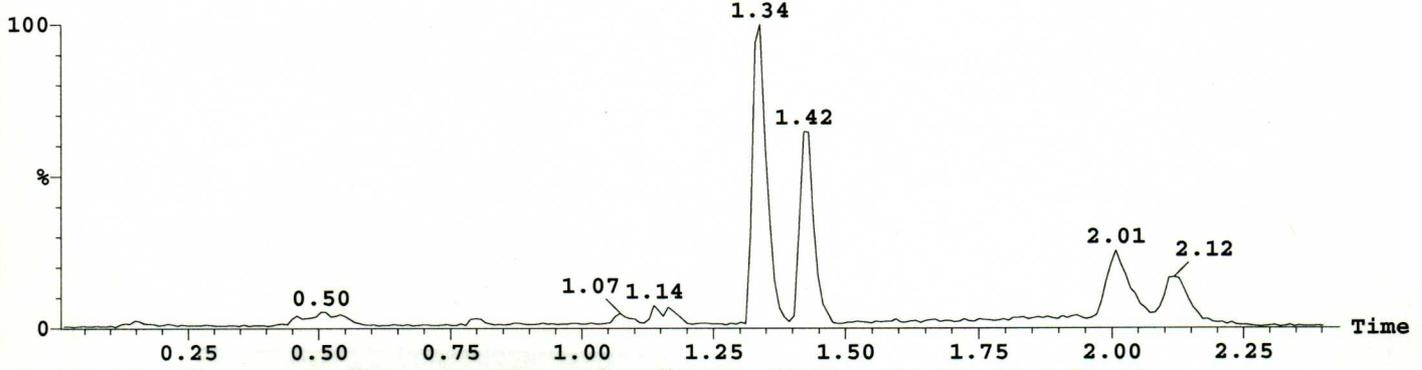
Printed: Mon Nov 07 09:40:41 2005

Sample Report:

Sample 14 Vial 6:15 ID A38450101C01-2298280 File N38450212 Date 20-Jul-2004 Time 21:08:17 Description 3484733

MS ES+ :BPI

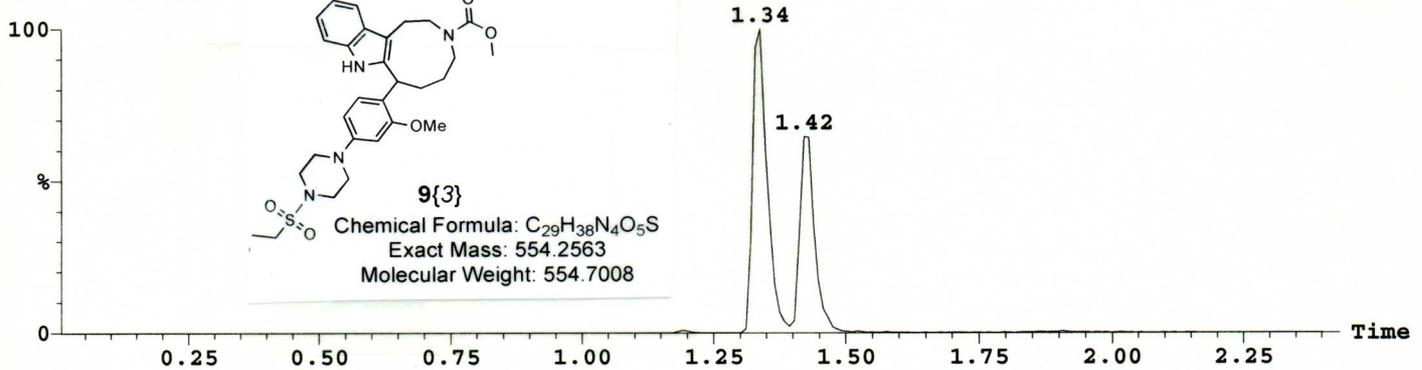
1.9e+007



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
-------------	----------	------	---------	-------------	-------	--------	------------

MS ES+ :555.26

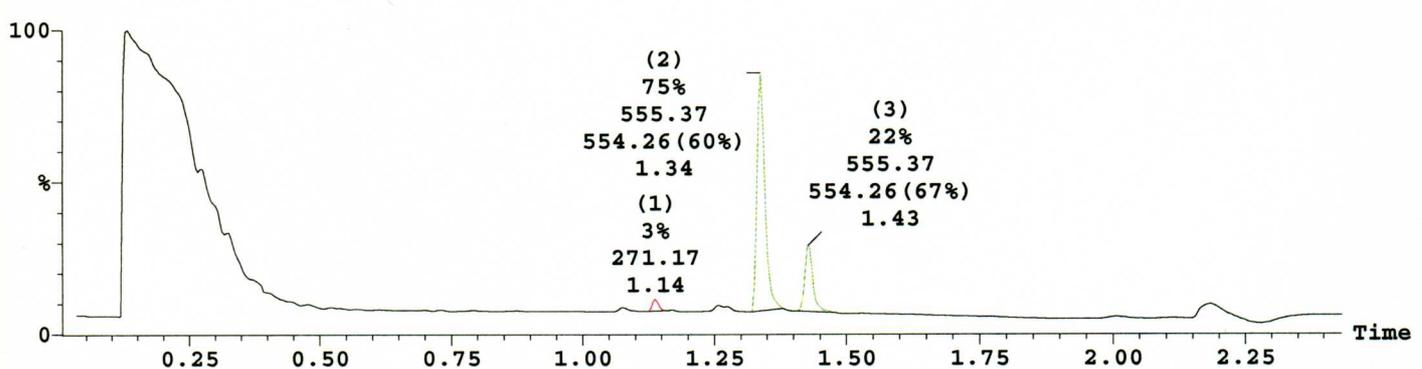
1.9e+007



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
-------------	----------	------	---------	-------------	-------	--------	------------

UV 214nm

3.6e+005

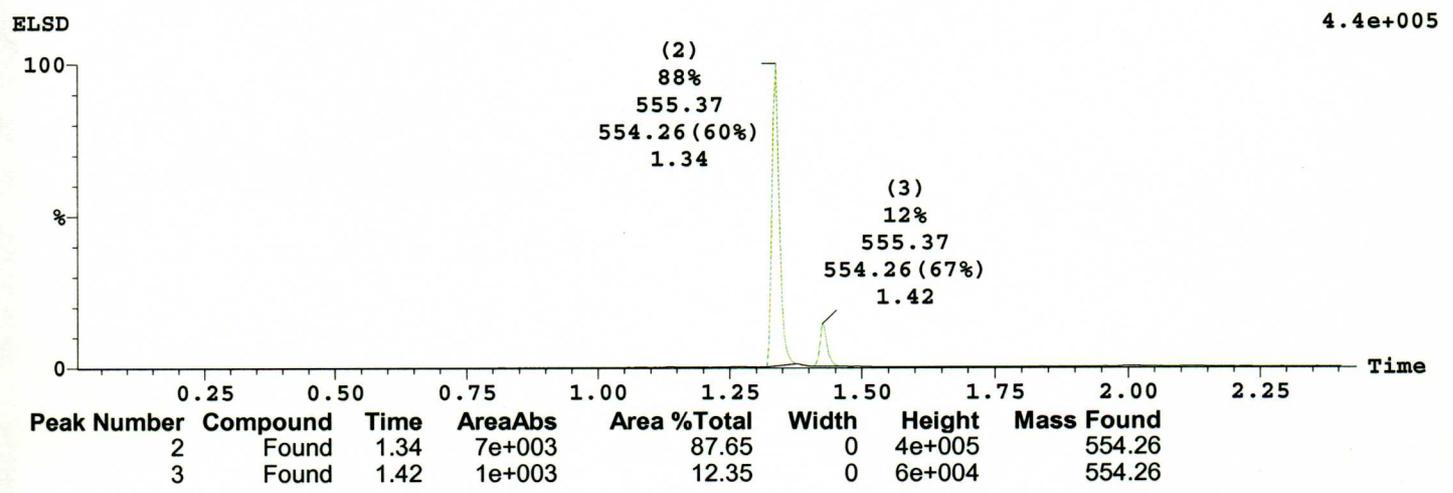


Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1		1.14	2e+002	3.02	0	1e+004	
2	Found	1.34	5e+003	74.83	0	3e+005	554.26
3	Found	1.43	1e+003	22.14	0	8e+004	554.26

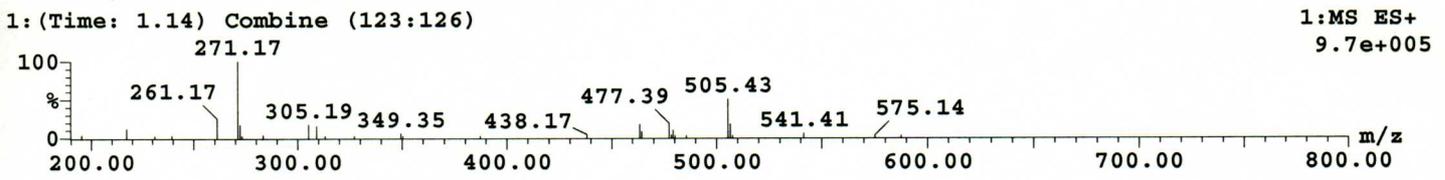
9533

Printed: Mon Nov 07 09:40:41 2005

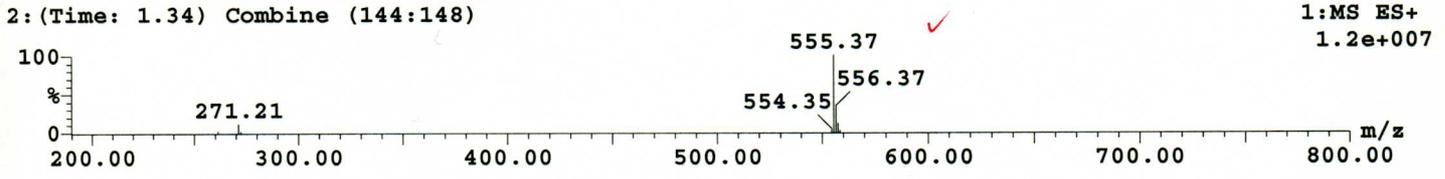
Sample Report (continued):



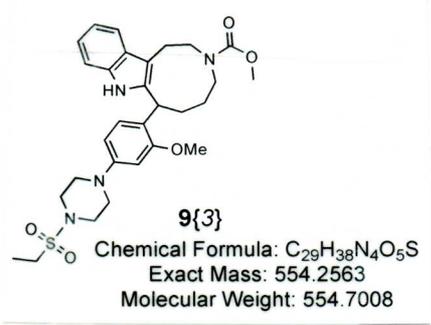
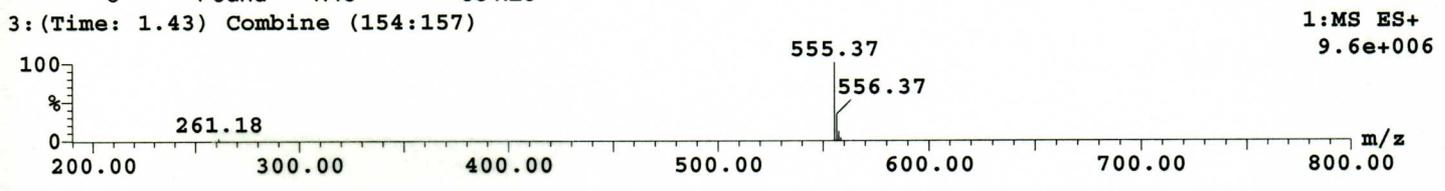
Peak ID Compound Time Mass Found  
1 1.14



Peak ID Compound Time Mass Found  
2 Found 1.34 554.26



Peak ID Compound Time Mass Found  
3 Found 1.43 554.26

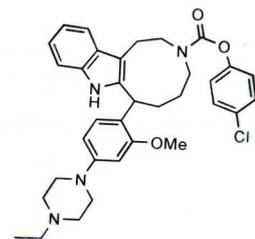


Printed: Wed Nov 02 14:40:24 2005

105173

Sample Report:

Sample 19 Vial 4:20 ID A38460101C05-2304701 File I38460217 Date 24-Jul-2004 T

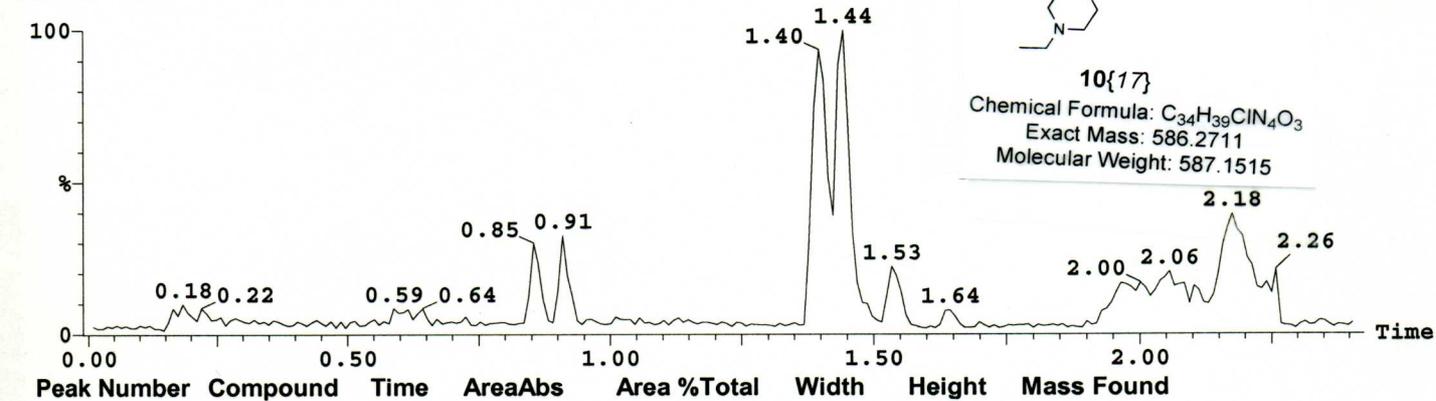


10{17}  
 Chemical Formula: C<sub>34</sub>H<sub>39</sub>ClN<sub>4</sub>O<sub>3</sub>  
 Exact Mass: 586.2711  
 Molecular Weight: 587.1515

4701

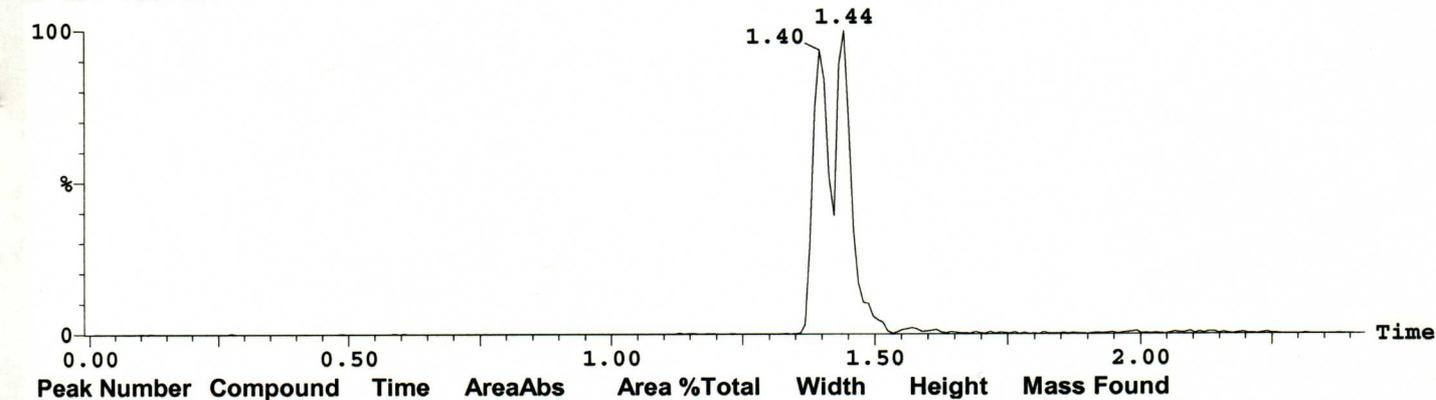
4.0e+006

MS ES+ : BPI



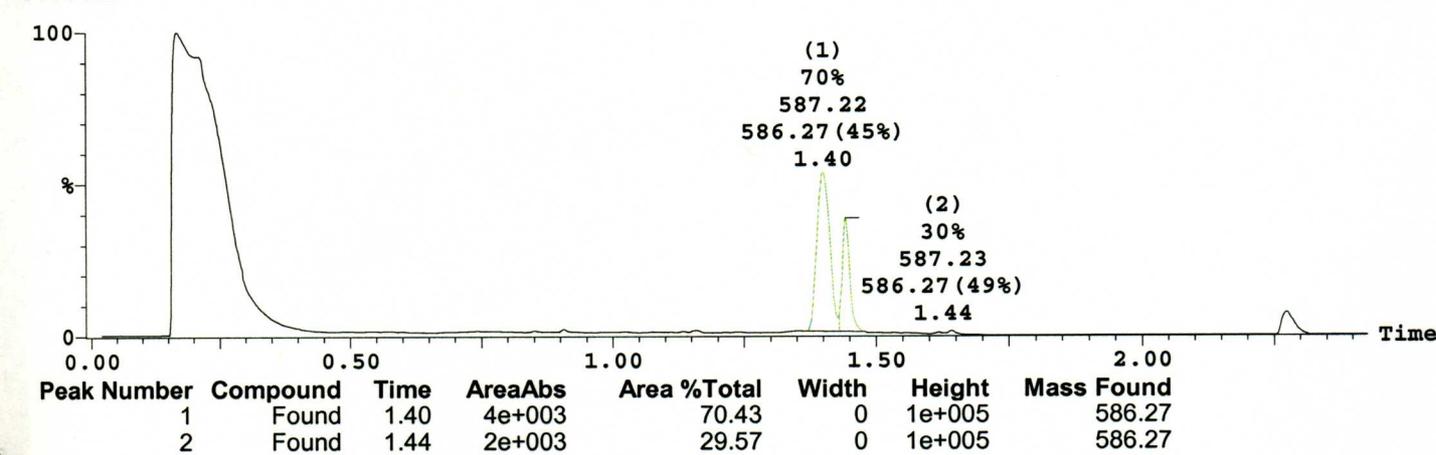
MS ES+ : 587.27

4.0e+006



UV214nm

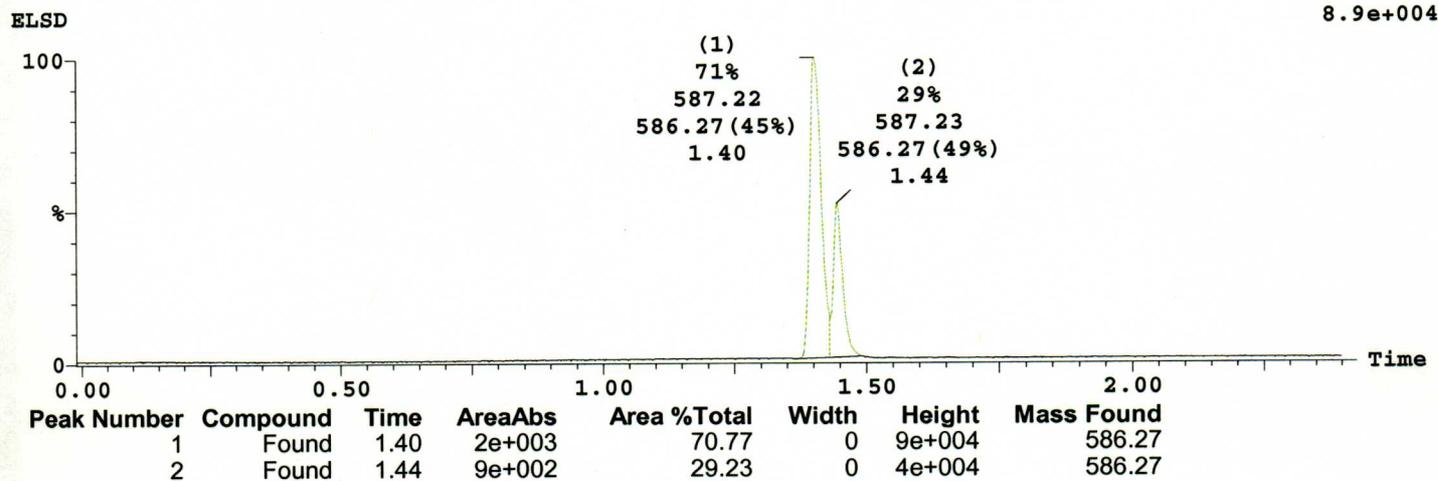
2.6e+005



10 {17}

Printed: Wed Nov 02 14:40:24 2005

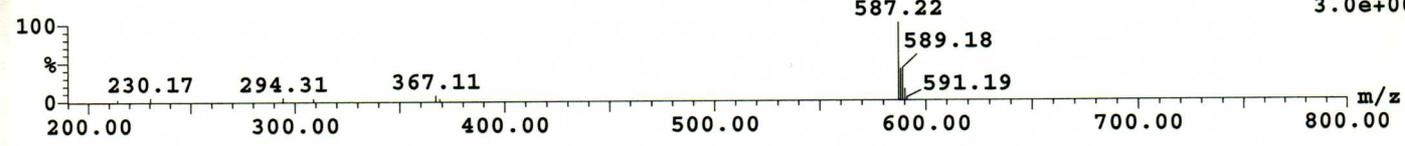
Sample Report (continued):



Peak ID	Compound	Time	Mass Found
1	Found	1.40	586.27

1: (Time: 1.40) Combine (151:154)

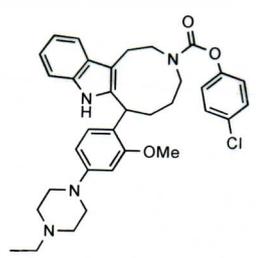
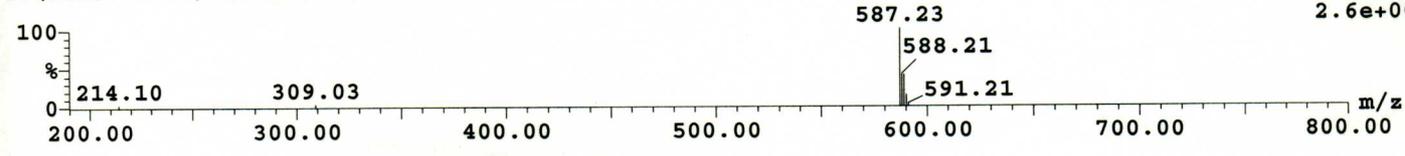
1: MS ES+  
3.0e+006



Peak ID	Compound	Time	Mass Found
2	Found	1.44	586.27

2: (Time: 1.44) Combine (155:159)

1: MS ES+  
2.6e+006



**10{17}**  
Chemical Formula: C<sub>34</sub>H<sub>39</sub>ClN<sub>4</sub>O<sub>3</sub>  
Exact Mass: 586.2711  
Molecular Weight: 587.1515

15{5}

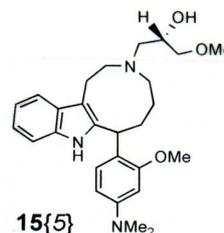
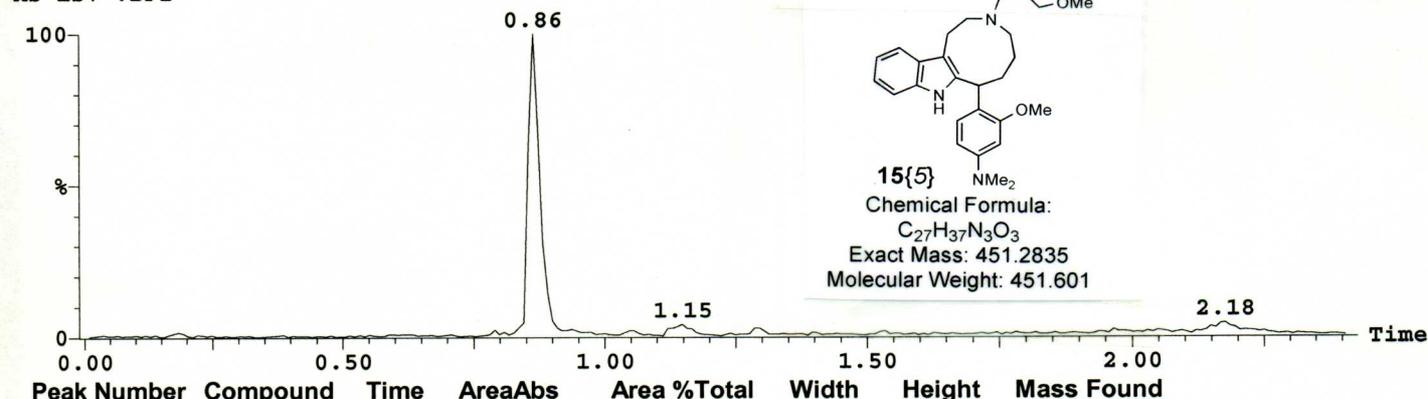
Printed: Mon Nov 07 09:46:49 2005

Sample Report:

Sample 6 Vial 5:5 ID A39120101A05-2305095 File I39120304 Date 24-Jul-2004 Time 05:09:31 Description 3493666

MS ES+ : BPI

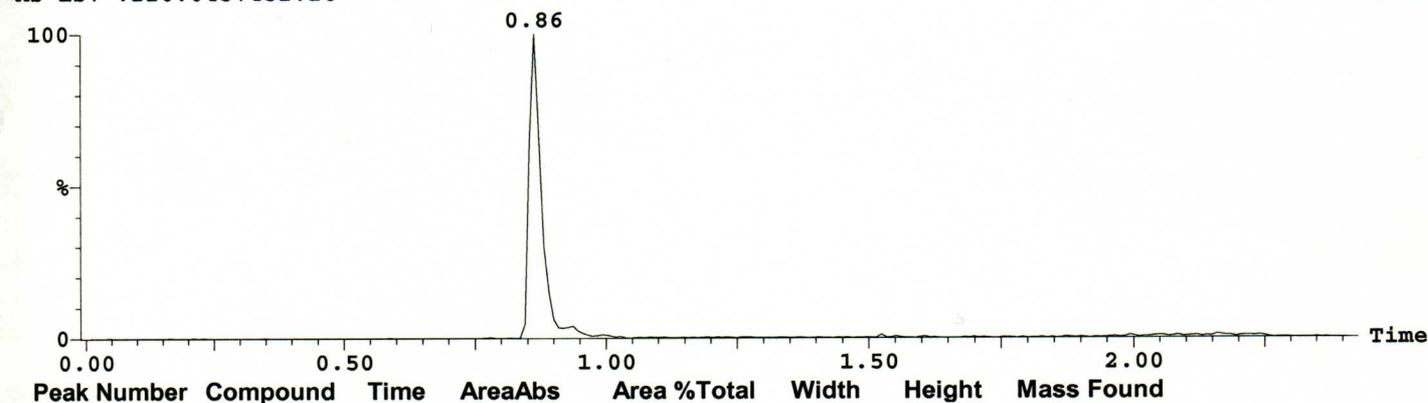
7.7e+006



Chemical Formula:  
C<sub>27</sub>H<sub>37</sub>N<sub>3</sub>O<sub>3</sub>  
Exact Mass: 451.2835  
Molecular Weight: 451.601

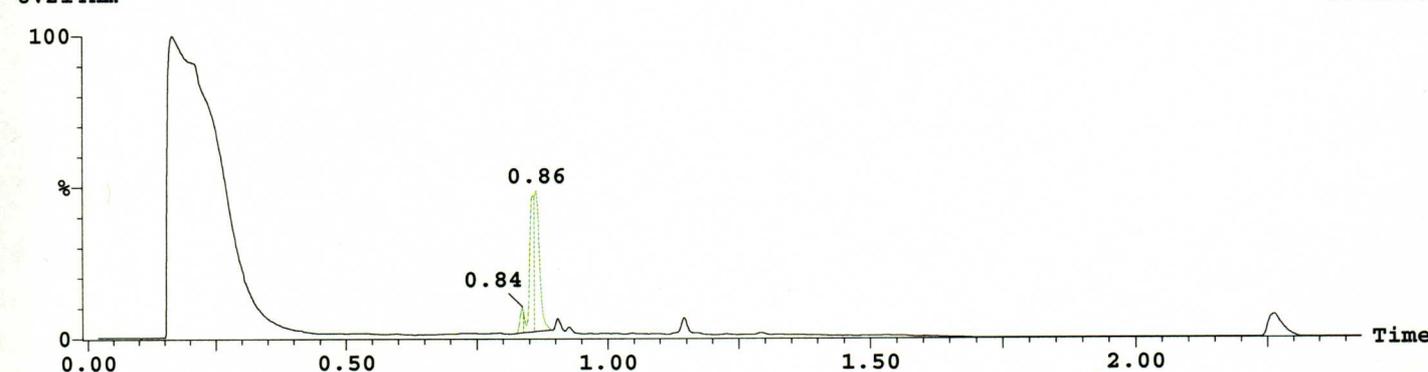
MS ES+ : 226.645+452.28

9.3e+006



UV214nm

2.6e+005



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1	Found	0.84	2e+002	8.01	0	2e+004	451.28
2	Found	0.86	1e+003	37.63	0	1e+005	451.28
3	Found	0.86	1e+003	54.37	0	1e+005	451.28

Sample: 6  
File: I39120304  
Description: 3493666

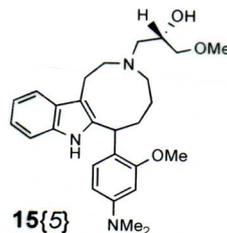
Vial: 5:5  
Date: 24-Jul-2004

ID: A39120101A05-2305095  
Time: 05:09:31

15{5}

Printed: Mon Nov 07 09:46:49 2005

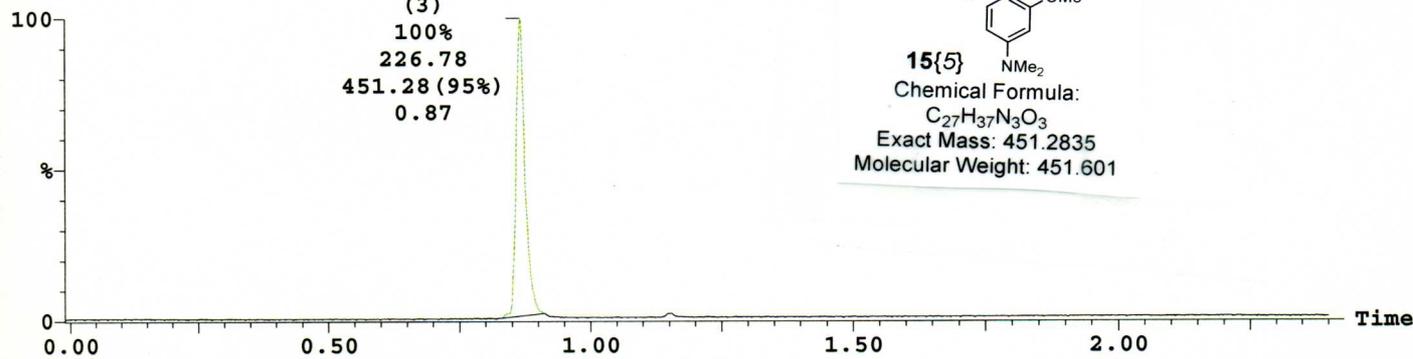
Sample Report (continued):



**15{5}**  
Chemical Formula:  
C<sub>27</sub>H<sub>37</sub>N<sub>3</sub>O<sub>3</sub>  
Exact Mass: 451.2835  
Molecular Weight: 451.601

1.0e+005

ELSD



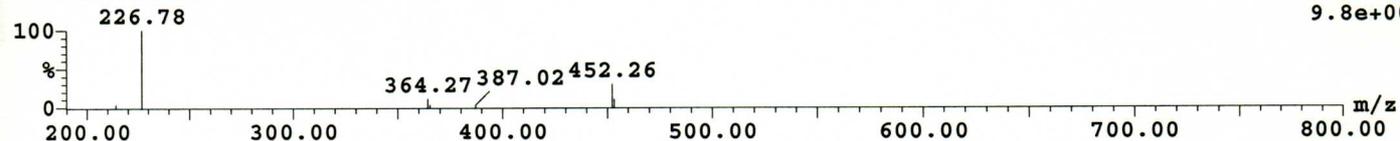
(3)  
100%  
226.78  
451.28 (95%)  
0.87

Peak Number	Compound Found	Time	AreaAbs	Area %Total	Width	Height	Mass Found
3	Found	0.86	2e+003	100.00	0	1e+005	451.28

Peak ID	Compound Found	Time	Mass Found
1	Found	0.84	451.28

1: (Time: 0.84) Combine (89:93)

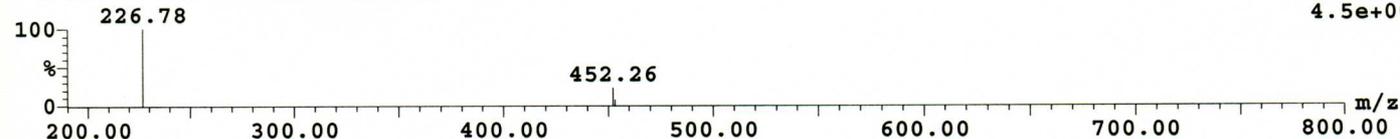
1: MS ES+  
9.8e+005



Peak ID	Compound Found	Time	Mass Found
2	Found	0.86	451.28

2: (Time: 0.86) Combine (92:95)

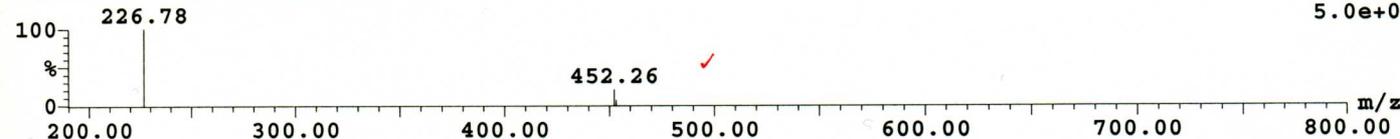
1: MS ES+  
4.5e+006



Peak ID	Compound Found	Time	Mass Found
3	Found	0.86	451.28

3: (Time: 0.86) Combine (93:96)

1: MS ES+  
5.0e+006



15{13}

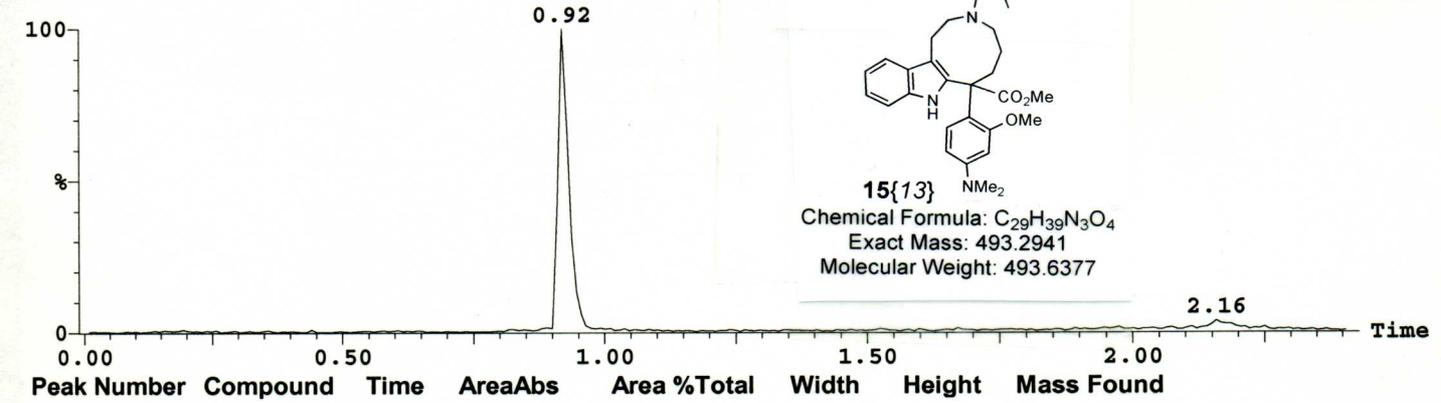
Printed: Wed Nov 02 14:18:01 2005

Sample Report:

Sample 13 Vial 5:14 ID A39120101C01-2305102 File I39120311 Date 24-Jul-2004 Time 05:27:28 Description 3493674

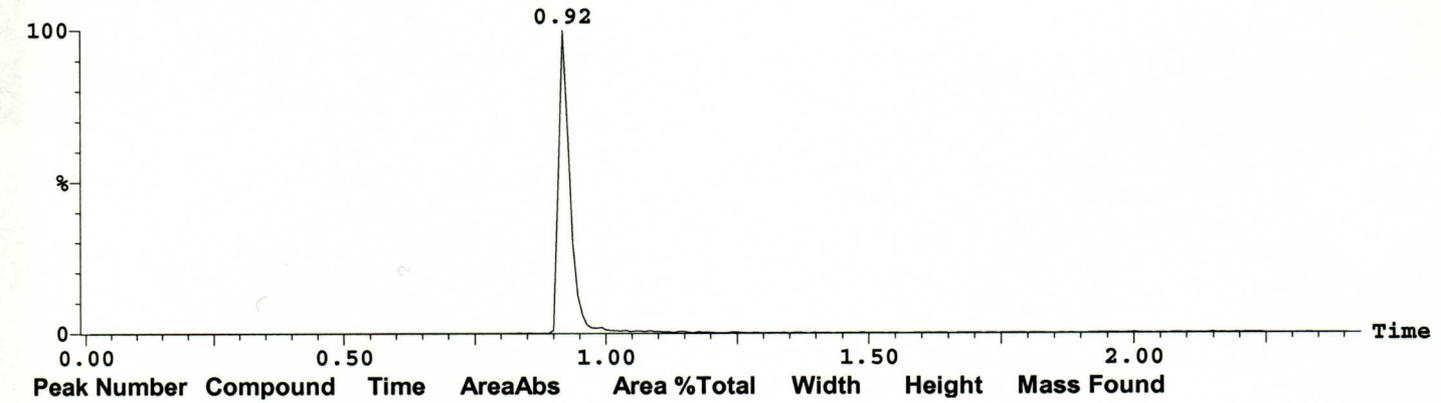
MS ES+ : BPI

1.1e+007



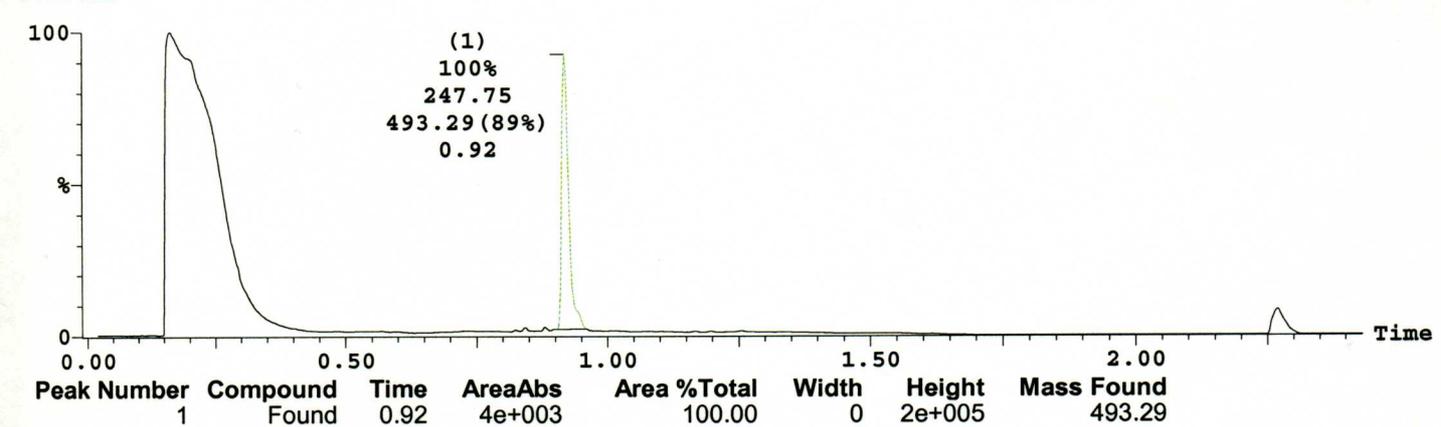
MS ES+ : 247.65+494.29

1.5e+007



UV214nm

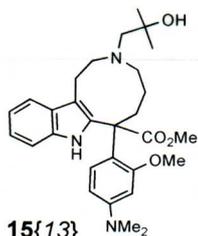
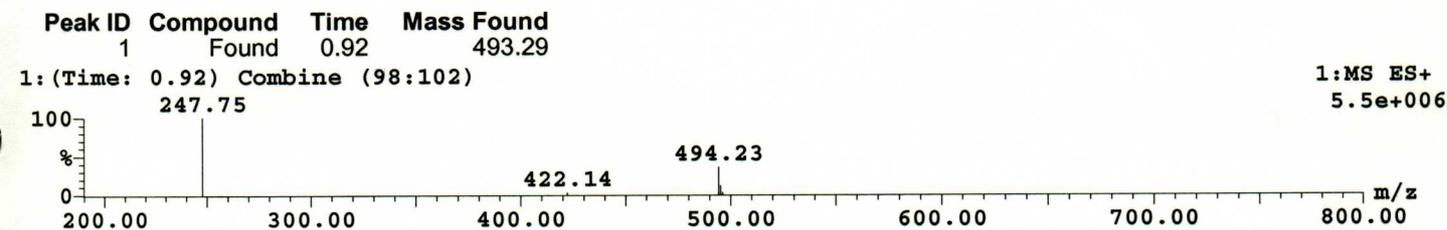
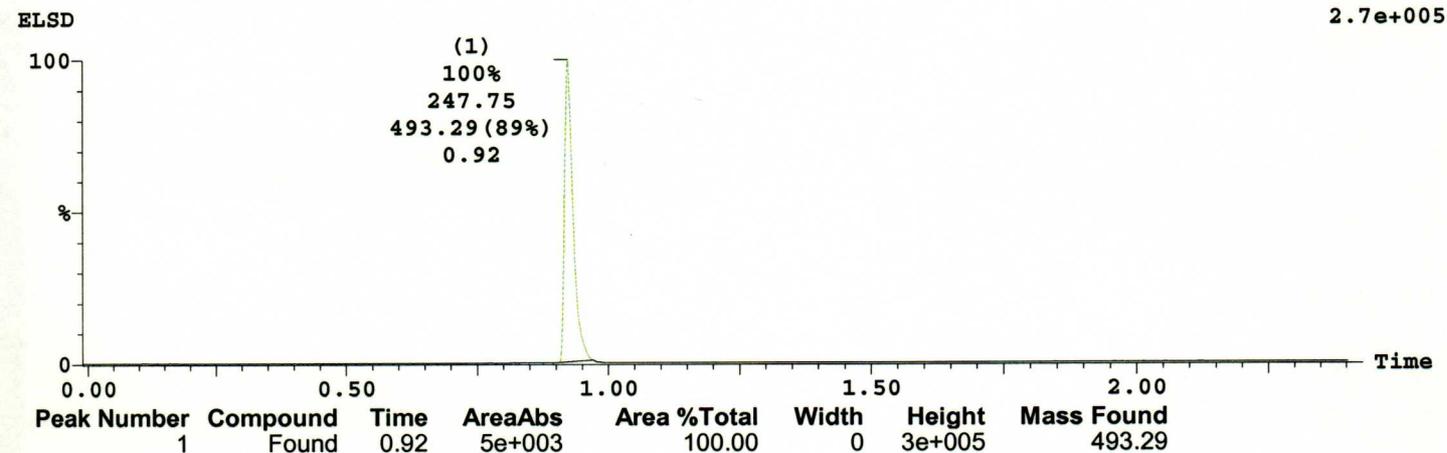
2.6e+005



15{13}

Printed: Wed Nov 02 14:18:01 2005

Sample Report (continued):



**15{13}**  
Chemical Formula: C<sub>29</sub>H<sub>39</sub>N<sub>3</sub>O<sub>4</sub>  
Exact Mass: 493.2941  
Molecular Weight: 493.6377

Printed: Wed Nov 02 14:20:15 2005

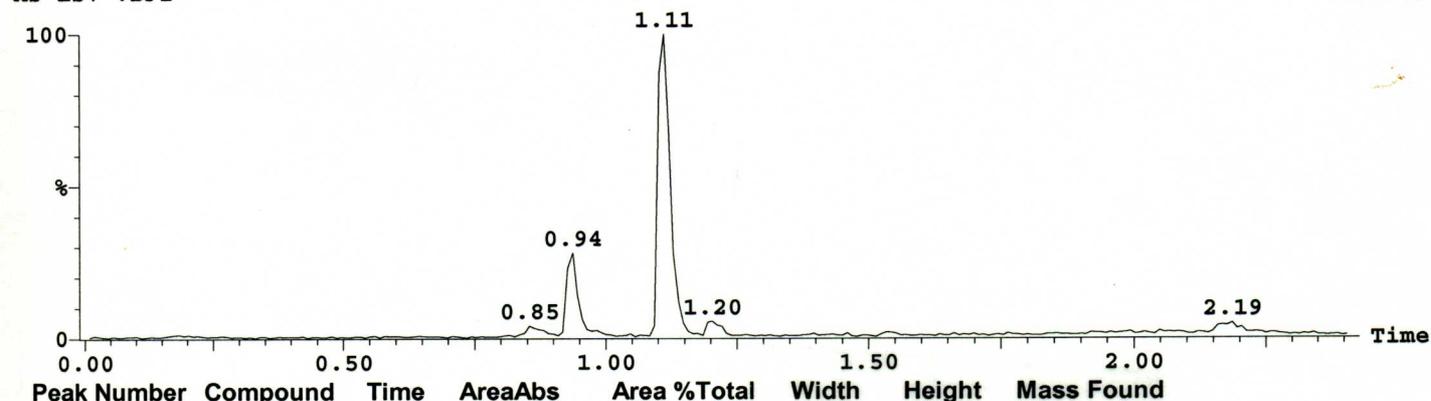
Sample Report:

155 233

Sample 21 Vial 5:22 ID A39120101D04-2305110 File I39120319 Date 24-Jul-2004 Time 05:48:02 Description 3493683

MS ES+ :BPI

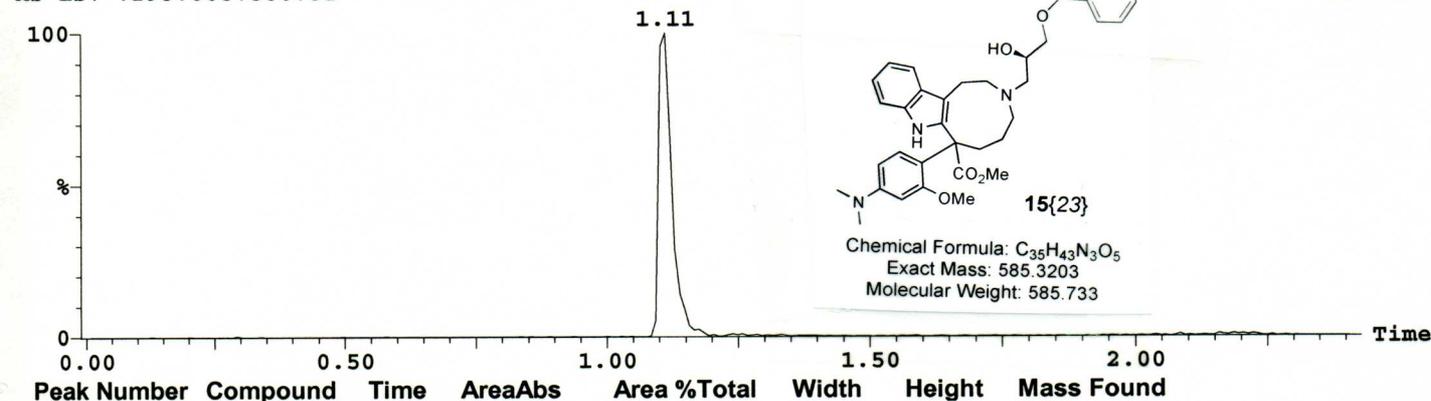
7.8e+006



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
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MS ES+ :293.665+586.32

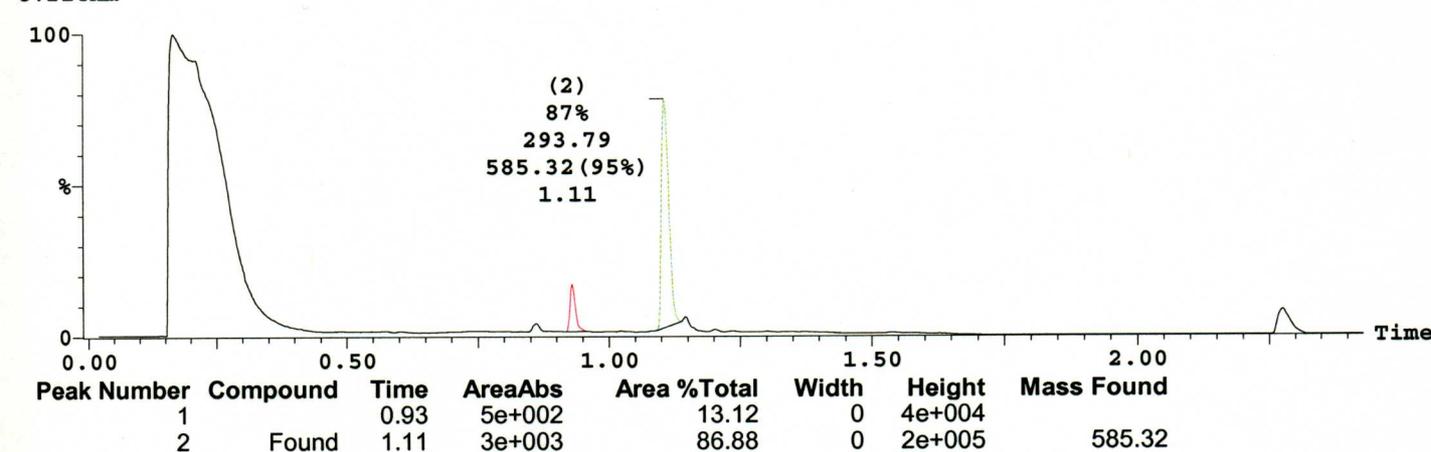
8.9e+006



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
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UV214nm

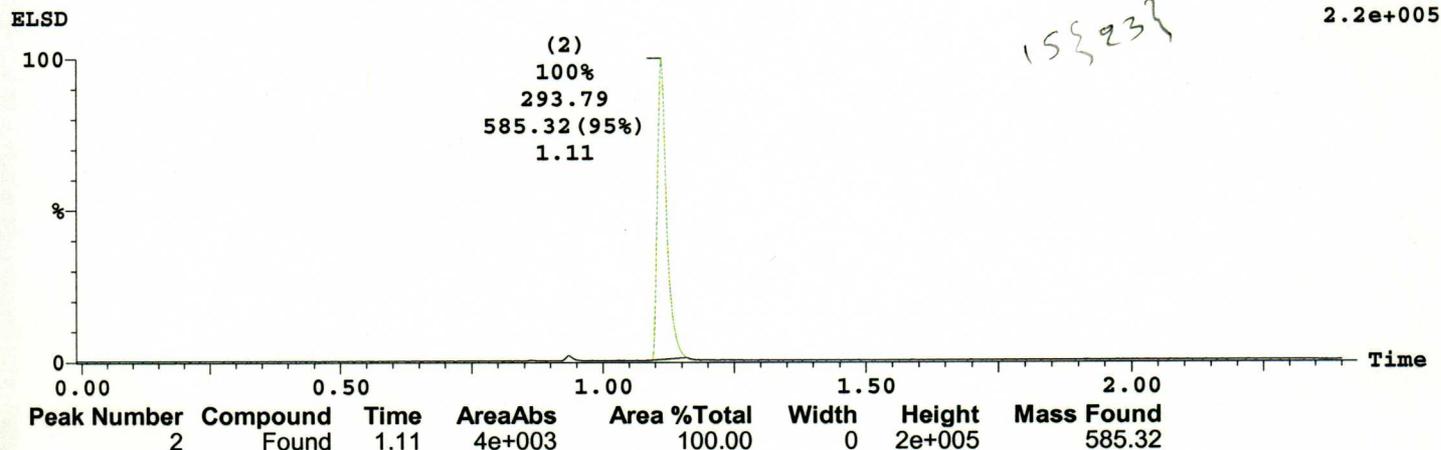
2.6e+005



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1		0.93	5e+002	13.12	0	4e+004	
2	Found	1.11	3e+003	86.88	0	2e+005	585.32

Printed: Wed Nov 02 14:20:15 2005

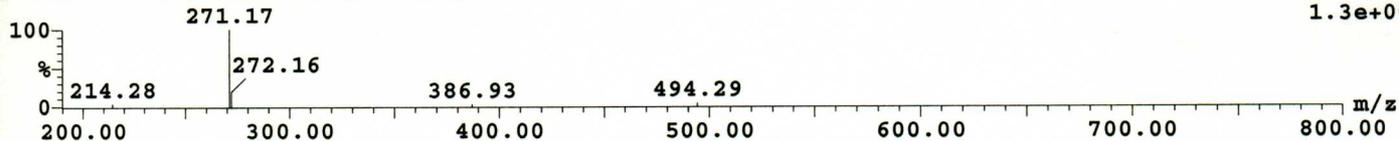
Sample Report (continued):



Peak ID Compound Time Mass Found  
1 0.93

1: (Time: 0.93) Combine (100:103)

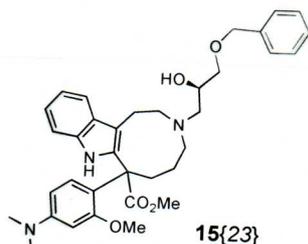
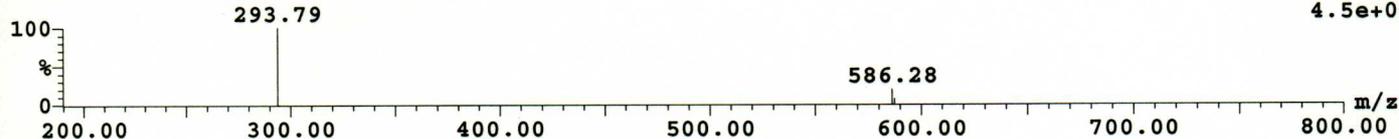
1: MS ES+  
1.3e+006



Peak ID Compound Time Mass Found  
2 Found 1.11 585.32

2: (Time: 1.11) Combine (119:123)

1: MS ES+  
4.5e+006



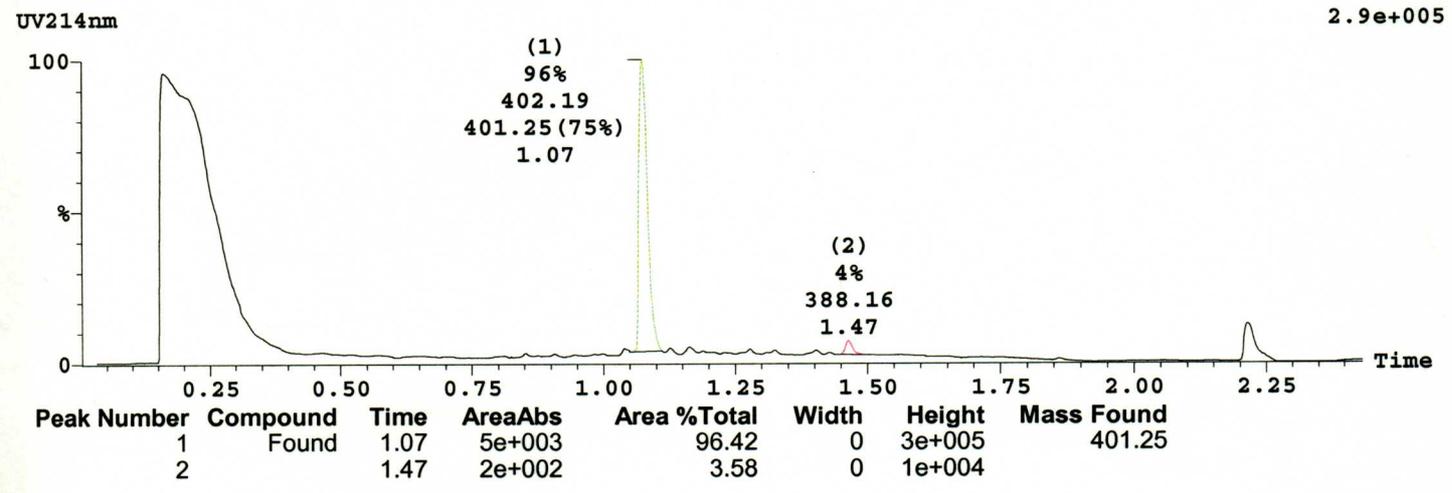
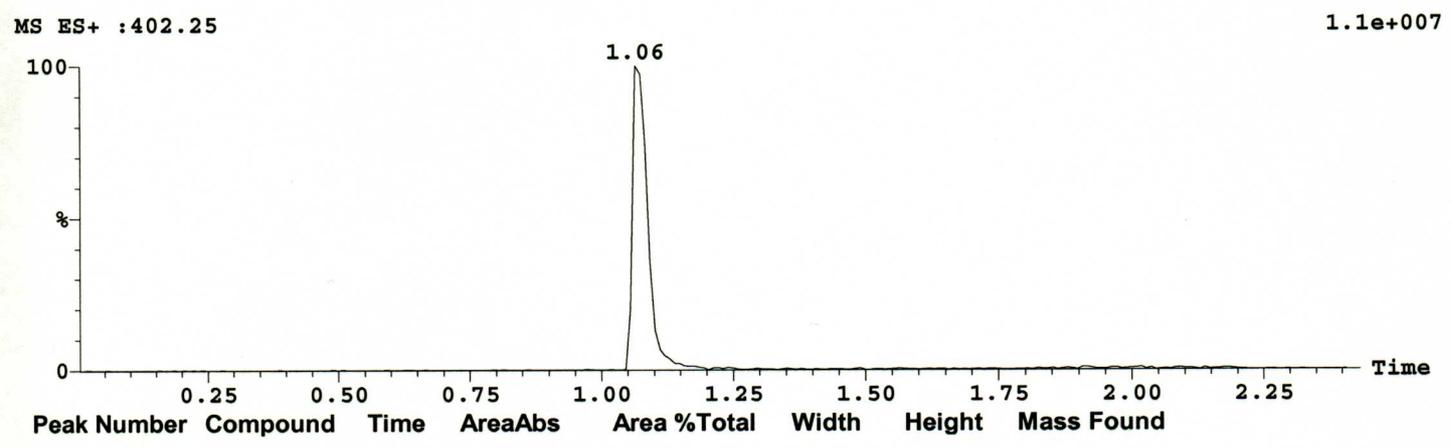
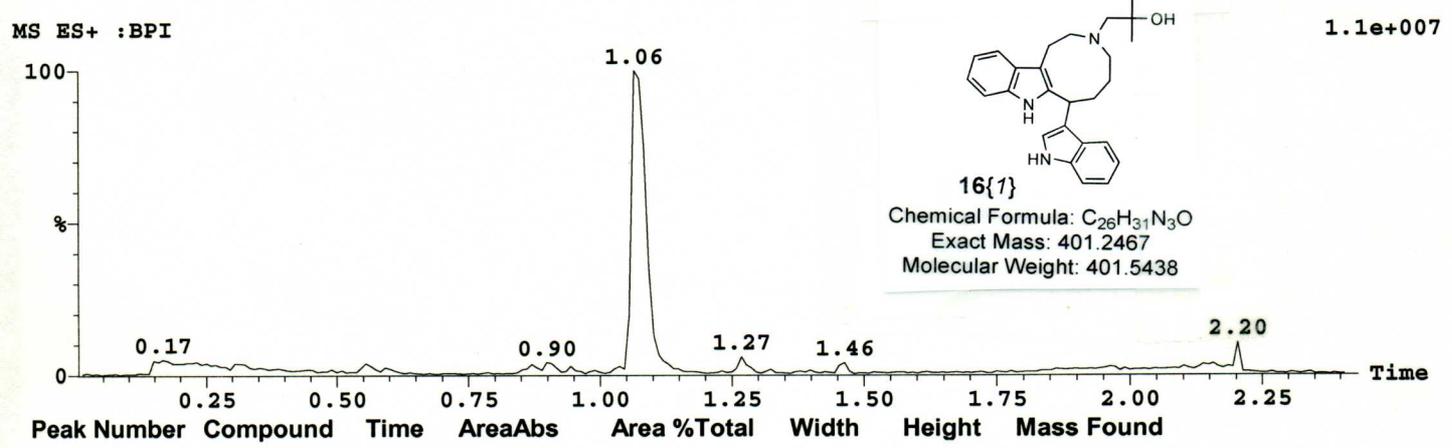
Chemical Formula: C<sub>35</sub>H<sub>43</sub>N<sub>3</sub>O<sub>5</sub>  
Exact Mass: 585.3203  
Molecular Weight: 585.733

16513

Printed: Wed Nov 02 14:29:43 2005

Sample Report:

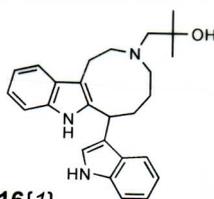
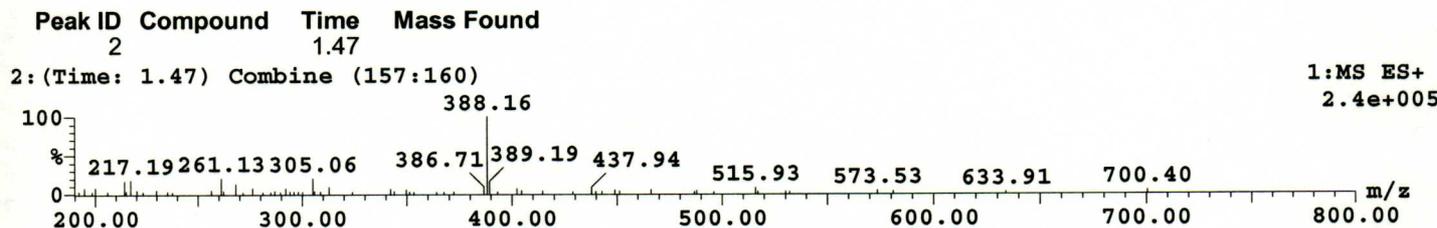
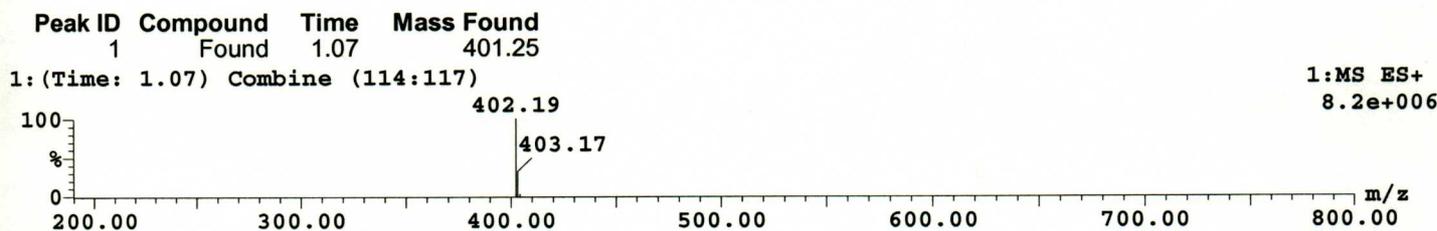
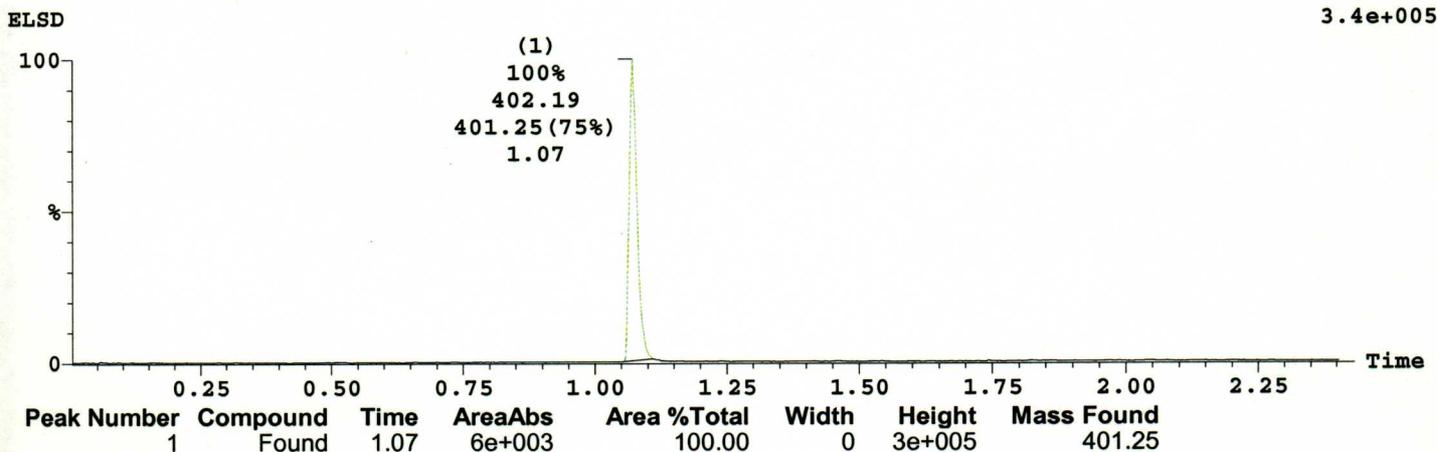
Sample 3 Vial 3:2 ID A39110101A01-2310983 File J39110201 Date 27-Jul-2004 Time 18:17:39 Description 3493638



16{1}

Printed: Wed Nov 02 14:29:43 2005

Sample Report (continued):



16{1}

Chemical Formula: C<sub>26</sub>H<sub>31</sub>N<sub>3</sub>O  
Exact Mass: 401.2467  
Molecular Weight: 401.5438

Printed: Wed Nov 02 14:30:15 2005

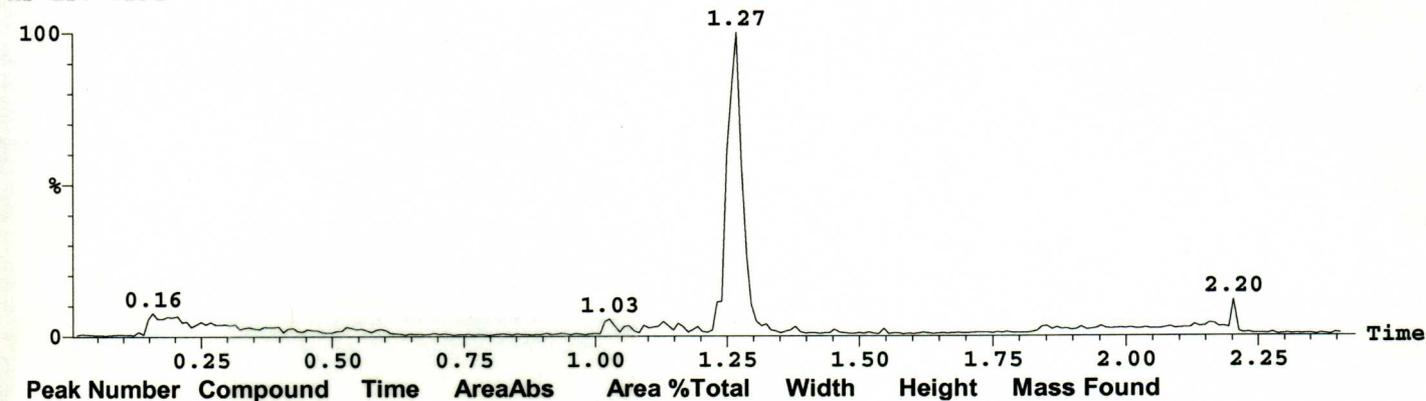
16{12}

Sample Report:

Sample 14 Vial 3:15 ID A39110101B06-2310994 File J39110212 Date 27-Jul-2004 Time 18:49:56 Description 3493649

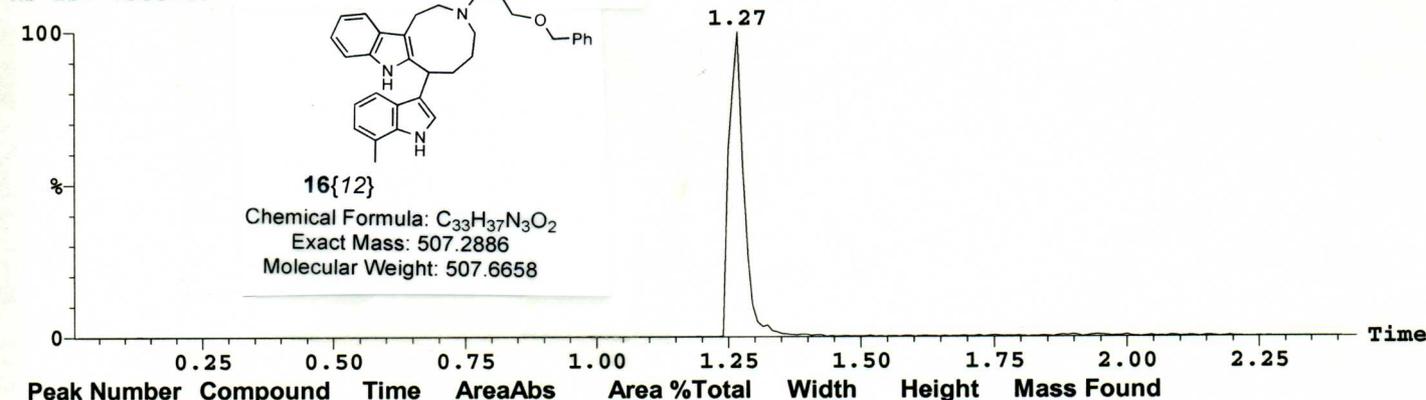
MS ES+ : BPI

1.0e+007



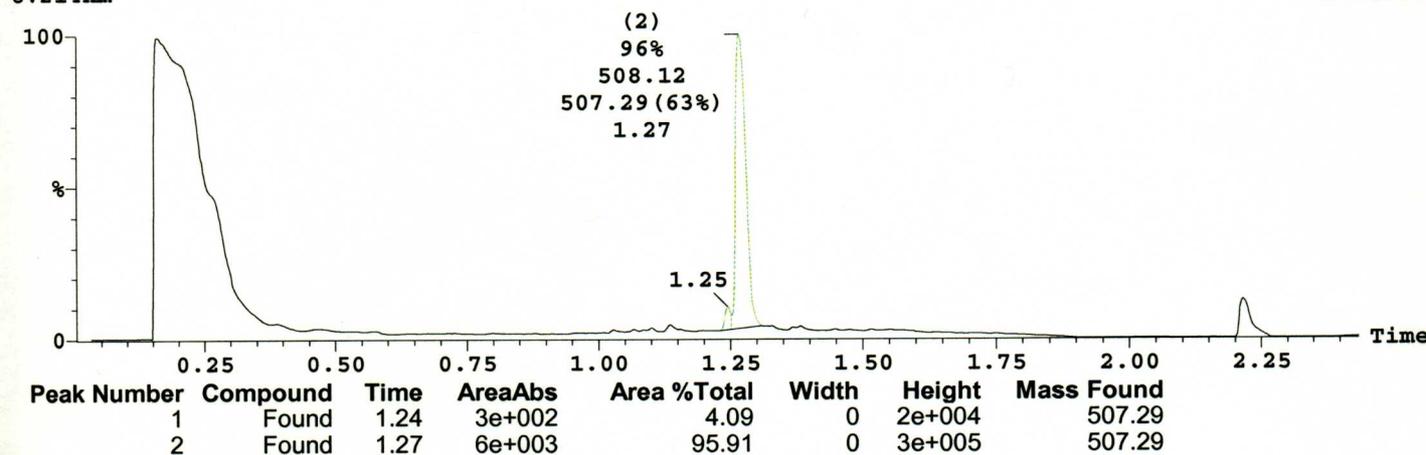
MS ES+ : 508.29

1.0e+007



UV214nm

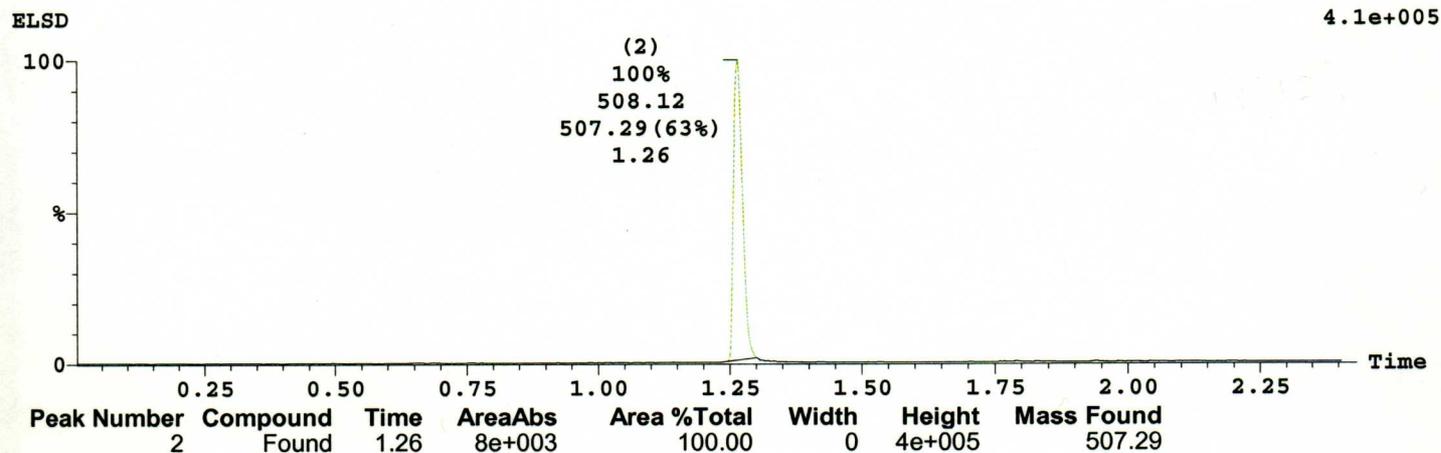
2.8e+005



165123

Printed: Wed Nov 02 14:30:15 2005

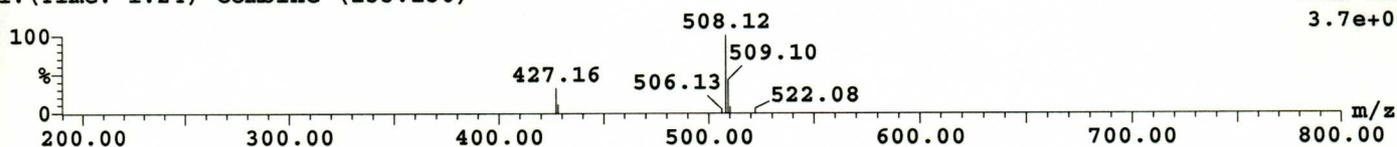
Sample Report (continued):



Peak ID Compound Time Mass Found  
1 Found 1.24 507.29

1: (Time: 1.24) Combine (133:136)

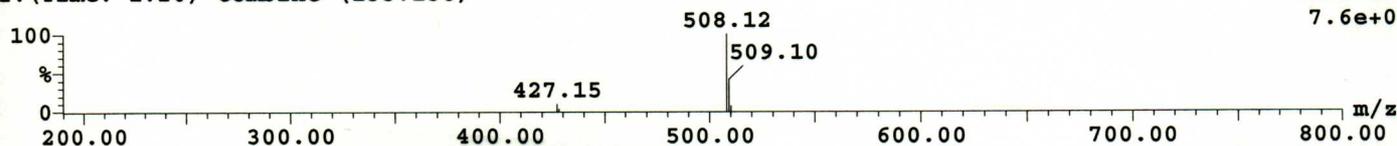
1: MS ES+  
3.7e+006



Peak ID Compound Time Mass Found  
2 Found 1.27 507.29

2: (Time: 1.26) Combine (135:138)

1: MS ES+  
7.6e+006



Chemical Formula: C<sub>33</sub>H<sub>37</sub>N<sub>3</sub>O<sub>2</sub>  
Exact Mass: 507.2886  
Molecular Weight: 507.6658

Sample: 17  
 File:K39300215  
 Description:3508964

Vial:7:18  
 Date:29-Jul-2004

ID:A39300101C03-2313949  
 Time:11:05:33

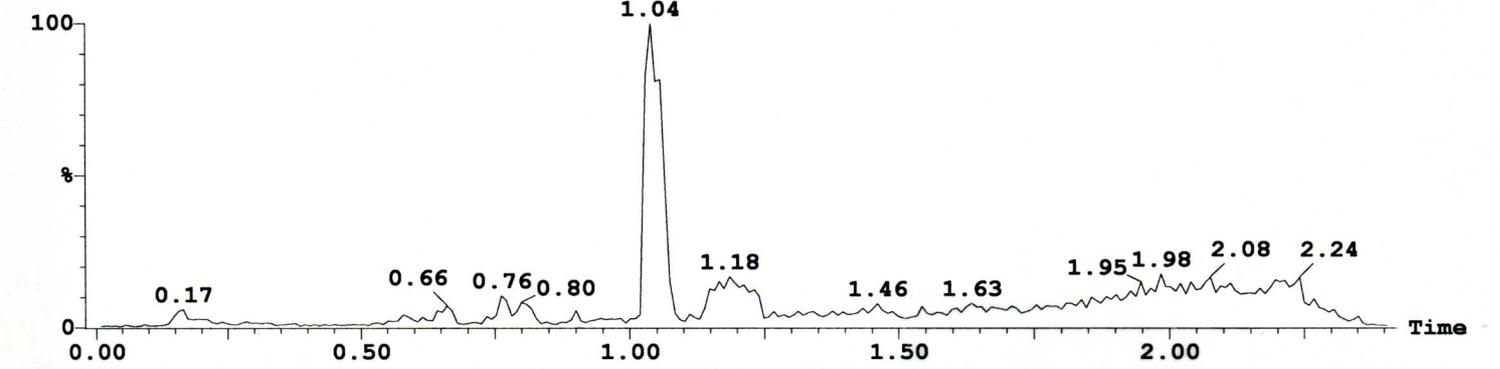
17{15}

Printed: Wed Nov 02 14:34:00 2005

Sample Report:

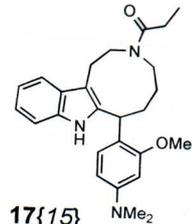
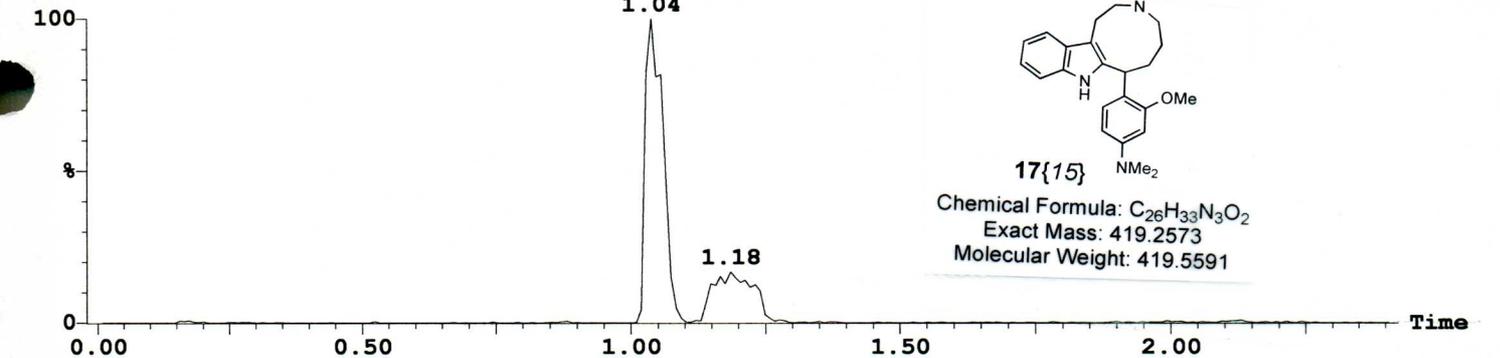
Sample 17 Vial 7:18 ID A39300101C03-2313949 File K39300215 Date 29-Jul-2004 Time 11:05:33 Description 3508964

MS ES+ :BPI 2.3e+006



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
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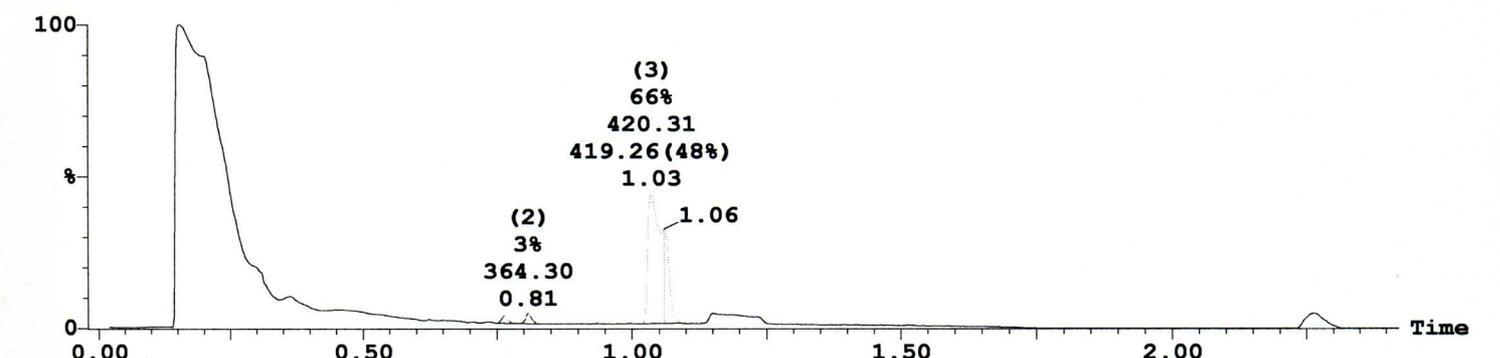
MS ES+ :420.26 2.3e+006



Chemical Formula: C<sub>26</sub>H<sub>33</sub>N<sub>3</sub>O<sub>2</sub>  
 Exact Mass: 419.2573  
 Molecular Weight: 419.5591

Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
-------------	----------	------	---------	-------------	-------	--------	------------

UV214nm 3.2e+005

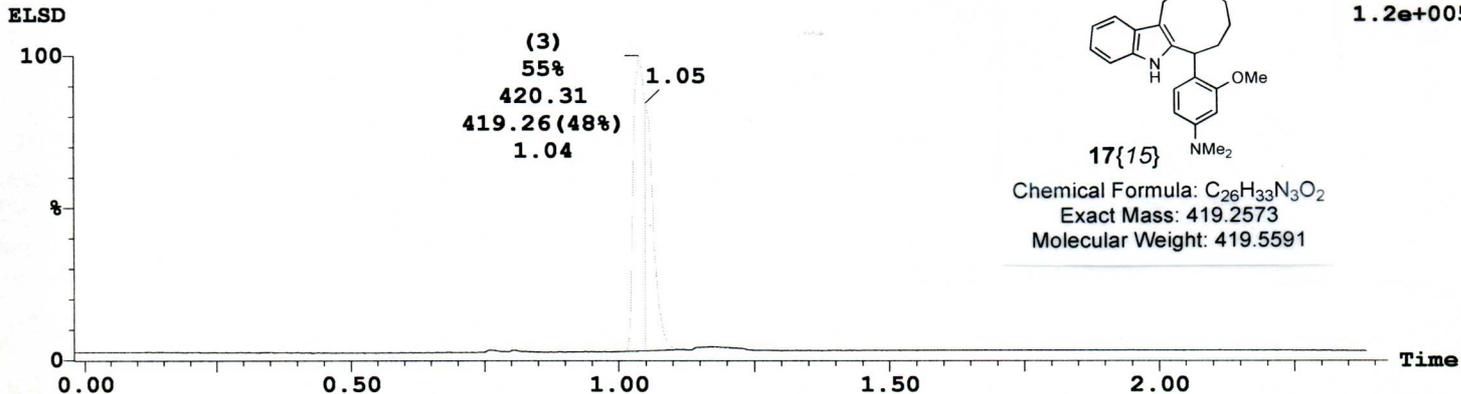


Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1		0.76	1e+002	2.04	0	8e+003	
2		0.81	1e+002	2.73	0	1e+004	
3	Found	1.03	3e+003	65.62	0	1e+005	419.26
5	Found	1.06	1e+003	29.60	0	1e+005	419.26

175153

Printed: Wed Nov 02 14:34:00 2005

Sample Report (continued):

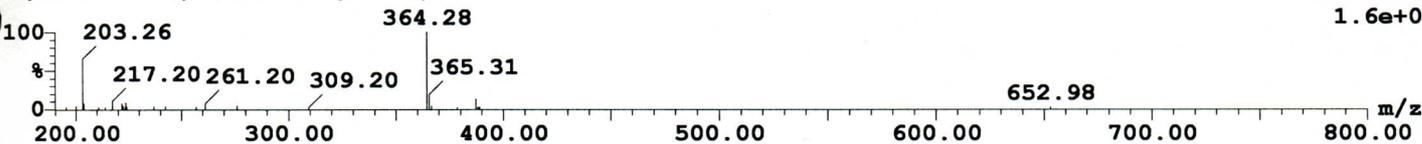


Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
3	Found	1.04	2e+003	54.81	0	1e+005	419.26
4	Found	1.05	2e+003	45.19	0	1e+005	419.26

Peak ID Compound Time Mass Found  
1 0.76

1: (Time: 0.76) Combine (82:85)

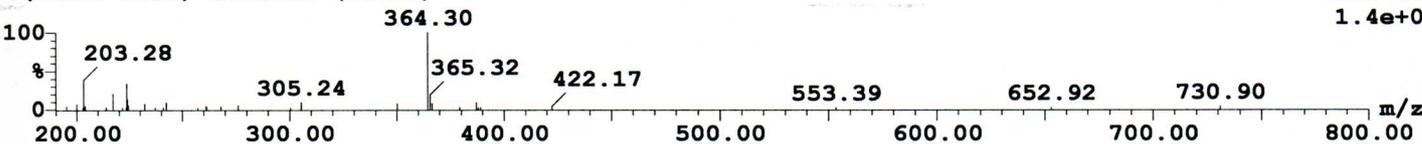
1:MS ES+  
1.6e+005



Peak ID Compound Time Mass Found  
2 0.81

2: (Time: 0.81) Combine (86:90)

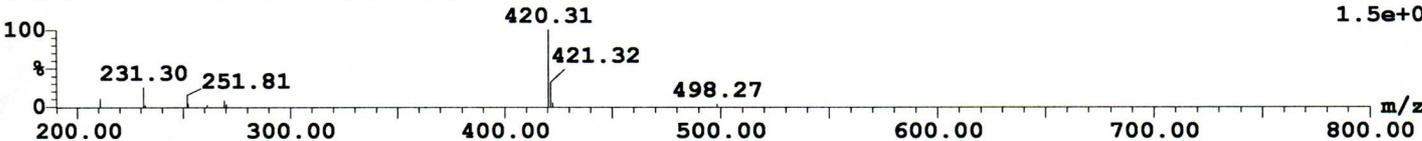
1:MS ES+  
1.4e+005



Peak ID Compound Time Mass Found  
3 Found 1.03 419.26

3: (Time: 1.03) Combine (111:114)

1:MS ES+  
1.5e+006



17{15}

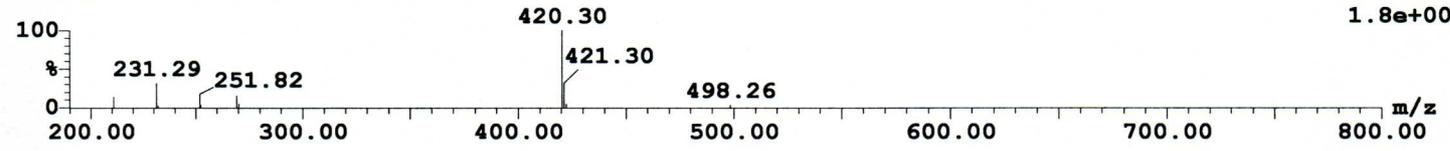
Printed: Wed Nov 02 14:34:00 2005

Sample Report (continued):

Peak ID Compound Time Mass Found  
4 Found 1.05 419.26

1:MS ES+  
1.8e+006

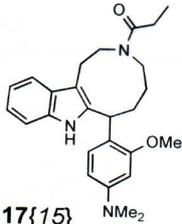
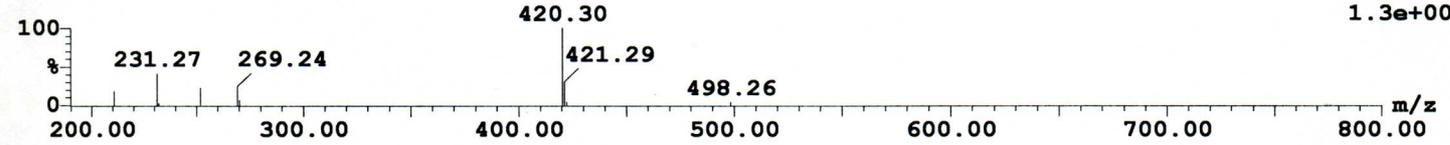
4:(Time: 1.05) Combine (112:116)



Peak ID Compound Time Mass Found  
5 Found 1.06 419.26

1:MS ES+  
1.3e+006

5:(Time: 1.06) Combine (114:117)



17{15}

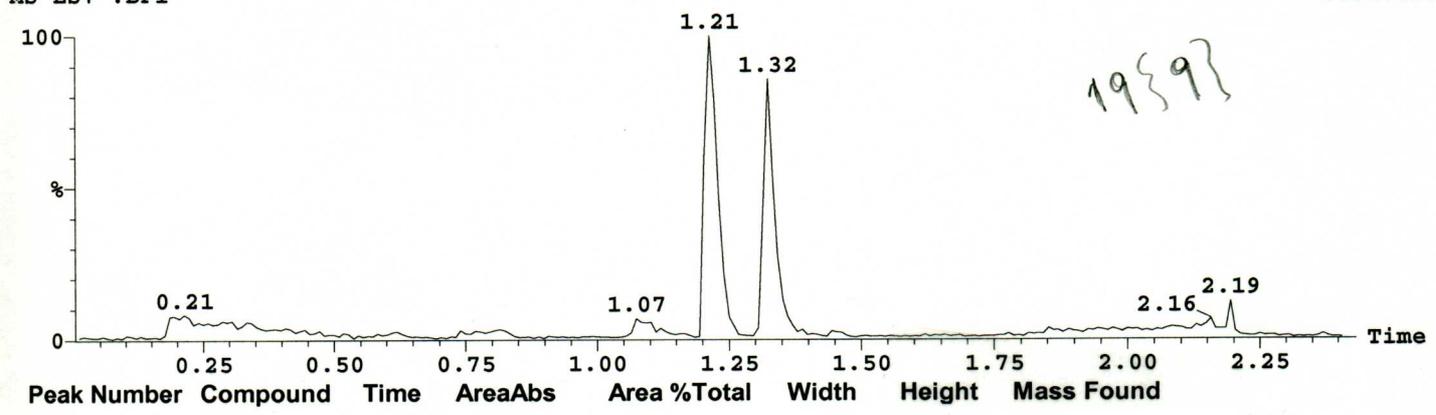
Chemical Formula: C<sub>26</sub>H<sub>33</sub>N<sub>3</sub>O<sub>2</sub>  
Exact Mass: 419.2573  
Molecular Weight: 419.5591

Printed: Wed Nov 02 15:17:32 2005

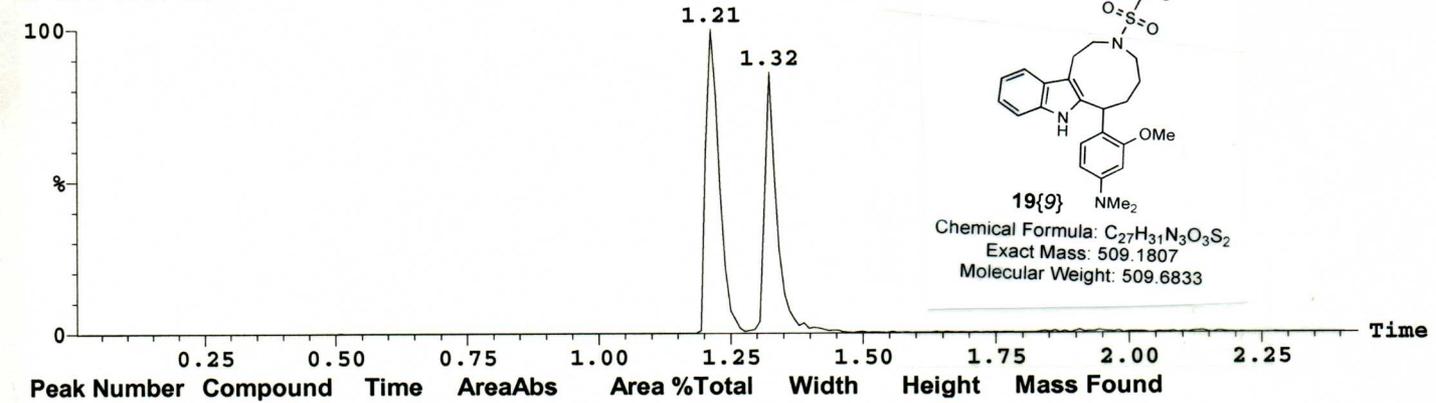
Sample Report:

Sample 11 Vial 4:10 ID A39310101B03-2311013 File J39310209 Date 27-Jul-2004 Time 19:56:44 Description 3508982

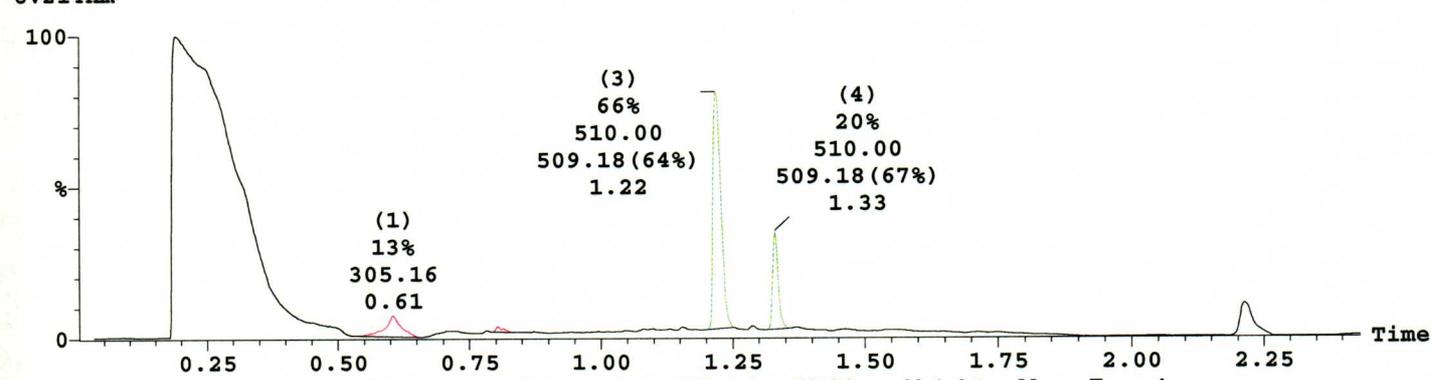
MS ES+ :BPI 8.0e+006



MS ES+ :510.18 8.0e+006



UV214nm 2.8e+005



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1		0.61	7e+002	12.81	0	2e+004	
2		0.80	9e+001	1.59	0	5e+003	
3	Found	1.22	4e+003	65.69	0	2e+005	509.18
4	Found	1.33	1e+003	19.92	0	9e+004	509.18

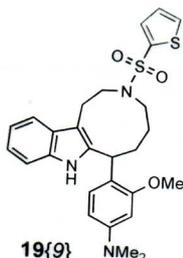
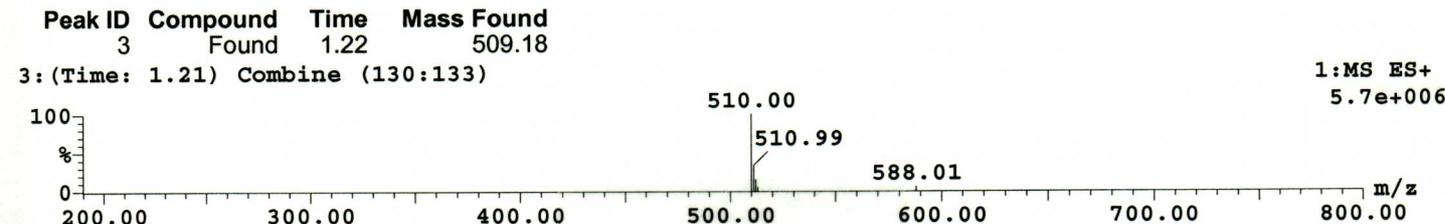
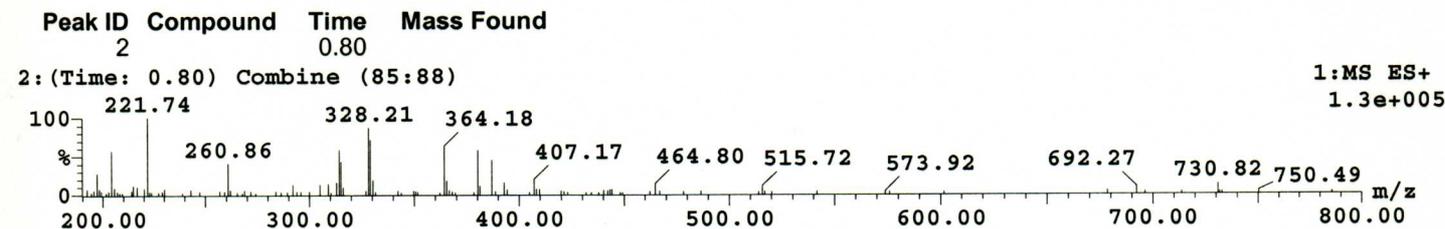
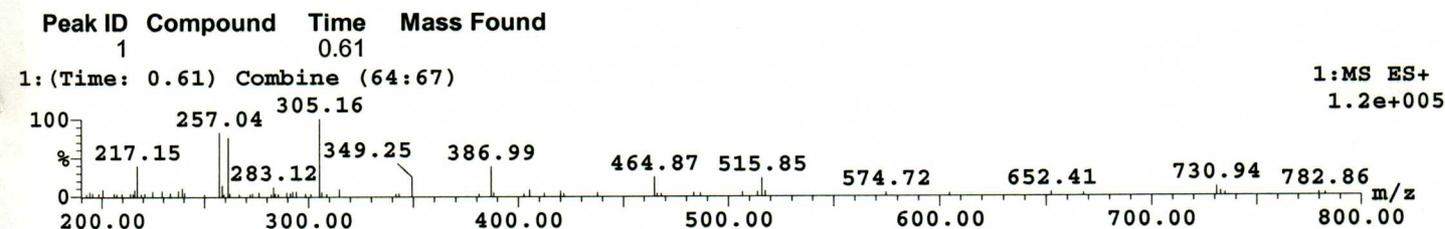
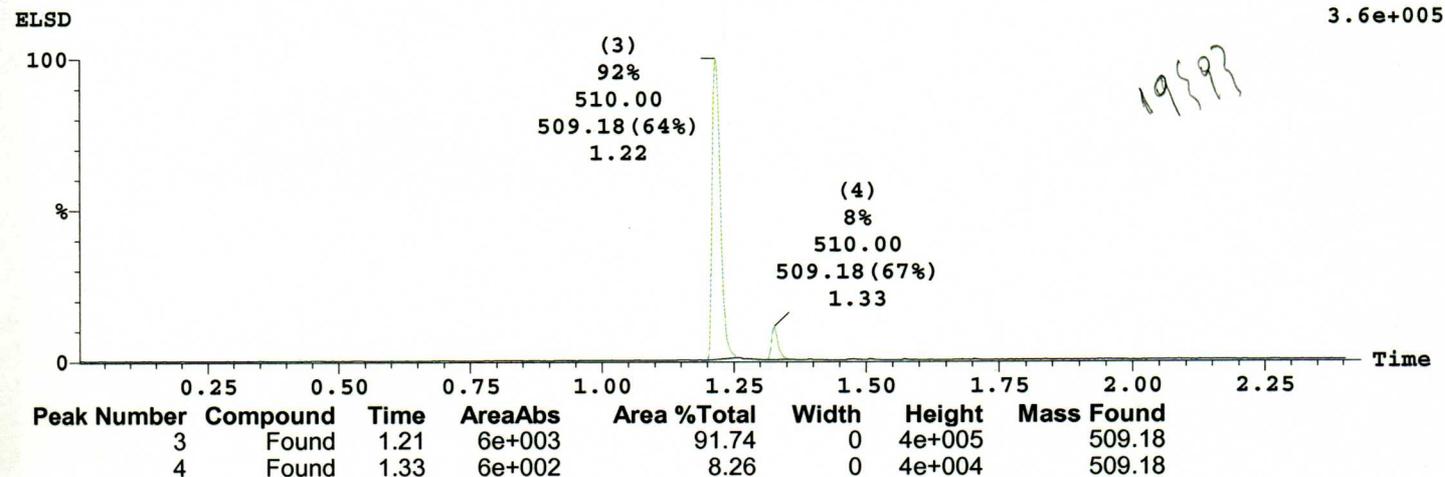
Sample: 11  
 File: J39310209  
 Description: 3508982

Vial: 4:10  
 Date: 27-Jul-2004

ID: A39310101B03-2311013  
 Time: 19:56:44

Printed: Wed Nov 02 15:17:32 2005

Sample Report (continued):



**19(9)**  
 Chemical Formula: C<sub>27</sub>H<sub>31</sub>N<sub>3</sub>O<sub>3</sub>S<sub>2</sub>  
 Exact Mass: 509.1807  
 Molecular Weight: 509.6833

19{93}

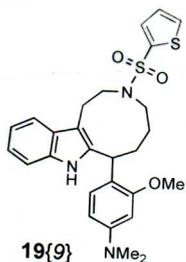
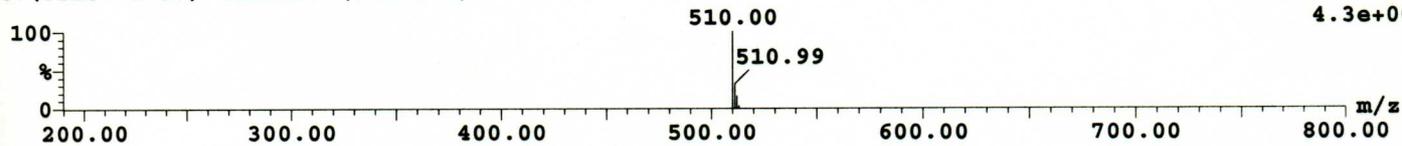
Printed: Wed Nov 02 15:17:32 2005

Sample Report (continued):

Peak ID	Compound	Time	Mass Found
4	Found	1.33	509.18

4: (Time: 1.33) Combine (142:145)

1:MS ES+  
4.3e+006



19{9}

Chemical Formula: C<sub>27</sub>H<sub>31</sub>N<sub>3</sub>O<sub>3</sub>S<sub>2</sub>  
Exact Mass: 509.1807  
Molecular Weight: 509.6833

195123

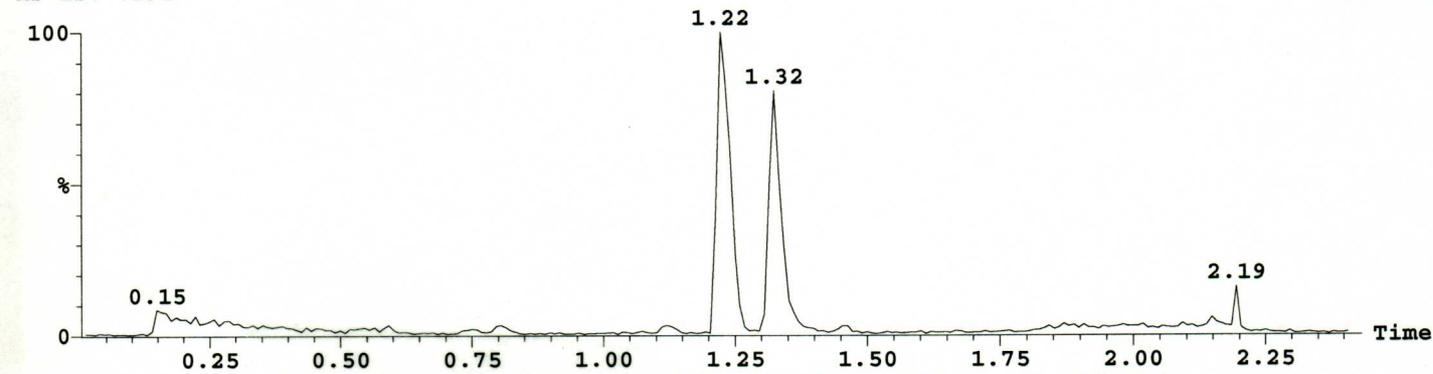
Printed: Wed Nov 02 15:17:59 2005

Sample Report:

Sample 14 Vial 4:15 ID A39310101B06-2311016 File J39310212 Date 27-Jul-2004 Time 20:05:33 Description 3508985

MS ES+ : BPI

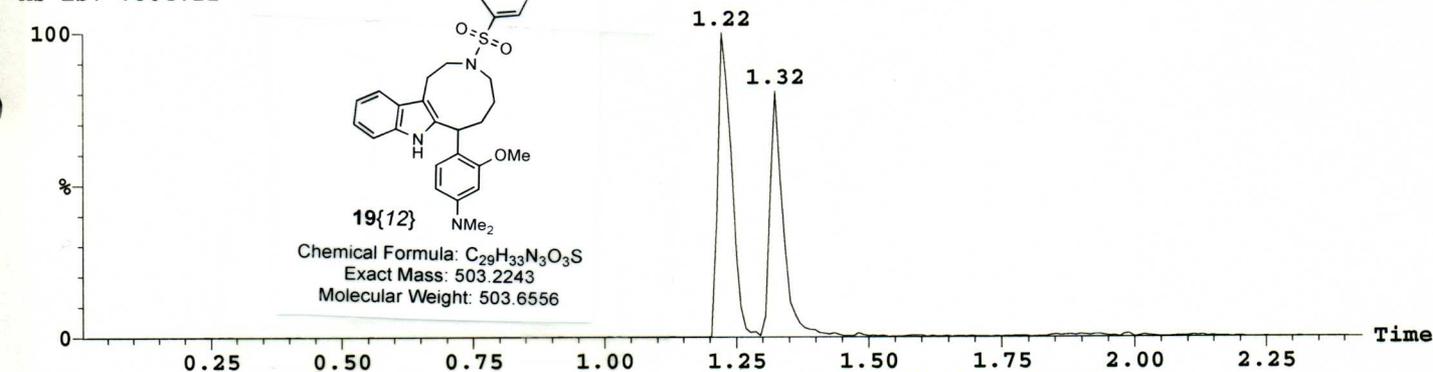
8.8e+006



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
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MS ES+ : 504.22

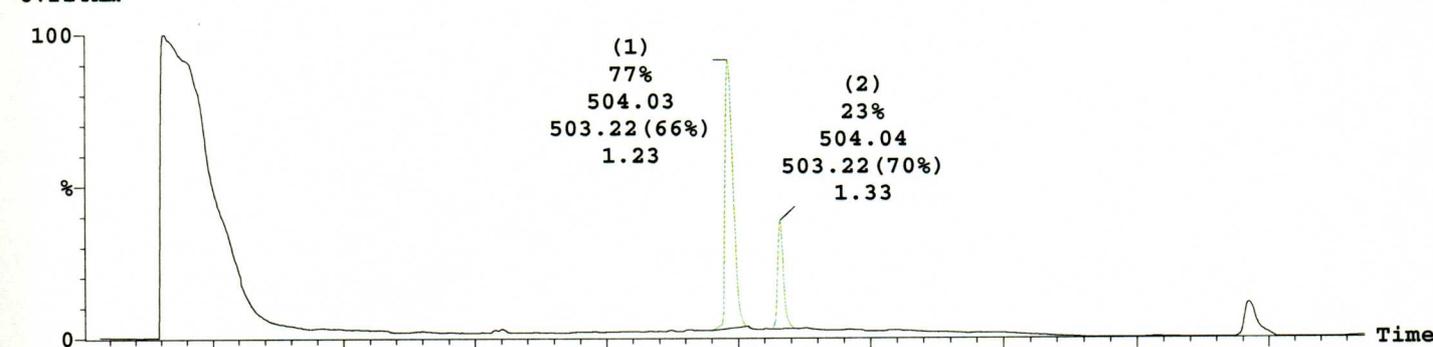
8.8e+006



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
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UV214nm

2.8e+005

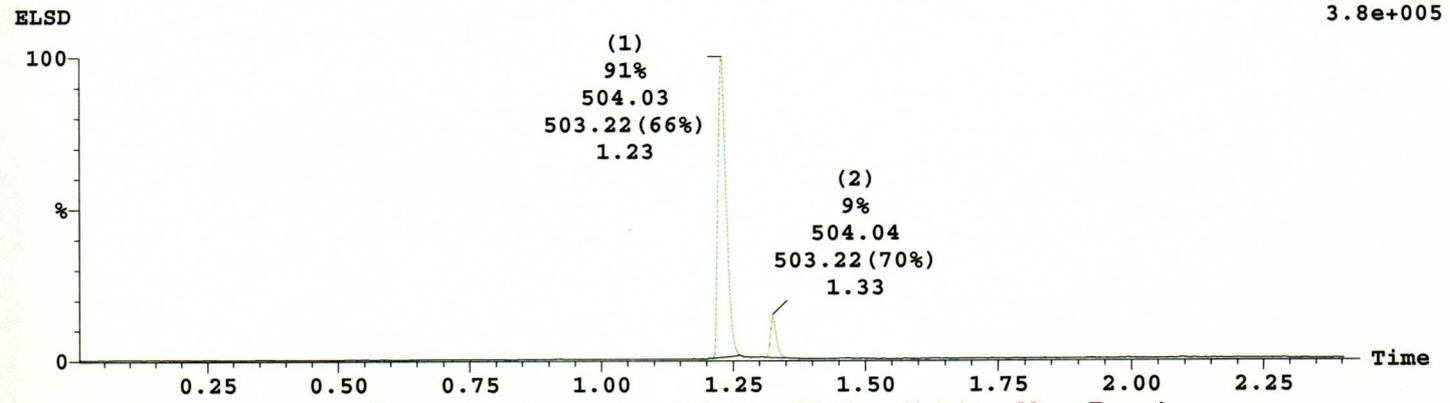


Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1	Found	1.23	4e+003	77.23	0	2e+005	503.22
2	Found	1.33	1e+003	22.77	0	1e+005	503.22

195123

Printed: Wed Nov 02 15:17:59 2005

Sample Report (continued):

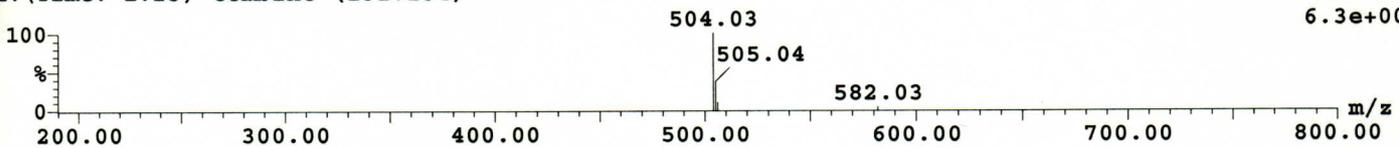


Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1	Found	1.23	7e+003	90.84	0	4e+005	503.22
2	Found	1.32	7e+002	9.16	0	5e+004	503.22

Peak ID Compound Time Mass Found  
1 Found 1.23 503.22

1: (Time: 1.23) Combine (131:134)

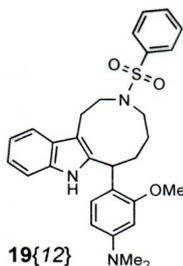
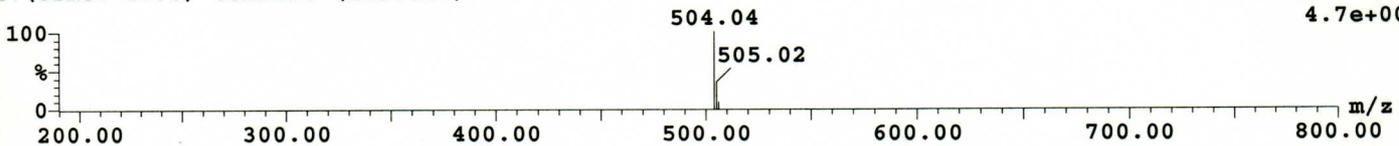
1: MS ES+  
6.3e+006



Peak ID Compound Time Mass Found  
2 Found 1.33 503.22

2: (Time: 1.33) Combine (142:145)

1: MS ES+  
4.7e+006



Chemical Formula: C<sub>29</sub>H<sub>33</sub>N<sub>3</sub>O<sub>3</sub>S  
Exact Mass: 503.2243  
Molecular Weight: 503.6556

19{20}

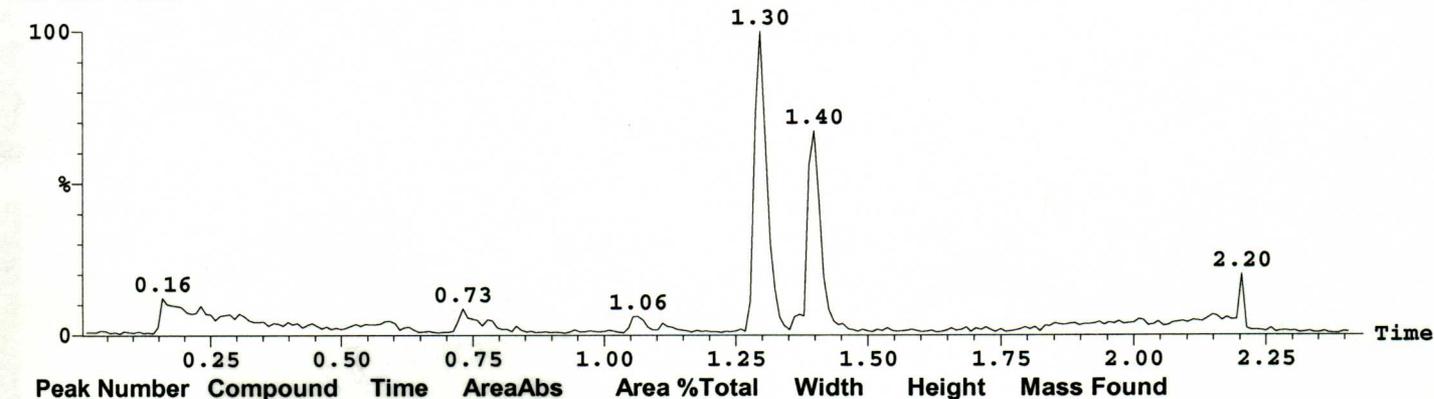
Printed: Wed Nov 02 15:18:18 2005

Sample Report:

Sample 22 Vial 4:23 ID A39310101D02-2311024 File J39310220 Date 27-Jul-2004 Time 20:29:02 Description 3508993

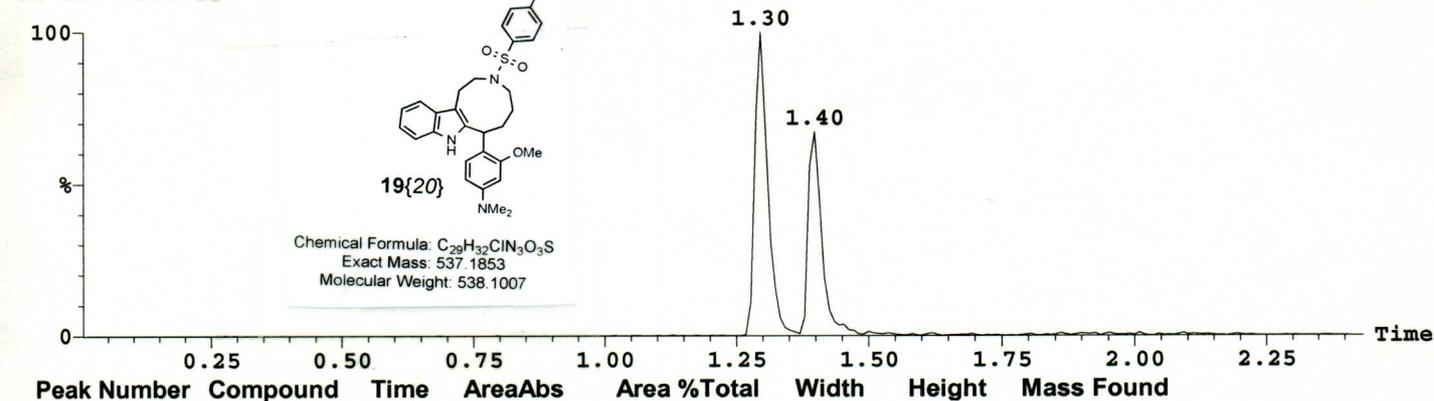
MS ES+ : BPI

6.0e+006



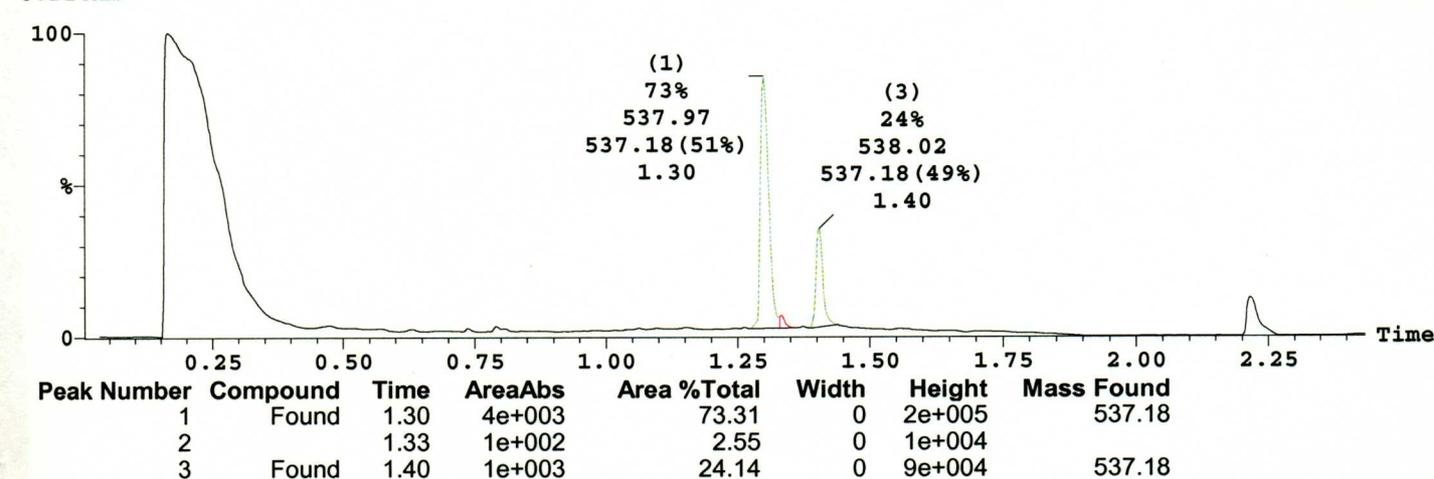
MS ES+ : 538.18

6.0e+006



UV214nm

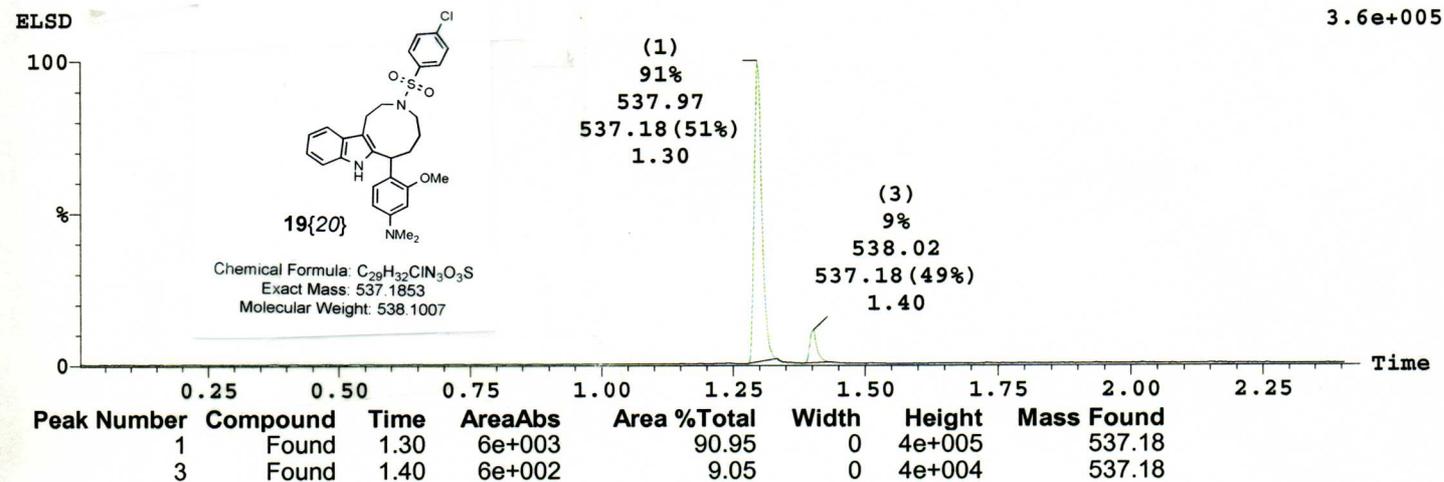
2.8e+005



19{20}

Printed: Wed Nov 02 15:18:18 2005

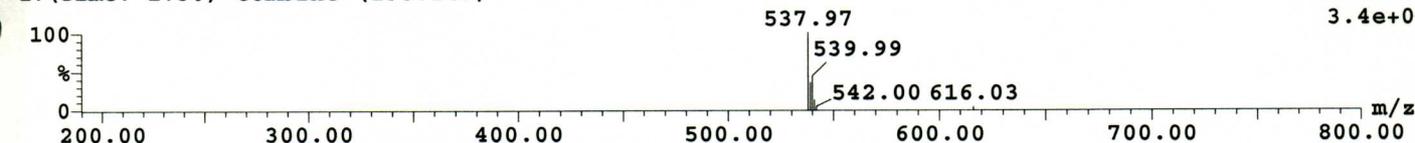
Sample Report (continued):



Peak ID Compound Time Mass Found  
 1 Found 1.30 537.18

1: (Time: 1.30) Combine (138:142)

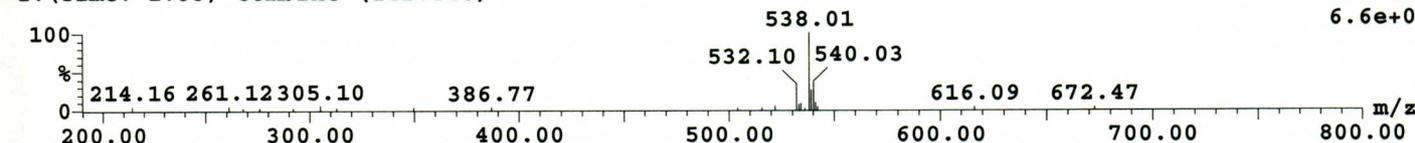
1: MS ES+  
 3.4e+006



Peak ID Compound Time Mass Found  
 2 Found 1.33

2: (Time: 1.33) Combine (142:146)

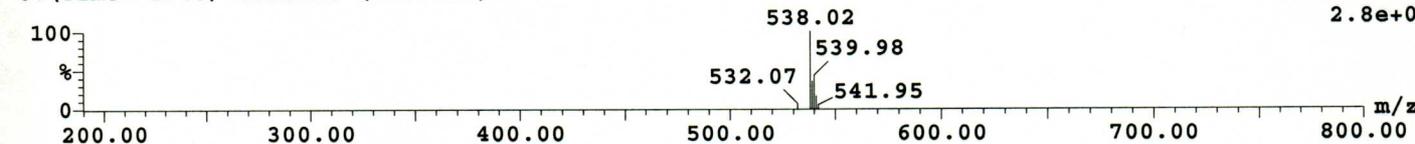
1: MS ES+  
 6.6e+005



Peak ID Compound Time Mass Found  
 3 Found 1.40 537.18

3: (Time: 1.40) Combine (150:153)

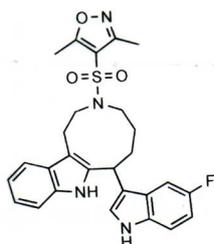
1: MS ES+  
 2.8e+006



205103

Printed: Mon Nov 07 09:48:03 2005

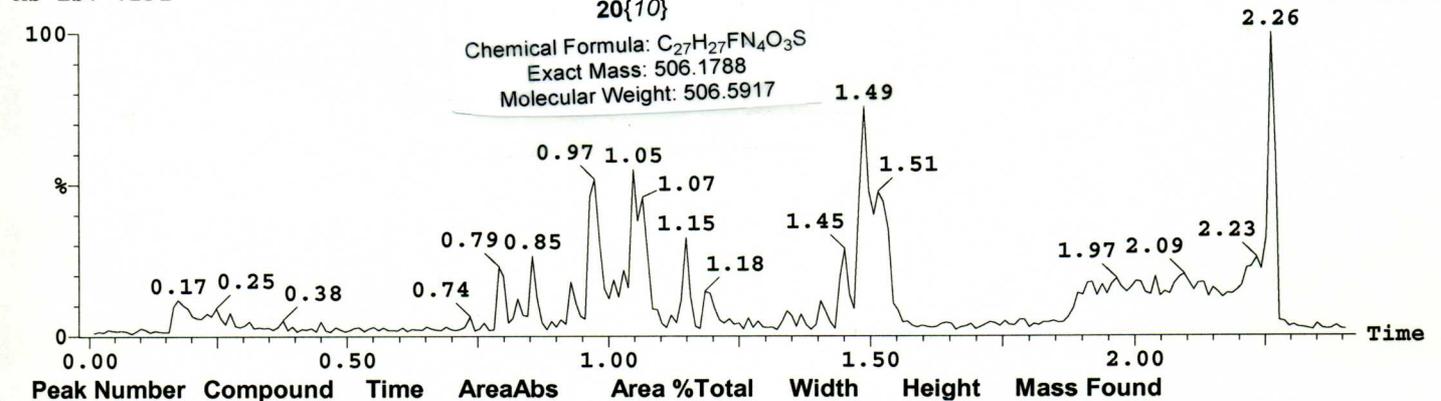
Sample Report:



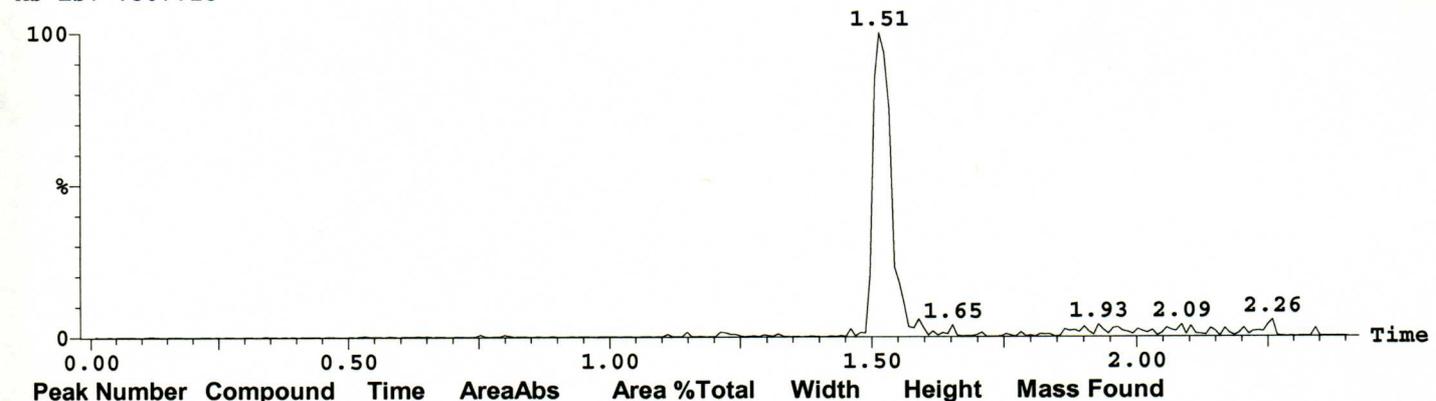
Sample 16 Vial 3:86 ID A39540101B04

17-Aug-2004 Time 01:08:13 Description 3546019

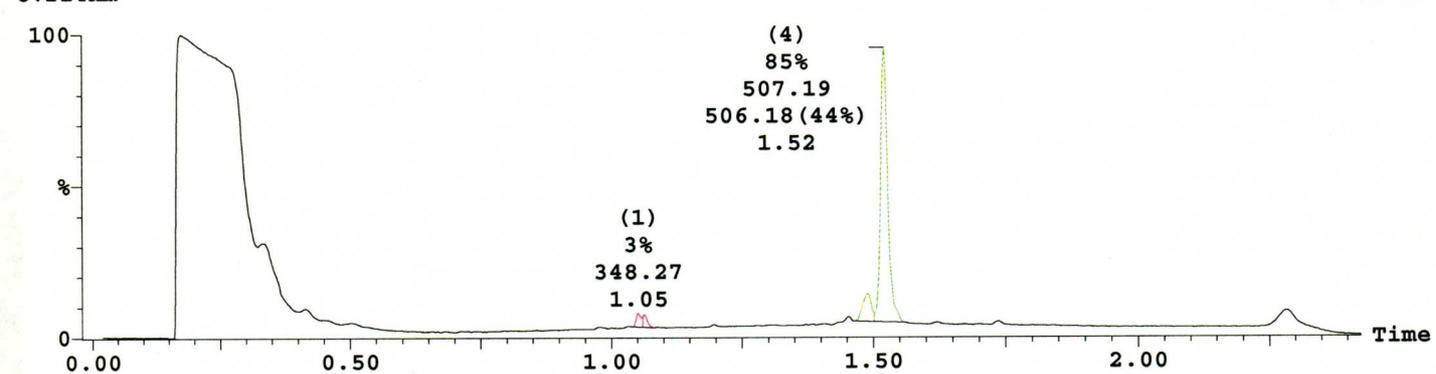
MS ES+ :BPI



MS ES+ :507.18



UV214nm



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1		1.05	2e+002	2.61	0	2e+004	
2		1.06	2e+002	2.75	0	1e+004	
3	Tentative	1.49	6e+002	10.13	0	3e+004	506.18
4	Found	1.52	5e+003	84.51	0	3e+005	506.18

Sample: 16  
File:K39540214  
Description:3546019

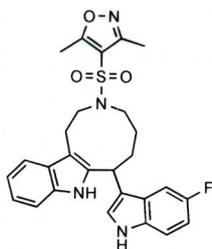
Vial:3:86  
Date:17-Aug-2004

ID:A39540101B04-2349193  
Time:01:08:13

205103

Printed: Mon Nov 07 09:48:03 2005

Sample Report (conti

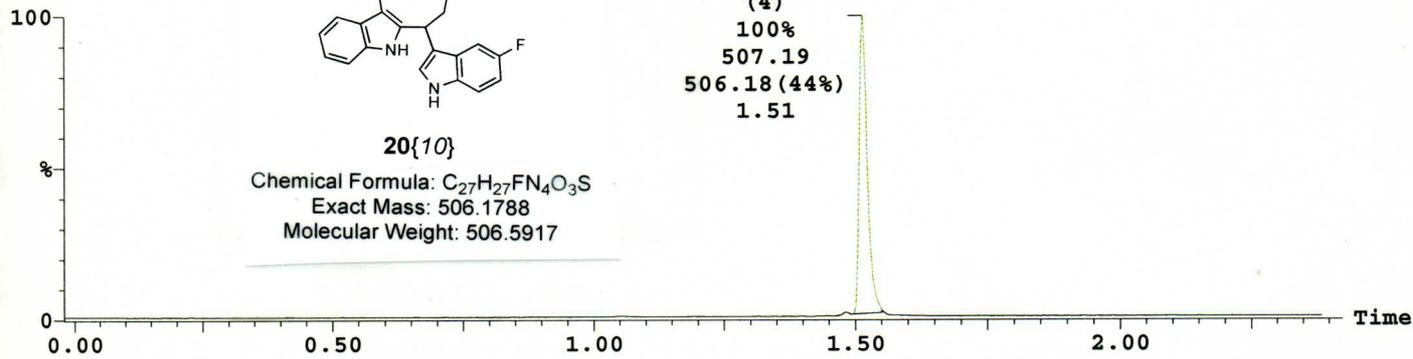


20{10}

Chemical Formula: C<sub>27</sub>H<sub>27</sub>FN<sub>4</sub>O<sub>3</sub>S  
Exact Mass: 506.1788  
Molecular Weight: 506.5917

3.3e+005

ELSD



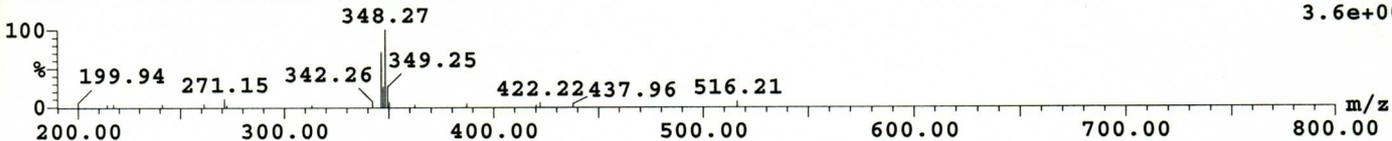
(4)  
100%  
507.19  
506.18 (44%)  
1.51

Peak Number	Compound Found	Time	AreaAbs	Area %Total	Width	Height	Mass Found
4	Found	1.51	6e+003	100.00	0	3e+005	506.18

Peak ID Compound Time Mass Found  
1 1.05

1:MS ES+  
3.6e+005

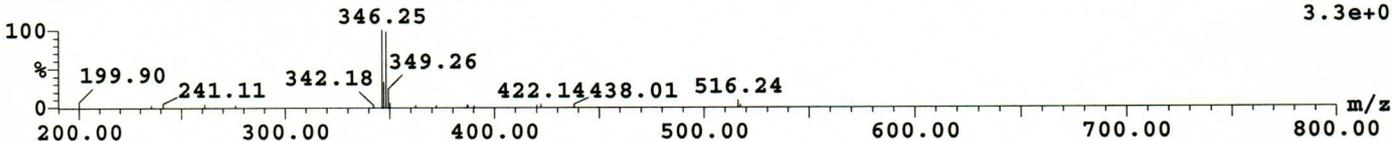
1:(Time: 1.05) Combine (113:116)



Peak ID Compound Time Mass Found  
2 1.06

1:MS ES+  
3.3e+005

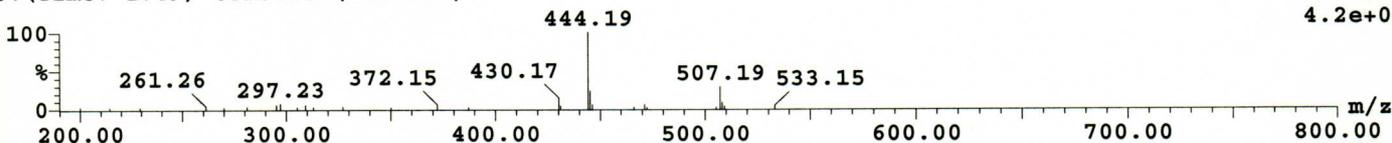
2:(Time: 1.06) Combine (114:117)



Peak ID Compound Time Mass Found  
3 Tentative 1.49 506.18

1:MS ES+  
4.2e+005

3:(Time: 1.49) Combine (160:164)



Peak ID Compound Time Mass Found  
4 Found 1.52 506.18

1:MS ES+  
4.2e+005

4:(Time: 1.51) Combine (163:166)

