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NMR 400 MHz CDCl3
Date: 25th March 2011

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**Elemental Composition Report**

**Single Mass Analysis**

Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

147 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

**Elements Used:**
- C: 0-35
- H: 0-35
- N: 0-6
- O: 0-6

UT0911_20 24 (0.541) Cm (24:26:75:78x0.010)

Aurigene Discovery Technologies, Hyderabad

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**Mass Table**

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>358.1541</td>
<td>358.1556</td>
<td>-1.5</td>
<td>-4.2</td>
<td>14.5</td>
<td>0.5</td>
<td>C22 H20 N3 O2</td>
</tr>
</tbody>
</table>

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1: TOF MS ES- 5.61e-06
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM  /  DBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
300 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35  H: 0-35  N: 0-6  O: 0-6  Br: 0-1

CPPS2
UT0911_1925 (0.579) Cm (25.28656.76x0.010)

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<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>436.0651</td>
<td>436.0661</td>
<td>-1.0</td>
<td>-2.3</td>
<td>14.5</td>
<td>2.8</td>
<td>C22 H19 N3 O2 Br</td>
</tr>
</tbody>
</table>
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
147 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35  H: 0-35  N: 0-6  O: 0-6

UT0911_18 26 (0.598) Cm (26:29-75:62x0.010)

Minimum: 5.0  5.0  0.0
Maximum: 50.0
Mass Calc. Mass mDa PPM DBE i-FIT Formula
372.1700 372.1712 -1.2 -3.2 14.5 4.5 C23 H22 N3 O2
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
147 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:
C: 0-35   H: 0-35   N: 0-6   O: 0-6

UT0911_17 25 (0.581) Cm (25:27-72.75x0.010)

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| Minimum: | 0.0 |
| Maximum: | 5.0 5.0 80.0 |
| Mass    | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 414.2174 | 414.2182 | -0.8 | -1.9 | 14.5 | 3.3 | C26 H28 N3 O2 |
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
147 formula(s) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:
C: 0-35  H: 0-35  N: 0-6  O: 0-6

CPPS5

UT0911_16 23 (0.525) Cm (23:28-71.76x0.010)

1: TOF MS ESI:
8.68e+00

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Minimum:  5.0  5.0  0.0
Maximum:  0.0

Mass  Calc. Mass  mDa  PPM  DBE  i-FIT  Formula
428.2336  428.2338  -0.2  -0.5  14.5  229.4  C27 H30 N3 O2
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
153 formula(s) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:
C: 0-30 H: 0-35 N: 0-4 O: 0-3 Cl: 0-3

UT0911_11 24 (0.541) Cm (24:28-74:62x0.010)

1: TOF MS ES- 2.53e+00

Aurigene Discovery Technologies, Hyderabad

Minimum:
Calc. Mass mDa PPM DBE i-FIT Formula
448.1773 448.1792 -1.9 -4.2 14.5 3.8 C26 H27 N3 O2 Cl

Maximum:
5.0 60.0
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
38 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-24    H: 0-25    N: 0-6    O: 0-3
CPPS-7

UT0911_10 21 (0.488) Cm (21:24-68.72x0.010)

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 Minimum: 5.0 5.0 0.0
Maximum: 80.0

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>344.1399</td>
<td>344.1382</td>
<td>-1.7</td>
<td>-4.9</td>
<td>14.5</td>
<td>6.6</td>
<td>C21 H18 N3 O2</td>
</tr>
</tbody>
</table>
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
25 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-24   H: 0-25   N: 0-5   O: 0-3
CPPS-8

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UT0911_05 19 (0.434) Cm (19:22:54:60:0.010)

Minimum:  5.0  5.0  0.0
Maximum:  5.0  5.0  80.0

Mass  Calc. Mass  mDa  PPM  DBE  i-FIT  Formula
360.1333  360.1348  -1.5  -4.2  14.5  1.8  C21 H18 N3 O3
## Elemental Composition Report

### Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
32 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-24   H: 0-25   N: 0-5   O: 0-3

![Chemical Structure](image)

UT0911_08 17 (0.399) Cm (17:22-64:71x0.010)

<table>
<thead>
<tr>
<th>Mass (m/z)</th>
<th>Calc. Mass</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>358.1543</td>
<td>358.1556</td>
<td>-1.2</td>
<td>-3.6</td>
<td>14.5</td>
<td>C22 H20 N3 O2</td>
</tr>
</tbody>
</table>

1: TOF MS ESI-
3.12e+0C
Elemental Composition Report

Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
185 formula(e) evaluated with 26 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35  H: 0-35  N: 0-5  O: 0-4  C: 0-1
CPPS-10

UT0911_07 20 (0.450) Cm (20:24-45:55x0.010)

Aurigene Discovery Technologies, Hyderabad

1: TOF MS ESI:
1.26e+00

Minimum: 5.0  100.0  80.0
Maximum: 378.0997  378.1009  -1.2  -3.2  14.5  2.1  C21 H17 N3 O2 Cl
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM  DBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
53 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0.25  H: 0.30  N: 0.4  O: 0.4  Br: 0.1

CPP21
UT0811_04 18 (0.415) Cm (18:23-56:60x0.010)

1: TOF MS ES- 3.25e+03

Aurigen Discovery Technologies, Hyderabad

Minimum:
Mass Calc. Mass mDa PPM DBE i-FIT Formula
436.0672 436.0666 1.1 2.5 14.5 897.9 C22 H19 N3 O2 Br
Elemental Composition Report

**Single Mass Analysis**

Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
52 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-24  H: 0-25  N: 0-6  O: 0-3

UT0911_02 17 (0.399) Cm (17:20-68:75x0.010)

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>286.1335</td>
<td>286.1344</td>
<td>-0.9</td>
<td>-3.1</td>
<td>13.5</td>
<td>1.4</td>
<td>C19 H16 N3</td>
</tr>
</tbody>
</table>
Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
51 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-24  H: 0-25  N: 0-5  O: 0-3
CPPS32

UT0911_03 19 (0.433) Cm (19:20)

Aurigene Discovery Technologies, Hyderabad

Minimum: 0.0  Maximum: 80.0

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>300.1490</td>
<td>300.1501</td>
<td>-2.1</td>
<td>-3.7</td>
<td>13.5</td>
<td>1.0</td>
<td>C20 H18 N3</td>
</tr>
</tbody>
</table>
**Elemental Composition Report**

**Single Mass Analysis**
- Tolerance: 5.0 PPM
- DBE: min = 0.0, max = 80.0
- Element prediction: Off
- Number of isotope peaks used for i-FIT = 3

**Monoisotopic Mass, Even Electron Ions**
- 77 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

<table>
<thead>
<tr>
<th>Elements Used:</th>
<th>C: 0-35</th>
<th>H: 0-35</th>
<th>N: 0-5</th>
<th>O: 0-4</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPPS-Suzuki</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

UT0911_05 20 (0.451) Cm (20:22:65:76x0.010)

![Chemical Structure](image)

Aurigene Discovery Technologies, Hyderabad

<table>
<thead>
<tr>
<th>Formula</th>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
</tr>
</thead>
<tbody>
<tr>
<td>C29 H25 N4 O3</td>
<td>477.1924</td>
<td>477.1927</td>
<td>-0.3</td>
<td>-0.6</td>
<td>19.5</td>
<td>3.6</td>
</tr>
</tbody>
</table>

Minimum: 5.0 5.0 0.0
Maximum: 5.0 80.0

1. TOF MS ES+ 8.55e+00
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
71 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35   H: 0-35   N: 0-5   O: 0-4

CPPS-SOG

UT0911_06 21 (0.490) Cm (21:26-43:56x0.010)

Aurigene Discovery Technologies, Hyderabad

1: TOF MS ES+ 1.45e+00

Minimum:
Maximum:
Mass  Calc. Mass  mDa  PPM  DBE  i-FIT  Formula
480.2276  480.2287  -1.1  -2.3  17.5  2.7  C30 H30 N3 O3