Copies of NMR spectra
Copies of NMR spectra
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Copies of NMR spectra
Copies of NMR spectra
Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications
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AR.No:ME0510/1520
Date:21st May 2010

5a

AR&D, Aurigene Discovery Technologies Ltd, Hyderabad
Instrument: Mercury Plus (Varian 400MHz)
Date & Time: Fri May 21 16:38:22 IST 2010

Copies of NMR spectra
Copies of NMR spectra
Copies of NMR spectra
Copies of NMR spectra
Copies of NMR spectra
Copies of NMR spectra
Copies of NMR spectra
Copies of NMR spectra
Copies of NMR spectra

[Image of NMR spectra with peaks labeled with chemical shifts, including 1H, 13C, and other resonances.]

5f

H O

ZN

O

C

Ph

NG-400 in CCl3

NMR: 0123/1132

Date: 13th Oct 2010
Copies of NMR spectra
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6b

[Chemical structure diagram of 6b]

ppm

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[Diagram of NMR spectra with various peaks labeled]
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Copies of NMR spectra
Copies of NMR spectra
Copies of NMR spectra
NMR-400 in CDCl₃
AR.No: ME0311/481
Date: 4th March, 2011

7i
**Mass Analysis Report**

**User Spectra**

<table>
<thead>
<tr>
<th>Fragmentor Voltage</th>
<th>Collision Energy</th>
<th>Ionization Mode</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>0</td>
<td>Esi</td>
</tr>
</tbody>
</table>

+ Scan (0.133 min) 100303015.d Subtract (1)

Counts (%) vs. Mass-to-Charge (m/z)

--- End Of Report ---
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
281 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-40  H: 0-55  N: 0-6  O: 0-6  Br: 0-1
APC-2
UT1210_109 11 (0.345) Cm (11:18-41:46)

![Chemical Structure](image)

<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>275.9984</td>
<td>275.9984</td>
<td>0.0</td>
<td>0.0</td>
<td>4.5</td>
<td>3.9</td>
<td>C8 H11 N3 O3 Br</td>
</tr>
</tbody>
</table>

Minimum: 1.0
Maximum: 5.0
Elemental Composition Report

**Single Mass Analysis**

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

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

Elements Used:
C: 0-30  H: 0-35  N: 0-5  O: 0-4  Br: 0-1

**UT1010_263** 9 (0.218) Cm (7:13-61:72)

<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>233.9874</td>
<td>233.9878</td>
<td>-0.4</td>
<td>-1.7</td>
<td>3.5</td>
<td>2.2</td>
<td>C6 H9 N3 O2 Br</td>
</tr>
</tbody>
</table>

Minimum: 5.0
Maximum: 5.0
80.0
Copies of HRMS spectra

Elemental Composition Report

Single Mass Analysis

Elemental composition analysis using the specified parameters.

1. **Elemental Composition**
   - C: 0.40
   - H: 0.55
   - N: 0.6
   - O: 0.6

2. **Formulas**
   - C11H14NO

3. **Isotope peaks**
   - Mass: 176.1078
   - Precision: ±0.0001

4. **Sample Information**
   - Formula: C11H14NO
   - Mass: 176.1078
   - Precision: ±0.0001

5. **Additional Information**
   - No further details provided in the image.

---

The image contains a chemical structure and a mass spectrum, indicating the analysis of a compound's elemental composition and mass accuracy.
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
111 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-40  H: 0-55  N: 0-6  O: 0-6
KSM-2B
UT1210_107 27 (0.841) Cm (24:27-57:91)

Minimum:
Maximum:
Mass         Calc. Mass  mDa  PPM  DBE  i-FIT  Formula
190.1240     190.1232    0.8  4.2  5.5  1.3  C12 H16 N O
**Elemental Composition Report**

**Single Mass Analysis**
Tolerance = 5.0 PPM  /  DBE: min = -1.0, max = 80.0  
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
244 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-40  H: 0-55  N: 0-6  O: 0-6  Br: 0-1
KSM-2C
UT1210_106 17 (0.547) Cm (17.26-49.56)

![Chemical Structure](attachment:structure.png)

**Mass**  **Calc. Mass**  **mDa**  **PPM**  **DBE**  **i-FIT**  **Formula**
248.1286  248.1287  -0.1  -0.4  6.5  2.6  C14 H18 N O3

Minimum:  5.0  5.0  -1.0
Maximum:  5.0  80.0

1: TOF MS ES+
5.72e+003

Copies of HRMS spectra
Elemental Composition Report

**Single Mass Analysis**

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron ions
214 formula(e) evaluated with 1 results within limits (up to 4 closest results for each mass)
Elements Used:
C: 0-25  H: 0-30  N: 0-5  O: 0-6  Br: 0-1

![Molecule Structure](image)

**Formula**

3a

<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>346.0190</td>
<td>346.0191</td>
<td>-0.1</td>
<td>-0.3</td>
<td>10.5</td>
<td>0.7</td>
<td>C15 H13 N3 O2 Br</td>
</tr>
</tbody>
</table>
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPm / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron ions
207 formula(e) evaluated with 2 results within limits (up to 4 closest results for each mass)
Elements Used:
C: 0-25  H: 0-30  N: 0-5  O: 0-6  Br: 0-1

MPPC-1
UT0910_103 21 (0.469) Cm (21:25-58:68)

```
<table>
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<tr>
<th>Mass</th>
<th>Calc. Mass</th>
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<th>FPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>360.0358</td>
<td>360.0348</td>
<td>1.0</td>
<td>2.8</td>
<td>10.5</td>
<td>1.1</td>
<td>C16 H15 N3 O2 Br</td>
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</tbody>
</table>
```
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
426 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-40  H: 0-55  N: 0-6  O: 0-6  Br: 0-1
BPPC-1C TDC-113
UT1210_105 13 (0.421) Cm (13:16-53:57)

Minimum:
Mass Calc. Mass mDa PPM DBE i-FIT  Formula
418.0415 418.0402 1.3 3.1 11.5 1.5  C18 H17 N3 O4 Br
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron ions
89 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30   H: 0-35   N: 0-5   O: 0-4
BPPC28001
UT1010_259 17 (0.399) Cm (17:21-67:72)

<table>
<thead>
<tr>
<th>Mass Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>376.2021</td>
<td>376.2025</td>
<td>-0.4</td>
<td>-1.1</td>
<td>12.5</td>
<td>C23 H26 N3 O2</td>
</tr>
</tbody>
</table>

Minimum: 5.0 5.0 -1.0
Maximum: 5.0 80.0

1: TOF MS ES+ 1.35e+00

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Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

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

Elements Used:
C: 0-30  H: 0-35  N: 0-5  O: 0-4
BPPC2/056
UT1010_254.20 (0.450) Cm (20:24:65:78)

Minimum: 5.0  Maximum: 5.0  Tolerance: 5.0

<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>362.1867</td>
<td>362.1869</td>
<td>-0.2</td>
<td>-0.6</td>
<td>12.5</td>
<td>0.3</td>
<td>C22 H24 N3 O2</td>
</tr>
</tbody>
</table>
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

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

Elements Used:
C: 0-30  H: 0-35  N: 0-5  O: 0-4

BPPC2002
UT1010_258 17 (0.398) Cm (17:22-65:74)

Minimum:  -1.0
Maximum:  5.0  5.0  80.0

Mass  Calc. Mass  mDa  PPM  DBE  i-FIT  Formula
368.1400  368.1399  0.1  0.3  16.5  20.1  C23 H18 N3 O2
## Elemental Composition Report

### Single Mass Analysis
- **Tolerance**: ±5.0 PPM  /  **DBE**: min = -1.0, max = 80.0
- **Element prediction**: Off
- **Number of isotope peaks used for i-FIT**: 3

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

Elements Used:
- C: 0-30
- H: 0-35
- N: 0-5
- O: 0-4

UT1010_253 17 (0.399) Cm (17:23-61:70)

<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>438.2169</td>
<td>438.2182</td>
<td>-1.3</td>
<td>-3.0</td>
<td>16.5</td>
<td>17.4</td>
<td>C28 H28 N3 O2</td>
</tr>
</tbody>
</table>
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

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

Elements Used:
C: 0-30   H: 0-35   N: 0-5  O: 0-4

BPPC2003
UT1010-257 20 (0.450) Cm (20:24-66:72)

Minimum:  
Maximum:  
Mass    Calc. Mass    mDa    PPM    DBE  i-FIT  Formula

372.1696  372.1712  -1.6  -4.3  14.5  1.4  C23 H22 N3 O2

Formula: C23 H22 N3 O2

1: TOF MS
2.57e
Elemental Composition Report

**Single Mass Analysis**

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
86 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30  H: 0-35  N: 0-5  O: 0-4

BPPC20004
UT1101_256 17 (0.399) Cm (17:17-66:74)

Minimum: 
Maximum: 

<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>390.1812</td>
<td>390.1818</td>
<td>-0.6</td>
<td>-1.5</td>
<td>13.5</td>
<td>2.2</td>
<td>C23 H24 N3 O3</td>
</tr>
</tbody>
</table>
**Elemental Composition Report**

**Single Mass Analysis**

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
90 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30   H: 0-35   N: 0-5   O: 0-4
BPPC2005
UT1010_255 18 (0.416) Cm (18:22-88:76)

![Structural formula](image)

<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>336.1346</td>
<td>336.1348</td>
<td>-0.2</td>
<td>-0.6</td>
<td>12.5</td>
<td>1.4</td>
<td>C19 H18 N3 O3</td>
</tr>
</tbody>
</table>
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

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

Elements Used:
C: 0-30  H: 0-35  N: 0-5  O: 0-4

MPPC21001
UT1010_259 17 (0.399) Cm (17.21-67.72)

Minimum:  Maximum:
5.0  5.0  -1.0  80.0

Mass  Calc. Mass  mDa  PPM  DBE  i-FIT  Formula
390.2103  390.2102  -0.4  -1.1  12.5  0.3  C24 H28 N3 O2
### Elemental Composition Report

**Single Mass Analysis**

- Tolerance = 100.0 PPM
- DBE: min = -1.0, max = 80.0
- Number of isotope peaks used for I-FIT = 3

**Monoisotopic Mass, Even Electron Ions**

<table>
<thead>
<tr>
<th>Mass (m/z)</th>
<th>PPM</th>
<th>I-FIT</th>
</tr>
</thead>
<tbody>
<tr>
<td>386.1884</td>
<td>0.00</td>
<td>1</td>
</tr>
<tr>
<td>386.1884</td>
<td>0.00</td>
<td>1</td>
</tr>
<tr>
<td>386.1884</td>
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</tr>
<tr>
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<td>1</td>
</tr>
<tr>
<td>386.1884</td>
<td>0.00</td>
<td>1</td>
</tr>
</tbody>
</table>

**Elements Used:**
- C: 0.30
- H: 0.36
- N: 0.05
- O: 0.4
- Si: 0.1

**178 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)**

**Formula:** C24H24N3O2

**Copies of HRMS spectra**
Elemental Composition Report

Single Mass Analysis
Tolerance = 10.0 PPM  /  DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron ions
179 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30  H: 0-35  N: 0-5  O: 0-4  I: 0-1

BPPC20001
UT1010_25017 (0.398) Cm (17:20-82:71)

Minimum:  -1.0
Maximum:   5.0  10.0  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>390.2181</td>
<td>390.2182</td>
<td>-0.1</td>
<td>-0.3</td>
<td>12.5</td>
<td>1.8</td>
<td>C24 H28 N3 O2</td>
</tr>
</tbody>
</table>
**Elemental Composition Report**

**Single Mass Analysis**
Tolerance = 5.0 PPM  /  DBE: min = -1.0, max = 80.0  
Element prediction: Off  
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
138 formula(e) evaluated with 1 results within limits (up to 4 closest results for each mass)
Elements Used:
C: 0-25  H: 0-30  N: 0-6  O: 0-6  : 0-1

BPPC3-001
UT0910_A1 31 (0.705) Cm (29:34:68:76)

<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>474.0664</td>
<td>474.0679</td>
<td>-1.5</td>
<td>-3.2</td>
<td>12.5</td>
<td>1.1</td>
<td>C21 H21 N3 O2 I</td>
</tr>
</tbody>
</table>
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
175 formula(e) evaluated with 1 results within limits (up to 4 closest results for each mass)
Elements Used:
C: 0-30   H: 0-30   N: 0-6   O: 0-6   I: 0-1

BPPC3-006
UT0910_A3 30 (0.688) Cm (30:34-72:80)

Minimum:  
Maximum:  5.0  5.0  80.0

Mass  Calc. Mass  mDa  PPM  DBE  i-FIT  Formula
460.0508  460.0522  -1.4  -3.0  12.5  0.4  C20 H19 N3 O2 I
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monocistotic Mass, Even Electron ions
172 formula(e) evaluated with 1 results within limits (up to 4 closest results for each mass)

Elements Used:
C: 0-30  H: 0-30  N: 0-5  O: 0-6  I: 0-1

BPPC3-02
UT0910_A7 25 (0.580) Cm (25:30-70:78)

Minimum:
Maximum:
Mass  Calc. Mass  mDa  PPM  DBE  i-FIT  Formula
466.0060  466.0053  0.7  1.5  16.5  0.1  C21 H13 N3 O2 I
Elemental Composition Report

**Single Mass Analysis**

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
266 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-40   H: 0-65   N: 0-4   O: 0-5   I: 0-1

BPPC3-007 TDC-113
UT1210_103 15 (0.469) Cm (15:20:49:55)

<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>536.0854</td>
<td>536.0835</td>
<td>1.9</td>
<td>3.5</td>
<td>16.5</td>
<td>1.2</td>
<td>C26H23N3O2I</td>
</tr>
</tbody>
</table>

Minimum: 5.0  Maximum: 80.0
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
188 formula(e) evaluated with 1 results within limits (up to 4 closest results for each mass)
Elements Used:
C: 0-30  H: 0-30  N: 0-5  O: 0-6  I: 0-1

BPPC3-003
UT0910_A4 23 (0.524) Cm (23:28-73:82)

<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>470.0374</td>
<td>470.0366</td>
<td>0.8</td>
<td>1.7</td>
<td>14.5</td>
<td>0.2</td>
<td>C21 H17 N3 O2 I</td>
</tr>
</tbody>
</table>
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DEBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
155 formula(e) evaluated with 1 results within limits (up to 4 closest results for each mass)
Elements Used:
C: 0-30   H: 0-30   N: 0-5   O: 0-6   I: 0-1

MPPC3-001
UTO910_A5 24 (0.541) Cm (24:29-78:83)

Minimum:
5.0 5.0  -1.0

Maximum:
5.0 5.0  80.0

Mass  Calc. Mass  mDa  PPM  DEBE  i-FIT  Formula
488.0836 488.0835 0.1 0.2 12.5 4.8  C22 H23 N3 O2 I

6f
Elemental Composition Report

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
122 formula(s) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30  H: 0-35  N: 0-5  O: 0-4  I: 0-1

MPPC3002
CT1010_249 25 (0.580) Cm (25:28:69:80)

Minimum: 5.0  10.0  80.0
Maximum: 1.0

<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>
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</thead>
<tbody>
<tr>
<td>484.0546</td>
<td>484.0522</td>
<td>2.4</td>
<td>5.0</td>
<td>14.5</td>
<td>1.6</td>
<td>C22 H19 N3 O2 I</td>
</tr>
</tbody>
</table>
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
128 formula(e) evaluated with 1 results within limits (up to 4 closest results for each mass)
Elements Used:
C: 0-30  H: 0-30  N: 0-5  O: 0-6  I: 0-1

BPPC3C-001
UT0910_A6 28 (0.632) Cm (27.36-69.80)

<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>
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<tbody>
<tr>
<td>548.0877</td>
<td>546.0890</td>
<td>-1.3</td>
<td>-2.4</td>
<td>13.5</td>
<td>0.6</td>
<td>C24 H25 N3 O4 I</td>
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</tbody>
</table>

548.0877
Elemental Composition Report

**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.0, 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 1 results within limits (up to 4 best isotopic matches for each mass)

**Elements Used:**
C: 0-35  H: 0-45  N: 0-6  O: 0-5
BPPC4-SOG-001
UT1010_270 14 (0.325) Cm (14.25-57.68)

![Chemical Structure](image)

**Peak Details:**

<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>442.2493</td>
<td>442.2495</td>
<td>-0.2</td>
<td>-0.5</td>
<td>14.5</td>
<td>0.3</td>
<td>C28 H32 N3 O2</td>
</tr>
</tbody>
</table>
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
186 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35  H: 0-45  N: 0-6  O: 0-6
BPPC4-SOG-002
UT1010_259 18 (0.416) Cm (17.26-57.67)

Mass  Calc. Mass  mDa  PPM  DBE  i-FIT  Formula
434.1855  434.1869  -1.4  -3.2  18.5  5.2  C28 H24 N3 O2

1: TOF MS ES+
3.90e-02
Copies of HRMS spectra

Elemental Composition Report

Single Mass Analysis

Elemental Mass Analysis

Tolerance = 5.0 PPM / DBE: min. = 10.0, max. = 80.0

Element prediction: Off

Number of isotope peaks used for I-FIT = 3

Monoisotopic Mass. Even Electron Loss

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

Elements Used:

C: 0-35, H: 0-45, N: 0-6, O: 0-6

BPPC4-SU-014 C10H10,N2 O2

UT0100,268.14 (0.328) Cn (14:20-54:93)

Minimum:

Mass Calcd. Mass m/e PPM DBE I-FIT

Maximum:

174.1286 212.0220 278.0340 317.4691 339.1282 467.2082

% 0

100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000

C28 327.94 03
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ion
188 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35  H: 0-45  N: 0-6  O: 0-6
BPPC4-SU-002
UT1010_267_15 (0.342) Cm (14:19-57:68)

Minimum: 5.0  5.0  -1.0
Maximum: 90.0

Mass  Calc. Mass  mDa  PPM  DBE  i-FIT  Formula
459.1449  459.1457  -0.8  -1.7  21.5  2.9  C28 H19 N4 O3
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM  DBE: min = -1.0  max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
112 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35  H: 0-45  N: 0-5  O: 0-4
BPPC4-HE-001
UT1010_265 16 (0.360) Cm (13:20:66:65)

Minimum:
Maximum:

Mass  Calc. Mass  mDa  FPP  DBE  i-FIT  Formula
446.2082  446.2080  0.2  0.4  14.5  0.9  C26 H28 N3 O4
Elemental Composition Report

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
99 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35  H: 0-45  N: 0-5  O: 0-4
BPPC4-HE-002
UT1010_26416 (0.380) Cm (16.20-66.84)

<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>474.2368</td>
<td>474.2393</td>
<td>-2.5</td>
<td>-5.3</td>
<td>14.5</td>
<td>6.0</td>
<td>C28 H32 N3 O4</td>
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</tbody>
</table>
Mass Analysis Report

User Spectra

Fragmentor Voltage  Collision Energy  Ionization Mode
135  0  ESI

+ Scan (0.258 min) 110224017.d Subtract (1)

Counts (%) vs. Mass-to-Charge (m/z)

--- End Of Report ---
Mass Analysis Report

User Spectra

--- End Of Report ---
Mass Analysis Report

User Spectra

--- End Of Report ---