Copies of spectra
Elemental Composition Report

Single Mass Analysis
Tolerance = 10.0 ppm * DBE: min = -5.0, max = 00.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoclonal Mass, Even Electron Ion
24 formulae calculated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-20 H: 0-20 O: 0-5 Na: 0-1

13191902413 (0.393) Cm (19.19)

Mass Calc. Mass PPM DBE i-FIT Formula
243.0613 243.0633 -2.0 -0.2 6.5 n/a C12 H12 O6 Na

TMS-408 Cyclic Ratio = 2 in DMSO

NMR-Green
ms: macromol/LCD
analysis: xiaodub
case: 11ch 6cm.3173

melting: 2115
m.p.: 44.12
exp.: 62 ppm
Elemental Composition Report

Single Mass Analysis

Tolerance = 6.0 PPM / DRE: min = -5.0, max = 80.0
Element prediction: OFF
Number of isotope peaks used for I/FIT = 4

Monodisperse Mass, Even Electron Ions
27 benzylidenevalerolactone within limits (up to 10 best isotopic matches for each mass)
Elements Used:
C: 0.0-20 H: 0.0-20 N: 0.2 O: 0.4
Cyclic Ether 3
151106924 7 (0.352) Cm (0.74)

---

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>Delta</th>
<th>ppm</th>
<th>Intensity</th>
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</thead>
<tbody>
<tr>
<td>233.0826</td>
<td>233.0824</td>
<td>1.2</td>
<td>5.1</td>
<td>9.5</td>
</tr>
</tbody>
</table>
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 ppm / DBE: min = -6.0, max = 80.0
Elemental prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron loss
4 formula(s) evaluated with 7 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:
C: 0-13  H: 0-12  O: 0-5

MC: EMER OF B13
113127505S 11 (0.34) C11 (11-12-33)

Mass: C11 O2

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc.</th>
<th>Exp.</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
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</thead>
<tbody>
<tr>
<td>119.0560</td>
<td>119.0560</td>
<td>119.0560</td>
<td>119.0560</td>
<td>119.0560</td>
<td>C11 O2</td>
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</tbody>
</table>
Elemental Composition Report

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

Monoisotopic Mass, Even Electron Ion
5 formula(s) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 1.04%  H: 0.15%  O: 0.0

Molecular Mass: 140.01612 12.01119 Cm [12:20:30]

Mass  Calc. Mass  mDa  PPM  DBE  I-FIT  Formula
219.0654  219.0657  -0.3  -1.4  7.5  12 8  C12 H16 O8
Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 50.0
Element precision: 18
Number of isotopic peaks used for I/FIT = 2

Monoisotopic Mass. From Electron Ionization

Elements Used:
C 0.0-15 H 0.4 O 0.4 Cl 0.1

THERMAL Mass 237.0322 (C10 H22 O3 Cl)

Isotopic Distribution

<table>
<thead>
<tr>
<th>Mass</th>
<th>Rel. Abundance</th>
</tr>
</thead>
<tbody>
<tr>
<td>237.0322</td>
<td>0.4</td>
</tr>
<tr>
<td>237.0318</td>
<td>1.7</td>
</tr>
<tr>
<td>237.3218</td>
<td>7.5</td>
</tr>
<tr>
<td>237.3222</td>
<td>1.1</td>
</tr>
</tbody>
</table>

C10 H22 O3 Cl
NMR-2D Data

Compound: Cyclic ketone-1 in DMSO

NMR Data:
- Nucleus: H1
- B0: 600.12
- TE: 4.0 µs

Chemical Shift (ppm):
- 10.0
- 9.0
- 8.0
- 7.0
- 6.0
- 5.0
- 4.0
- 3.0
- 2.0
- 1.0

Structural Formula:

\[
\text{HO} - \text{C} - \text{O}
\]

[Image of an NMR spectrum with peaks and chemical shifts]
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DDBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for I-FIT = 4

Monoisotopic Mass, Even Electron Ions
9 formula(s) evaluated with 1 results within limits (up to 10 best isotopic matches for each mass)
Elements Used:
C: 0.20  H: 0.20  O: 0.40
Cyclc: Ketone
131/106/89 12.0.400 Cm (11.92-1.2)

<table>
<thead>
<tr>
<th>Mass</th>
<th>C</th>
<th>H</th>
<th>O</th>
<th>PPM</th>
<th>DDBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
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<td>173.0601</td>
<td>173.0603</td>
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<td>-1.3</td>
<td>7.5</td>
<td>n/a</td>
<td>C13 H9 O2</td>
<td></td>
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</tbody>
</table>

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Elemental Composition Report

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

Monoisotopic Mass, Even Electron Ions
8 formula(e) evaluated with 1 results within limits (up to 4 best isotope matches for each mass)
Elements Used:
C: 0-15  H: 0-15  O: 0-4
CYCLIC KETONE=2
140.01018 (0.212) C11 (7.8)

Minimum:
Maximum:

<table>
<thead>
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<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>I-FIT</th>
<th>Formulas</th>
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<td>2.5</td>
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<td>0.5</td>
<td>C12 H11 O3</td>
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</tbody>
</table>
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 ppm / DBE: min = -5.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Loss
44 formulas evaluated with 1 results within limits (up to 10 best isotope matches for each mass)
Elements Used:
C: 0-25  H: 0-35  N: 0-2  O: 0-4
Cyclic

Molecular Formula: C10 H8 N O2

Mass  Calcd. Mass  Delta ppm  i-FIT  Formula
174.0548  174.0555  -0.4  7.5  C10 H8 N O2
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 ppm / DDBE: min = 5.0, max = 80.0
Element prediction: SW
Number of isotopes peaks used for i-FIT = 3

Monoisotopic Mass, Exact Mass, Low abundance ions
17 formula(s) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used: C 0.15, H 0.15, N 0.2, O 0.4

Calc. Molar %: 1.072 Molar wt: 2.036 Gm (g)

[Further analysis details]
Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM  DBE: min = 5.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for IIT = 4

Monoisotopic Mass, Even Electron ions
273 formulas evaluated with 1 results within limits (up to 10 best isotope matches for each mass)
Elements Used:
C: 0-40  H: 0-40  N: 0-6  O: 0-6  Cl: 0-1
CYCLIC AMINE - X

Minimum:
Maximum:
Mass  Calc. Mass  MDL  PPM  DBE  I-FIT  Formula
204.0664  204.0661  0.3  1.5  7.5  4.3  C11 H10 N O3
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0
Element prediction: Off

Monochromatic Mass, Even Electron Ions
20 formula(s) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-15  H: 0-15  N: 0-2  O: 0-4
N-Me sample of 40
131286068 (1.17) Cm (8-10)

Minimum: Mass
Maximum: 5.0  5.0  80.0

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc.</th>
<th>Mean</th>
<th>Min</th>
<th>PPM</th>
<th>Error</th>
<th>Formula</th>
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<tbody>
<tr>
<td>188.0703</td>
<td>188.0712</td>
<td>-0.9</td>
<td>-4.8</td>
<td>7.5</td>
<td>C11 N10 H O2</td>
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</table>
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for S/IR = 4
Monoisotopic Mass, Even Electron Ions
20 formulas evaluated with 1 results within limits (up to 10 best isotopic matches for each mass)
Elements Used:
C: 2.0; H: 0.0; N: 0.0; O: 0.0
Name of S/CMe
1311/1825 17 (8.81%) Cn (7.19-1.17)

- Mass Calc. Mass ppm DBE 1-FIT Formula
  - 216.0836 216.0837 0.9 4.1 7.5 10.1 Cl2 H12 N03