Copies of spectra

Methyl 2-(2-chloro-1H-indol-3-yl)-2-oxoacetate

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = 4.5, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monosaccharide Mass, Even Electron ion
36 formula(s) evaluated with 1 results within limits (up to 4 best isotope matches for each mass)
Elements Used:
C: 0.15  H: 0.14  N: 0.2  O: 0.5  Cl: 0.1
1002/1806 15 (0.205) Cn (16.17-37.46) 500

Mass Calc. Mass Error DBE i-PIC Formula
238.0260  238.0271 -0.6  9.0  DHE 5  [M+H] Cl

Methyl 2-(2-Chloro-1H-indol-3-yl)-2-oxoacetate
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
23 formula(cq) evaluated with 1 results within limits (up to 4 best isobaric matches for each mass)
Elements Used:
C: 9.20 H: 0.15 N: 0.5 Cl: 0.3
308.0409
466.5854
308.0409
308.0406
9.0 0.3 11.5 5.3 Cl7 H12 N3 Cl3

NMR-610 C1360/CA79/011

Analyser: Rackham
Date: 06/06/2014

NMR: 600
Sp (MHz): 400.22
Sp: 400m
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 = 3

Monoisotopic Mass, Even Electron Ions
3 formula(s) evaluated with 1 results within limits (up to 10 best isotopic matches for each mass)
Elements Used:
C: 0.24
H: 0.20
N: 0.4

C10H6Cl2N2O (10.2718) cm (9.11-2831.83)

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>ppm</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>349.1463</td>
<td>349.1453</td>
<td>-1.0</td>
<td>-1.5</td>
<td>17.5</td>
<td>C12 H17 N4</td>
</tr>
</tbody>
</table>
Elemental Composition Report

Single Mass Analysis
Tolerance = 50 PPM
Element prediction: Off
Number of isotopic peaks used for i-FIT = 4

MassSpectrum Mass: Even Electron Ions
291 formula(s) evaluated with 1 results within limits (up to 10 best isotopic matches for each mass)
Elements Used:
C: 0.25  H: 0.25  N: 0.2  O: 0.2  S: 0.1  Br: 0.3

100%

Minimum: 5.0  Maximum: 80.0

Calc. Mass  PPM  DBE  i-FIT  Formula
345.1701  345.1715  -1.4  -0.1  13.5  2.1  C21 H21 N4 O

DMSO

NMR-639Hz
Ac:0.67  Me:0.85  Ac:0.65
Date: 30th Aug 2014
Elemental Composition Report

Mass Analysis

Element: C

Monoisotopic Mass, Even Electron Ions
9 formula(e) evaluated with 1 results within limits (up to 10 best isotopic matches for each mass)

Elements Used:
C: 0.75 H: 0.35 N: 0.5 O: 0.1

C10H11N1O1Cl1

Mass: 379.1543
Calc. Mass: 379.1559
Moa: 5.0
PPM: -2.6
DBS: 37.5
i-FIT: 5.2

Formula: C20 H19 N4 O
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-58  H: 0-24  N: 0-5
C18H13ClN3O4
14(30500)  M (8.05) Cn (41.53-110.132)

Minimum: -1.5
Maximum:  5.0  5.0  5.0
Mass Calc. Mass eDa  PPM  DBE  i-FIT  Formula
315.1609  315.1610  -0.1  -0.3  13.5  671.2  C20 H19 N4

HPLC:  81
PDF (mol%):  491.12
EQ  :  a2py1
Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for I-FIT = 3

Monoisotopic Mass, Even Electron Ions
5 formula(s) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-28   H: 0-20   N: 0-5
C10H11N4F4O2
1,412101217 (M+3) On (17.45)

1: TCP ME ES+
2.3Me+CO3

Minimum: -1.5
Maximum: 10.0

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>%DA</th>
<th>PPM</th>
<th>DBE</th>
<th>I-FIT</th>
<th>Formula</th>
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<tbody>
<tr>
<td>363.1621</td>
<td>363.1610</td>
<td>1.1</td>
<td>3.0</td>
<td>17.5</td>
<td>34.7</td>
<td>C24 H19 N4</td>
</tr>
</tbody>
</table>
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
3 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0.17  H: 0.12  N: 0.3  O: 0.1

Mass Calc. Mass mDa PPM DBE i-FIT Formula
260.0832 260.0824 0.8 3.1 13.5 2.1 C16 H10 N3 O
# Elemental Composition Report

## Single Mass Analysis
- **Tolerance:** 5.0 PPM  
- **DBE:** min = -1.5, max = 80.0
- **Element prediction:** Off
- **Number of isotope peaks used for i-FIT = 2**

### Monoisotopic Mass, Even Electron Ions
122 formula(e) evaluated with 1 result within limits (up to 10 best isotopic matches for each mass)

<table>
<thead>
<tr>
<th>Elements Used</th>
<th>C: 0-21 H: 5-13 N: 0-6 O: 0-5 S: 0-2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Canvas</td>
<td>C156H130N6O6S9 (6.5177) C11 (5.9372/6.508)</td>
</tr>
</tbody>
</table>

### Minimum
- **Mass**
- **Calc. Mass**
- **m/ε**
- **DBE**
- **i-FIT**
- **Formula**

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>m/ε</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>290.0751</td>
<td>290.0752</td>
<td>-0.1</td>
<td>-0.3</td>
<td>13.5</td>
<td>Cl7 H12 N3 S</td>
</tr>
</tbody>
</table>

**TOC-190-C108-C000C-027**

- **AX No:** HE1214.2514
- **Analyst:** WAMS B
- **Date:** May 10, 2014
- **Method:** 81
- **PMU (Imp):** 419.22
- **MS:** 39/210
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monosotopic Mass, Even Electron ions
28 formula(s) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)
Elements Used:
C: 0-24  H: 0-20  N: 0-5  Cl: 0-3
C21H20ClN2O2

Minimum:  5.0  5.0  80.0

Mass  Calcd. Mass  ppm  DBE  i-FIT  Formula
385.1207  385.1220  -1.3  -3.4  16.5  1.9  C21 H18 N4 Cl

Elemental Composition Report

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