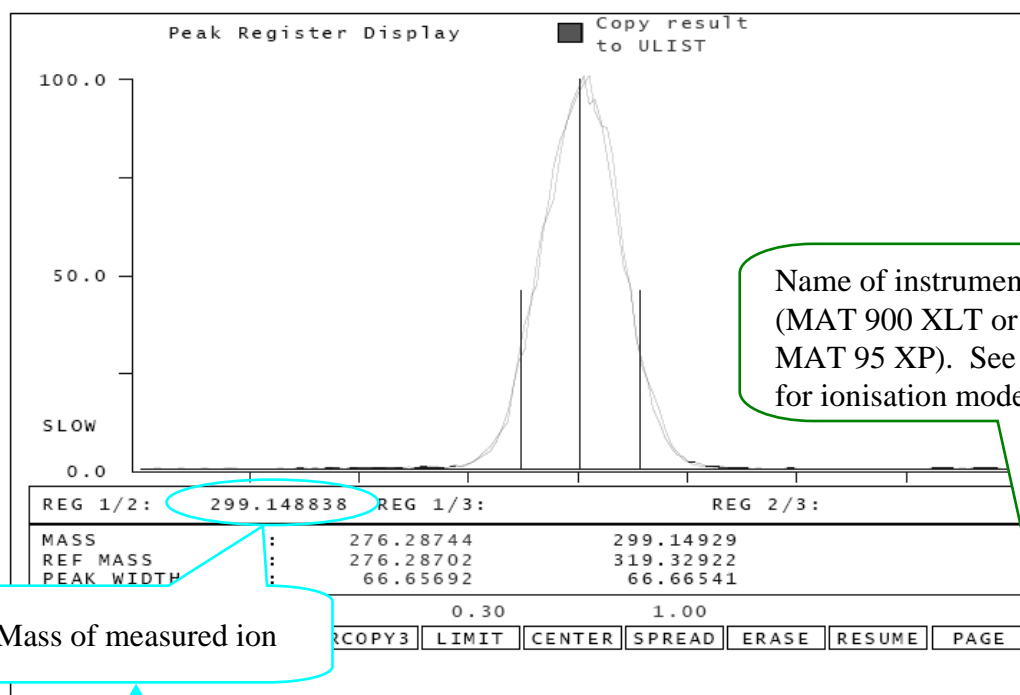


## Understanding your ESI, EI, CI and LSIMS (FAB) accurate mass data



Name of instrument (MAT 900 XLT or MAT 95 XP). See filename for ionisation mode.

Mass of measured ion

01/08/2008 9:43:56 AM

CMEP755MAT900

MAT 900 XLT

Expected elements of measured ion

Elemental limits

Charge state of measured ion.  
**Note:** To a calculated neutral mass, subtract the mass of the electron for the positive ion, add the mass of the electron for the negative ion!

Isotope:  
14 N  
16 O  
12 C  
1 H

| Min.                    | Max. |
|-------------------------|------|
| 0...                    | 10   |
| 0...                    | 15   |
| 0...                    | 30   |
| 0...                    | 60   |
| +- 5.00 ppm             |      |
| Tolerance Window:       |      |
| Db/Ring Equiv: -2.. 100 |      |
| Fits: 1000              |      |

N-Rule: Do not use  
Charge: 1

Calculated mass of ion will appear here

| Mass     | Theoretical Mass | Delta [ppm] | RDB  | Composition   |
|----------|------------------|-------------|------|---|
| 299.1488 | 299.1489         | -0.4        | 10.0 | C <sub>14</sub> H <sub>17</sub> C <sub>1</sub> N <sub>7</sub> |
|          | 299.1489         | -0.4        | 4.5  | C <sub>15</sub> H <sub>23</sub> C <sub>2</sub>                |
|          | 299.1476         | 4.1         | 5.0  | C <sub>13</sub> H <sub>21</sub> C <sub>2</sub> N <sub>3</sub> |
|          | 299.1476         | 4.1         | 10.5 | C <sub>12</sub> H <sub>15</sub> N <sub>10</sub>               |
|          | 299.1503         | -4.9        | 9.5  | C <sub>16</sub> H <sub>19</sub> C <sub>2</sub> N <sub>4</sub> |

Mass of measured ion

Difference between measured and calc. mass\*

RDB – rings and double bonds equivalent value

Possible formulae of measured ion. Your compound should be listed here!

\*Calculating the ppm error:

(Measured mass - Theoretical mass)

Theoretical mass

x 1,000,000