Intro to MS Resolution & Accuracy

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CHEM-5181  
Mass Spectrometry & Chromatography  
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Mass Spectrum

Signal intensity vs mass-to-charge ratio
Mass Analyzer Resolving Power

**Figure 1:** Mass accuracy determination and the FWHM method for determining resolution for a mass spectrometer measured at a given ion.

<table>
<thead>
<tr>
<th>True mass</th>
<th>400.00000</th>
</tr>
</thead>
<tbody>
<tr>
<td>Measured mass</td>
<td>400.0020</td>
</tr>
<tr>
<td>Difference</td>
<td>0.0020 or 2 mnu</td>
</tr>
<tr>
<td>Error</td>
<td>0.0020 / 400 = 5 ppm</td>
</tr>
<tr>
<td>Mass</td>
<td>500</td>
</tr>
<tr>
<td>Peak width (50%)</td>
<td>0.1</td>
</tr>
<tr>
<td>Resolution (FWHM)</td>
<td>500 / 0.1 = 5000</td>
</tr>
</tbody>
</table>

**Mass peak width (Δm_{50%})**
Full width of mass spectral peak at half-maximum peak height

**Mass resolution / Resolving Power (m / Δm_{50%})**
Quantifies ability to isolated single mass spectral peak

**Mass accuracy**
Mass accuracy is the difference between measured and actual mass

Figure from: M. P. Balogh, *LC-GC Europe*, 17(3), 152–159 (2004)

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**Argon**
Atomic Weight (Da): 39.948

<table>
<thead>
<tr>
<th>Atomic mass (m/u)</th>
<th>Abundance</th>
</tr>
</thead>
<tbody>
<tr>
<td>35.96754552</td>
<td>0.33%</td>
</tr>
<tr>
<td>37.9627325</td>
<td>0.06%</td>
</tr>
<tr>
<td>39.9623837</td>
<td>99.6%</td>
</tr>
</tbody>
</table>

**Calculate resolution and accuracy**
Mass Analyzer Resolution II

- Question: what is the resolution (FWHM definition) in both cases
  - if $m_1 = 50$ Da?
  - If $m_1 = 2500$ Da?

$(m_2 = m_1 + 1$ amu$)$

What Resolution do we really need?

- What resolution is really needed to distinguish these two overlapping ions, if we know that only these two ions are present?

A. $\chi = 0.4$
B. $\chi = 0.8$
C. $\chi = 1.2$
D. $\chi = 1.6$
E. $\chi = 2.0$

$\chi = \frac{\text{peak separation}}{\text{HWHM}}$
What Resolution do you really need?

\[ \chi = \text{peak separation} / \text{HWHM} \]

Clicker Q: A mass spectrometer with a resolution of 5000 should be capable of resolving isotopic peaks (e.g. \(^{12}\text{CH}_4\) vs \(^{13}\text{CH}_4\)) for singly charged species with \(m/z\):

(a) Of any value  
(b) Less than \(m/z\) 5000  
(c) Greater than \(m/z\) 5000  
(d) It depends on the type of mass spectrometer  
(e) I don’t know