Step 1: Custom peptide threshold setting for Orbitrap data (MS1 30,000 resolution) in Scaffold

Click on drop down arrow next to Peptide Threshold, select ‘Custom’

Note: select ‘Exclusive Spectrum Count’ for display of peptides per protein in Samples view (v 4.2.1)
Step 2: Custom peptide threshold setting for Orbitrap data (MS1 30,000 resolution) in Scaffold

Click on ‘New Threshold’
Step 3: Custom peptide threshold setting for Orbitrap data (MS1 30,000 resolution) in Scaffold

Configure threshold settings as shown; type name in ‘Name Peptide Threshold’ field and click on ‘Okay’ (settings will be saved for future use)

Note: select mass tolerance check box and enter ‘10’
Step 1: Custom peptide threshold setting for Low Resolution LTQ Ion Trap Data in Scaffold

- Click on drop down arrow next to Peptide Threshold, select ‘95%’
- Set ‘Min # Peptide’ to 2
- Note: select ‘Exclusive Spectrum Count’ for display of peptides per protein in Samples view (v 4.2.1)
# Measured Mass Deviation

## Example Calculations

<table>
<thead>
<tr>
<th>Error Expression</th>
<th>Fractional Error Expression</th>
<th>Multiply by:</th>
</tr>
</thead>
<tbody>
<tr>
<td>ppm</td>
<td>( \Delta / \text{Theoretical value} )</td>
<td>1,000,000</td>
</tr>
<tr>
<td>%</td>
<td>( \Delta / \text{Theoretical value} )</td>
<td>100</td>
</tr>
</tbody>
</table>

where \( \Delta = \text{Experimental (or observed) – Theoretical } m/z \) value

**Example:**

**Experimental/observed value** (*i.e.*, the data acquired by the mass spectrometer) = 1480.107 m/z

**Theoretical value** (calculated from periodic table, after the peak is identified) = 1480.028 m/z

**Delta** (\( \Delta \)) = 0.079

<table>
<thead>
<tr>
<th>Error Expression</th>
<th>Error Equation</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>ppm</td>
<td>((0.079/1480.028) \times 1,000,000)</td>
<td>53 ppm</td>
</tr>
<tr>
<td>%</td>
<td>((0.079/1480.028) \times 100)</td>
<td>0.0053%</td>
</tr>
</tbody>
</table>

A USEFUL REFERENCE: