Week 10- Advanced Imaging & Measurement Technology

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Waters- Part I: Molecular Weight

After selecting two adjacent charge-state peaks from Figure 1, the values used were **903.7148** and **875.4421 m/z**.

1) Calculate the charge state *z*

Using the adjacent Using the adjacent charge-state equation from the handout, with the peaks ordered as higher m/z first:

$$z = \frac{m_{Zn+1}}{m_{Zn} - m_{Zn+1}}$$

Substituting the values:

$$z = \frac{875.4421}{903.7148 - 875.4421}$$

$$z = \frac{875.4421}{28.2727}$$

$$z \approx 30.96 \approx 31$$

So:

- the peak at **903.7148** corresponds to $z = 31$
- the adjacent peak at **875.4421** corresponds to $z = 32$

2) Calculate the molecular weight of the protein

Use:

$$MW = z\left(\frac{m}{z} - 1.0073\right)$$

Using the peak at **903.7148** with $z = 31$:

$$MW = 31\ (903.7148 - 1.0073)$$

$$MW = 31\ (902.7075)$$

$$MW = 27983.93\ Da$$

Using the peak at **875.4421** peak with $z = 32$:

$$MW = 32\ (875.4421 - 1.0073)$$

$$MW = 32\ (874.4348)$$

$$MW = 27981.91\ Da$$

The experimental MW is around 2.798×10^4 Da

3) Calculate the accuracy

The theorical MW from Expasy was:

$$MW_{theorical} = 28006.60\ Da$$

We use the formula:

$$Accuracy = \frac{\left|MW_{experimental} - MW_{Theorical}\right|}{MW_{theorical}}$$

The MW experimental used is from z= 31 (27983.93 Da)

$$Accuracy = \frac{|27983.93 - 28006.60|}{28006.60}$$

$$Accuracy = \frac{|22.67|}{28006.60}$$

$$Accuracy = 8.094\ x\ 10^{-4}$$

$$Accuracy = 0.00081$$

As a percentage:

$$0.00081\ x\ 100 = 0.081\%$$

The value of 0.081% corresponds to the error.

Waters- Part II: Charge state

As calculated before, MW was around 28000 Da and the charge state of the peak is approximately 2800 m/z

So:

$$z \approx \frac{28000}{2800} \approx 10$$

Based on the formula:

$$m/z = \frac{MW + zH}{z}$$

Waters- Part III: Peptide Mapping - primary structure

Calculus for the figures 5b, 5c, and 6.

Figure 5b:

The principal peak value is: **525.76712 m/z**

The mass-to-charge ratio (m/z) of the peptide shown in Figure 5b is **525.77**

Charge state (z)

$$\Delta\,(m/z) = 526.25918 - 525.76712 = 0.49206$$

Calculus for (z)

$$z = \frac{1}{\Delta(m/z)}$$

$$z = \frac{1}{0.492} \approx 2$$

Peptide Mass (Single Charged)

Based on the formula:

$$MW = z\,(m/z\ - 1.0073)$$

So:

$$MW = 2(525.76712 - 1.0073)$$

$$MW = 2(524.75982)$$

$$MW = 1049.52\ Da$$

The molecular weight of a singly charged peptide was:

$$MW = 2(525.76712 - 1.0073) \approx 1049.52\ Da$$

Error (ppm)

Based on the formula:

$$Error\ (ppm) = \frac{|MW_{exp} - MW_t|}{MW_t}\ x\ 10^6$$

Calculus:

$$Error\ (ppm) = \frac{|1049.52 - 1050.52|}{1050.52}\ x\ 10^6$$

$$Error\ (ppm)\ \approx\ 952\ ppm$$

Waters IV- Oligomers

Calculus of CDMS and expected oligomers masses

Polypeptide Subunit Name	Calculus	Subunit Mass (kDa)	Subunit Mass (MDa)
7FU Decamer	$10\ x\ 340$	3400	3.4
8FU Didecamer	$20\ x\ 400$	8000	8.0
8FU 3-Decamer	$30\ x\ 400$	12000	12.0
8FU 4-Decamer	$40\ x\ 400$	16000	16.0

Waters V- Did I make GFP?

Based on previous questions, the values I obtained are:

- Theorical MW: 28006.60 Da → 28.0066 kDa ≈ 28.01 kDa
- Experimental MW: 27983.93 Da → 27.98393 kDa ≈ 27.98 kDa
- Accuracy (%): 0.081%

Transform accuracy error to ppm

$$1\% = 10\ 000\ ppm$$

So:

$$0.081\ x\ 10\ 000 = 810\ ppm$$

Or by using the Error ppm formula:

$$Error\ (ppm) = \frac{|MW_{exp} - MW_t|}{MW_t}\ x\ 10^6$$

$$= \frac{22.67}{28006.60}\ x\ 10^6 \approx 809\ ppm$$