SAMPLE MASS SPECTROMETRY

1. Principle of mass spectrometry

A student is asked to explain how a mass spectrometer can separate ions produced from a sample.

Question: Describe how mass spectrometry separates ions and explain why ions with different masses are detected at different positions on the detector.
Learning outcome: Understanding the basic principle of mass spectrometry.

2. Identifying the molecular ion peak

A compound gives a spectrum with a small peak at
m/z=74 and several smaller fragment peaks at lower
m/z values.

Question: Which peak is most likely the molecular ion peak, and why is it important in determining the identity of the compound?
Learning outcome: Identifying the molecular ion peak.

3. Determining relative molecular mass

A sample of an organic compound produces a molecular ion peak at m/z=88.

Question: What is the relative molecular mass of the compound, and what does this suggest about the size of the molecule?
Learning outcome: Using the molecular ion peak to determine relative molecular mass.

4. Fragmentation pattern analysis

A spectrum shows strong peaks at
m/z=15, 29, and 43, with a molecular ion peak at
m/z=58.

Question: What do the fragment peaks suggest about the structure of the compound, and how can fragmentation help identify functional groups?
Learning outcome: Interpreting fragmentation patterns.

5. Isotope pattern recognition

A compound containing chlorine gives two molecular ion peaks at

m/z=78 and
m/z=80 in a 3:1 ratio.

Question: What does this isotope pattern suggest about the element present, and how can this be used to support identification of the compound?
Learning outcome: Recognising isotopic patterns.

6. Isotopes and relative atomic mass

A bromine-containing compound produces two molecular ion peaks of similar intensity separated by 2 mass units.

Question: Explain why bromine gives this pattern and how it differs from the pattern produced by chlorine-containing compounds.
Learning outcome: Understanding isotopes and their effect on spectra.
7. Unknown compound identification
An unknown compound has a molecular ion peak at
m/z=46 and fragment peaks at m/z=31 and
m/z=29.

Question: Suggest a possible identity for the compound and justify your answer using the spectrum.
Learning outcome: Applying mass spectral data to identify an unknown substance.
8. Comparison of two compounds
Two compounds have the same molecular formula but different fragmentation patterns.

Question: What does this tell you about the structure of the compounds, and how can mass spectrometry distinguish between structural isomers?
Learning outcome: Understanding structural isomerism through fragmentation.
9. Effect of ionisation on samples
A student notices that only charged particles are detected in the mass spectrometer.

Question: Why must the sample be ionised before analysis, and what would happen if neutral molecules were not converted to ions?
Learning outcome: Understanding the role of ionisation.
10. Evaluating a spectrum in context
A forensics laboratory analyses a sample from a crime scene and obtains a spectrum matching a known compound.

Question: Explain how mass spectrometry can be used as an analytical tool in forensic science and why it is reliable for identifying substances.
Learning outcome: Applying mass spectrometry to a real-world context.