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# Quantitative Elemental and Functional-Group Analysis

Practical 19 - Practical study

## Aim

To connect elemental and functional-group measurements to a justified structural assignment.

## Principle

Elemental composition constrains a molecular formula; group-selective chemical or instrumental tests provide additional evidence. A positive qualitative test alone cannot establish an entire structure or quantify all functional groups.

## Materials and Requirements

- Certified or supplied elemental-analysis data
- Approved group-selective assays and blanks
- Candidate structures and spectral data
- Approved method or teaching-data pack and a dated record sheet

## Procedure

1. Define the preparation or dataset, study question and method version. Record identities, units and the criteria to be used before examining the outcome.
2. Calculate the proposed elemental percentages and compare them with measured values, accounting for salt, water and solvent form.
3. Choose selective quantitative tests for the relevant acid, hydroxyl, amino or other groups and state reaction equivalents.
4. Review positive and negative controls and identify interfering functionalities.
5. Combine equivalent content, elemental evidence and spectra; record inconsistent evidence rather than forcing a match.
6. Retain the original observations and calculations. State deviations, missing information and the limits of the conclusion; do not replace measured values with expected results.

## Observations and Record

Enter actual measurements or the supplied teaching data. Record the method, material identity, conditions and units.

| Evidence | Expected / model | Measured | Interpretation |
|---|---|---|---|
| Elemental content | Calculate | Enter | Compare |
| Group equivalents | Calculate | Enter | Compare |
| Orthogonal spectrum | Assign | Enter | Assess |

## Calculations

- Element mass (%) = number of atoms x atomic mass / molecular mass x 100
- Equivalent content follows the validated group-reaction stoichiometry.

### Worked Example

Illustrative C8H9NO2 with molar mass about 151.16 g/mol has carbon percentage about 63.56%.
A close carbon result cannot distinguish constitutional isomers with the same formula.

## Result and Interpretation

• Provide a supported assignment and identify evidence that remains insufficient.

## Precautions

• Use validated group chemistry and suitable blanks.
• Avoid hazardous classical elemental-decomposition experiments outside an approved setup.
• Account for hydrates, salts and residual solvent.

## Viva Questions and Answers

### Can elemental analysis distinguish isomers?

Not when the molecular formula is identical.

### Why use a blank in group analysis?

Reagents and matrix can contribute to the measurement.

### Why combine methods?

Independent evidence reduces ambiguity.

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