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Education Services

Pre-IB Chemical Research Skills Programme

Chemical Research Skills

A Skills-Building Programme for Independent Chemical Investigation



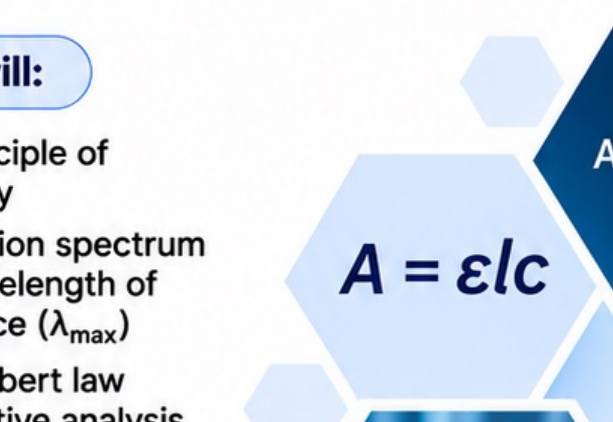
Module 8

Spectroscopic Analysis: UV-Vis in Chemical Investigation

Principles, Applications and Data Interpretation

In this module, you will:

- Understand the principle of UV-Vis spectroscopy
- Interpret an absorption spectrum and identify the wavelength of maximum absorbance (λ_{max})
- Apply the Beer–Lambert law ($A = \varepsilon lc$) in quantitative analysis
- Use UV-Vis to determine the concentration of an unknown solution
- Recognise limitations, sources of error and good experimental practice



$$A = \varepsilon lc$$



- A = Absorbance
- ε = Molar absorptivity (L mol^{-1} cm^{-1})
- l = Path length (cm)
- c = Concentration (mol L^{-1})

Sunny Chiam

IB Chemistry Specialist & Examiner-Level Educator
Founder, LearningSparks Education Services
Creator of the CHIAM Framework™

REFACE

Learning to Think Like a Chemical Researcher

Pre-IB Chemical Research Skills Programme | Modules 1–10

Chemistry is more than the study of substances, reactions, and scientific principles. It is also a discipline built upon observation, questioning, experimentation, measurement, and evidence-based reasoning. For many students, learning chemistry begins with understanding concepts, applying equations, and performing laboratory experiments according to established instructions. These are essential foundations. However, there is an important difference between following an experimental procedure and understanding how to design one.

This distinction becomes particularly significant when students progress into the International Baccalaureate Diploma Programme (IBDP), where independent scientific investigation forms an important part of their learning experience. Students are increasingly expected to formulate meaningful research questions, select appropriate analytical techniques, justify experimental decisions, evaluate the quality of their measurements, and draw conclusions supported by scientific evidence. Yet these research skills do not necessarily develop simply through learning more chemistry content or completing more laboratory experiments. They require deliberate preparation.

The **Pre-IB Chemical Research Skills Programme** was developed to address this need.
Drawing upon my experience as an IB Chemistry educator and examiner, I have observed that students may possess a reasonable understanding of chemical concepts yet encounter considerable difficulty when asked to translate those concepts into an independent investigation.

A student may understand concentration but struggle to prepare a suitable series of standard solutions. Another may know the Beer–Lambert law but remain uncertain about constructing and interpreting a calibration curve. Others may be familiar with experimental procedures yet find it challenging to explain why a particular analytical technique is appropriate, how many measurements are necessary, or whether their results are sufficiently reliable to support a conclusion.

These difficulties are not always the result of insufficient chemical knowledge. Often, they reflect a missing connection between conceptual understanding and experimental research design. This programme seeks to build that connection.

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Organised into ten progressive modules, the programme introduces students to the essential thinking processes and practical skills involved in chemical research. Beginning with the formulation of research questions, students gradually develop their understanding of quantitative solution preparation, dilution, calibration, analytical techniques, standardisation, measurement reliability, and experimental planning.

Each module builds upon the skills established in the preceding modules, encouraging students to recognise that scientific research is not a collection of isolated laboratory techniques. Rather, it is a connected process in which every experimental decision must serve a clear scientific purpose.

Throughout the programme, particular emphasis is placed on a fundamental principle:
A sophisticated-looking experiment is not necessarily a good experiment. A simple experiment that is thoughtfully designed, carefully measured, and critically evaluated can be an excellent scientific investigation.

Students are therefore encouraged not merely to ask *what should I do?* but also *why should I do it this way?*

Why is a volumetric flask preferable to a measuring cylinder when preparing a standard solution? Why might several smaller extractions be more effective than a single extraction? Why is a calibration curve necessary? Why can repeated measurements still produce inaccurate results? How can we determine whether an experimental method is capable of answering a research question?

These questions represent the foundations of scientific reasoning.
Importantly, this programme is not intended to replace the IB Chemistry syllabus, nor is it a shortcut to completing an Internal Assessment (IA) or Extended Essay (EE). Instead, it provides an early introduction to the research skills that students will eventually need when undertaking more demanding independent investigations.

The intention is to help students enter the IB Diploma Programme with greater confidence, stronger experimental awareness, and a more structured approach to scientific problem-solving. By the end of these ten modules, students should begin to appreciate that successful chemical research does not start with selecting an impressive experiment or sophisticated instrument.

It begins with a meaningful question, followed by careful consideration of the evidence required to answer it.

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Ultimately, the purpose of this programme is not simply to teach students how to conduct experiments. It is to develop their ability to think independently, make scientifically justified decisions, and approach chemical investigations with clarity, confidence, and intellectual curiosity.That is where meaningful scientific research begins.

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Founder, LearningSparks Education Services
Creator of the CHIAM Framework™
Think Chemistry. Think Structurally.

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Module 8 — Reliability, Accuracy & Data Quality
How Do We Know Whether Our Experimental Results Can Be Trusted?
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Related 1-Minute Chemical Research Skills episodes:

- **Episode 19:** Why Do We Repeat Measurements?
- **Episode 20:** Accuracy vs Precision — What's the Difference?
- **Episode 21:** What Should We Do with Anomalous Results?

Module Overview

In Modules 1–7, students learned how to:

- formulate research questions
- identify experimental variables
- prepare standard solutions
- perform dilutions
- construct calibration curves
- use UV–Vis spectroscopy
- determine unknown concentrations
- perform liquid–liquid extraction
- standardise solutions using titration

These techniques allow chemists to generate quantitative data.
However, an important question remains:
Just because an experiment produces numbers, does that mean those numbers are trustworthy?
Consider two students investigating the concentration of an unknown solution.
Student A reports:

$$c = 0.1047 \text{ mol dm}^{-3}$$

Student B reports:

$$c = 0.105 \text{ mol dm}^{-3}$$

Which result is better?
We cannot decide from the number of decimal places alone.
We need to know:

- How were the measurements obtained?
- Were measurements repeated?
- How consistent were the results?
- Were the instruments appropriate?
- Were systematic errors considered?
- Were unusual results investigated?

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- Was the reported precision justified?
- Does the evidence support the conclusion?

This module introduces students to **the evaluation of experimental data**.

The central progression is:

Collect Data → Repeat → Analyse Variation → Identify Errors → Evaluate Uncertainty → Defend Conclusion

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Part A — Why Data Quality Matters

1. A Measurement Is Not Automatically the True Value

Suppose the actual concentration of a reference solution is:

$$0.1000\ \text{mol dm}^{-3}$$

A student measures:

$$0.1032\ \text{mol dm}^{-3}$$

The measurement differs from the reference value.

The difference could arise from:

- instrument limitations
- incorrect calibration
- experimental technique
- sample preparation
- chemical interference
- random measurement variation
- systematic bias

Therefore:

Measured value ≠ necessarily true/reference value

A good scientist does not merely report the measurement.

A good scientist evaluates how much confidence can reasonably be placed in it.

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2. What Do We Mean by Data Quality?

Data quality describes how suitable experimental data are for answering the research question.

High-quality data should ideally be:

Relevant: The measurement actually addresses the research question.

Valid: The method measures what it is intended to measure.

Precise: Repeated measurements show sufficiently small variation.

Accurate: Results are close to a reliable reference value, where one is available.

Traceable: The reported result can be connected to identifiable measurements, standards and calculations.

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Reproducible: The method can produce consistent findings when appropriately repeated under specified conditions.

These properties are related but not identical.

A dataset can be precise without being accurate.

A dataset can also be repeatable while measuring the wrong chemical quantity.

Key principle

Good data quality requires more than attractive numbers.

Part B — Episode 19: Why Do We Repeat Measurements?

3. Why Is One Measurement Usually Insufficient?

Imagine measuring the concentration of a solution once.

You obtain:

$$0.102\ \text{mol dm}^{-3}$$

Is this result reliable?

We cannot determine its repeatability from one measurement.

Now suppose the experiment is repeated:

$$0.101,\ 0.102,\ 0.103\ \text{mol dm}^{-3}$$

These results show relatively little variation.

Repeating measurements provides information about the consistency of the method.

Main purposes of repeated measurements

1. Assess random variation.
2. Estimate a representative result.
3. Identify potentially anomalous measurements.
4. Improve the precision of an estimated mean.
5. Provide evidence about experimental repeatability.

However:

Repeated measurements do not automatically eliminate systematic error.

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4. Repeated Readings vs Independent Repeats

This is an especially important distinction for future IB Chemistry investigations.

Consider a student using UV–Vis spectroscopy.

Method A

Prepare one solution.

Measure its absorbance five times using the same cuvette.

Method B

Prepare five independent solutions using the same procedure.

Measure each solution once.

Are these equivalent?

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No.

Method A mainly assesses the repeatability of the measurement process for that particular prepared solution.

Method B additionally captures variation arising from:

- weighing
- solution preparation
- dilution
- transfer
- mixing
- sample handling

Therefore, Method B generally provides stronger evidence about the repeatability of the **overall preparation-and-measurement method**.

Important distinction

Repeated instrument readings ≠ independent experimental repeats

Both can be useful, but they answer different questions.

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5. What Is a Replicate?

A replicate is a repeated experimental unit or determination conducted under defined conditions.

The meaning depends on the investigation.

For example:

Investigation	**Possible replicate**
UV–Vis measurement	Independent sample preparation and measurement
Titration	Fresh aliquot titrated independently
Extraction	Separate extraction performed on a fresh equivalent sample
Reaction-rate experiment	Independently repeated reaction under the same conditions
Calibration curve	Independently prepared standard solution or calibration series

Students should specify exactly what was repeated.

Simply writing:

“The experiment was repeated three times.”

may be insufficient.

A better statement is:

“Three independent 25.00 cm^3 aliquots were titrated under the same conditions.”

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6. Why Three Repeats?

Students often assume that three repeats are always sufficient.

There is no universal rule that three repeats guarantee reliable results.

The appropriate number depends on:

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- expected variation
- measurement uncertainty
- available resources
- experimental complexity
- required confidence
- the size of the effect being investigated

Three repeats are often a practical starting point in school experiments.
However:

$$\boxed{n = 3 \neq \text{automatic reliability}}$$

A method with substantial variability may require more repeats.

Part C — Describing Variation in Data

7. Calculating the Mean

Consider five concentration measurements:

$$0.101,\ 0.103,\ 0.102,\ 0.104,\ 0.100$$

all in:

$$\text{mol dm}^{-3}$$

The arithmetic mean is:

$$\boxed{\bar{x} = \frac{\sum x_i}{n}}$$

Therefore:

$$\bar{x} = \frac{0.101 + 0.103 + 0.102 + 0.104 + 0.100}{5}$$

$$\boxed{\bar{x} = 0.102\ \text{mol dm}^{-3}}$$

The mean provides a central estimate of the measured quantity.
However, it does not show how widely the individual measurements vary.

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8. Why the Mean Alone Is Insufficient

Consider two datasets.

Dataset A

$$0.101,\ 0.102,\ 0.103$$

Dataset B

$$0.092,\ 0.102,\ 0.112$$

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Both have the same mean:

$$\boxed{0.102\ \text{mol dm}^{-3}}$$

But the spread differs substantially.
Dataset A shows much better repeatability.
Therefore:

$$\boxed{\text{Same mean} \neq \text{same precision}}$$

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9. Range

The range is:

$$\boxed{\text{Range} = x_{\text{max}} - x_{\text{min}}}$$

For Dataset A:

$$0.103 - 0.101 = \boxed{0.002\ \text{mol dm}^{-3}}$$

For Dataset B:

$$0.112 - 0.092 = \boxed{0.020\ \text{mol dm}^{-3}}$$

Dataset B has ten times the range.
The range is simple to calculate but has limitations.
It depends only on the highest and lowest values and does not describe how all measurements are distributed.

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10. Standard Deviation

Standard deviation provides a more informative measure of variation.
For a sample of repeated measurements:

$$\boxed{s = \sqrt{\frac{\sum (x_i - \bar{x})^2}{n - 1}}}$$

where:

- s= sample standard deviation
- x_i= individual measurement
- $\bar{x}$= sample mean
- n= number of measurements

A smaller standard deviation indicates that the measurements are more closely grouped.

Important distinction

Standard deviation describes variation among measurements.
It does not directly establish whether their mean is close to the true value.

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11. Worked Example — Standard Deviation

Consider:

$$10.1,\ 10.2,\ 10.3$$

Step 1 — Calculate the mean

$$\bar{x} = \frac{10.1 + 10.2 + 10.3}{3}$$

$$\boxed{\bar{x} = 10.2}$$

Step 2 — Calculate deviations

$$10.1 - 10.2 = -0.1$$
$$10.2 - 10.2 = 0$$
$$10.3 - 10.2 = +0.1$$

Step 3 — Square deviations

$$(-0.1)^2 = 0.01$$
$$0^2 = 0$$
$$(+0.1)^2 = 0.01$$

Step 4 — Calculate sample standard deviation

$$s = \sqrt{\frac{0.01 + 0 + 0.01}{3 - 1}}$$

$$= \sqrt{0.01}$$

$$\boxed{s = 0.10}$$

A suitable descriptive report is:

$$\boxed{10.2 \pm 0.1}$$

where 0.1represents the **sample standard deviation**, not necessarily the measurement uncertainty.

The meaning of the ± value must always be stated.

12. Relative Standard Deviation

When comparing datasets with different mean values, relative standard deviation can be useful.

$$\boxed{\text{RSD} = \frac{s}{\bar{x}} \times 100\%}$$

For:

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