LearningSparks®
Education Services

Pre-IB Chemical Research Skills Programme

Chemical Research Skills

A Skills-Building Programme for Independent Chemical Investigation



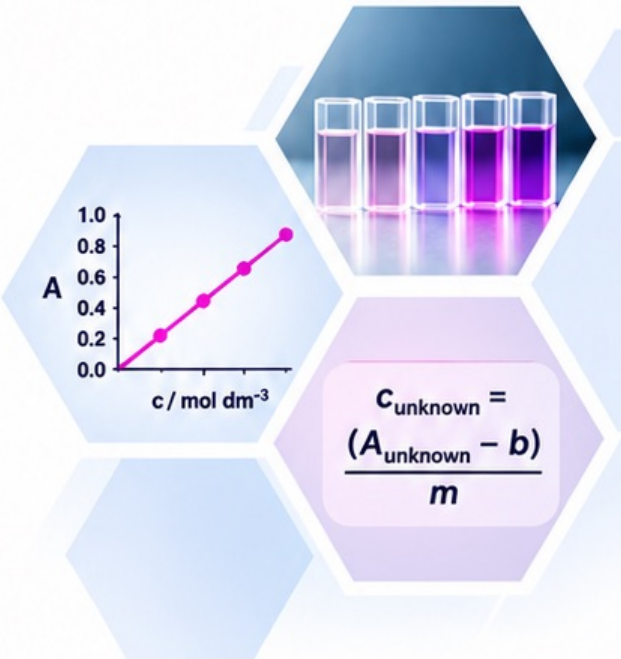
Module 5

From Calibration to Unknown Concentration

Applying Quantitative Analysis in Practice

In this module, you will:

- Use a calibration curve to determine an unknown concentration
- Carry out dilution and calculation steps with confidence
- Interpret results and evaluate reliability and uncertainty
- Apply the method in a realistic, research-style investigation



Sunny Chiam

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

PREFACE

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.

LEARNINGSPARKS Education Services

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.

LEARNINGSPARKS Education Services

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.

Sunny Chiam
IB Chemistry Specialist & Examiner-Level Educator
Founder, LearningSparks Education Services
Creator of the CHIAM Framework™
Think Chemistry. Think Structurally.

LEARNINGSPARKS Education Services

Module 5 — From Calibration to Unknown Concentration

Calibration Quality, Unknowns & Defensible Results

Learning objectives

By the end of this module, you should be able to:

- evaluate whether a calibration curve is suitable for quantitative analysis
- recognise common problems in calibration data
- distinguish between random variation, anomalous results and systematic problems
- explain why a high R^2alone does not prove calibration quality
- use a calibration equation to determine an unknown concentration
- distinguish between interpolation and extrapolation
- decide when an unknown should be diluted and remeasured
- apply dilution factors correctly
- recognise when an unknown may require additional sample preparation
- evaluate repeated measurements of an unknown
- distinguish between instrument precision and overall analytical accuracy
- identify possible causes of an unexpected calibration intercept
- justify whether an anomalous calibration point should be retained, repeated or excluded
- report an unknown concentration with scientifically defensible reasoning

---

1. Calibration is only useful if we can trust it

In Module 4, we established:

Known concentration → Measured signal

For example:

$$A = 6.24c + 0.004$$

We can then use an unknown absorbance to calculate concentration.

But there is an important question before doing that:

Is the calibration relationship reliable enough to use?

A regression equation produced by software is not automatically a valid chemical calibration.

---

2. What makes a good calibration?

A useful calibration should normally have:

- accurately prepared standards
- an appropriate concentration range
- enough calibration points
- consistent measurement conditions
- an appropriate blank
- suitable instrumental settings
- a scientifically reasonable relationship

LEARNINGSPARKS Education Services

- no unexplained major anomalies
- an unknown that falls within the calibrated range, where possible

Therefore:

$$\boxed{\text{Good calibration} \neq \text{simply a high } R^2}$$

It is the result of an entire **chain of reliable experimental decisions**.

---

3. First inspect the data

Consider:

c/ mol dm⁻³	Absorbance
0.020	0.124
0.040	0.249
0.060	0.371
0.080	0.498
0.100	0.622

There is a clear increasing trend.

The change in absorbance is approximately consistent as concentration increases.

This looks reasonable.

Now consider:

c/ mol dm⁻³	Absorbance
0.020	0.124
0.040	0.249
0.060	0.371
0.080	**0.912**
0.100	0.622

Something is clearly unusual.

The:

$$0.080 \text{ mol dm}^{-3}$$

point deserves investigation.

---

4. An unusual point is not automatically an outlier

Students sometimes think:

"That point doesn't fit my line, so I'll delete it."

This is not scientifically defensible.

A point that appears inconsistent may result from:

- incorrect standard preparation
- incorrect dilution
- contaminated sample

LEARNINGSPARKS Education Services

- dirty cuvette
- bubble in the light path
- transcription error
- wrong wavelength
- incorrect blank
- instrument problem
- genuine experimental variation

The correct first response is:

Investigate

not:

Delete

---

5. Repeat before you reject

Suppose the 0.080 mol dm^{-3} standard gives:

$$A = 0.912$$

when approximately 0.50 is expected from the overall trend.

If possible:

1. remeasure the same solution
2. inspect the cuvette
3. check for bubbles or contamination
4. check the recorded value
5. check the preparation records
6. prepare the standard again if necessary

Suppose the repeated preparation gives:

$$A = 0.497$$

Now there is evidence that the original 0.912 result may have arisen from an experimental problem.

The decision to exclude a value should therefore be based on **evidence**, not on whether exclusion improves the graph.

---

6. Random variation vs systematic error

These are different problems.

Random variation

Measurements vary unpredictably around a value.

For example:

$$0.491,\ 0.498,\ 0.494$$

Small differences may arise from normal experimental uncertainty.

Repeated measurements help us assess this variation.

LEARNINGSPARKS Education Services

Systematic error

Measurements are shifted consistently in one direction.

For example, suppose every standard was prepared using a volumetric flask that produced a larger actual volume than assumed.

All concentrations could be systematically different from the stated values.

Repeating the absorbance measurement may produce highly consistent results but will not correct the concentration error.

Therefore:

Repeatability does not guarantee accuracy

---

7. Precision can hide a problem

Suppose an unknown gives:

$$A_1 = 0.521$$
$$A_2 = 0.522$$
$$A_3 = 0.521$$

These measurements are highly **precise**.

But suppose the blank was incorrect.

Then all three measurements could still be systematically biased.

So:

High precision ≠ high accuracy

This principle appeared in Module 2 and becomes even more important in analytical chemistry.

---

8. What does R^2 actually tell us?

Suppose:

$$R^2 = 0.9997$$

This suggests that the observed data conform very closely to the fitted linear regression.

That is useful information.

But it does **not** tell us whether:

- concentrations were prepared correctly
- the correct chemical species was measured
- the blank was appropriate
- the wavelength was appropriate
- the instrument was properly used
- systematic errors were present
- the unknown lies inside the valid range

Therefore:

R^2 is evidence about the fit of the model—not proof of the validity of the entire experiment.

LEARNINGSPARKS Education Services

9. A beautiful calibration can still be wrong

Imagine that every standard concentration is actually 10% lower than the value written on the label.

The absorbances may still increase beautifully and produce:

$$R^2 = 0.9999$$

But the x-axis values are wrong.

The resulting equation may therefore produce incorrect concentrations for unknown samples.

This gives us a crucial principle:

$$\boxed{\text{Mathematical quality} \neq \text{chemical validity}}$$

Both are required.

---

10. Using the calibration equation

Suppose:

$$\boxed{A = 6.24c + 0.004}$$

An unknown gives:

$$A = 0.441$$

Substitute:

$$0.441 = 6.24c + 0.004$$
$$0.437 = 6.24c$$
$$c = \frac{0.437}{6.24}$$
$$\boxed{c = 0.0700 \text{ mol dm}^{-3}}$$

But calculation is only the first step.

We must now ask:

Is 0.0700 mol dm^{-3} within the calibration range?

---

11. Interpolation

Suppose the standards cover:

$$0.020 - 0.100 \text{ mol dm}^{-3}$$

Our unknown is:

$$0.0700 \text{ mol dm}^{-3}$$

This lies inside the experimentally tested range.

Therefore, we are using:

$$\boxed{\text{interpolation}}$$

Interpolation is generally preferred because the result is supported by calibration data on both sides of the unknown.

LEARNINGSPARKS Education Services

12. Extrapolation

Suppose the calculated concentration is:

$$0.180\ \text{mol dm}^{-3}$$

This lies outside:

$$0.020 - 0.100\ \text{mol dm}^{-3}$$

Therefore:

$$\boxed{\text{extrapolation}}$$

The problem is that we are assuming the relationship continues into a region we have not experimentally validated.

The response may no longer remain linear.

Therefore, strong extrapolation should generally be avoided in quantitative calibration.

---

13. What should we do instead?

Suppose an unknown gives an absorbance far above the calibration range.

One solution is:

$$\boxed{\text{Dilute the unknown}}$$

Measure the diluted sample so that its response falls within the calibration range.

Then:

$$\text{calibration} \rightarrow c_{\text{diluted}}$$

and:

$$\boxed{c_{\text{original}} = c_{\text{diluted}} \times \text{dilution factor}}$$

This reconnects directly with Module 3.

---

14. Worked example — Diluting an unknown

Calibration:

$$A = 5.80c + 0.010$$

An unknown initially gives:

$$A = 1.72$$

This lies well above the calibrated absorbance range.

The student performs a five-fold dilution.

The diluted sample gives:

$$A = 0.474$$

Calculate:

$$0.474 = 5.80c + 0.010$$
$$0.464 = 5.80c$$
$$c_{\text{diluted}} = 0.0800\ \text{mol dm}^{-3}$$

Since the sample was diluted five-fold:

$$c_{\text{original}} = 5(0.0800)$$
$$\boxed{c_{\text{original}} = 0.400\ \text{mol dm}^{-3}}$$

LEARNINGSPARKS Education Services

15. Do not forget the dilution factor

This is a common analytical error.

Suppose the calibration gives:

$$0.0800\ \text{mol dm}^{-3}$$

for the diluted sample.

Reporting:

$$\boxed{0.0800\ \text{mol dm}^{-3}}$$

as the concentration of the original sample would be wrong.

The calibration determines the concentration of the **solution actually placed in the instrument**.

If that solution was diluted beforehand, we must work backwards.

---

16. Unknown samples should be repeated too

Calibration standards are not the only measurements that can vary.

Suppose an unknown is measured three times:

$$A = 0.438,\ 0.441,\ 0.439$$

These are reasonably consistent.

Mean:

$$\bar{A} = \frac{0.438 + 0.441 + 0.439}{3}$$

$$\boxed{\bar{A} = 0.439}$$

Using repeated measurements gives us more information about the precision of the measurement than a single reading.

---

17. But what exactly are we repeating?

There is an important distinction.

Repeat instrumental reading

The same prepared sample is measured several times.

This mainly tests:

instrumental/measurement repeatability

Repeat sample preparation

Independent samples are prepared and measured separately.

This tests more of the entire analytical procedure:

$$\boxed{\text{preparation} + \text{measurement}}$$

Therefore, three readings from the same cuvette are not equivalent to three independently prepared samples.

This is an important research-design distinction.

LEARNINGSPARKS Education Services