



AI as a tool for adaptive learning: promoting critical thinking rather than replacing it

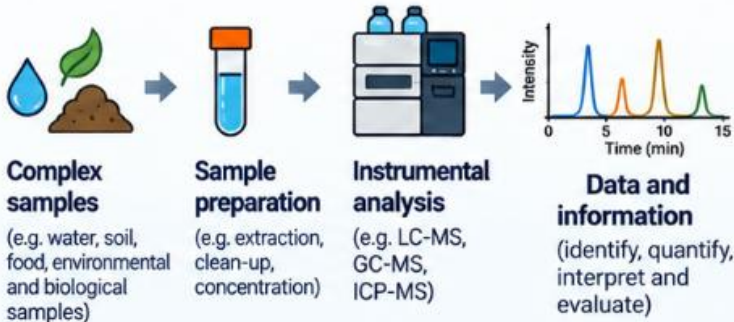


Victor Castro-Alves and Leo Yeung



What is analytical chemistry?

Analytical chemistry is the science of **obtaining, identifying and quantifying information** about the chemical composition of materials.



Key questions in analytical chemistry

- What substances are present?
- How much are they present?
- How reliable are the results?
- What do the results mean in a real-world context?

Typical tasks in the course



Understand analytical principles

e.g. chromatography, mass spectrometry, spectroscopy, sample preparation



Interpret analytical data

e.g. chromatograms, mass spectra, calibration curves, QA/QC results



Perform calculations

e.g. concentration, dilution, recovery, LOD/LOQ, mass accuracy, DBE



Evaluate methods and results

e.g. method selection, matrix effects, uncertainty, QA/QC, advantages and limitations



Solve analytical problems

e.g. identify unknowns, compare methods, choose appropriate analytical strategies

What we did?

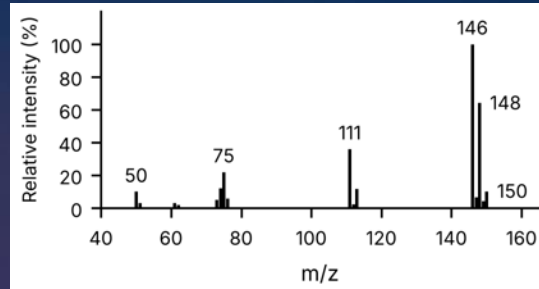
Integrating AI in 2 undergraduate courses

Our question: can AI help students evaluate analytical reasoning after they have solved a problem themselves?

Instrumental Analytical Methods

(KE308G – 3rd year BSc course)

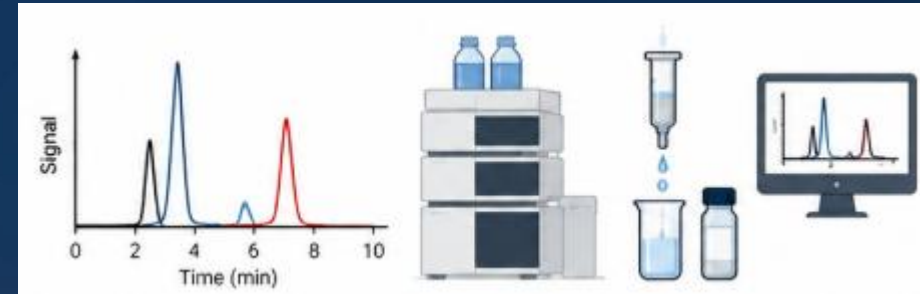
Focus: Mass spectrum interpretation



Analytical Chemistry

(KE306G – 2nd year BSc course)

Focus: Chromatography, sample preparation, QA/QC and method development

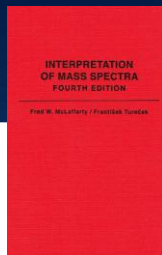


KE308G

Context: McLafferty's Interpretation of Mass Spectra



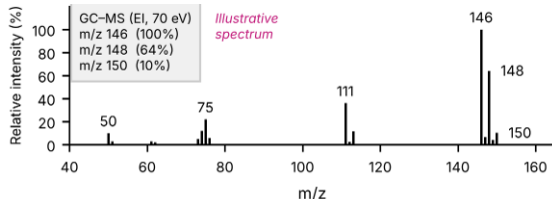
THE BOOK



F. W. McLafferty, Interpretation of Mass Spectra. 1st ed. **1966**, 2nd 1973, 3rd 1980; 4th ed. 1993 with F. Tureček.

- Reference text for KE308G
- Written in the style of its time: students call it “old English”

EXPLAIN SPECTRA FROM THE PHYSICS



LEARNING BY SOLVING UNKNOWN

Step-by-step deduction, practised on “unknown” spectra with worked solutions at the back of the book.

- Rule-based and calculation-driven
- Clean test: One correct molecular formula, checkable by calculation
- We can judge AI's answer and its reasoning

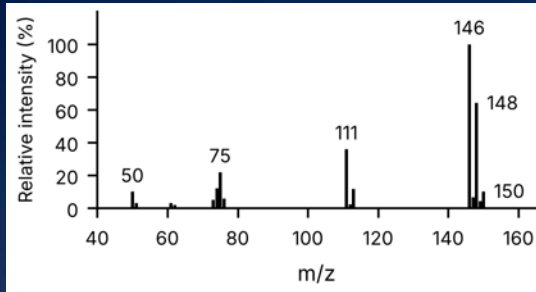
Formula deduction is exact: the same data always give the same answer, so AI's output can be checked.

What we did:

Integrating AI in 2 undergraduate courses

Instrumental Analytical Methods

(KE308G – 3rd year BSc course)



The test

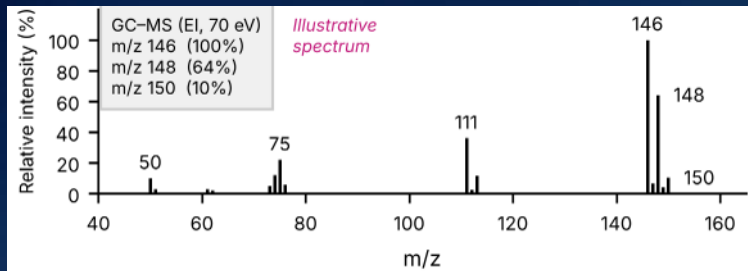
1. Read the fingerprint: the peak pattern reveals key atoms
2. Use the weight: find atom combinations that fit
3. Apply simple chemical and physical rules: drop impossible ones
4. Count rings and double bonds: check the shape
5. Propose the molecular formula

AI task

1. Solve the questions independently
2. Discuss in class; correct answers given
3. Use AI to verify the solution
4. Evaluate the AI's explanation against the course method

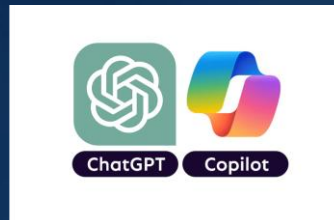
AI can produce the right answer. But does the student understand why?

Interpret the mass spectra



Answer: $\text{C}_6\text{H}_4\text{Cl}_2$

Let's ask AI



Is it correct?

“What is the most likely molecular formula for a compound with a molecular ion at m/z 146 and isotope peaks at m/z 148 and 150 (100 : 64 : 10)? (GC-MS, EI)”

Answer: $\text{C}_6\text{H}_4\text{Cl}_2$

What KE308G students told us

AI always got the answer right

Correct molecular formulas for every spectrum, on every platform, even when students just uploaded the homework.

- ChatGPT (free) and Microsoft Copilot
- Correctness described as “very high”
- Minimal prompting was enough

...but explanations varied

Some explanations followed the course’s rule-based procedure; others were disorganised or incomplete.

- Correct answer ≠ correct reasoning
- Steps did not always match course method
- Unclear how to get there

Study companion, not a replacement

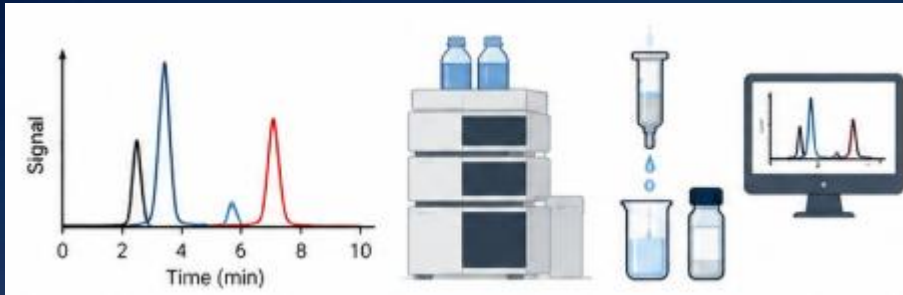
Most saw AI as a “good study companion”; a minority felt it could “replace the need for lectures”.

- Useful for checking work and quick support
- Helped paraphrase McLafferty’s “old English”
- Not enough to learn the method itself

KE306G – 2nd year BSc course

Analytical Chemistry

Focus: Chromatography, sample preparation, QA/QC and method development



1. AI as a tutor

- Explain how changing the flow rate affects chromatographic efficiency

2. AI as a laboratory assistant

- What could cause peak broadening in my LC method, and how can I trouble-shoot it?

3. AI as a problem generator

- Give me addition HPLC calculation or new method.development scenario

4. AI as a thinking partner

- Compare 2 analytical workflows for PFAS in water and justify which one is better

How students used AI in KE306G:

From answer-seeking to reasoning-seeking prompts

Factual/answer-seeking prompts

"What is HPLC?"

- Useful for quick definition and general explanations
- Limited analytical reasoning
- Similar to textbook information

Verification prompts

"I calculated the number of theoretical plates. Is it correct?"

- Good for checking calculations and confirming results
- Help to identify simple mistakes
- Do not deepen understanding

Problem-solving prompts

"My chromatographic peaks are broad and tailing. What could be the possible causes and how could I fix it?"

- More analytical and context-specific
- Support trouble-shooting and method development
- Provides multiple possible solutions
- Explore and compare approaches

Analytical and reflective prompts

"We need to analyze PFAS in wastewater. Compare SPE and LLE for this application including advantages, limitations, and relevant QA/QC

- Support comparison and critical evaluation different approaches
- Encourage discussion of QA/QC and uncertainty
- Promote deeper analytical reasoning

What did we learn?



AI supported understanding

Students used AI to explain concepts, check their reasoning and explore alternative approaches.

- Explain difficult analytical concepts
- Verify calculations and interpretations
- Explore alternative analytical approaches
- Support independent learning

Critical evaluation was essential

Students could not simply accept AI responses; they needed to check the reasoning and assumptions.

- AI explanations sometimes omitted reasoning steps
- Responses could be too general or simplified
- Students needed to question assumptions
- Compare responses with course material and principles

Better questions → deeper learning

The way students formulated questions strongly influenced the educational value of AI.

- Move from factual to analytical questions
- Ask for comparison and justification
- Use AI as a discussion and thinking partner
- Focus on scientific decision-making

We want

“Think first, then use AI” is how both courses ran
The full five steps are our recommendation

Think First

- Solve the analytical problem independently or with your peer
 - Lecture notes
 - Textbook
 - Understand what you know and discuss with peer/teachers in lectures

Use AI

- Ask AI to explain or verify or compare
 - Use AI after their attempt
 - Ask specific, well-defined questions
 - Request explanations, not just the final answer

Challenge

- Evaluate the AI response
 - Are there any steps missing
 - Is the reasoning correct
 - Could there be alternative explanations or methods?

Verify

- Compare with analytical principles and course materials
 - Check against lecture notes and textbook
 - Confirm or identify inconsistencies

Reflect

- What did I learn?
 - What did AI help me understand better?
 - Where was my reasoning correct or incorrect?
 - How should I apply this learning next time?

Lessons learned and future development

Key lessons

Students benefit when AI is integrated into the learning process, **not used as a shortcut**.

The **quality of the question** influences the usefulness of the AI response.

AI responses need **critical evaluation** and verification against analytical principles.

AI can **stimulate deeper discussion** and comparison of analytical approaches.

Challenges and limitations

AI responses can be **incomplete, oversimplified or contain incorrect reasoning**.

Students may focus on the **answer** rather than the analytical reasoning process.

AI needs to be verified using lecture material, textbooks and established scientific knowledge.

Effectiveness depends on **well-designed exercises and guidance** on appropriate AI use.

Implications for teaching

Provide a clear framework:
Think first → Use AI →
Challenge → Verify → Reflect.

Design tasks that require **reasoning, comparison, justification and critical evaluation**.

Give examples of effective prompting and show both useful and problematic AI responses.

Integrate AI across different learning activities, including individual and practical work.

Future development

Expand the approach to more topics and advanced analytical case studies.

Develop structured guidance and example prompts for students.

Incorporate reflective AI-based assignments into teaching.

Collect more systematic evidence of learning outcomes through questionnaires and course evaluations.

Lessons learned and future development

Key lessons

Students benefit when AI is

Challenges and limitations

AI responses can be

Implications for teaching

Provide a clear framework

Future development

Different AI models give different results and students need to notice this!
As a teacher, we do not have all resources to test and show!

AI responses need critical evaluation and verification against analytical principles.

AI can stimulate deeper discussion and comparison of analytical approaches.

AI needs to be verified using lecture material, textbooks and established scientific knowledge.

Effectiveness depends on well-designed exercises and guidance on appropriate AI use.

evaluation.

Give examples of effective prompting and show both useful and problematic AI responses.

Integrate AI across different learning activities, including individual and practical work.

Incorporate reflective AI-based assignments into teaching.

Collect more systematic evidence of learning outcomes through questionnaires and course evaluations.

Thank you