Personalised Journeys Through Chemistry

The ChemTrack Project

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Motivation for change

BSc Chemistry
- 440 hours in the teaching labs

MSci Chemistry
- 570 hours

500 hours lectures etc. in years 1-3
Chemical synthesis from design to application

Make It!  Measure It!  Hack It!  Prove It!

ChemTrack Modules

Hypothesise and challenge

LDA manifold of fragment data and energy targets

Aquiring data, curating data, analysing data

Post-it plans to prototype
ChemTrack Skills Passport
ChemTrack Skills Passport

The Skills Passport contains 6 distinct categories:

- Consulting the literature and formulating a research question
- Designing the Experiment
- Doing the Experiment
- Processing and analysis of data
- Concluding with respect to the hypothesis
- Communicating results and defending claims

...Each containing one or more descriptors...

Addressing the research question
Planning the implementation of the work
Managing risks and hazards
...which break down into levels of achievement, level criteria
e.g. for Addressing the research question:

5. Design experiment from first principles and evaluate several different approaches.

4. Evaluation of different options, with fall back plans also developed; or design from first principles a single experimental approach.

3. Able to explain how all decisions (or instructions) address the hypothesis with appreciation of the limitations of the planned work.

2. Able to explain how some decisions (or instructions) address the hypothesis.

1. Able to explain how some decisions (or instructions) address the hypothesis.

0. No opportunity to design the experiment or no understanding of how decisions about considerations relate to addressing the hypothesis.

ChemTrack Skills Passport
Remember
Understand
Apply
Analyse
Evaluate
Create
ChemTrack Skills Passport

A profile of learning across experiments
160 year 3 students asked to complete “a further, formative, lab learning evaluation”

20 submitted a first attempt and received feedback

2 completed the process...

2017-18: a Blackboard-based prototype
### Rubric Description

Your reflective statement should be written in the free-text box provided and focus on addressing each of the descriptors within the category. For each descriptor you should clearly indicate the level corresponding to the criteria you believe that you have demonstrated. Your lab tutor will review your statement and assigned levels and provide feedback, and confirm the overall level for each category after agreeing this with you. The levels are not a mark out of 5, a 3 does not correspond to a mark of 60%; the level numbers merely provide a convenient way of mapping progression and achievement through the specific criteria.

<table>
<thead>
<tr>
<th>Grid View</th>
<th>List View</th>
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<tbody>
<tr>
<td><strong>Addressing the research question</strong></td>
<td><strong>Level 0</strong></td>
</tr>
<tr>
<td>No opportunity to design the experiment or no understanding of how decisions about considerations relate to addressing the hypothesis (no understanding of why).</td>
<td>Able to explain how some decisions (or instructions) address the hypothesis.</td>
</tr>
<tr>
<td><strong>Planning the implementation of the work</strong></td>
<td>No opportunity or no planning of work.</td>
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Addressing the research question

I have mainly analysed and evaluated multiple routes of synthesis to form my target molecule, but ultimately chose one suitable route to be implemented whilst ruling out others (e.g., reacting 1-cyclohexenyl)methanol with triethyl orthoacetate) through reasoned arguments. However, I kept in mind reactions for enamine formation using the same starting materials (cyclohexanone and pyrrolidine) but with different reaction conditions as an alternative to the main reaction.

Level 3

Planning the implementation of the work

My initial choice of reaction by refluxing cyclohexanone and pyrrolidine in toluene with an acid catalyst using a Dean-Stark apparatus did not give NMR data that correlated with desired enamine and thus I made changes and looked up the literature for a more recent reaction as back-up that only required overnight stirring of the starting materials in a MgSO₄ drying agent at room temperature, which drove my reaction to completion and showed positive results in the NMR.

Level 4

Managing risks and hazards

After going through the experimental sections for each step in literature articles, I listed all the reagents needed, printed out the MSDS for the chemicals and tabulated their hazards into the respective COSHH forms along with a detailed quantity of reagents to be used and work-up procedure required to purify my samples. These considerations were subsequently approved by my lab mentor during the proposal viva.
Student: “Understanding the context of the work - Level 4
For Experiment 4SP, my goal was to plan and carry out a multi-step synthesis of the target molecule, Ethyl-(2-methylene cyclohexyl)ethanoate. By comparing and evaluating various research papers, I have reasoned out and formulated a feasible synthesis route to obtain the target compound, taking into account the technical ease of the reaction, overall yield, cost of reagents, rate of reaction and any hazards associated.

The theoretical basis of the route I selected involved enamine formation using cyclohexanone and pyrrolidine, followed by alkylation at the alpha-carbon with ethyl bromoacetate and subsequent hydrolysis with water to form a keto ester. Methylenation of the ketone group in the keto ester via a Wittig reaction formed the final product and a further epoxidation of the alkene formed a 1-Oxaspiro[2.5]octane racemix compound as part of my extension.”

3 Understanding of the theoretical basis and context for the experiment and how it relates to the wider field.
4 Understanding of the theoretical basis and context for the experiment with reference to research literature.

Feedback: “As written this statement supports level 3, your description of the general form of the reactions you planned demonstrates understanding of how your experiment relates to the wider field. Your reference to the literature is rather restricted to the specific target molecule, to support level 4 you would need to use the research literature to establish your understanding of the context, eg. what is a recent research application of the chemistry you are using?”
Lessons learned from the pilot

160 year 3 students asked to complete “a further, formative, lab learning evaluation”

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2 completed the process...

• Outcomes:
  • level criteria (and some descriptors) still lacking clarity
  • appreciation of the workload (student and lab tutor)
  • appreciation of student attitudes
  • a better understanding of technical requirements, how the passport should work

(Blackboard is *!#$&!ing stupid...)

2017-18: a Blackboard-based prototype
ChemTrack next steps

Blackboard-based prototype

Tailor-made software
- More iteration-friendly
- Reflective statement key words function
  → UG student summer project on machine learning
Lab Learning Assessment

2. Review and approval
Module: Prove it! 2.3

Designing the experiment
Novice
Because...

Doing the experiment
Distillation  Competent

Select:
- Approve
- Discuss and edit

ChemTrack Skills Passport
ChemTrack next steps

New lab activities

• UG summer students developing experiments

... a new labs curriculum