

CH-400 Automated and data-driven chemistry

General comments on first project reports (P.Miéville, 11.10.2024)

First of all : it was globally a very good job and was mostly well aligned with requirements.

Some more detailed comments and recommendations

Be synthetic :

- Your report is destined to chemists, IT specialists and robotics specialists. No need to convince them that this method is the best :)
- Describe clearly your goals but no need to re-explain the FTIR or the LC. Just focus on the essential information to make the project feasible and efficient.
- Be careful with the GPT typical language hyperbolism -> you don't sell nothing, you describe a process in precise terms and should always avoid the bullshit effect.
- If your workflow is really large and complex, treat it in subsegments or sections.

Additional general comments :

- Respect the 3 pages consign
- Be careful with the title naming instructions - this can be the reason for a grant proposal rejection
- Always remind the name of the project at the beginning of each report sections and also the name of the authors and group letter (easier for us to orientate the comments to the right persons)
- Always start with a small intro (5-10 lines) to describe the goal of this section/ chapter. A global intro (10-20 lines) will have to be planed at the beginning of the global report to describe the project and the components of the report.
- Always date (useful for your archives and also patenting) and page numbers (easier to read larger documents and slides)

For automation project report :

- try to avoid a too restrictive approach from the beginning. It is clearly easier to automate something very well defined and restrictive (typical engineer strategy -> give me an exact requirements list). In our case the goal is to explore the possible. The restrictions will come progressively by the technical possibilities.
- Explain clearly your choices in terms of automations and also the work hypothesis you use (e.g. : we work only we pre-solubilized molecules) - justify these choices in terms of automation rationality and also demonstrate that the loss induced is not critical for the chemistry that has to be performed on the system.