Scientific Reports at LCSO

Oral and written communications are important in the scientific world. For this reason, a great care is taken at LCSO to learn how to write scientific reports, which can then serve as basis for PhD thesis or publications. Scientific writing is not easy, it will take you years to be able to write a good report or publication. The hints given below will help you in this process.

Reports are required yearly by the doctoral school, but the standards are lower than those of LCSO. The high level of quality for reports will be very helpful for you later when writing publications or your thesis. The reports at LCSO will be expected on fixed deadline: for PhD: 6 months, 12 months (first year exam), then yearly short reports for the doctoral school; for postdocs at the end of the stay. The thesis redaction usually takes place in months 45 to 47, but here flexibility is certainly possible. The 6 months report is not required by the doctoral school, but it has been introduced to help first year students: for many students, writing a report on one full year of research was just so difficult that a lot of sleepless nights resulted. With the training on a shorter report after six months, it becomes easier. The fix deadlines are a good preparation to the time pressure omnipresent in the "real" world. First year students will get intensive support from my side to help them prepare the report on time.

1. General Remarks

Every student joining the group for a project, a master or a PhD thesis will be taught how to write a high quality scientific report. The difference will reside in the length of the work.

- **Language**: Reports are written in English at LCSO. It is important to remember that scientific English favors short sentences. In part 1-3 (see below), care has to be taken of the structure of the text, the flow of concepts and to avoid repetitions. The goal is to communicate all (but only) the relevant information in a concise but correct way. Plagiarism (copying from publications or reports from other persons) is absolutely forbidden. Self-plagiarism is tolerated (copying his own text from previous reports or publications), excepted for published text and pictures, when writing a new publication. In this case however, the used text has to be clearly indicated by a footnote. In the experimental part (section 4), standard repetitive sentences can be used. Copy paste from previous reports is encouraged to speed up writing. The goal of this part is to ensure reproducibility.
- **Illustrations**: Illustrations are classified as Figure (no reaction arrows), Equation (1 reaction arrow), Scheme (>1 reaction arrows) and Table and are numbered. In general, Figures, Schemes and Tables should have a legend. All illustrations should be referred to at least one time in the text, and the relevant text should come before the illustration. All chemical drawings have to be realized using ACS 1996 template. No caption is needed in the experimental part. All drawings need to have the same font size and the font in the drawings should be close to the font size in the text.
- **Numbering of Structures**: All exactly defined structures are numbered in order of appearance in the main text using Arabic numbering and each structure should be designed by a single number. General structures (with R's) and structures above/below reaction arrows can be numbered, but it is not absolutely required. Reactive intermediates and transition states are numbered either as Roman numbers or letters, starting by A or I again in each new illustration. All numbers are in bold in the text. If the exact name of a structure is used, the number is given in parenthesis.
- **Headings**: Heading numbering should be Arabic: 1.1, 2.1.2, …Heading titles are capitalized in English.
- The text should be justified.

2. Structure of the Report

0. Title page, including title of the work, name and time of the work. For long reports: Table of content, list of abbreviations.
1. Introduction
2. Results and Discussion
3. Conclusion and Outlook
4. Experimental Part
5. Acknowledgments
6. References: as endnote in short reports, as footnote in longer ones.

3. Introduction

- **Structure**: Introduction should include the following sections: 1) General introduction, 2) Relevant work of other groups in the field 3) Relevant work at LCSO 4) Goal of the project (for example development of new reactions, extension of scope, synthesis of substrates, retrosynthesis Scheme can be included here).
- The introduction should start from broad concepts, and then becomes more and more focused to the project. It is the most difficult and time-consuming part to write. Particular care has to be taken to include references to all relevant works.
- At the end of the introduction, the answers to following questions should be clear to the reader: **What has been done?**, **What do you want to do?** and **Why do you want to do it?**
- **Often occurring mistakes:** Long introduction without relevance to the work. Fragmented introduction without logic. Relevant works omitted. Not relevant works described. Difference between past of future not clear (what has already been done, what is new?).

4. Results and Discussion

- **Structure**: There are no fixed structure for this part, as it is highly dependent of the kind of the project (example for methodological work: discovery of reaction/optimization/scope/application, example of synthetic work: synthesis of fragment A, Synthesis of Fragment B, coupling and completion of the synthesis).
- **Form**: This part is a descriptive part in a story-telling way. The relevance of the results has to be clear for the reader. All details are not described in this part, but the results are discussed and explained. Care has to be taken to emphasize new or unexpected results, and standard reactions that perform well are just shortly mentioned. (Example: TBS protection proceeded well under standard conditions (Scheme X). But: When TBS protection was attempted under standard conditions, no product was obtained (Scheme X). We think that is due to… Consequently, the methods of X, Y and Z were examined. Finally, Method Z was successful, probably because…). It is very important to speak about the attempts that did not work.
- Extended descriptions of other works should not take place in this section: It is reserved to your own work. Short description of other works can be needed, but should be clearly recognizable as such.
- Particular care has to be taken to explain the results in a logical way, even if the real work was often much less logic-driven. It is always easier to see the logic after than during the work. The flow of the text from one section to the other should be good. It should never look like a simple list of results, like an experimental part.
- **Tables**: Notes concerning the tables are added directly at the foot of the tables in a smaller font and are numbered as a, b, c. The first column of tables is labeled as entry. All tables should have a note giving experimental details.
- **Illustrations**: All illustrations should be in the format **in-line with text**. All illustrations should be **the same size**. The legend of the illustration should specify the type (Figure, Equation, Scheme), be numbered and have a **clear enough title** to be self-understood (e.g. not just "Optimization", but "Optimization of the reduction of ketone **XX**"). Illustrations can have also notes if needed.
- **Often occurring mistakes:** Mixed up of styles with the experimental part (too many details, looks like a list), own work is not clearly distinguished from other's work, flow of text is not logical, expected results are described in details and unexpected ones not enough. Illustrations are not well described and of varying style and size.

5. Conclusion and Outlook

- **Conclusion**: The conclusion should make clear, how many of the project's goals have been met. Unexpected results have to be highlighted again. Where the hypothesis formulated in the introduction correct? How much novelty has been generated in this work and what is its relevance for the advancement of the field?
- **Outlook**: Which future works has been made possible by this research? Is it still going in the same general direction, or do unexpected results lead to new ideas for research?
- **Often occurring mistakes:** Personal impressions do not belong here, but to the acknowledgement section.

6. Experimental Part (See also file 7b for a template)

- **General Remarks**: The experimental part is an essential part of any scientific work, as it is the proof of what you affirm and it allows the reproduction of your work. Consequently, extreme care is needed when preparing it. There are very strict rules of syntax and representation, in order to facilitate comparison of results and reproducibility.

- **Structure**: 1) General methods 2) General procedures 3) Detailed experimental procedures and characterization 4) Spectra

6.1 General Methods

- This section includes all common techniques that are used for synthesis, purification and analysis. The equipment and the chemical used are described in details. It can be copied from other reports and adapted if needed.

6.2 General Procedures

- If a reaction procedure has been followed exactly more than three times, then a general procedure for this reaction can be prepared. This protocol should be the smallest common denominator of the reactions. The detailed section will then contain only the details that change every time (usually quantities of starting material, yield of product and purification methods).
- General procedures have to be numbered and referenced to (For example as **GP1**)

6.3 Detailed Experimental Procedures and Characterization

- Help for the redaction of this very important part of the report is given in the file **7a/7b** Experimental-Labbook.

7. Acknowledgments

- This section is the only part of the work that is completely free. No corrections will be done and if desired it can be added after the report has been accepted. It is also the right place to put personal impression, what you personally learned, what is the impression you get for your internship. Your advice is important to further improve the quality of work at LCSO.

8. References

- Endnote or footnote can be used. Footnote is best for long reports.
- **All References have to be in ACS style**. Use superscript in text, parenthesis in footnote or endnote. A fast way to obtain the references is to export them from web of science to endnote, then choose the correct format. There are abbreviation mistakes, however.
- Cluster of reference can be separated as a, b,…
- Font for references should be smaller than the main text.
- Example:[1,2,3,4]

(1) (a) Pelay-Gimeno, M.; Glas, A.; Koch, O.; Grossmann, T. N., Structure-Based Design of Inhibitors of Protein–Protein Interactions: Mimicking Peptide Binding Epitopes. *Angew. Chem., Int. Ed.* **2015**, *54*, 8896-8927. (b) Wang, H.; Dawber, R. S.; Zhang, P.; Walko, M.; Wilson, A. J.; Wang, X., Peptide-based inhibitors of protein–protein interactions: biophysical, structural and cellular consequences of introducing a constraint. *Chem. Sci.* **2021**, *12*, 5977-5993.

(2) (a) Villar, E. A.; Beglov, D.; Chennamadhavuni, S.; Porco, J. A.; Kozakov, D.; Vajda, S.; Whitty, A., How proteins bind macrocycles. *Nat. Chem. Biol.* **2014**, *10*, 723-731. (b) Cromm, P. M.; Spiegel, J.; Grossmann, T. N., Hydrocarbon Stapled Peptides as Modulators of Biological Function. *ACS Chem. Biol.* **2015**, *10*, 1362-1375. (c) Lau, J. L.; Dunn, M. K., Therapeutic peptides: Historical perspectives, current development trends, and future directions. *Biorg. Med. Chem.* **2018**, *26*, 2700-2707. (d) Henninot, A.; Collins, J. C.; Nuss, J. M., The Current State of Peptide Drug Discovery: Back to the Future? *J. Med. Chem.* **2018**, *61*, 1382-1414. (e) Vinogradov, A. A.; Yin, Y.; Suga, H., Macrocyclic Peptides as Drug Candidates: Recent Progress and Remaining Challenges. *J. Am. Chem. Soc.* **2019**, *141*, 4167-4181.

(3) (a) White, C. J.; Yudin, A. K., Contemporary strategies for peptide macrocyclization. *Nat. Chem.* **2011**, *3*, 509-524. (b) Mortensen, K. T.; Osberger, T. J.; King, T. A.; Sore, H. F.; Spring, D. R., Strategies for the Diversity-Oriented Synthesis of Macrocycles. *Chem. Rev.* **2019**, *119*, 10288-10317. (c) Reguera, L.; Rivera, D. G., Multicomponent Reaction Toolbox for Peptide Macrocyclization and Stapling. *Chem. Rev.* **2019**, *119*, 9836-9860.

(4) (a) Bechtler, C.; Lamers, C., Macrocyclization strategies for cyclic peptides and peptidomimetics. *RSC Med. Chem.* **2021**, *12*, 1325-1351. (b) Posada, L.; Serra, G., Three Methods for Peptide Cyclization: Peptide Cyclization Via Lactamization. In *Peptide Macrocycles: Methods and Protocols*, Coppock, M. B.; Winton, A. J., Eds. Springer US: New York, NY, 2022; pp 3-17.