**Computer-assisted drug discovery – startup challenge**

**Company name and logo**

| *Name 1* | Email 1 | *Name 5* | Email 5 |
| --- | --- | --- | --- |
| *Name 2* | Email 2 | *Name 6* | Email 6 |
| *Name 3* | Email 3 | *Name 7* | Email 7 |
| *Name 4* | Email 4 |  |  |

**Instructions:** How to use this template:

* Fill out the company name (and the logo if available).
* Fill out the names of the participants and their emails.
* Follow the guidelines in each section of this template, and remove/replace everything that is written in blue.
* Follow the maximum allowed number of pages and words for the document. If a document does not respect this, it will not be considered for grading.
* Changing font, spacing, or document layout is not allowed.

**Materials and methods** (max 600 words)

Max **600** words in total. This section is aimed to provide a brief overview of the methodological steps and choices undertaken to solve the challenge.

Molecular descriptor calculation. Use this part to write what descriptors you decided to compute and with what settings. Extensive info can also go to the appendix.

Data analysis. Briefly summarize the steps undertaken to perform the task. The corresponding results and the discussion can go in the “Results and Discussion” session. You can also use diagrams if this makes your life easier.

Software and code. Write the packages (and their versions) used to solve the assignment. There’s no need to mention classical packages like *numpy* and *pandas*.

Link to the company’s GitHub. Linking a GitHub repository for this project is **mandatory** to pass this assignment.

**Wordcount: \_\_**

**Results and discussion** (max 3 pages, with figures and tables included)

This section will collect information about how you came up with a solution, using your programming and data analysis skills. In particular, here you will provide an answer to the following questions:

* How have you decided to tackle the challenge?
* What is the motivation behind the chosen steps?
* What does your analysis suggest about the problem at hand?
* How have you defined and measured the success of your approach?
* What are the limitations and/or gaps in your approach?

Only discuss the essential steps and the corresponding results and put everything else in the Appendix (see below). Feel free to create subsections if necessary. Figures/tables in the appendix can also be referenced (*e.g.*, Supporting Figure S1).

=============================== Max 3 pages ============================

**Author contribution according to CRediT**

This section does not count toward the page limit. This section will help us understand who contributed to what. Make sure that the contributions of each and every one of you are mentioned truthfully where appropriate. Have a look at <https://credit.niso.org/> to know more about the meaning of these roles.

Note: we expect all the group members to contribute to a significant part of this report. Authors that play only a minor role in this research will not receive a grade!

| *Conceptualization* | Write the initials here, *e.g.*, “M.R. with contributions from D.B.”, “F.G. and M.R.”, or “all authors” when it is the case. |
| --- | --- |
| *Methodology* |  |
| *Software* |  |
| *Validation* |  |
| *Formal analysis* |  |
| *Investigation* |  |
| *Data Curation* |  |
| *Writing - Original Draft* |  |
| *Writing - Review & Editing* |  |
| *Visualization* |  |

**Usage of ChatGPT**

This section does not count toward the page limit. Report how and for what you have used ChatGPT to solve the challenge.

**References**

This section does not count toward the page limit. Consider using automated tools to create references, such as [Zotero](https://www.zotero.org/).

**Appendix**

This section does not count toward the page limit. You can use this part in a “free form” to report anything that is useful to your discussion but does not fit the main story and/or the template above. Remember to reference this material appropriately (e.g., Supporting Figure S1, Supporting Table S1). If something is not referenced in the main text, then it might not be necessary at all ;) Keep your story short and to the point.