Final Project: Putting it all together…

Title: *"It's not just code, it's mindset"*

Objectives:

- Employ all what you have learned in the past weeks to produce a coherent talktorial.

Deliverables:

- A talktorial on the task you have been working on for the whole semester
  - Group 1: Predicting aqueous solubility from molecules' SMILES notation
  - Group 2: Predicting binding affinity of the D2 receptors from molecules' SMILES notation.
  - **Push a talktorial to the GitHub repo by 6 PM the Wednesday before next session**
- A walkthrough-presentation for your talktorial (45 minutes)

Description

You went through quite the journey with your CEO. She thought that replacing humans with AI was going to be an easy task, but it turned out to be a tricky one!

To replace humans, we need to "understand" humans. And, hopefully, by now you know that there is no way to replace humans yet. If we remove them from the manual work, they will still be needed for the cognitive work.

And cognitive work is not easy. Not at all…

You understand the humility needed for conducting your task. Now, instead of expecting one's code to fly to the moon and back, one only acknowledges the presence of limitations and yearns to spot them. Because… each limitation acknowledged, is a door opened to the next solution!

You decide to create a talktorial to show your CEO. In this code, you will not claim superiority of an ML model or promise anything. You will simply state what you have, state what was good about it, what was missing, what looks promising, and what would be a

good next step. **Remember that this is an open problem that might or might not have definitive answers, and your added value to the company is the critical thinking you bring to the table.**

The talktorial will include the 5 topics you have been exploring this semester; chemistry, data, representation, modeling, and evaluation.

- Your talktorial will contain a section for each of these topics.
- In each section, you will explain
    1. Its premise: e.g., what is the known chemistry of your problem? What would you expect to find in your data? What features are needed to describe your molecules for your problem?
    2. Its state: What actually exists in your data? What features are available?
    3. Its limitations: What is missing? How would it affect your analysis?
    4. Its prognosis: What is expected given what one has and does not have?
    5. Its results: Did you get what you expected? If yes, show evidence. If not, propose hypotheses.
- Your talktorial will be your presentation. So, make sure it contains coherent and easy-to-read text alongside enough good figures to help you explain your points to the CEO.