**Minutes from meeting 2023.09.07**

* Caio has collected a number of ”seed” CBCs: 15 with 3D structure from bacteria, plant, fungi and animal from a 2015 review paper plus the 7 that he has been working with.
* It would be good to have additional seeds from for example archaea, mycetes, protozoans.
* The CBC structures have a domain which superimpose nicely between all of them. Some have additional domains. It would be good to get an idea of what the extra stuff is, and whether we should trim the sequences for the clustering (for example only use the pfam domain).
* We decided to blast the seeds against Genbank, because the non-redundant database is too big and not well-curated. After that, we’ll cluster them, and then we’ll link the clustering with activity.
* We have several “layers” of activity: mono- or diphenolase, substrate preference (0, 1 or 2 methoxylations), and nitrosation (I’m not completely sure about this part 😅)
* Paper 2 will be simulating some reactions for different CPCs to explain their difference in activity/substrate preference. According to Albert it’s not possible to simulate a reaction with normal MD, and QMD takes a long time. We’ll set up a meeting with him later.

**Ida tasks:** Retrieve sequences from the PDBs and make multiple sequence alignment. Start table with seeds and activity information. Talk with Ulla about end date of sick leave. Write research aims for paper 1. Start writing new project description for the half year report.

**Caio tasks:** Look for characterized CBCs from other taxonomies (on a website which I forgot the name of) when he returns from holidays.