**Minutes from meeting 2023.08.29**

Jane + Caio introduced Lignin Biotechnology and PPOs. Some of the major research questions at this point:

1. Why does some enzymes prefer non-substituted phenols (tyrosinases) over guaiacyls (single subst)? What are the structural differences/determinants for these differences?
2. Why can some enzymes only perform the diphenolase activity (2 e abstraction) while others can perform both monophenolase (monooxygenase) and the diphenolase reactions?
3. Why and how does a subset of “short” PPOs oxidize the syringol unit (S-unit, with two methoxylations)?

Discussions concerning potential paths for Ida’s future project.

1. Classificaition/phylogeny of CBC (coupled binuclear copper) enzymes. They exist in all branches of life. How did they evolve? How can we classify any biochemical differences in differences in sequence/fold/structures? What are the speculations (?) of potential biological roles in various life forms?
2. Reclassification/organization of VAO-enzymes (flavoenzymes). Big ambrella-collection of enzymes that are currently containing a number of different activities that are unrelated. Contains among others AA7s and AA4s. Is it possible to obtain a better differentiation between flavo-enzymes and thereby classification that resembles their activity?
3. MD simulations used on carefully selected PPOs to investigate differences in ligand binding and catalysis of PPOs that display different catalytic behavior. Several very open questions like; how can we explain based on enzyme-substrate interactions that some enzymes can perform both monophenolase and diphenolase activity? How can we explain the differences in interactions between substrates with one or two methoxylations (G- or S-unit) compared to non-substituted phenols?

Decision to follow track #1 and #3, starting with #1. Aim is to identify key determinants for structural/sequence-based variations that can lead to high-resolution differentiation of enzymes, which can then lead to phrasing relevant questions to MD simulations. Each track should preferably result in one paper.

**Ida tasks**: Focus and finish work on paper 1. Gradually start building the frame for does sequence based classification of CBC-enzymes; aka identify know/characterized members from as many different phylum as possible. Identify structurally characterized members of CBCs in PDB. Start collection of sequence data of CBCs.

**Caio tasks**: Support Ida in the above (except paper 1).

**Jane tasks**: Finalize formal supervisor change procedure. Start prolongation process.