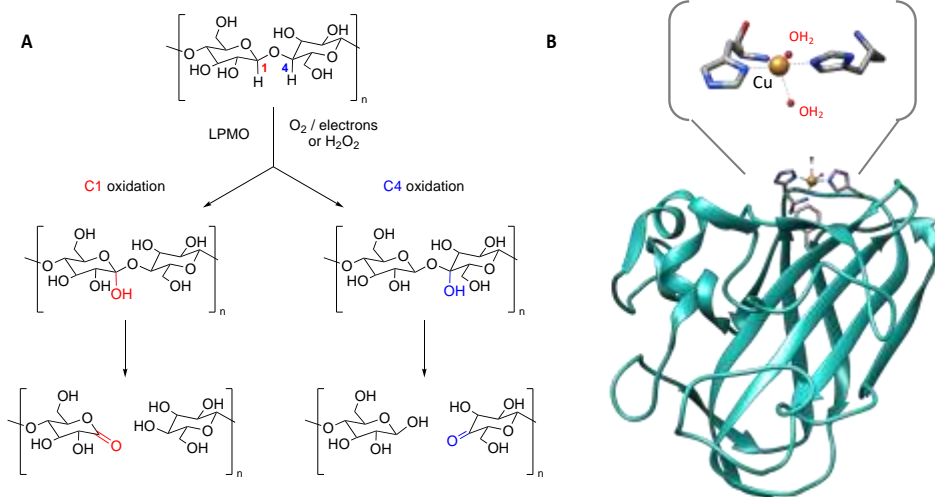


## Structural and catalytic peptide models of the Cu-LPMO enzyme.

Lignocellulosic biomass is increasingly considered as a renewable feedstock to produce bio-sourced chemicals, biomaterials and advanced biofuels. In this context, Copper-dependent Lytic Polysaccharide Monooxygenases (Cu-LPMO), discovered in 2010, have attracted attention given their ability to initiate the degradation of recalcitrant polysaccharides from biomass. LPMO are mono-copper enzymes able to promote extended polysaccharides cleavage (e.g. cellulose or chitin) using oxidative mechanisms. More precisely, LPMO catalyze the hydroxylation of an inert C-H bond at the glycosidic linkage (either at C1 or C4 position) at the surface of recalcitrant polysaccharide polymers further leading to glycosidic bond cleavage (Fig A).



In collaboration with the BioSciences group (Jalila Simaan from ISM2) in Marseille, we have recently started to structurally and functionally characterized peptide-based models of Cu-LPMO. The peptide scaffold chosen, although quite simple in design, is able to reproduce the key features of the Cu(II) coordination site (shown in Fig. 1B) and the Cu-peptide complexes thus obtained show interesting catalytic activity towards a model substrate. The aim of the internship is to widen the peptide family, with rationale modifications to improve the catalytic activity of the Cu-peptide complexes.

During the internship, the student will be involved in a multidisciplinary project, going from peptide synthesis to the measurements of catalytic activity via investigations of the reaction mechanism at play using a variety of spectroscopic tools.

Environment: The successful candidate will work in a dynamic and international environment at the CNRS, Laboratoire de Chimie de Coordination in Toulouse, team [ALAMBIC](#). The technical and scientific environment of the laboratory and the host team is ideally suited to the project. The successful candidate will be trained in peptide synthesis and characterizations and advanced spectroscopic techniques such as NMR, EPR, UV-Visible, circular dichroism, fluorescence.

Profile: We are looking for a highly motivated student with a background in molecular chemistry and excellent grades. Candidates should have a keen interest in multidisciplinary projects in the field of bioinorganic chemistry. They should also be able to work autonomously and as part of a team. There will be an open PhD position on the same topic in 2024.

Supervisors : Christelle Hureau [christelle.hureau@lcc-toulouse.fr](mailto:christelle.hureau@lcc-toulouse.fr) & Jalila Simaan [jalila.simaan@univ-amu.fr](mailto:jalila.simaan@univ-amu.fr)

Applications (CV and academic transcripts) should be sent to Dr. Hureau, no later than the 30<sup>th</sup> of November.

### Bibliography:

[1] Singhvi, M. S.; Gokhale, D. V. Lignocellulosic Biomass: Hurdles and Challenges in Its Valorization. *Appl Microbiol Biotechnol* 2019, *103* (23–24), 9305–9320. <https://doi.org/10.1007/s00253-019-10212-7>

[2] Forsberg, Z.; Sørli, M.; Petrović, D.; Courtade, G.; Aachmann, F. L.; Vaaje-Kolstad, G.; Bissaro, B.; Røhr, Å. K.; Eijsink, V. G. Polysaccharide Degradation by Lytic Polysaccharide Monooxygenases. *Cur Op Struct Biol* 2019, *59*, 54–64. <https://doi.org/10.1016/j.sbi.2019.02.015>

[3] Wang, B.; Wang, Z.; Davies, G. J.; Walton, P. H.; Rovira, C. Activation of O<sub>2</sub> and H<sub>2</sub>O<sub>2</sub> by Lytic Polysaccharide Monooxygenases. *ACS Catal* 2020, *10* (21), 12760–12769. <https://doi.org/10.1021/acscatal.0c02914>