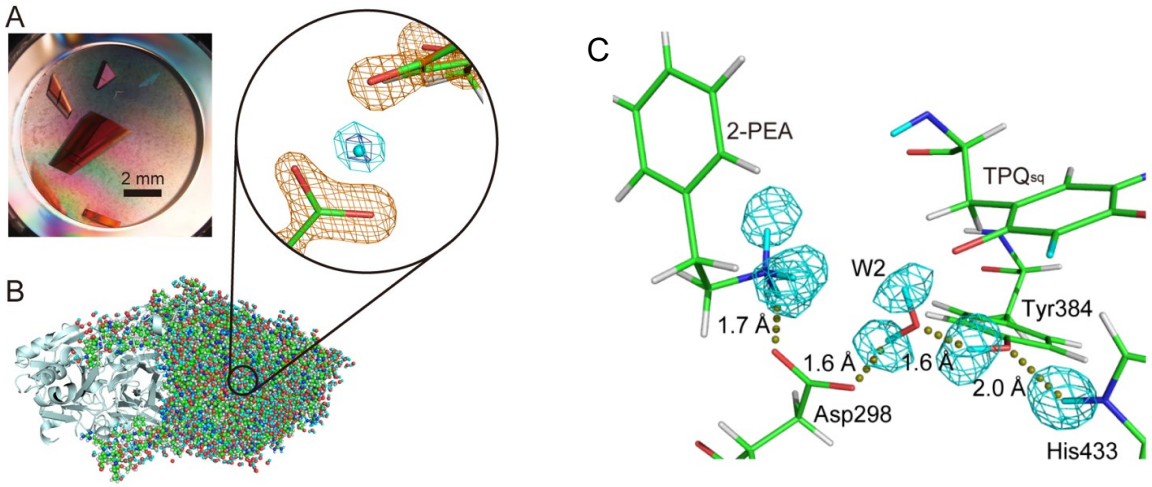
# Neutron crystallography of bacterial copper amine oxidase: Real active-site structures based on the positions of hydrogen atoms

T. Okajima

*SANKEN, Osaka University, Ibaraki, Osaka 567-0047, Japan*

Neutron crystallography is a powerful diffraction method to specify the positions of hydrogen atoms in protein structures. Our group has elucidated the enzyme-catalytic mechanism of a bacterial copper amine oxidase (CAO) based on the hydrogen/proton coordinates determined by neutron crystallography. CAOs contain a redox cofactor, topa quinone (TPQ), and copper ion in the active site. In redox enzymes including CAO, the change of the protonation state of the active site or hydrogen/proton transfer from/to the substrate is a key of the catalysis. In addition, the valence and geometry of bound hydrogen atoms provide essential information to identify chemical species of the cofactor or bound ligands. Here we will introduce recent progress of our group, indicating novel and unique structural information of the active site of the resting oxidized form and the semiquinone radical intermediate.

[1] T. Murakawa, Proc. Natl. Acad. Sci. U. S. A. 117, 10818 (2020).
[2] T. Murakawa, ACS Catal. 13, 12403 (2023).




Neutron crystallography of a copper amine oxidase from *Arthrobacter globiformis*. A) Extra-large crystal for neutron diffraction. B) Overall structure and an unusual "levitated" proton in the resting state. C) Active-site structure of the semiquinone radical intermediate. The next-cycle amine substrate has been bound to the substrate-binding pocket during the reaction cycle.