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**BioSim Talk 2025 #1**  
**Yuri Tulchinsky, PhD.**

Hebrew University of Jerusalem, Israel

**May 30<sup>th</sup> 2025 (Friday), 16:30-18:00**

Institute for Protein Research,  
The University of Osaka (Suita Campus)  
4<sup>th</sup> floor conference room (415)

**Genie in a Bottle – Formation and Reactivity of an Elusive Monomeric Mn(IV)-Oxo Species Inside a Cavitand Pore**

Metal-functionalized cavitands are promising scaffolds for mimicking the hydrophobic environments of metalloenzymes, but integrating their supramolecular features with transition metal reactivity remains challenging. This study introduces a cavitand embedding a coordinatively-unsaturated Mn(II) center, enabling formation of a Mn(IV)-oxo species (high-valent Mn=O complex involved in oxidation) within the cavity. The complex was fully characterized by UV-vis, EPR, HRMS, and, for the first time in a pseudo-octahedral Mn(IV)-oxo species, by XRD. Despite steric shielding, the Mn(IV)-oxo center remains highly reactive in hydrogen atom abstraction (HAA) and oxygen atom transfer (OAT). The cavitand framework enforces steric control, allowing substrate discrimination and regioselective oxidation, mimicking enzymatic selectivity.

Link for online participation via Zoom:

Meeting ID: 862 4686 7061

Passcode: 642880

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