PAN
POLSKA AKADEMIA NAUK

Oddział
we Wrocławiu

Komisja Chemii Teoretycznej i Obliczeniowej Oddziału Polskiej Akademii Nauk we Wrocławiu

uprzejmie zaprasza na otwarte posiedzenie i mikrosympozjum,

które odbędzie się

w dniu 23 września 2026 r., o godz. 10:00

w siedzibie Oddziału Polskiej Akademii Nauk we Wrocławiu

ul. Podwale 75 (sala konferencyjna – parter).

Podczas mikrosympozjum wykład pt.:

„From Static Pockets to Dynamic Binding Sites: A Prediction Perspective" wygłosi

Prof. David Hoksza, Kierownik Katedry Inżynierii Oprogramowania, Wydział Matematyki i Fizyki, Uniwersytet Karola (Praga, Republika Czeska).

Streszczenie wykładu: Most protein functions begin with recognizing a small molecule, making it essential to identify this interaction for tasks such as virtual screening, druggability assessment, functional annotation, and others. Since experimental techniques often lag behind the rapid increase in new proteins, in silico prediction of binding sites has become vital in structural bioinformatics. This presentation will highlight our group's work in this area. We begin with structure-based pocket detection, using machine learning to identify potential pockets on the protein surface. Developing these predictors prompted us to analyze the underlying data, as most reference binding sites are derived from ligand-bound protein conformations. Comparing bound and unbound forms led us to create a benchmark for sites that are difficult to detect in unbound states. This inspired exploration of protein language model representations, which rely only on sequence data and are unaffected by conformational changes. I will show how these compare to traditional methods that use structural and evolutionary data, and conclude with our efforts to combine both approaches, allowing sequence data to inform about spatial pockets and provide new insights.

Przewodniczący Komisji

Chemii Teoretycznej i Obliczeniowej

Prof. dr hab. Robert Wieczorek