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in kemijsko tehnologijo

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VABILO NA PREDAVANJE
V OKVIRU DOKTORSKEGA ŠTUDIJA
KEMIJSKE ZNANOSTI

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z naslovom:

Macromolecular structure and dynamics from computational integration of multiple experimental methods

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Vljudno vabljeni!

Abstract:

Proteins generally populate multiple structural states in solution. Transitions between these states are important for function, such as allosteric signaling and enzyme catalysis. Structures solved by X-ray crystallography provide valuable, but static, atomic resolution structural information. In contrast, Small angle X-ray scattering (SAXS) profiles, while limited in resolution, contain information about conformational and compositional states of the system in solution. Moreover, SAXS profiles can be rapidly collected for a variety of experimental conditions, such as ligand-bound and unbound protein samples, ligand titration series, different temperatures, or pH values. The challenge lies in data interpretation since the profiles provide rotationally, conformationally, and compositionally averaged information about protein shape in solution. I will describe a novel computational method, MultiFoXS, that simultaneously uncovers the set of structural states that exist across multiple input SAXS profiles as well as their population weights in each sample. Moreover, comparison of conformations and their weights between the ligand-bound and unbound SAXS profiles can help in determining the allosteric mechanism. The method was benchmarked on over 30 cases with experimental SAXS profiles, including large multi-domain proteins and proteins with long disordered fragments. The applicability of the method extends beyond SAXS datasets. It has been applied to datasets from Small Angle Neutron Scattering (SANS), Electron Microscopy, and residual dipolar couplings (RDCs).