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VABILO NA PREDAVANJE
V OKVIRU DOKTORSKEGA ŠTUDIJA
KEMIJSKE ZNANOSTI / INVITATION TO THE
LECTURE WITHIN DOCTORAL PROGRAMME IN
CHEMICAL SCIENCES

Prof. Marie Skepö

*Lund University, Department of Chemistry
Division of Theoretical Chemistry, Sweden*

z naslovom / title:

**Application of a coarse-grained model using
intrinsically disordered Histatin 5 as model
protein**

v sredo, 4. 5. 2022 ob 15. uri /

on Wednesday, 4. 5. 2022 at 15.00

preko spletnega orodja Zoom / via Zoom:

[https://uni-lj-
si.zoom.us/j/96899033530?pwd=UmZmT1A1a2xlQkIITHNGMD
bzR283QT09](https://uni-lj-si.zoom.us/j/96899033530?pwd=UmZmT1A1a2xlQkIITHNGMDbzR283QT09)

(Meeting ID: 968 9903 3530, Passcode: 633038)

Vljudno vabljeni! | Kindly invited!

Abstract:

For more than 30 years, a coarse-grained model based on the primitive model, in combination with Monte Carlo simulations, has been used to model polyelectrolytes and polyampholytes under various conditions. Sometimes this model is also referred to as the bead-necklace model. In this model, each monomer corresponds to a bead with a radius and furthermore, it can be appointed a charge. The water is always treated as a dielectric continuum. Our aim is to apply this model to intrinsically disordered proteins, and thereby, be able to study conformational properties of the proteins and intermolecular interactions with other macromolecules as well as solid surfaces and membranes.

To validate our model and to obtain a molecular understanding of the system, we are utilizing a combination of atomistic molecular dynamics simulations as well as experimental techniques. In this talk I will present the coarse-grained model, its possibilities, and limitations, using Histatin 5, an anti- microbial saliva peptide, as a model system. More specifically, the focus will be on oligomerization and reentrant condensation upon the addition of multivalent ions.