Opis delovnega mesta mladega raziskovalca/ke (D*escription of the Young Researcher's position)*

1. Članica UL (*UL member)*:

Fakulteta za kemijo in kemijsko tehnologijo/Faculty of Chemistry and Chemical Technology

2. Ime, priimek in elektronski naslov mentorja/ice (*Mentor's name, surname and email*):

Barbara Hribar Lee (barbara.hribar@fkkt.uni-lj.si)

3. Raziskovalno področje (*Research field*):

Fizikalna kemija (Physical Chemistry)

4. Opis delovnega mesta mladega raziskovalca/ke (D*escription of the Young Researcher's position)*: Vključuje morebitne dodatne pogoje, ki jih mora izpolnjevati kandidat/ka za mladega raziskovalca/ko, ki niso navedeni v razpisu za mlade raziskovalce.

slo: Proteini so aktivni samo v svoji nativni konformaciji, ki je dana tako z lastnostmi proteina, kot tudi z okolico, v kateri se nahaja. Za pravilno zvitje proteina je tako ključna njegova solvatacija oz. hidratacija, saj se večina proteinov nahaja v vodnem okolju. Čeprav vemo, da različni sotopljenci v raztopin na hidratacijo vplivajo, je mehanizem teh procesov slabo raziskan, predvsem zaradi težav z modeliranjem samega topila. Prav tako se proteini v celicah nahajajo v močno nagnetenem prostoru, ki na hidratacijo vpliva že samo po sebi. V okviru doktorskega dela bo kandidat/kandidatka raziskal vpliv različnih vrst sotopljencev (različne soli, hidrofobni topljenci, ...) na hidratacijo globularnih proteinov in kako le-ta vpliva na stabilnost njihove nativne konformacije ter agregacijo. Le-ta namreč predstavlja enega glavnih problemov pri pripravi formulacij bioloških zdravil. Pri svojem delu bo kandidat/kandidatka uporabil kombinacijo eksperimentalnih tehnik ter teoretičnih metod in računalniških simulacij. Te omogočajo študij hidratacije tako v raztopinah kot tudi v utesnjenem okolju in so ključne za razumevanje procesov na mikroskopskem nivoju ter s tem za njihovo načrtovanje. Na podlagi dobljenih rezultatov bo kandidat/kandidatka poskusil hidratacijo vključiti v potencial srednje sile za opis interakcije med proteini ter proteini in drugimi makromolekulami s svojo okolico, pri čemer se bo, poleg zgoraj že omenjenih pristopov, poslužil tudi metod strojnega učenja.

eng: Proteins are only active in their native conformation that is determined by the properties of the protein, as well as by its surrounding. On of the main driving forces in protein folding is its solvation, where water is the most frequent solvent. Even though it is known that cosolutes affect the protein solvation, the mechanism of the process is still not well understood, mostly due to the problems with water modelling. Further, the proteins in the cells are exposed to extremly crowding conditions that influence the solvation. Within the doctoral work the candidate will investigate the influence of different cosolutes (different salt types, hydrophobic solutes ...) on the solvation of the globular proteins, and

thus on the stability of the protein native structure, and their aggregation. He/she will use different experimental techniques to study the protein conformation, while the mechanism of (de)solvation will be investigated on the micro level by theoretical methods and computer simulations. The methods will be applied to bulk solutions, as well as to the proteins in crowded environment. Using the obtained results he/she will, with the help of machine learning approaches, make an attempt to include solvation into the potential of mean fore describing the interaction of the proteins and other macromolecules with their surroundings.