1. Raziskovalna organizacija (*Research organisation)*:

Univerza v Ljubljani, *Fakulteta za kemijo in kemijsko tehnologijo*

2. Ime in priimek mentorja (*Name and surname of a mentor*):

Barbara Hribar Lee

3. Področje znanosti iz šifranta ARRS (*Primary research field*):

1.04.01 Naravoslovje/Kemija/Fizikalna kemija

4. Kontaktni e-naslov mentorja (*Contact of a mentor)*:

barbara.hribar@fkkt.uni-lj.si

5. Kratek opis programa usposabljanja (*Short description of the program)*:

Lastnosti biološko pomembnih molekul, kot so njihova nativna struktura, asociacija, topnost, stabilnost ... so odvisne od intra in intermolekulskih interakcij. Zaradi ključnega pomena teh lastnosti v medicini, farmacevtski industriji in različnih tehnoloških procesih je poznavanje interakcij v raztopinah biološko pomembnih molekul eden večjih izzivov današnjih raziskav.

Mladi raziskovalec bo pri svojem delu raziskal medsebojno odvisnost različnih prispevkov (elektrostatski, hidrofobni, izključeni volumen) k efektivnim medmolekulskim interakcijam. Ustrezno izbranim proteinom s poznano nativno strukturo bo najprej določil fazni diagram v vodnih raztopinah, pri tem bo posebej pozoren na parametre razvitja proteina ter na območje steklastega prehoda. Preveril bo reverzibilnost sprememb v strukturi proteina in njegovih asociatov. Podatke bo izmeril pri različnih parametrih (temperatura, tlak, ...), ki določajo pomembnost posameznih prispevkov k meddelčnim interakcijam. Pri tem bo še posebej pozoren na določitev množine hidratirane vode na proteinu. Poskusil bo konstruirati asociativni hamiltonian, s katerim bi lahko teoretično reproduciral fazni diagram.

V drugem delu bo raziskal jakost vezanja skupine ligandov na protein. Eksperimentalno določeno stabilnost kompleksov bo primerjal s teoretičnimi napovedmi.

The properties of biologically important molecules, such as their native structure, association tendency, solubility, stability etc. are determined by inter- and intra- molecular interactions. Due to the importance of these characteristics in medicine, pharmacy, as well as in various technological processes, the study of molecular interactions in solutions of biologically important molecules represent a great challange for today's researchers.

During the program, the MR will study the interplay of different contributions (electrostatic, hydrophobic, excluded volume effect) to the effective potential between molecules in solution. He/she will, using different experimental techniques, measure the phase diagram

of aqueous solutions of different proteins with the known native structure. He/she will pay special attention locating the folding and glass transition of proteins in question. The reversibility of the protein structure, as well as that of the associates will be checked. The phase diagram will be studied at different parameters that are known to affect the interactions (temperature, pressure, ...). The amount of the hydration water will be determined. An attempt will be made to construct the associative hamiltonian, which will be used to reproduce the phase diagram via theoretical methods.

In the second part of his/her work, the MR will study the binding of different ligands to a chosen protein with a known structure. The experimentally determined stability will be compared with theoretical predictions.