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*):

Iztok Turel

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

1.04 Kemija

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

iztok.turel@fkkt.uni-lj.si

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

SLO

Rutenij je kovina prehoda, ki ima v obliki spojin številne možnosti uporabe. Mnogi raziskovalci se ukvarjajo s pripravo novih rutenijevih spojin kot možnih zdravil, za konverzijo sončne energije, za katalizo raznih organskih reakcij in razkroj vode.
Spojine, ki vsebujejo kovinske ione se v medicini uporabljajo za različne namene (npr. kot terapija za zdravljenje različnih bolezni, v diagnostiki). Dve rutenijevi spojini sta že vstopili v klinična testiranja kot možni protirakavi spojini, saj imata določene prednosti pred spojinami platine, ki se sicer v klinični rabi uporabljajo v ta namen. Mnoge rutenijeve spojine se uporabljajo tudi kot katalizatorji za pretvorbe v organski sintezi (za raziskave na tem področju je bilo podeljenih že nekaj Nobelovih nagrad za kemijo!). Znano je tudi, da kovinske spojine lahko katalizirajo tudi določene procese v celicah, a mnoge podrobnosti zaenkrat še niso znane. Uporaba kovinskih spojin kot katalitičnih zdravil bi omogočila uporabo zelo nizkega, netoksičnega odmerka. Raziskave povezav med biološkimi in katalitskimi lastnostmi so zato zelo aktualne.

Za vsako od omenjenih področij je bistvenega pomena, da se spojine pred praktično uporabo popolnoma fizikalno-kemijsko okarakterizira in s tem bolje razume njihovo naravo. Spojine, ki so kandidati za uporabo na naštetih področjih, morajo imeti še mnoge druge lastnosti (recimo topnost, stabilnost, primerno reaktivnost, itd). Njihovo topnost lahko izboljšamo tudi s kemijsko modifikacijo (vezavo določene skupine ali zamenjavo protiiona) ali pa z vezavo v/na razne nosilce (polimere, liposome). Mladi raziskovalec bo na osnovi sistematičnega pristopa poskušal izolirati nove rutenijeve komplekse, ki bodo čimbolj ustrezali omenjenim zahtevam. V naših laboratorijih smo v zadnjih letih pripravili številne rutenijeve komplekse z β-diketonatnimi, hidroksikinolatnimi, kinolonskimi, fosfinskimi in drugimi ligandi. Tudi trenutne raziskave se najbolj odvijajo v teh sistemih, saj želimo z večjim naborom spojin dobiti boljšo sliko o povezavi strukture z aktivnostjo (SAR).

Kot izhodne spojine za pripravo kompleksov bo mladi raziskovalec uporabil različne rutenijeve prekurzorje. Od ligandov bo uporabil različne dvovezne (N,N-; N,O- in O,O-) kot tudi enovezne donorske ligande. V primeru da bodo fizikalno-kemijski in/ali biološki rezultati določenih produktov zanimivi, bomo poskusili rezultate obogatiti tudi z drugimi kovinskimi ioni. Poleg izolacije koordinacijskih in organokovinskih spojin, bo raziskovalec po potrebi z organskimi sintezami pripravil tudi ligande, ki niso komercialno dostopni.

Definirane produkte bo doktorand okarakteriziral s standardnimi fizikalno-kemijskimi metodami (elementna analiza, infrardeča, UV-VIS, fluorescenčna, NMR, masna spektroskopija, itd.), ki so na voljo na Fakulteti za kemijo in kemijsko tehnologijo v Ljubljani. V vsakem primeru bo cilj tudi priprava primernih kristalov, ki jim bomo z rentgensko difrakcijo določili kristalne strukture. Za dosego tega cilja bodo uporabljene različne sintezne tehnike (tudi solvotermalna in mikrovalovna sinteza) in pogoji. Druge lastnosti vzorcev bomo po potrebi nadalje raziskovali tudi v sodelovanju z laboratoriji s katerimi imamo utečeno sodelovanje (tako doma kot tudi v tujini) in kjer so na voljo tudi druge tehnike, ki jih pri nas nimamo. Tovrstne laboratorije bo imel doktorand možnost tudi obiskati, dobil pa bo tudi možnost sodelovanja v domačih in mednarodnih projektih v katerih sodelujemo.

ANG

Ruthenium is a transition metal and its compounds have many interesting applications. Many researchers are dealing with isolation of novel ruthenium compounds as potential drugs, as components of solar cells, as catalysts for organic reactions and decomposition of water.
Metal ion containing compounds are used in medicine for different purposes (e.g. as therapy for the treatment in many diseases, in diagnostics). Two ruthenium compounds are currently involved in clinical tests as potential anticancer agents. These compounds exert many advantages in comparison to standard platinum drugs that are currently used in clinical practice. Many ruthenium compounds

are also used as catalysts for a variety of organic reactions (few Nobel prizes in the field of chemistry were awarded for such discoveries). It is known that metal compounds can catalyze certain processes in the cells but many details on the exact reaction mechanisms remain unclear at this moment. The use of metal compounds as catalytic drugs would enable uses of low non-toxic dosages. Therefore studies dealing with relationships between biological and catalytic properties are currently a hot research topic.

For all of the described fields it is of essential meaning that compounds are characterized in detail by physico-chemical methods. This enables to better understand their nature. The candidate compounds for applications must bear also many other properties (solubility, stability, appropriate reactivity, etc). Their solubility can be improved by chemical modifiactions (introduction of chemical functionalities or counterion exchange) or by the use of drug delivery systems (polymeric carriers, liposomes). With the use of a systematic approach, young researcher will try to prepare novel ruthenium complexes that meet the above mentioned requests. In last years our lab has reported the synthesis of numerous ruthenium complexes with β-diketonate, hydroxyquinolate, quinolone, phosphine and other ligands.These systems are also involved in an ongoing study to determine structure-activity relationships (SAR).

Different ruthenium precursors will be used as starting materials in synthetic work carried out by the young researcher. Various bidentate (N,N-; N,O- in O,O-) as well as monodentate ligands will be used for preparation of metal complexes. In case that interesting physico-chemical and/or biological results of certain isolated products are obtained, reactions might be extended to other metal ions. Researcher will mainly be involved in the isolation of coordination and organometallic compounds. If necessary, part of work could be devoted to organic syntheses (preparation of ligands that are commercially not available).

Defined products will be characterized by standard physico-chemical methods (elemental analysis, infrared, UV-VIS, fluorescence, mass spectroscopy, NMR, etc) which are all available at the Faculty of Chemistry and Chemical Technology in Ljubljana (UL FCCT). One of main goals will also be a preparation of suitable crystals to determine the structure by X-ray structure analysis. Different synthetic approaches will be used to achieve this goal including solvothermal and microwave synthesis. To study other properties of isolated compounds (with techniques not available at UL FCCT) existing cooperations with domestic and foreign research labs will be used. The young researcher will also get the opportunity to visit such groups and to be involved in the current national and international research projects.