

V 3. letniku so “na voljo” naslednji strokovni izbirni predmeti iz področja organske kemije:

## UŠP Kemija:

Izbirni predmeti 3. letnika - strokovni		Kontaktne ure					Σ	ECTS
		P	S	SV	LV	DO		
M. Jereb	Principi zelene kemije	15	15		45		75	5
J. Svete	Kemija heterocikličnih spojin	30	15		30		75	5

## VŠP Kemijska tehnologija:

J. Košmrlj	Organska analitika in spektroskopija	45		30			75	5
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# **Mentorji diplomantom na Katedri za organsko kemijo**

**prof. dr. Janez Cerkovnik**

**prof. dr. Darko Dolenc**

**doc. dr. Uroš Grošelj**

**prof. dr. Marjan Jereb**

**prof. dr. Marijan Kočever**

**prof. dr. Janez Košmrlj**

**prof. dr. Franci Kovač**

**doc. dr. Krištof Kranjc**

**prof. dr. Andrej Petrič**

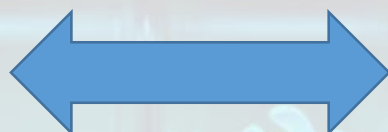
**doc. dr. Franc Požgan**

**prof. dr. Jurij Svete**

**doc. dr. Bogdan Štefane**

# Področja organske kemije, ki jih pokrivamo na Katedri za organsko kemijo:

**Organska sinteza**



**Organska analiza**



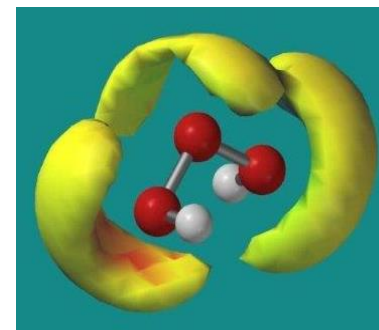
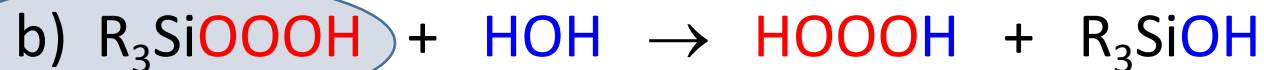
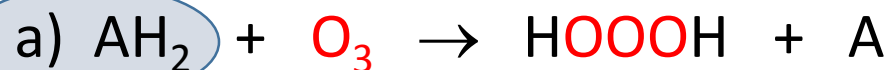
- Heterociklične spojine (sinteza, struktura, lastnosti, uporaba)
- Sinteza biološko aktivnih spojin in njihovih analogov
- Organokovinska kemija
- Pretvorbe pod vplivom mikrovalov oz. pod visokim pritiskom
- Moderne metode NMR spektroskopije
- Organska fotokemija
- Zelena kemija
- Selektivno halogeniranje
- Oksidacije modelnih spojin z reaktivnimi kisikovimi zvrstmi (ozon, dioksirani, peroksidi)
- Stereoselektivna in “high-throughput” sinteza

izr. prof. dr. Janez Cerkovnik  
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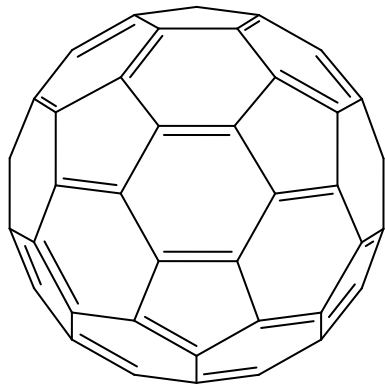
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1) Sinteza izhodnih spojin za pripravo HOOOH:

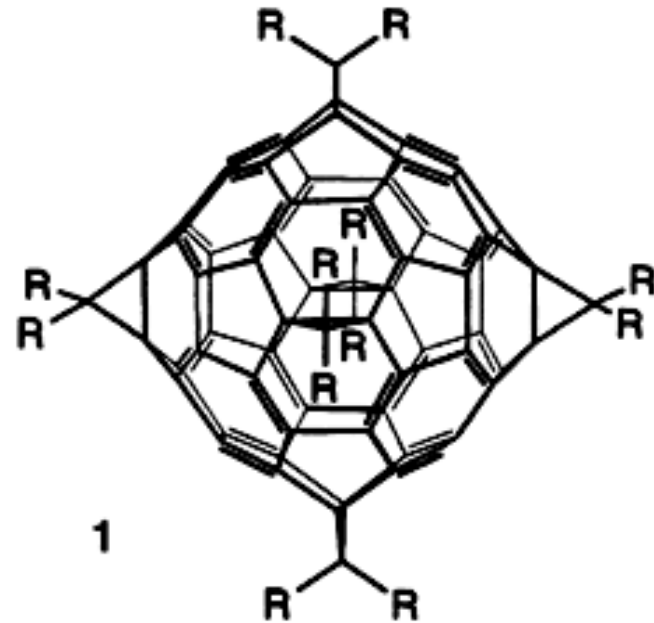
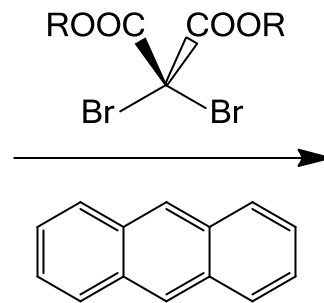


## 2) Sinteza, izolacija in karakterizacija malonatnih aduktov na C<sub>60</sub>

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C<sub>60</sub>



heksaadukt  $T_h$ -C<sub>60</sub>(COOR)<sub>12</sub>

R = alkil, H

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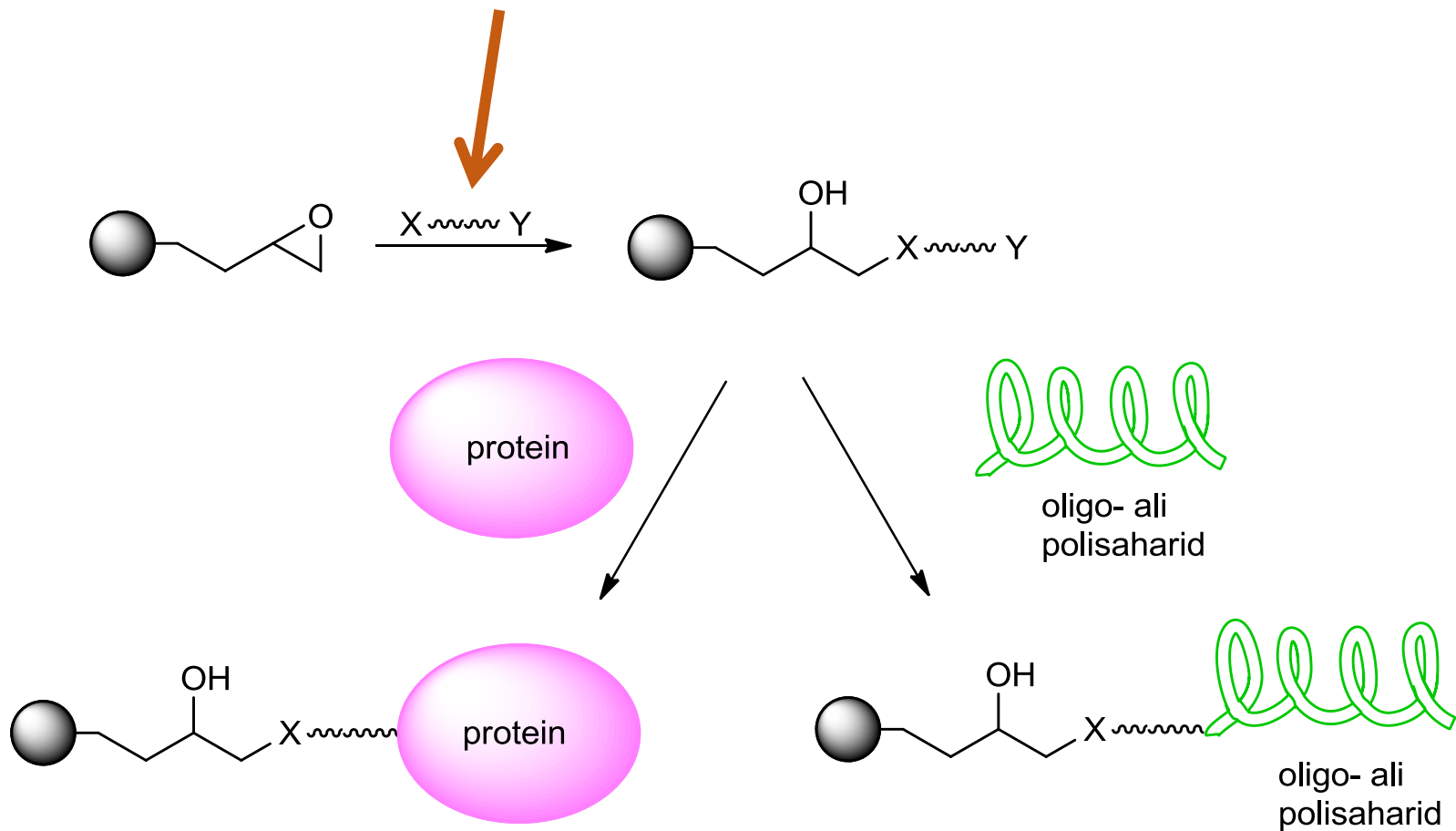
**prof. dr. Darko Dolenc**

## **Razvoj metod za vezavo bioloških makromolekul na epoksi funkcionalizirane polimerne nosilce**

Netopni polimerni nosilci, funkcionalizirani z različnimi funkcionalnimi skupinami se uporabljajo med drugim za separacijo in čiščenje bioloških makromolekul.

- Posebno pomembni postajajo taki nosilci v proizvodnji biofarmacevtikov, kot so monoklonska protitelesa, proizvodnja cepiv, bakteriofagi, plazmidna DNK itn.

- Za vezavo bioloških makromolekul je treba razviti primerne bifunkcionalne "ročice".









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## 1. Asimetrična organokataliza

- Sinteza in strukturna karakterizacija reakcijskih intermediatov
- Sinteza novih imidazolidinonskih katalizatorjev
- Sinteza potencialnih organokatalizatorjev na osnovi pirazolidin-3-onov in tetrahidropiridazin-3-onov
- Sinteza potencialnih organokatalizatorjev na osnovi kafe

## 2. Sinteza heterocikličnih sistemov

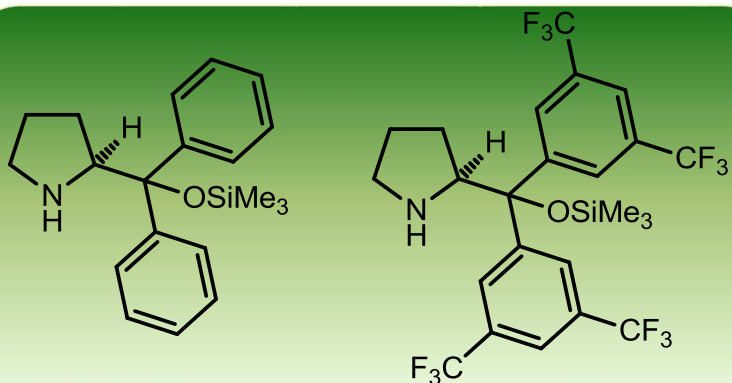
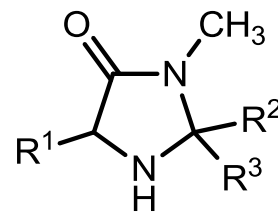
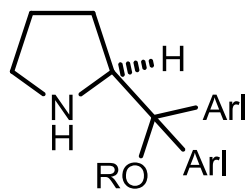
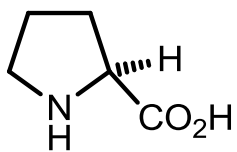
- Sinteza funkcionaliziranih pirolov in nadaljnje pretvorbe
- Transformacije enaminonskih intermediatov, pripravljenih iz *N*-zaščitenih  $\alpha$ -amino kislin
- Sinteza novih heterocikličnih gradnikov/sistemov

# ASIMETRIČNA ORGANOKATALIZA

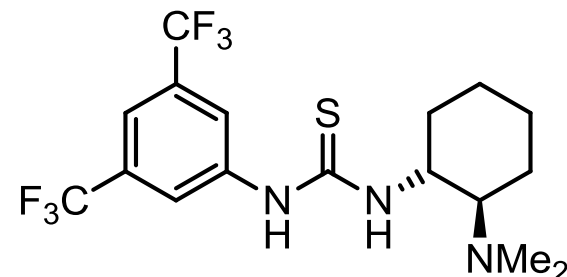
## Kovalentna organokataliza

1. Enaminska kataliza
2. Iminijeva kataliza

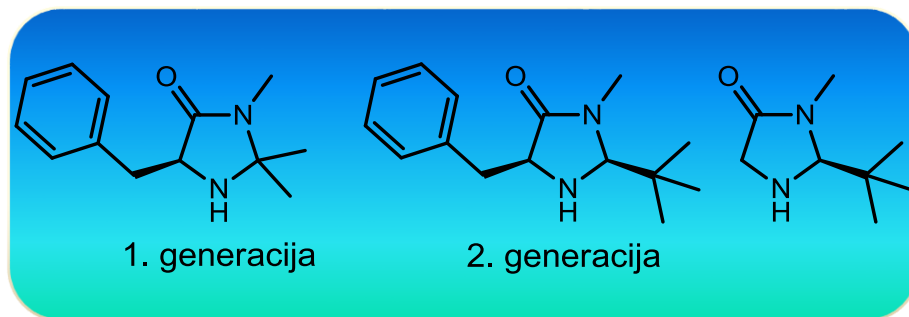
Ciklični sekundarni  
amini kot organokatalizatorji



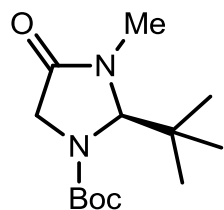
## Ne-kovalentna organokataliza



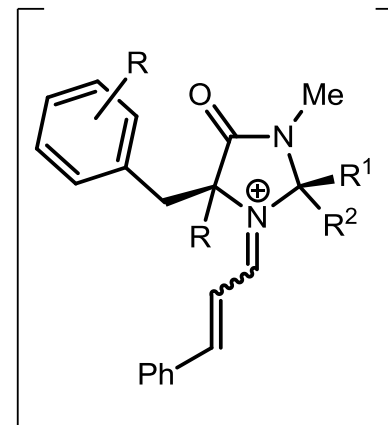
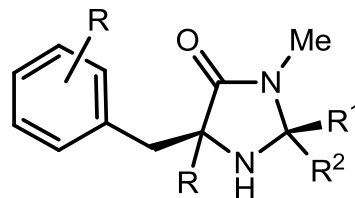
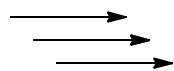
*Takemoto-jev katalizator*



- **Sinteza novih imidazolidinonskih katalizatorjev in karakterizacija reakcijskih intermediatov – iminijevih soli**



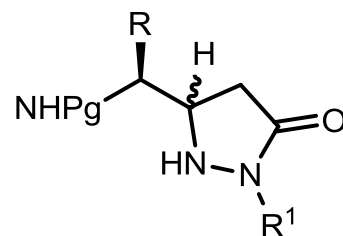
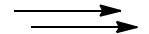
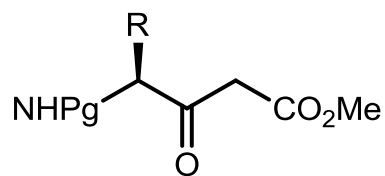
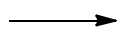
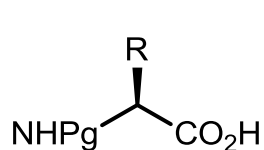
**(S)-Boc-BMI**



**Testna stereoselektivna pretvorba: adicija 1-metilindola na *trans*-cinamaldehyd**

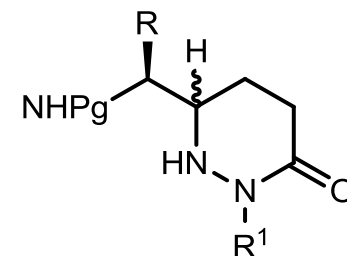
1. U. Grošelj, W. B. Schweizer, M.-O. Ebert, D. Seebach, *Helv. Chim. Acta* **2009**, *92*, 1-13.
2. U. Grošelj, Č. Podlipnik, J. Bezenšek, J. Svete, B. Stanovnik, D. Seebach, *Helv. Chim. Acta* **2013**, *96*, 1815-1821.

- **Sinteza potencialnih organokatalizatorjev na osnovi pirazolidin-3-onov in tetrahidropiridazin-3-onov**



**A**

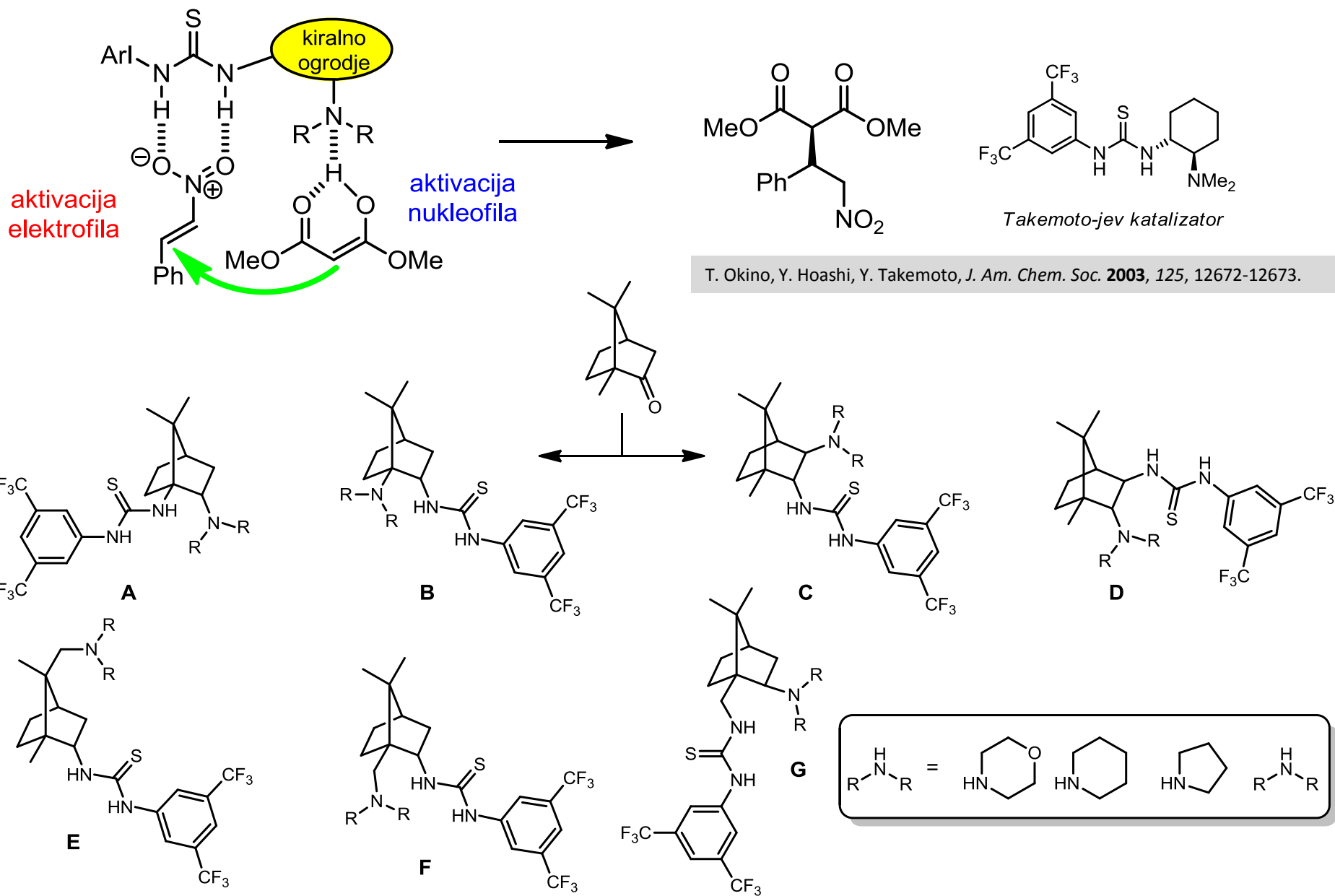
ali



**B**

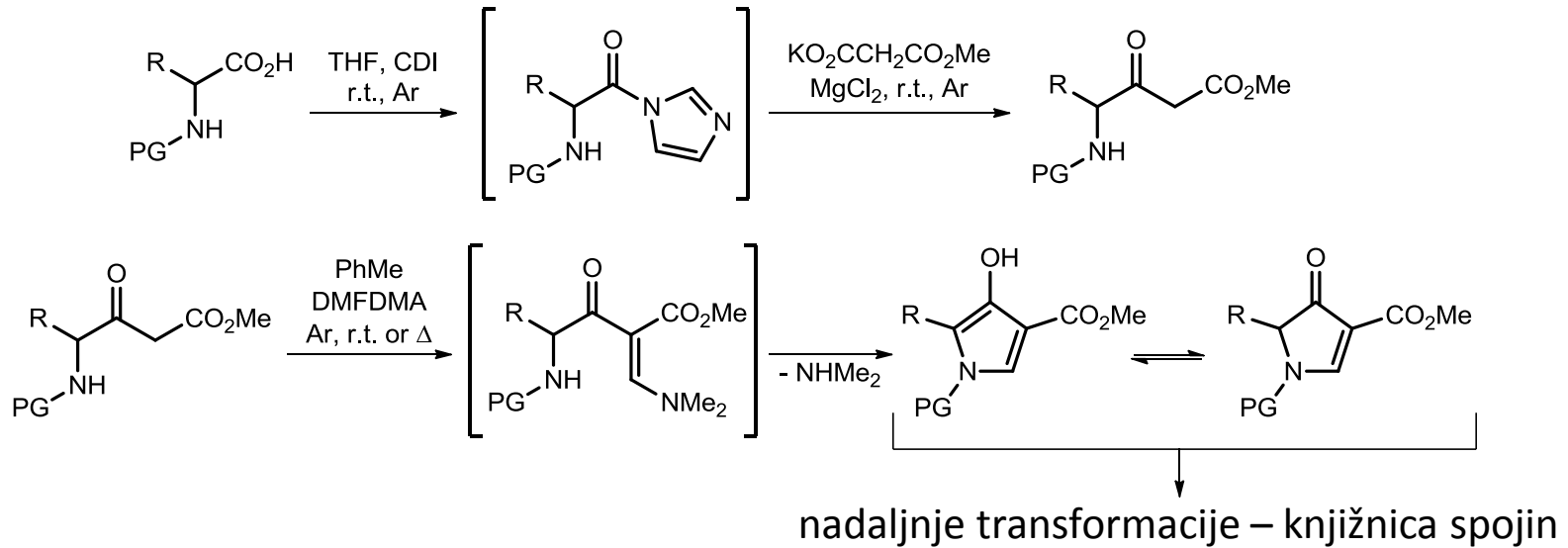
U. Grošelj, A. Golobič, J. Svete, B. Stanovnik, *Chirality*, **2013**, *25*, 541–555.

# Sinteza potencialnih organokatalizatorjev na osnovi kafe



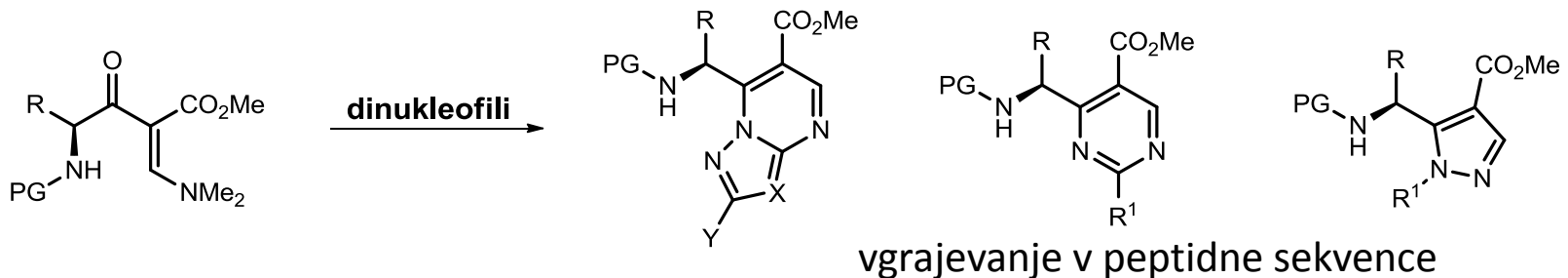
# Sinteza heterocikličnih sistemov

## Sinteza funkcionaliziranih pirolov



U. Grošelj, M. Žorž, A. Golobič, B. Stanovnik, J. Svete, *Tetrahedron*, **2013**, *69*, 11092-11108.

## Transformacije enaminonskih intermediatov, pripravljenih iz *N*-zaščitenih $\alpha$ -amino kislin



## Sinteza novih heterocikličnih gradnikov/sistemov

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**Marjan.jereb@fkkt.uni-lj.si**  
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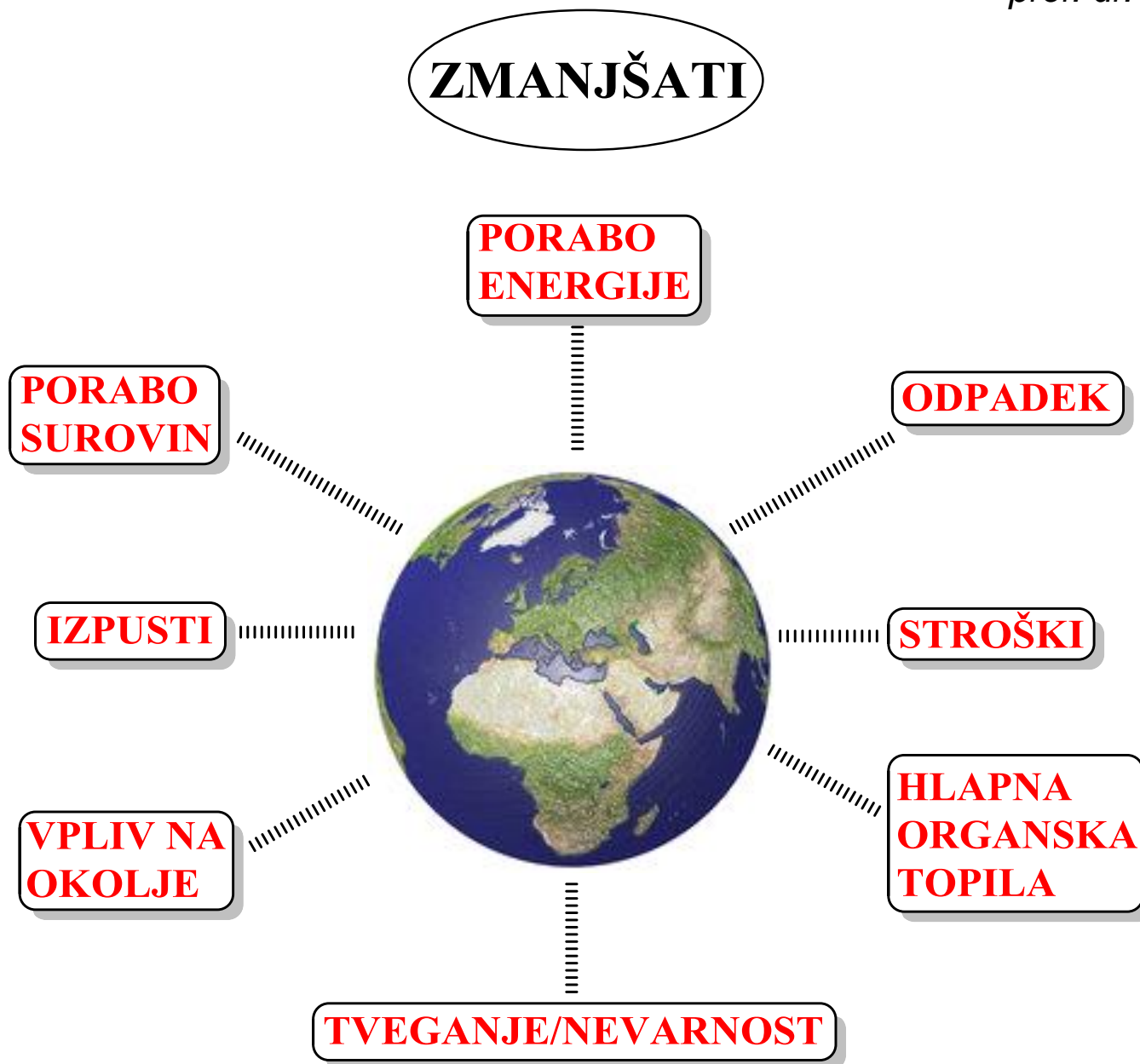
# Bioorganska kemija

**Program Bioanorganska in Bioorganska kemija**

**Selektivna uvedba halogenov v  
organske molekule**

**Zelena kemija**

**Halogeni kot mediatorji transformacij  
organskih molekul**



# **ZELENA KEMIJA**

**REAKCIJE POD POGOJI BREZ TOPILA**

**REAKCIJE NA VODI**

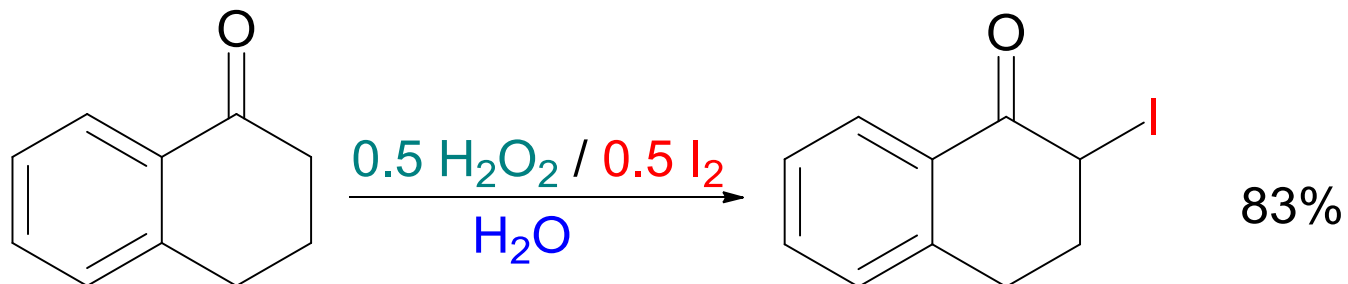
**OBNOVLJIVI REAKCIJSKI MEDIJI**

**ATOMSKA EKONOMIJA**

**MANJ STRUPENI, MANJ NEVARNI REAKTANTI**

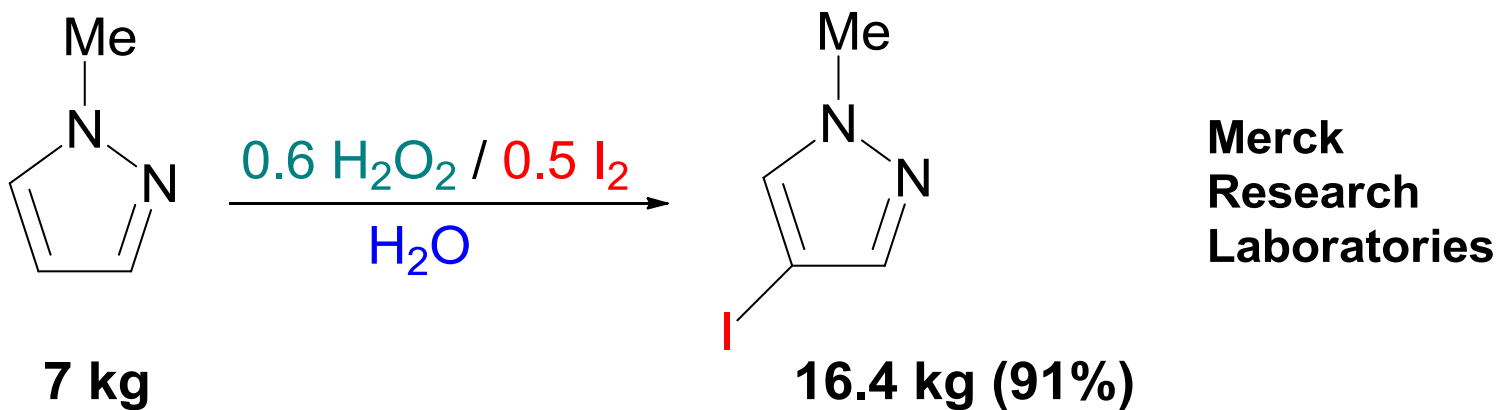


# JODIRANJE NA VODI S 30% RAZTOPINO H<sub>2</sub>O<sub>2</sub> in JODOM



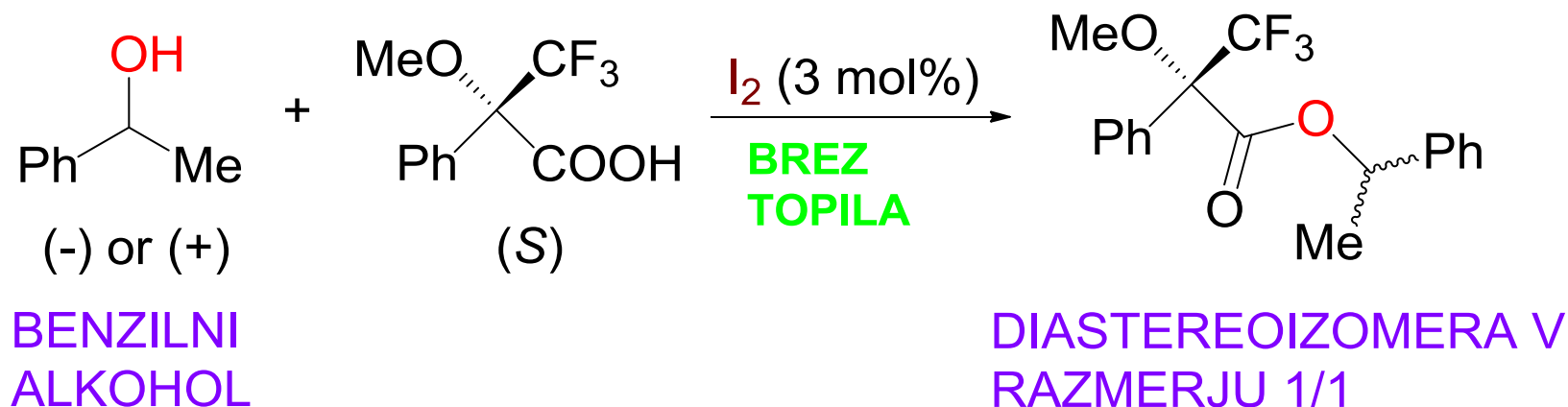
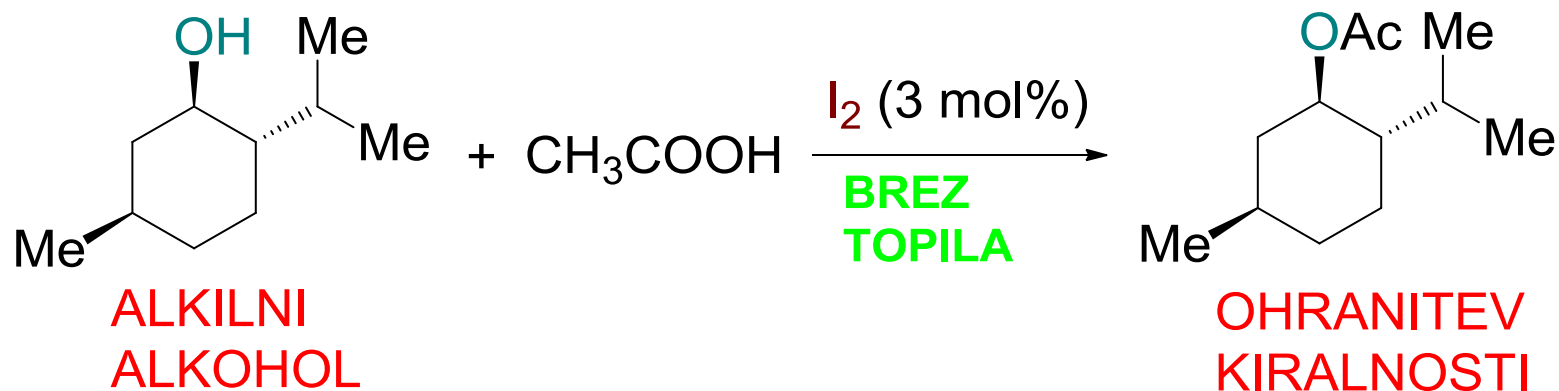
M. Jereb et. al., *Chem. Commun.* 2004, 2614.

## UPORABA: JODIRANJE PIRAZOLOV



M. M. Kim et. al., *Tetrahedron Lett.* 2008, 49, 4026

## ESTRENJE POD VPLIVOM I<sub>2</sub>: DVOJNO OBNAŠANJE ALKOHOLOV

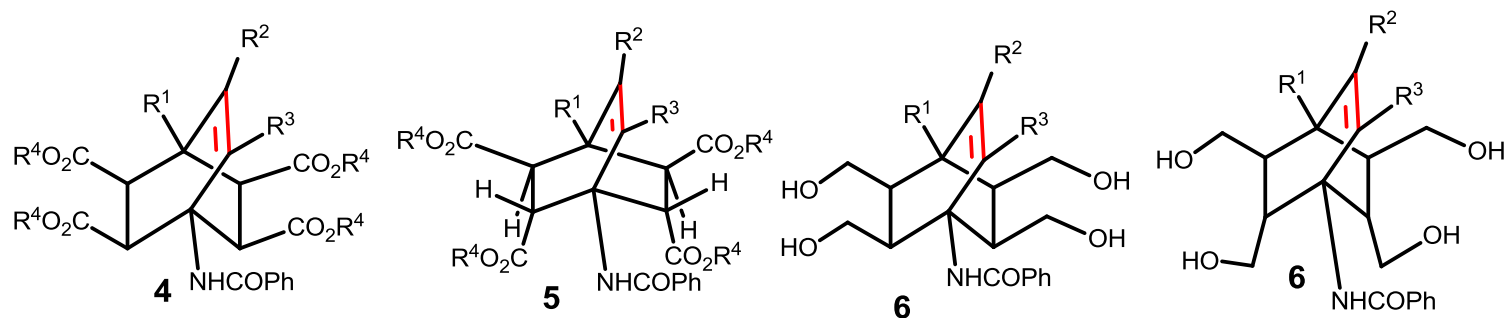
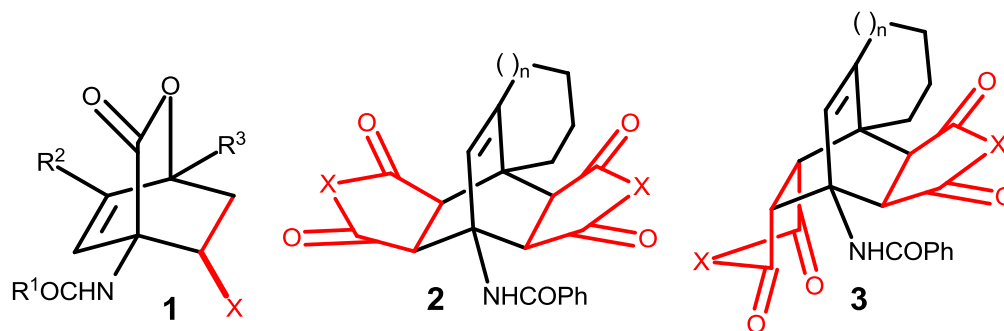


M. Jereb et. al., *Tetrahedron Lett.* 2009, 50, 2347.

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## IZBRANE TARČNE SPOJINE (PROKIRALNE IN KIRALNE) ZA UPORABO V KATALIZI

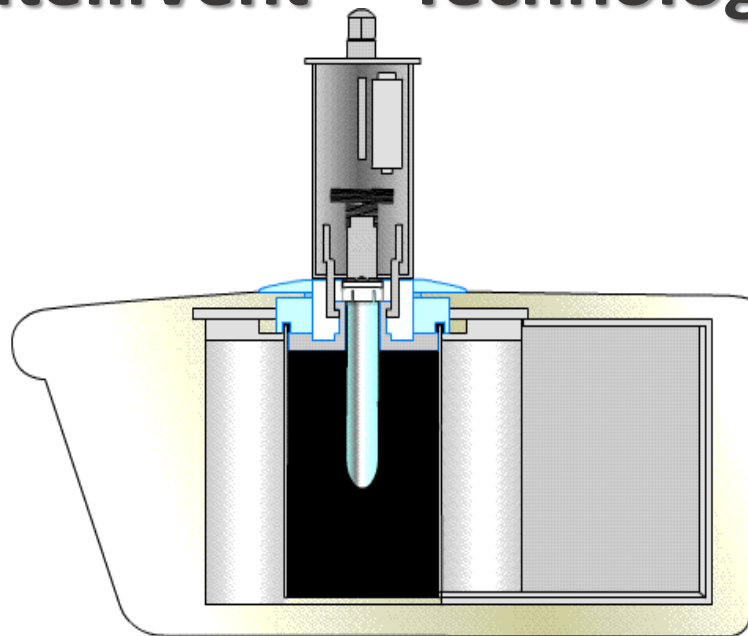


# CEM MICROWAVE DISCOVER SYSTEM

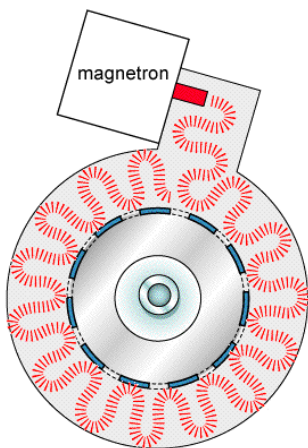
## IntelliVent™ Vial Sealing System



## IntelliVent™ Technology



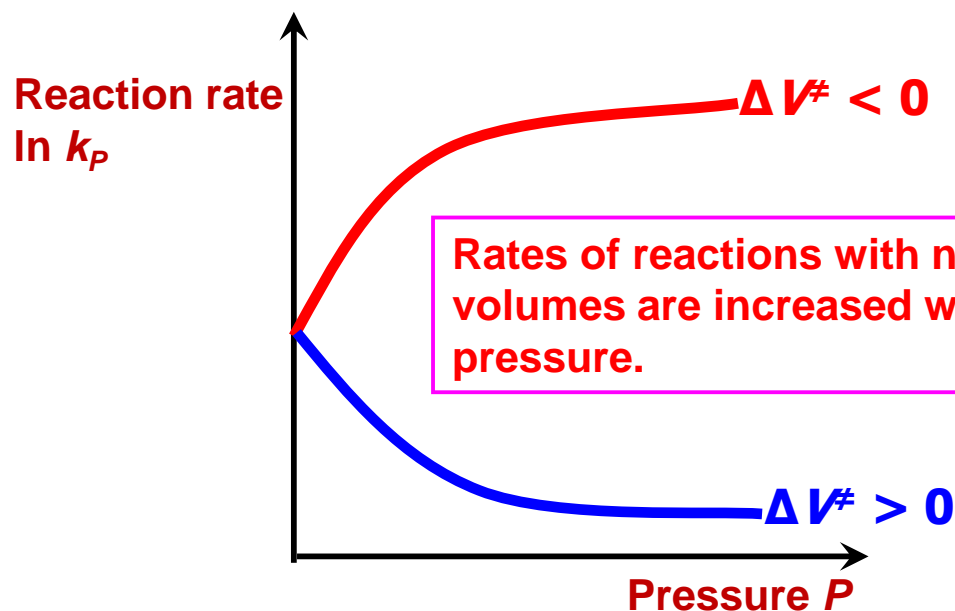
## Self-Tuning Single Mode Microwave Cavity



# HIGH-PRESSURE CONDITIONS

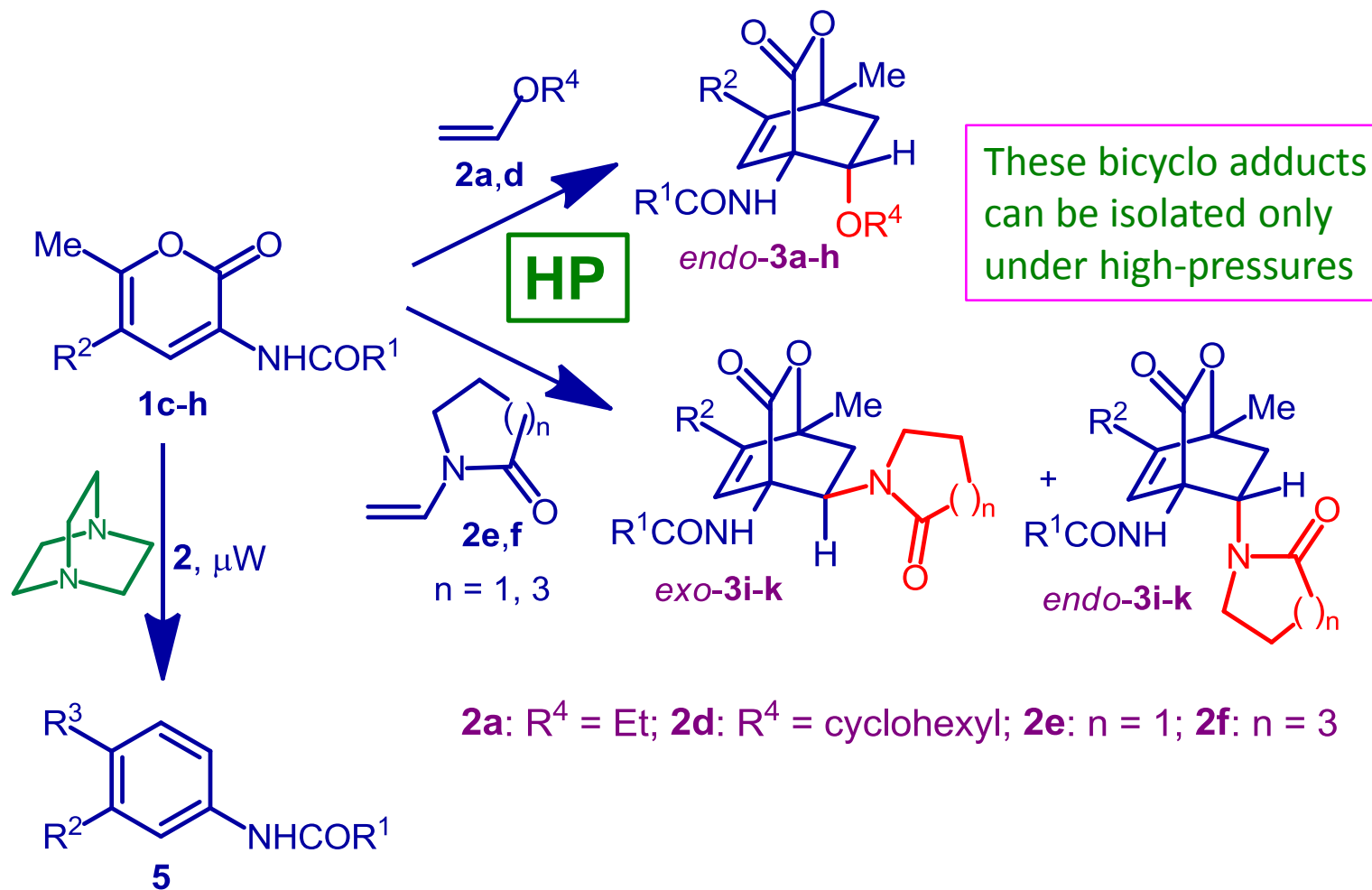
## Experimental:

- usual pressures between 10 and 20 kbar (1-2 GPa); HP effects are detected above 7 kbar);
- appropriate choice of solvents (should not freeze), such as  $\text{CH}_2\text{Cl}_2$ ,  $\text{Et}_2\text{O}$ ,  $\text{PrOH}$  etc.
- relatively small reaction volumes (2-10 mL).

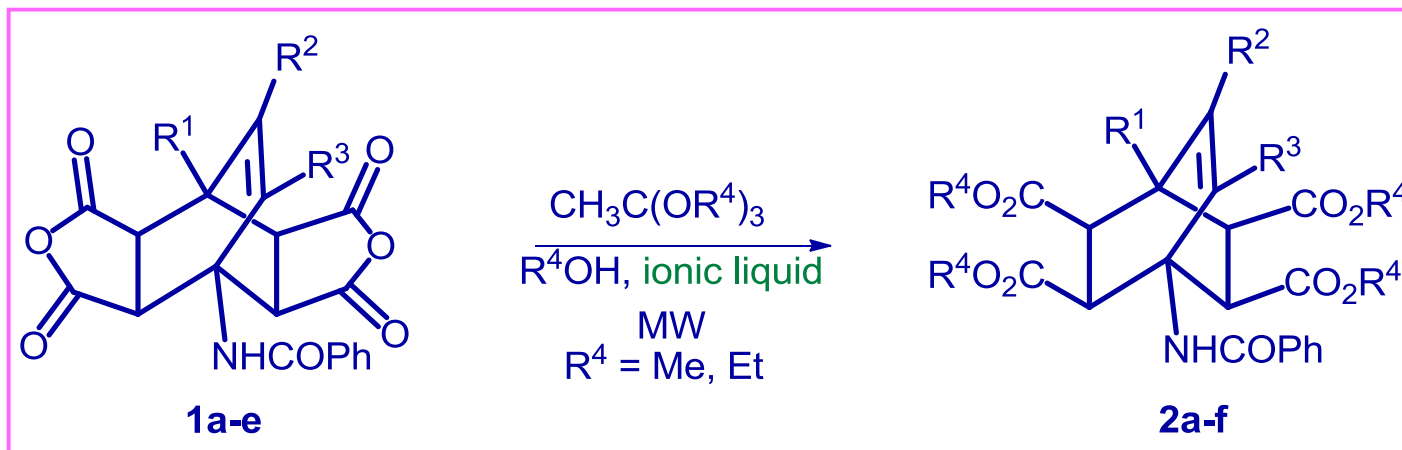


Rates of reactions with negative activation volumes are increased with increasing pressure.

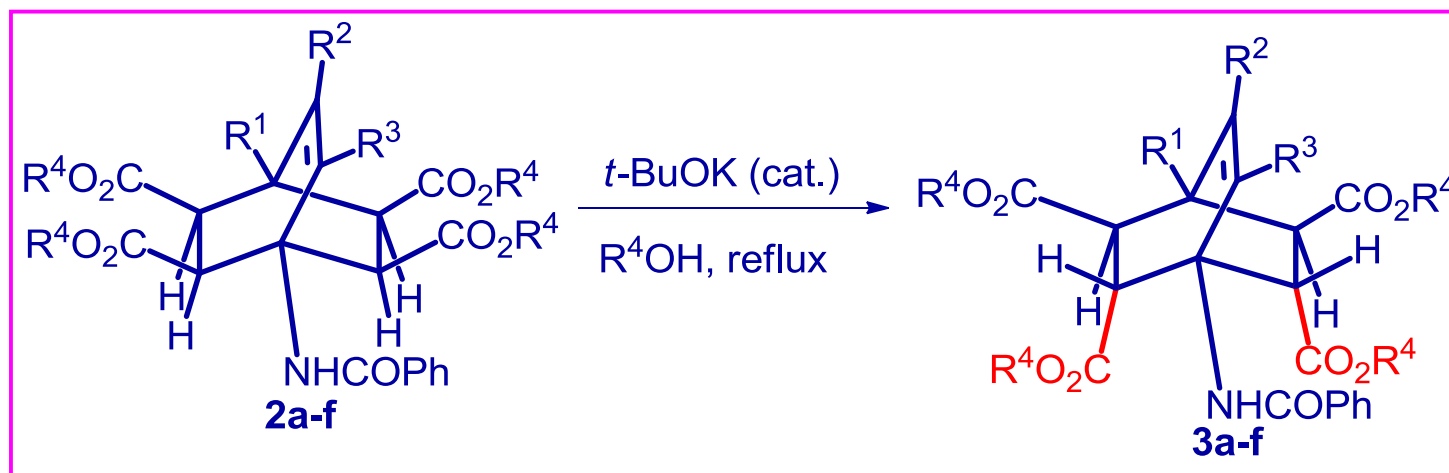
# DABCO-Catalyzed Microwave-Assisted Diels–Alder Reaction/-Elimination Reaction Sequence and High-Pressure (15 kbar) Reactions Starting from 2H-Pyran-2-ones



## PREPARATION OF PROCHIRAL SUBSTRATES: MW-ASSISTED AND IONIC LIQUIDS CATALYZED ESTERIFICATION OF ANHYDRIDE DERIVATIVES



### ISOMERISATION OF TETRAESTERS 2





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**tel: 01-24-19-256**

***Izbrane publikacije:***

- J. Org. Chem.* **2001**, 66, 6394.  
*J. Am. Chem. Soc.* **2002**, 124, 3951.  
*J. Am. Chem. Soc.* **2003**, 125, 3208.  
*J. Org. Chem.* **2003**, 68, 3291.  
*Dalton Trans.* **2003**, 420.  
*J. Org. Chem.* **2004**, 69, 5646.  
*Magn. Reson. Chem.* **2007**, 45, 700.  
*J. Comb. Chem.* **2008**, 10, 981.  
*Synlett* **2009**, 1144.  
*Synlett* **2009**, 2217.  
*Inorg. Chem.* **2010**, 49, 4820.  
*Inorg. Chim. Acta* **2010**, 363, 3817.  
*J. Org. Chem.* **2010**, 75, 6681.  
*Cryst. Growth Des.* **2010**, 10, 4920.  
*Eur. J. Inorg. Chem.* **2011**, 1921.  
*Dalton Trans.* **2011**, 40, 5188.  
*Polyhedron* **2011**, Accepted.

***Patentna prijava:***

WO 2010/086438 A1 (5.08.2010).

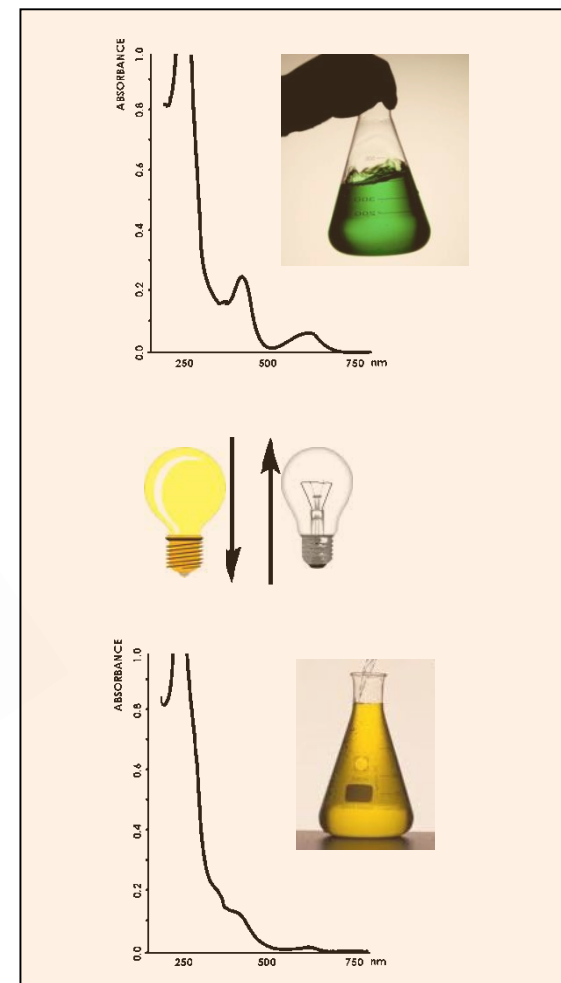
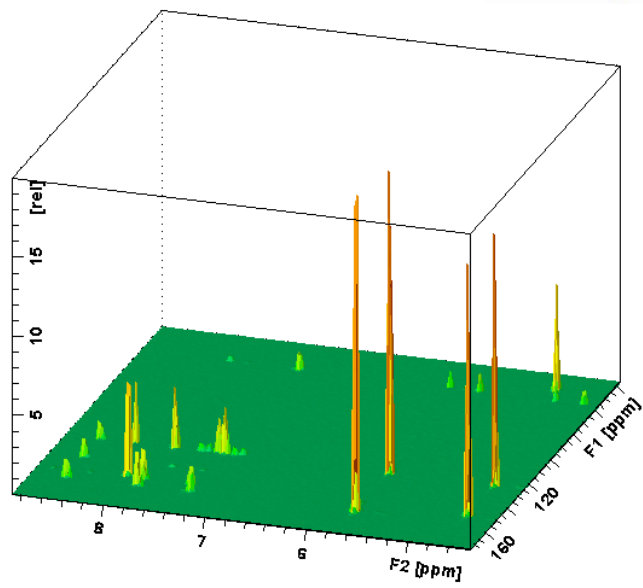
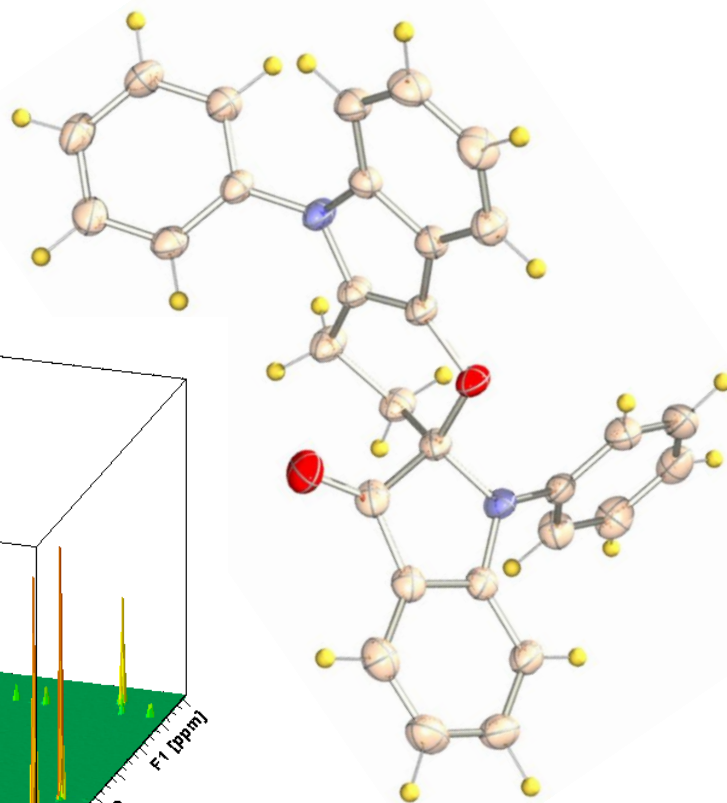
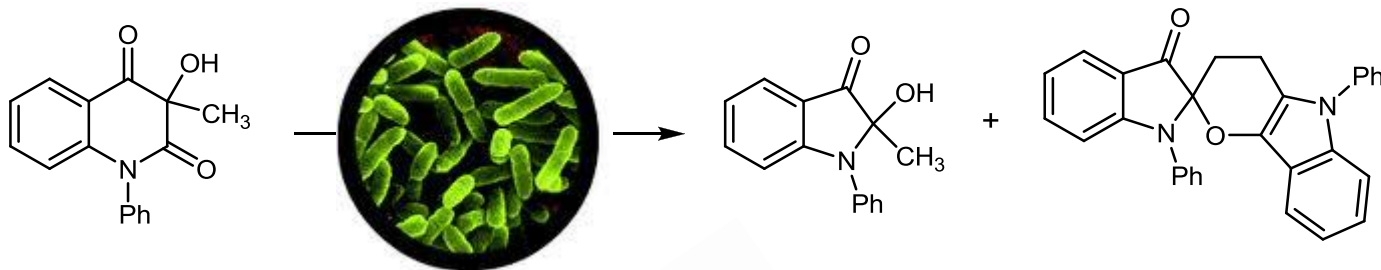
***Trenutni sodelujoči partnerji:***

- |                 |  |
|-----------------|--|
| dr. Časar       | Lek/Sandoz, <b>Slovenija</b>   |
| prof. De Proft  | Vrije Universiteit Brussel (VUB), Brussels, <b>Belgium</b>                 |
| prof. Maes      | University of Antwerp, <b>Belgium</b>                                      |
| prof. Britovsek | Imperial College London, <b>UK</b>   |
| prof. Lakshman  | The City College and The City University of New York, New York, <b>USA</b> |
| prof. Kafka     | Tomas Bata University in Zlin, <b>Czech Republic</b>                       |
| dr. Osmak       | Ruder Bošković Institute, Division of Molecular Biology, <b>Croatia</b>    |



# Moderne spektroskopske metode v strukturi analizi

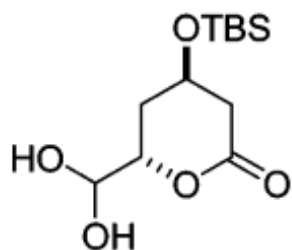
prof. dr. Janez Košmrlj



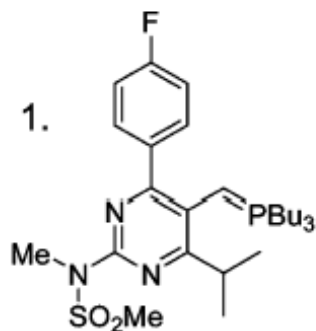


# Lek je prvi v Sloveniji ponudil generični rosuvastatin za zniževanje holesterola

## Sinteza učinkovin: rosuvastatin

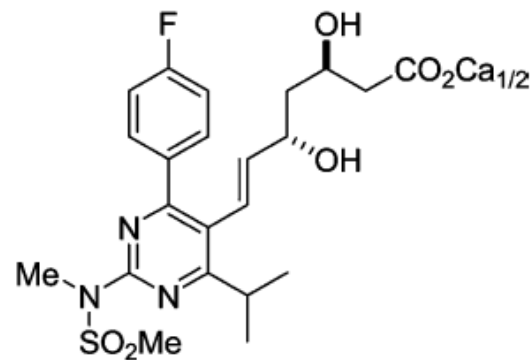


lactone hydrate



toluene, 110 °C

2. *n*-Bu<sub>4</sub>NF, AcOH, THF  
 3. aq. NaOH, THF, 30 °C  
 4. Ca(OAc)<sub>2</sub>, 40 °C



Rosuvastatin calcium

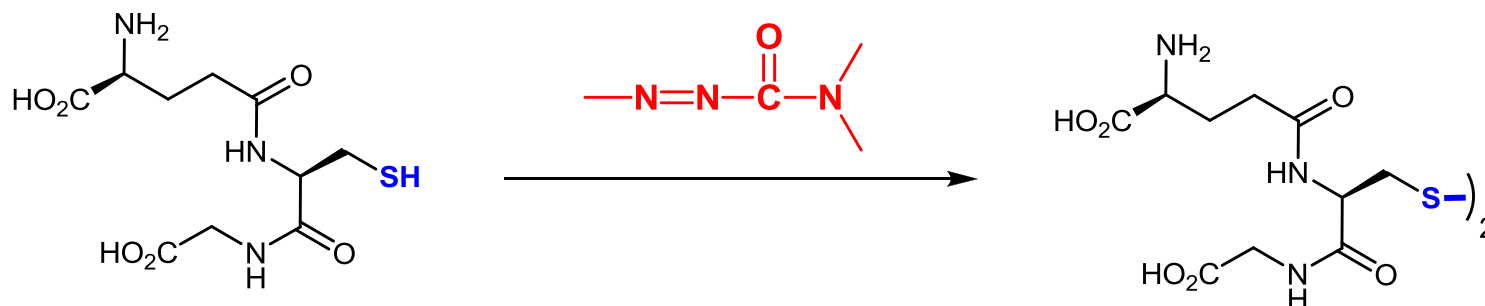
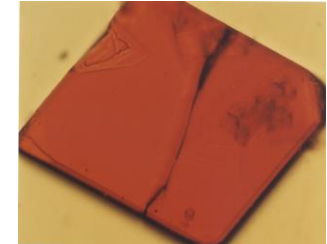


Časar, Košmrlj, *Synlett* **2009**, 1144.

Časar, Steinbücher, Košmrlj, *J. Org. Chem.* **2010**, 75, 6681.

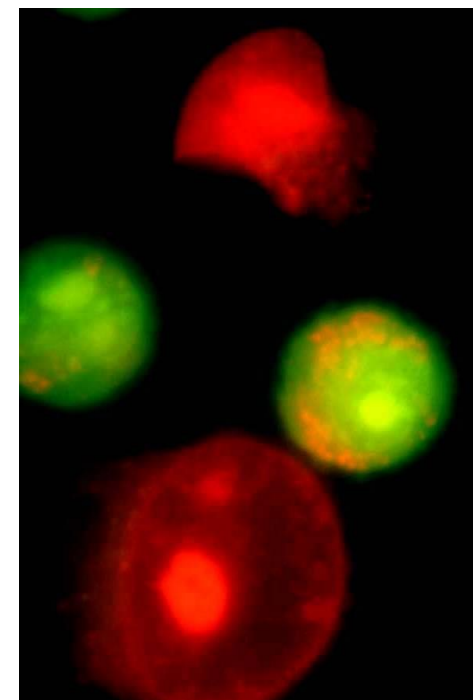
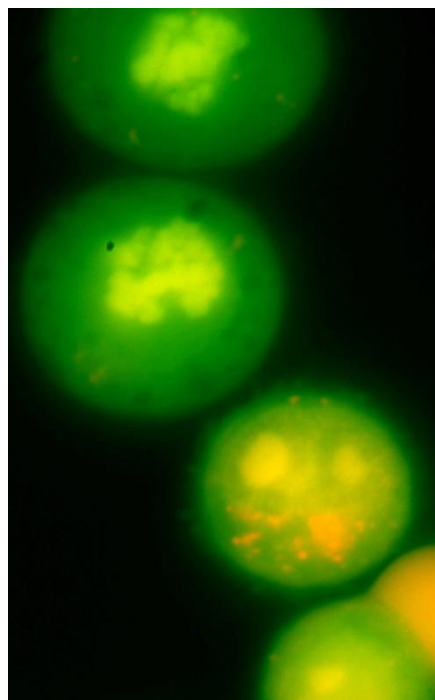
Časar, Košmrlj, International patent application: WO 2010/086438 A1.

# Biološko aktivne spojine: citotoksične lastnosti diazenkarboksamidov:



## Celične linije:

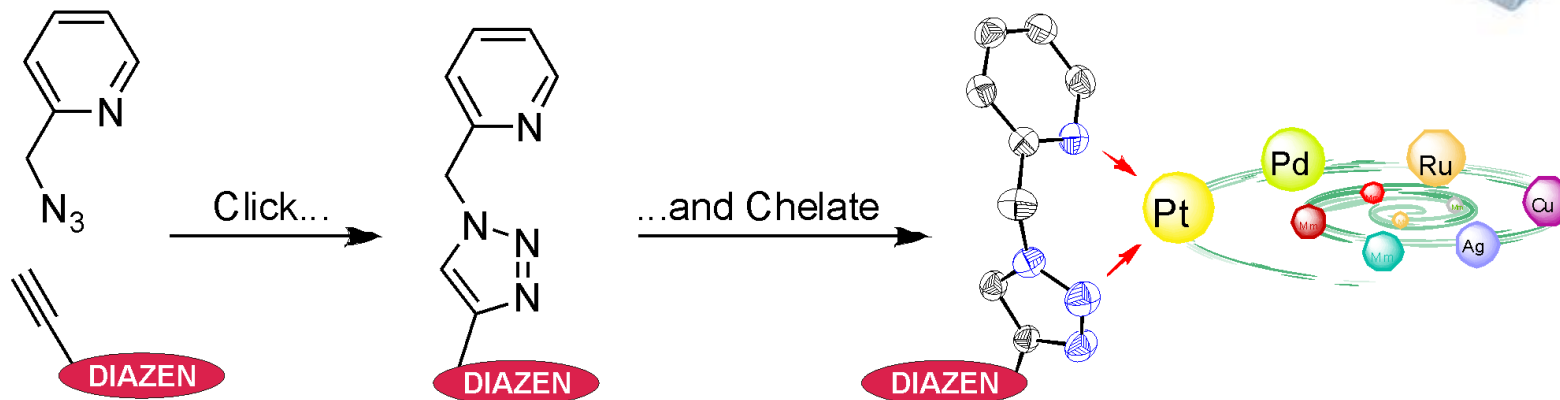
- cervical carcinoma cells (**HeLa**)
- glioblastoma cells (**A1235**)
- laryngeal carcinoma cells (**HEp2**)
- mammary carcinoma cells (**MCF-7**)
- breast adenocarcinoma cells (**SK-BR-3**)
- non-small cell lung cancer (**NCI-H460**)
- central nervous system cancer (**SF-268**)
- prostate adenocarcinoma cells (**PC-3**)
- leukemic cell lines **NALM-1** , **JURKAT** , **HL-60** , **K-562** , **CCRF-CEM**).



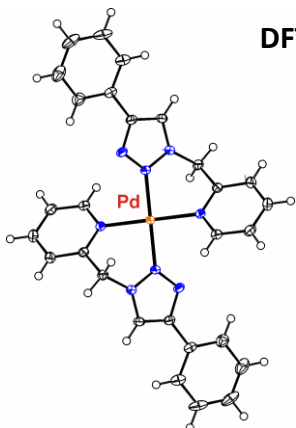
# Koordinacijske spojine:

od potencialnih učinkovin do katalizatorjev

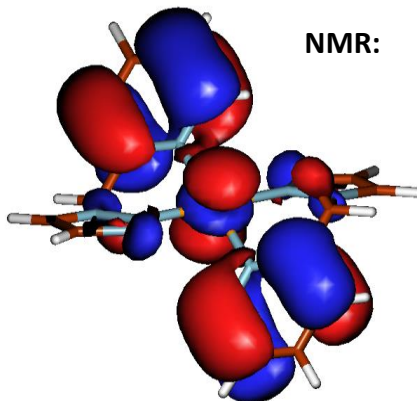
prof. dr. Janez Košmrlj



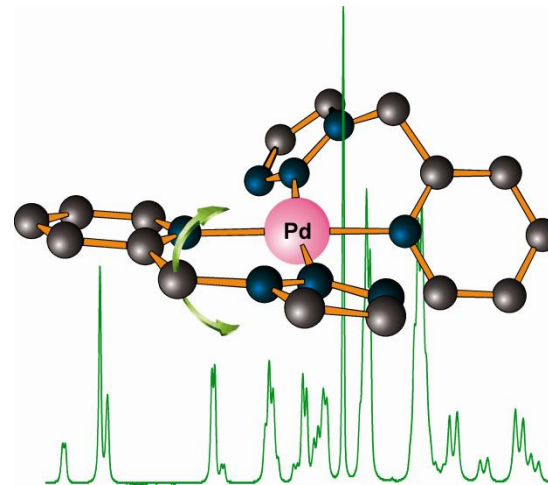
X-ray:



DFT:



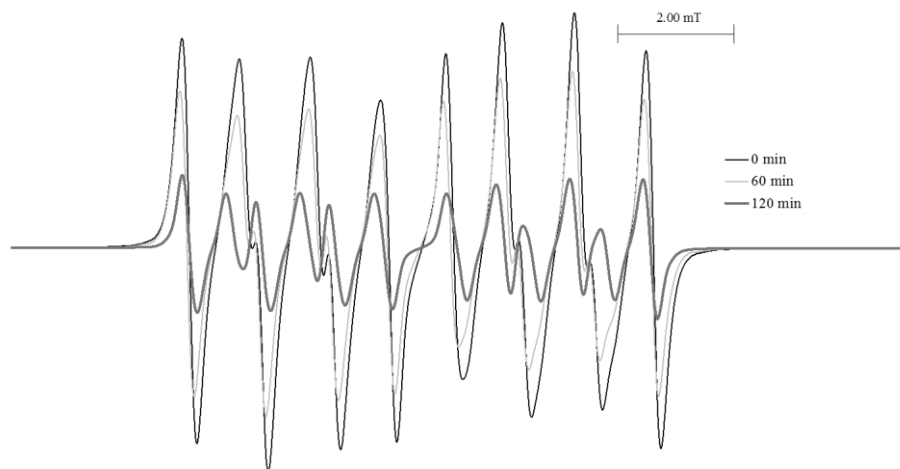
NMR:

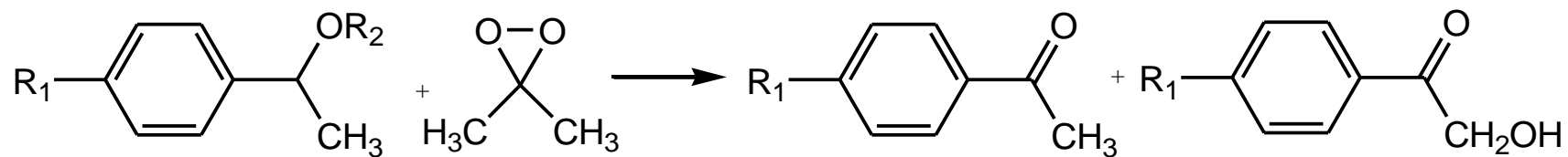
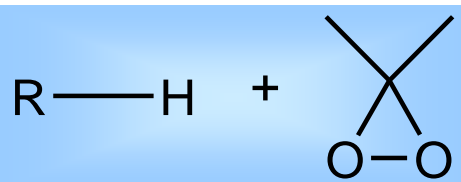


Izr. prof. dr. Franci Kovač  
franci.kovac@fkkt.uni-lj.si  
tel: 01-24-19-252



# Študij oksidacije organskih substratov z dioksidirani in ozonom



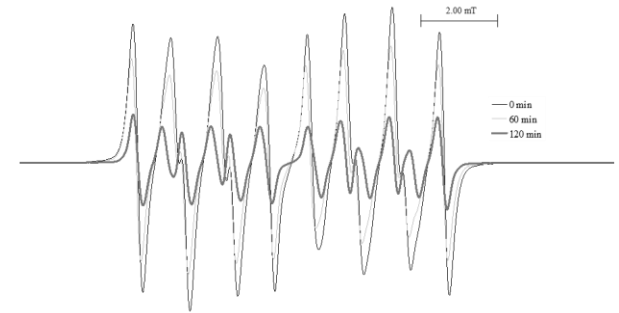
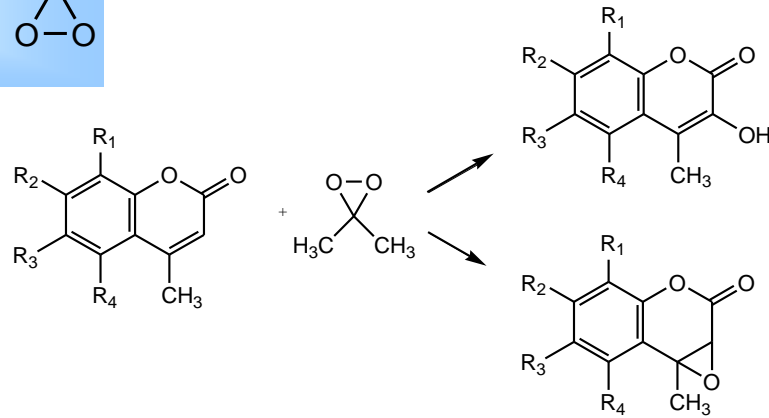
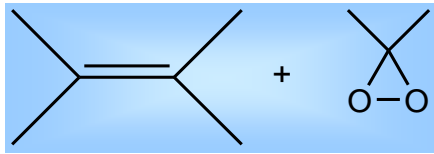


UV/VIS-Instrument



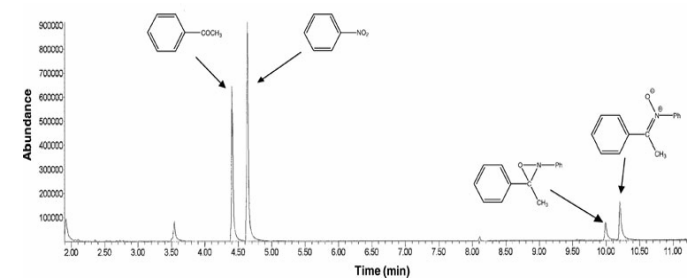
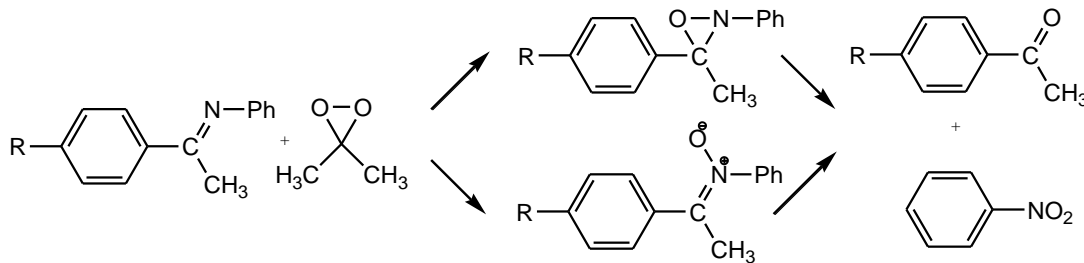
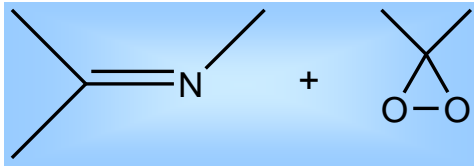
UV/VIS-Eksperiment

Kovač F., Baumstark Alfons L. Oxidation of  $\alpha$ -methylbenzyl alcohols by dimethyldioxirane, *Tetrahedron Lett.*, **1994**, 35, 8751-8754



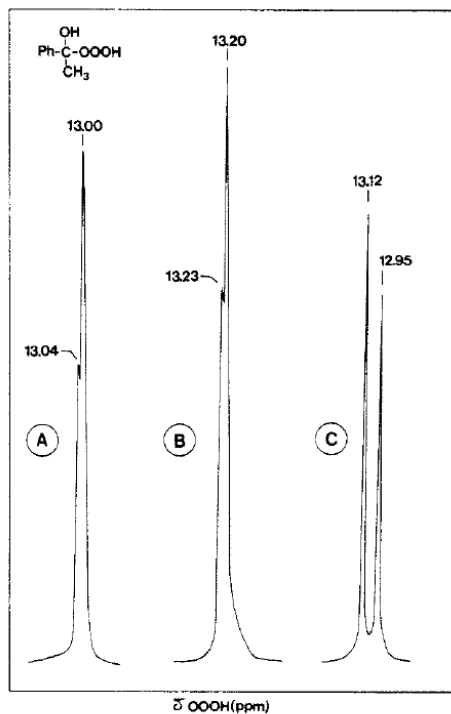
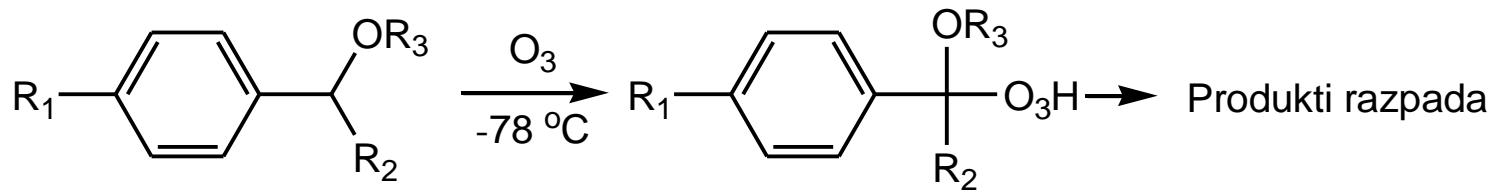
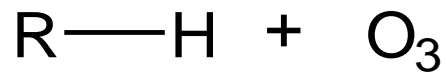
EPR

Cavar S., Kovac F. The oxyfunctionalization of 4-methylcoumarins using dimethyldioxirane. *International Journal of Chemical Kinetics* (2009), 41(6), 414-420.; Cavar S., Kovac F. Maksimovic M. Synthesis and antioxidant activity of selected 4-methylcoumarins. *Food Chemistry* (2009), 117(1), 135-142.

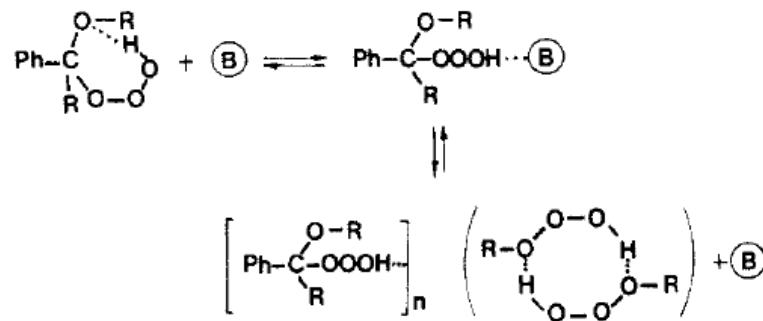


GC/MS

Nose Z.; Kovac F. Kinetic study of oxidation of N-( $\alpha$ -methylbenzylidene) anilines by dimethyldioxirane. *International Journal of Chemical Kinetics* (2007), 39(9), 492-497.



**Figure 2.** Segments of  $^1\text{H}$  NMR (100 MHz) spectra of **6a** at  $-60\text{ }^\circ\text{C}$ : (A) in ethyl acetate; (B) in acetone- $d_6$ ; (C) in diethyl ether.



Kovač Franci, Plesničar Božo. The substituent effect on the thermal decomposition of acetal hydrotrioxides. Polar and radical decomposition paths, *J.Am.Chem.Soc.*, **1979**, *101*, 2677-2681, Plesničar Božo, Kovač Franci, Schara Milan Valter. Chemistry of hydrotrioxides. Preparation, characterization and thermal decomposition of hydrotrioxides of alkyl- $\alpha$ -methylbenzyl ethers and  $\alpha$ -methylbenzyl alcohol. Attempted spin trapping of trioxyl radicals, *J.Am.Chem.Soc.*, **1988**, *110*, 214-222, Plesničar Božo, Cerkovnik Janez, Koller Jože, Kovač Franci. Chemistry of hydrotrioxides. Preparation, characterization and reactivity of dimethylphenylsilyl hydrotrioxides. Hydrogen trioxide (HOOH), a reactive intermediate in their thermal decomposition?, *J.Am.Chem.Soc.*, **1991**, *113*, 4946-4953



# METODE DELA

- sinteza izhodnih spojin
- oksidativna pretvorba
- kinetske študije oksidacije
- analiza produktov
- analitika (GC/MS; NMR; UV/VIS; IR; EPR; HPLC)

# DIELS-ALDERJEVE REAKCIJE

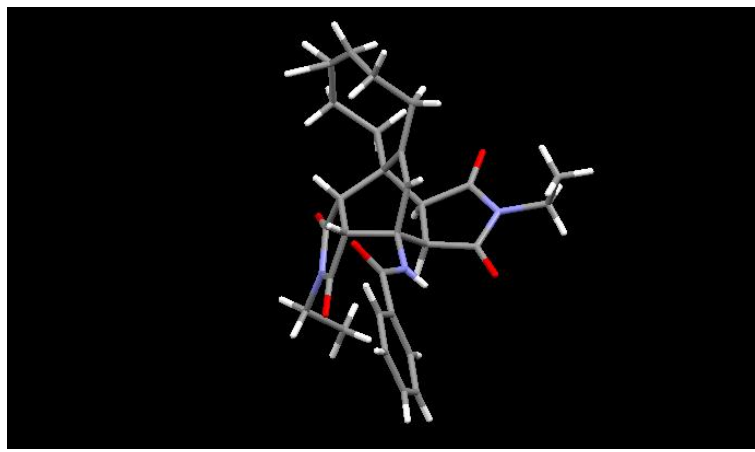
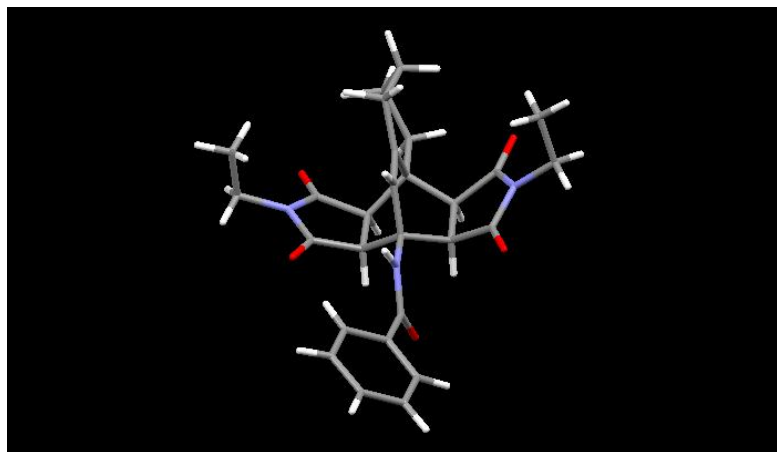
doc. dr. Krištof Kranjc  
kristof.kranjc@fkkt.uni-lj.si  
tel.: (01) 2419 230 ali 260  
lab. 424 ali 409



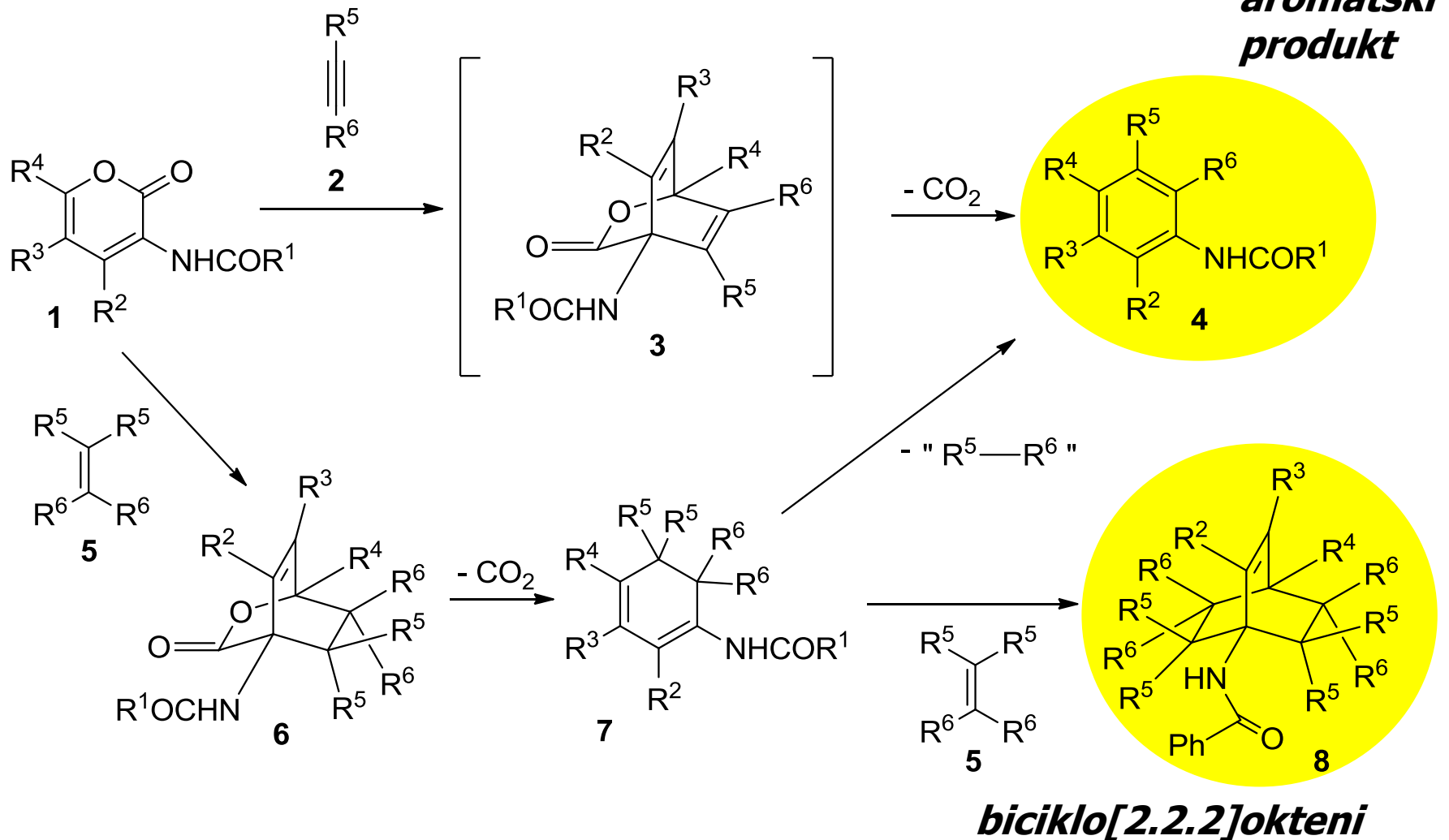
za pregledne članke o dosedanjih rezultatih gl.:

- 1) *Curr. Org. Chem.* **2010**, *14*, 1050.
- 2) *Curr. Org. Chem.* **2013**, *17*, 448 in 457.
- 3) *Arkivoc* **2013**, (*1*), v tisku.

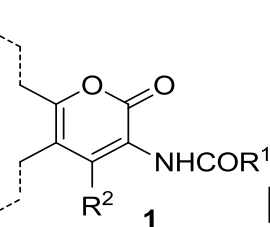
*simetrični ali asimetrični?*



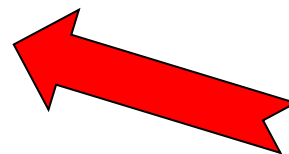
# SPLOŠNA POT DIELS-ALDERJEVE REAKCIJE 2H-PIRAN-2-ONOV



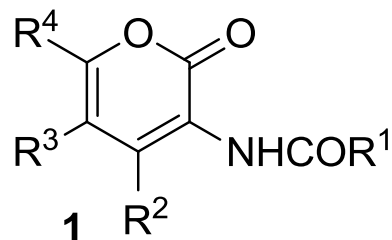
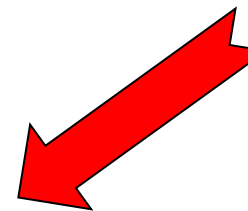
# BICIKLO[2.2.2]OKTENI



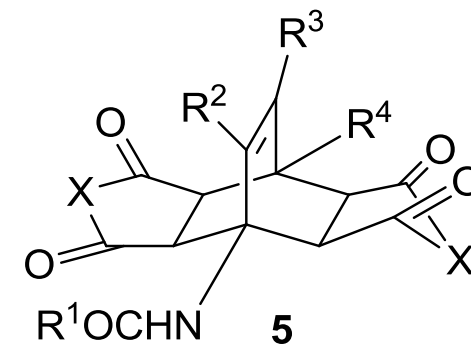
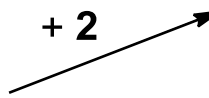
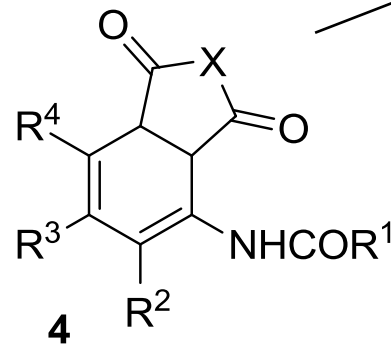
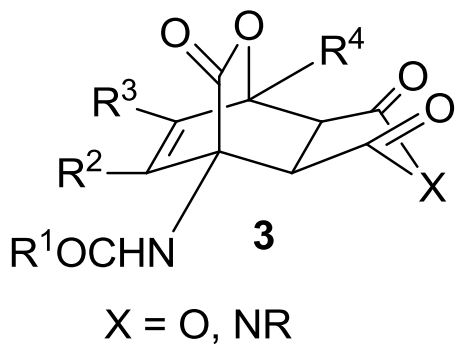
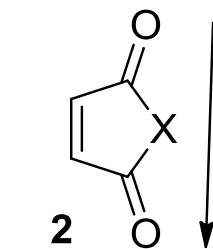
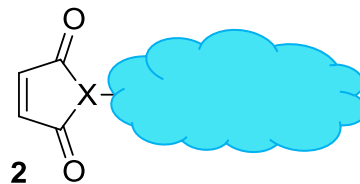
povečati dien **1**  
(pripojiti 8-členski  
obroč)



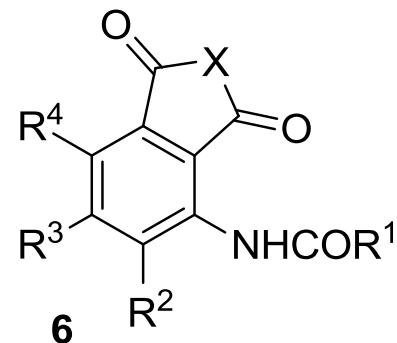
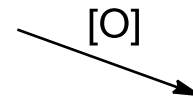
*kako do  
asimetričnih?*



povečati dienofil **2**

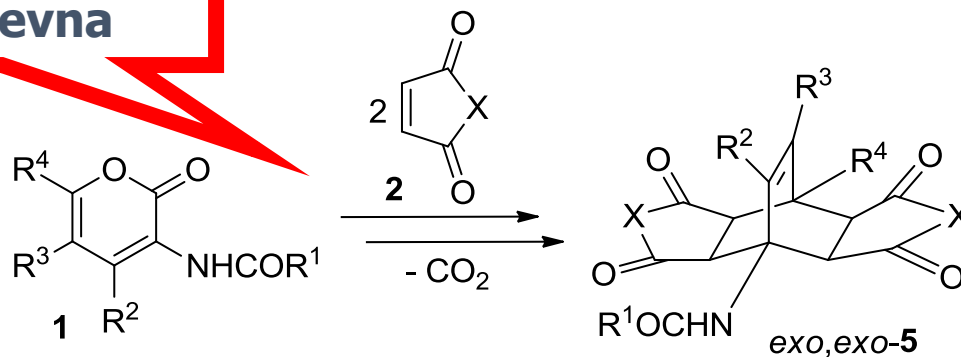


*sim. ali asim.?*

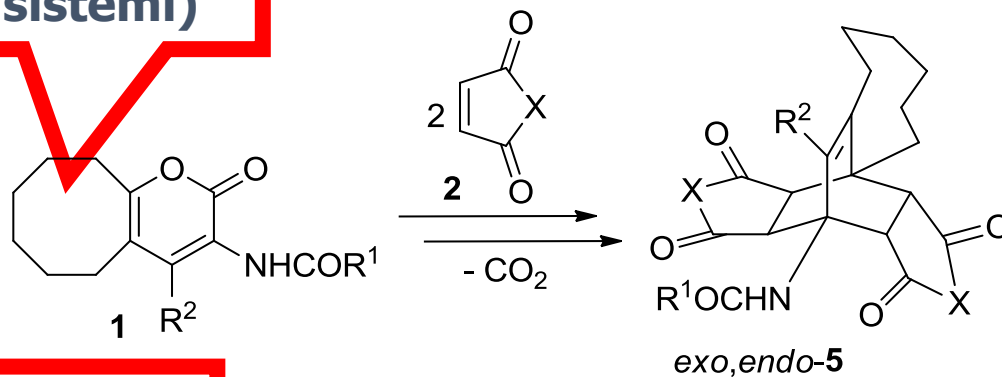


**R<sup>3</sup>, R<sup>4</sup> in X sterično nezahtevna**

doc. dr. Krištof Kranjc

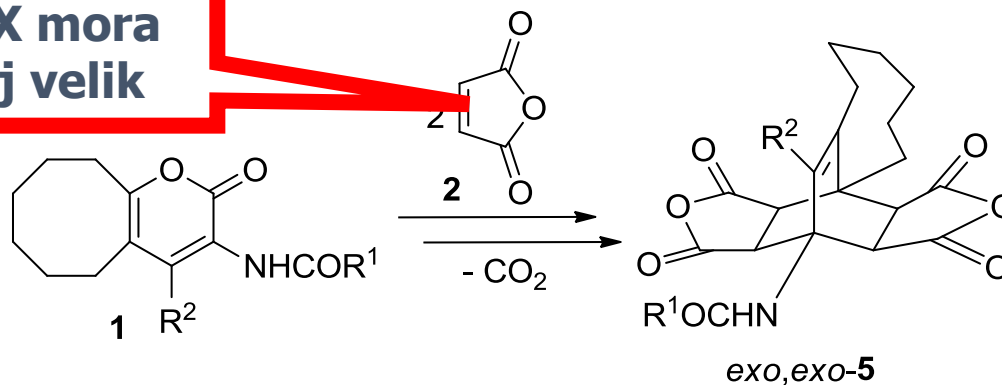


**povečamo R<sup>3</sup>, R<sup>4</sup> (pripojeni sistemi)**



... X je vsaj NMe (ali NEt, NPh)...

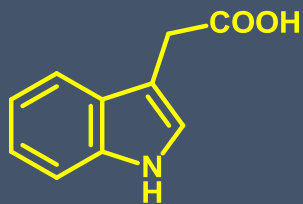
**toda tudi X mora biti dovolj velik**



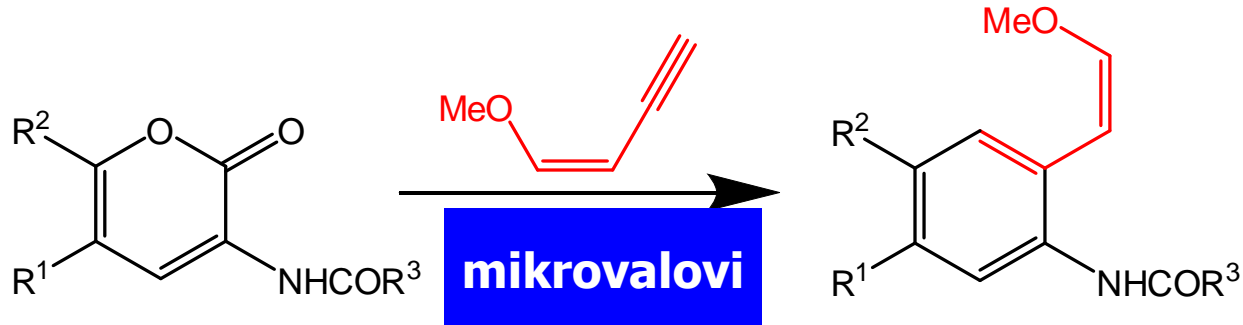
... če X = O, pa spet...

K. Kranjc, F. Perdih, M. Kočevar, *J. Org. Chem.* **2009**, 74, 6303.

# SINTEZA INDOLOV



indol-3-ocetna  
kislina (*auksin* - hormon  
regulacije rasti rastlin)



90-180 min v toluenu, 150 °C;  
izkor. 69-84%

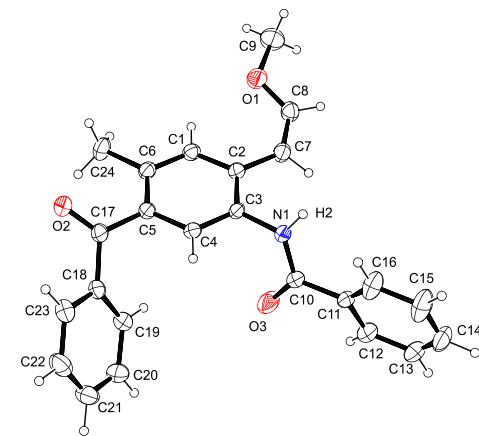
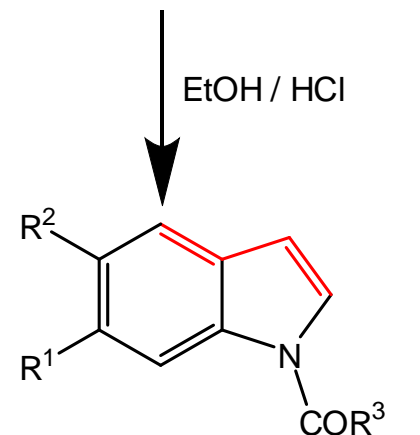
R<sup>1</sup> = COMe, CPh, CO<sub>2</sub>Me, CO<sub>2</sub>Et;

R<sup>2</sup> = Me, CH<sub>2</sub>CO<sub>2</sub>Me, CH<sub>2</sub>CO<sub>2</sub>Et;

R<sup>3</sup> = Me, Ph, CH<sub>2</sub>Ph;

(*Z*)-1-metoksibut-1-en-3-in (50%  
raztopina v MeOH).

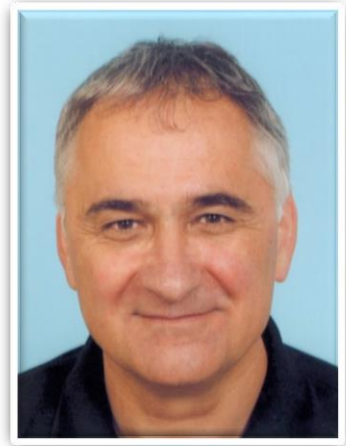
K. Kranjc, M. Kočevar *Tetrahedron* **2008**,  
64, 45-52.



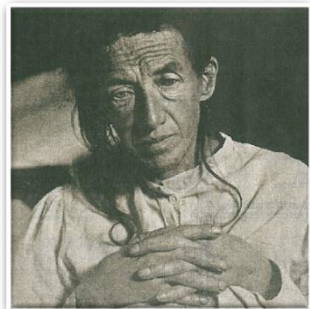
prof. dr. Andrej Petrič

[andrej.petric@fkkt.uni-lj.si](mailto:andrej.petric@fkkt.uni-lj.si)

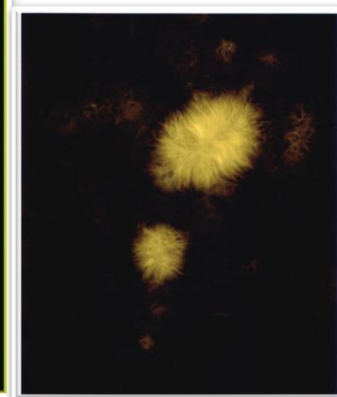
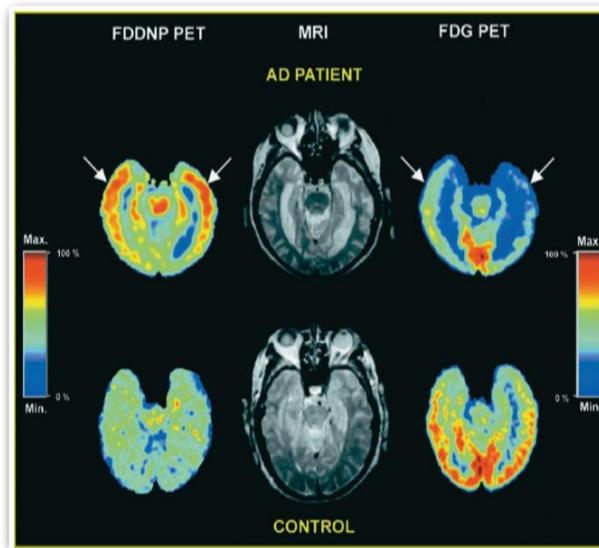
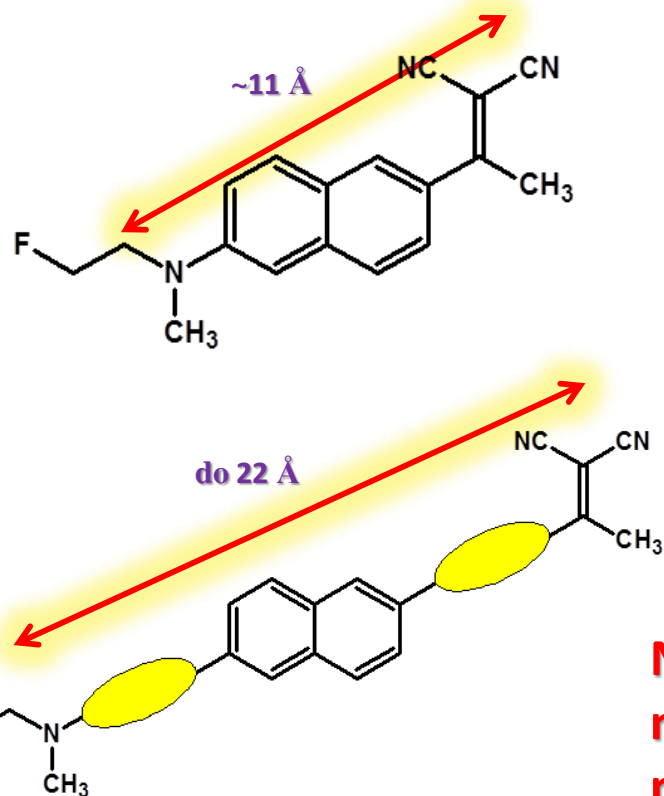
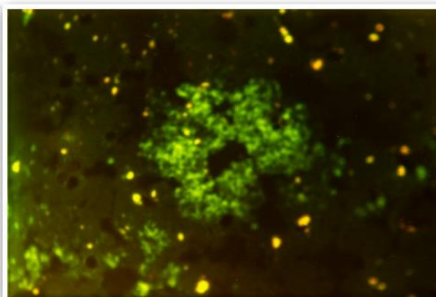
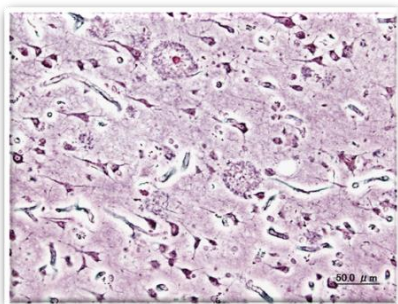
tel: 01-24-19-232



## FDDNP kot molekularna sonda pri Alzheimerjevi in varianti Creutzfeld-Jacobove bolezni



†1906



**Naloga diplomantov bodo sinteza in karakterizacija novih analogov FDDNP z uporabo klasičnih in modernih sinteznih ter analitskih metod.**



doc. dr. Franc Požgan

franc.pozgan@fkkt.uni-lj.si

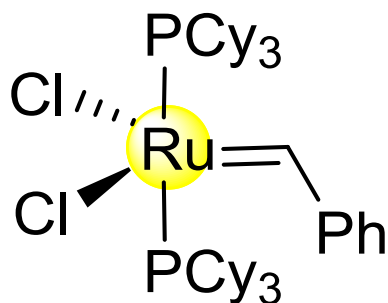
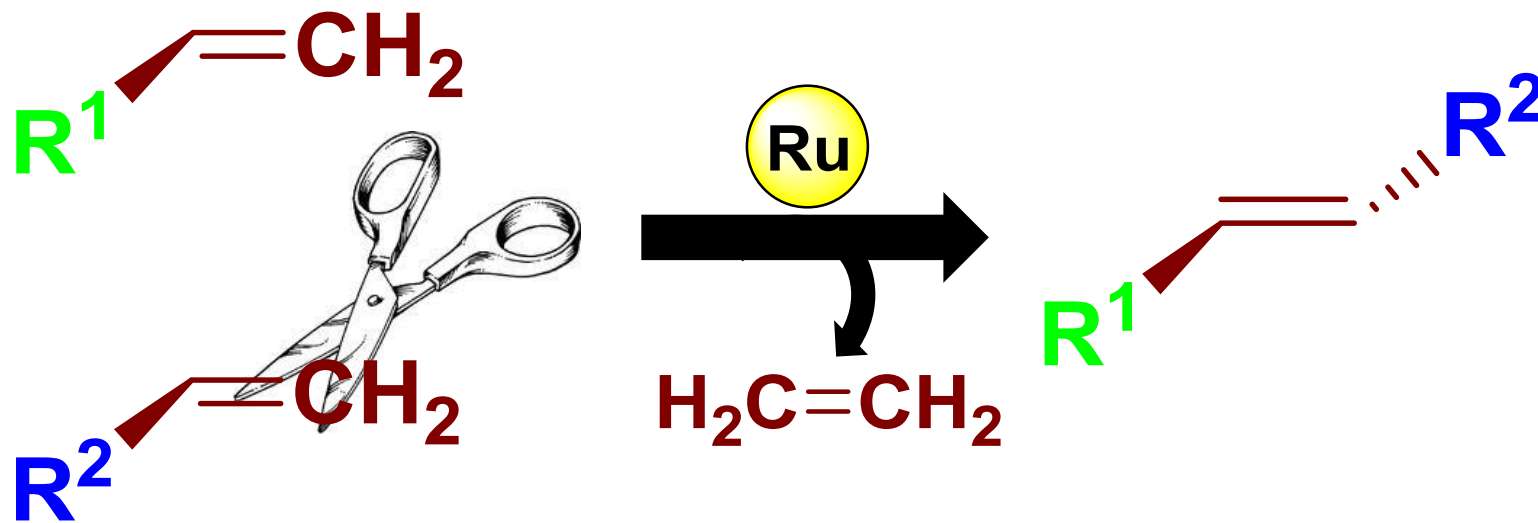
tel: 01-24-19-261



## Kataliza s kovinami prehoda – uporabno orodje v moderni organski sintezi

- Načrtovanje **katalizatorjev** (sinteza ligandov in njihova kompleksacija s kovinami prehoda)
- Uporaba kompleksov kovin prehoda za **katalitske pretvorbe organskih molekul**
- **Kataliza s kovinami prehoda:**
  - omogoča učinkovito tvorbo C-C enojnih, dvojnih vezi...
  - atomsko bolj ekonomična
  - omogoča reakcije, ki sicer ne bi potekle
  - omogoča selektivne pretvorbe
  - milejši reakcijski pogoji
  - tolerira vrsto funkcionalnih skupin

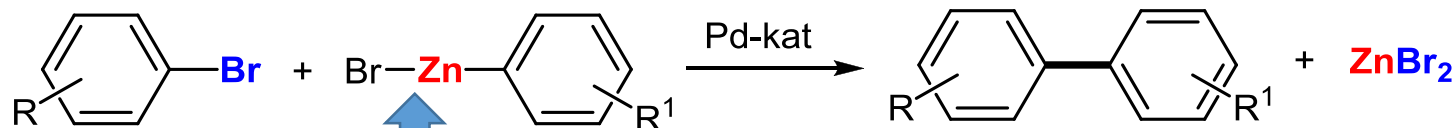
# Alkenska metateza (Nobelova nagrada 2005: Y. Chauvin, R. H. Grubbs, R. R. Schrock)



F. POŽGAN, P. H. DIXNEUF. Recent applications of alkene metathesis for fine chemicals and supramolecular system synthesis. V: İMAMOĞLU, Yavuz (ur.), DRAGUTAN, Valerian (ur.). *Metathesis chemistry: from nanostructure design to synthesis of advanced materials*. Vol. 243, Dordrecht; London: Springer, 2007.

# C–H vez kot funkcionalna skupina – aktivacija s kovinami prehoda

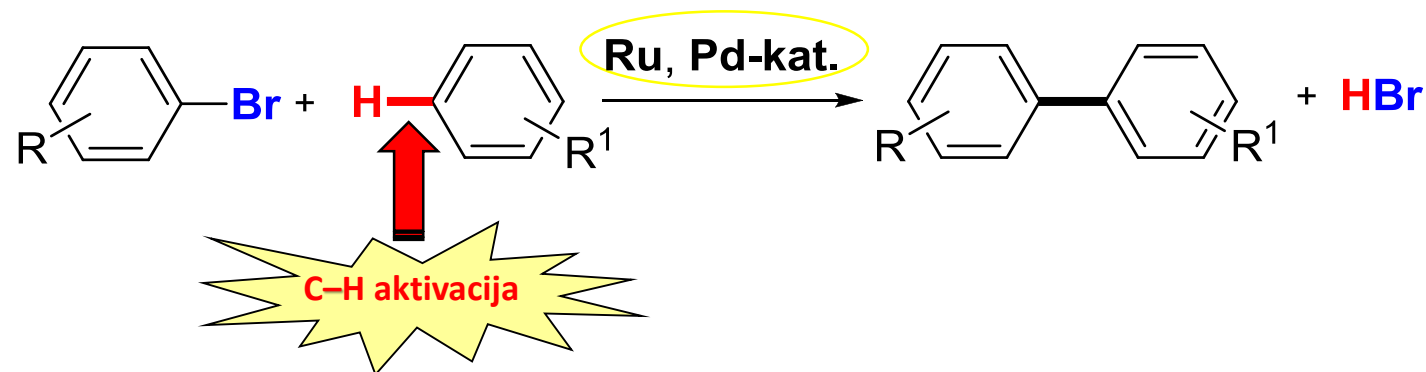
Klasične reakcije pripajanja



Organokovinski reagenti:

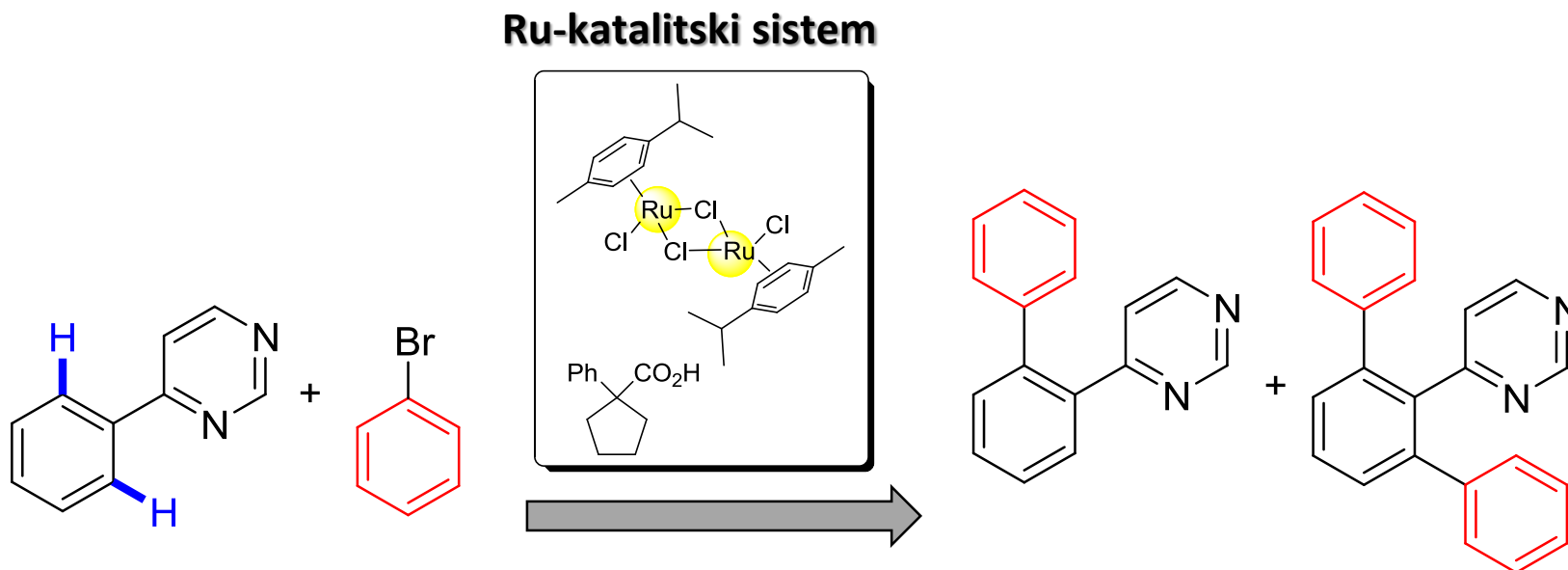
- nekateri zelo reaktivni
- neželene stranske reakcije
- dostikrat nekupljivi
- priprava lahko težavna

Aktivacija C–H vezi s kovinami prehoda



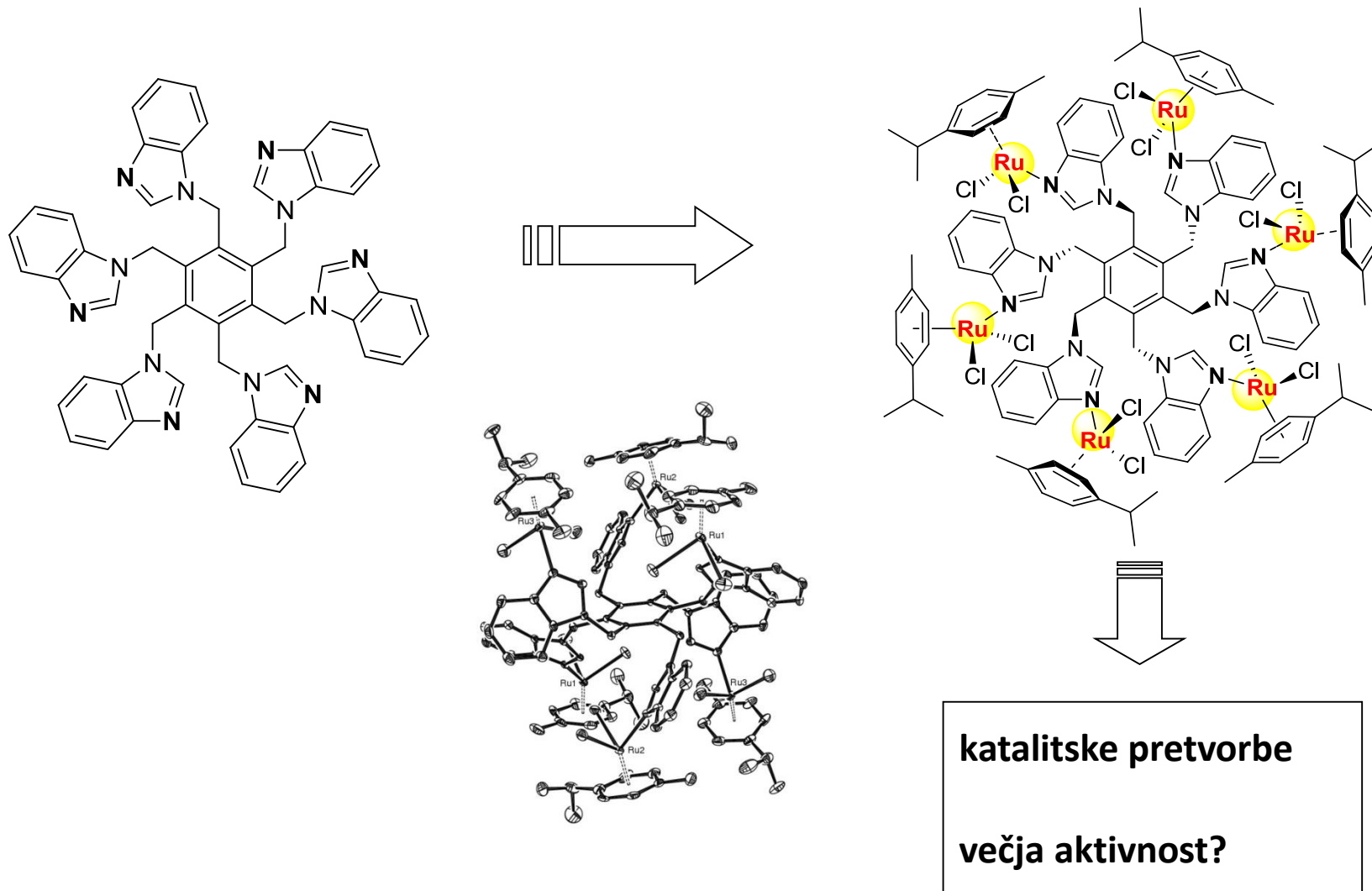
# Selektivna direktna funkcionalizacija

## C–H vezi v heterocikličnih sistemih



B. ŠTEFANE, J. FABRIS, F. POŽGAN. C–H Bond functionalization of arylpyrimidines catalyzed by an in situ generated ruthenium(II) carboxylate system and the construction of tris(heteroaryl)-substituted benzenes. *Eur. J. Org. Chem.* 2011.

# Multidentatni ligandi in večjedrni kompleksi



F. POŽGAN, L. TOUPET, P. H. DIXNEUF. Preparation of hexacoordinating benzimidazole containing ligand and hexakis(benzimidazole-ruthenium(II)) complex. Molecular structure of  $C_6\{CH_2-(N-benzimidazole-RuCl_2(p-cymene))\}_6$ . *Dalton Trans.* 2011.

**prof. dr. Jurij Svete**  
**jurij.svete@fkkt.uni-lj.si**  
**tel: 01-24-19-254**



## **Heterociklične spojine: sinteza, struktura, lastnosti in uporaba Stereoselektivna in »high-throughput« organska sinteza**

### **Mentorstva diplomskim študentom 2009-2014:**

Miha Friedrich (2009), Sonja Kiraly-Potpara (2009), Monika Janjić (2009), Darja Žerovnik (2009), Urban Feguš (2010), Rok Prebil (2010), Peter Perdih (2010), Bojana Črček (2011), Mladena Milošević (2011), Luka Šenica (2011), Ana Testen (2011), Matej Štefanič (2012), Anja Podlogar (2012), Jaka Glavač (2012), Klara Lombar (2012), Barbara Andolšek (2013), Urša Šraj (2013), Sizana Ahmetaj (2013), Eva Pušavec (2013), Nina Velikanje (2013), Mojca Žorž (2013), Miha Drev (2013), Ines Šterbal (2013).

V teku: Janja Štrekelj, Karmen Stopar, Špela Mevec, Nejc Petek, Karmen Verdenik, Maja Brinovec.

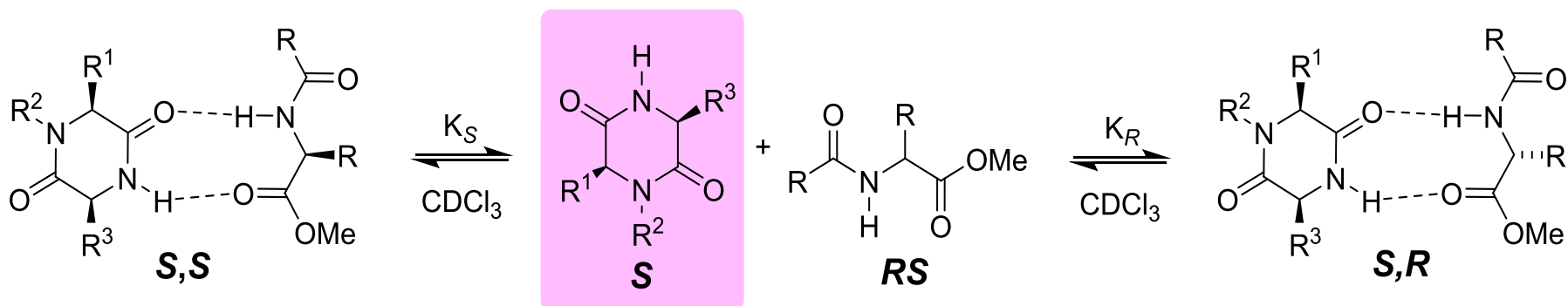
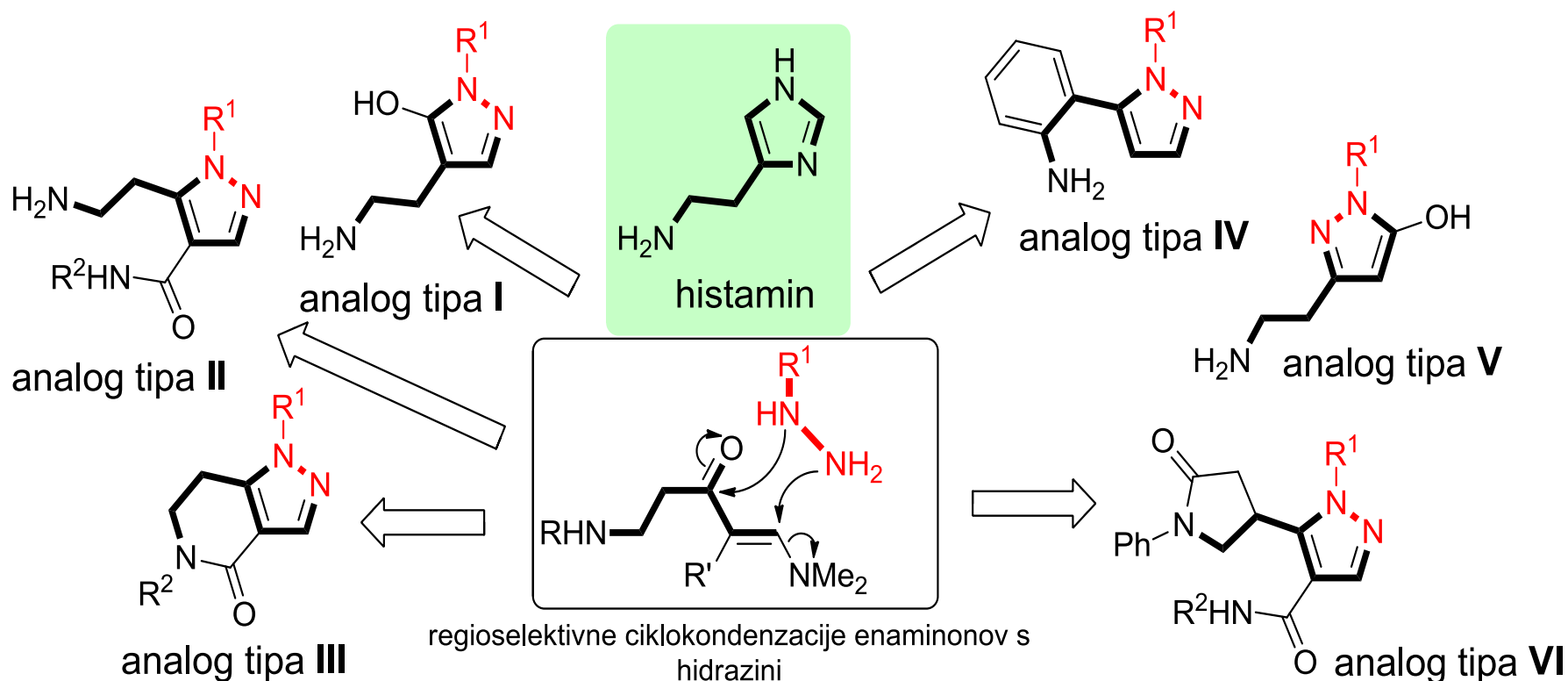
### **Mentorstva podiplomskim študentom in mladim raziskovalcem 2008-2014:**

dr. Lidija Pezdirc (2003-2008), dr. David Kralj (2004-2008), dr. Črt Malavašič (2006-2011), dr. Ana Novak (2009-2013), Luka Šenica (od 2011), Jona Mirnik (od 2012), Eva Pušavec (2013), odobren MR za 2014.

Testiranje na inhibicijo encimov (skupaj s FFA-prof.dr. Stanislav Gobec)



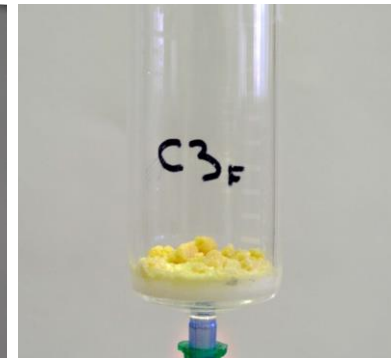
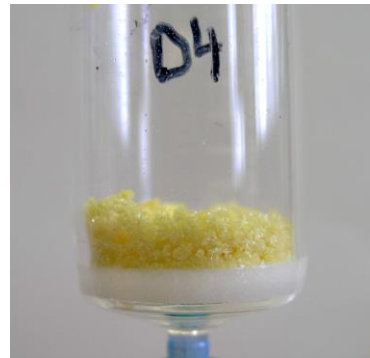
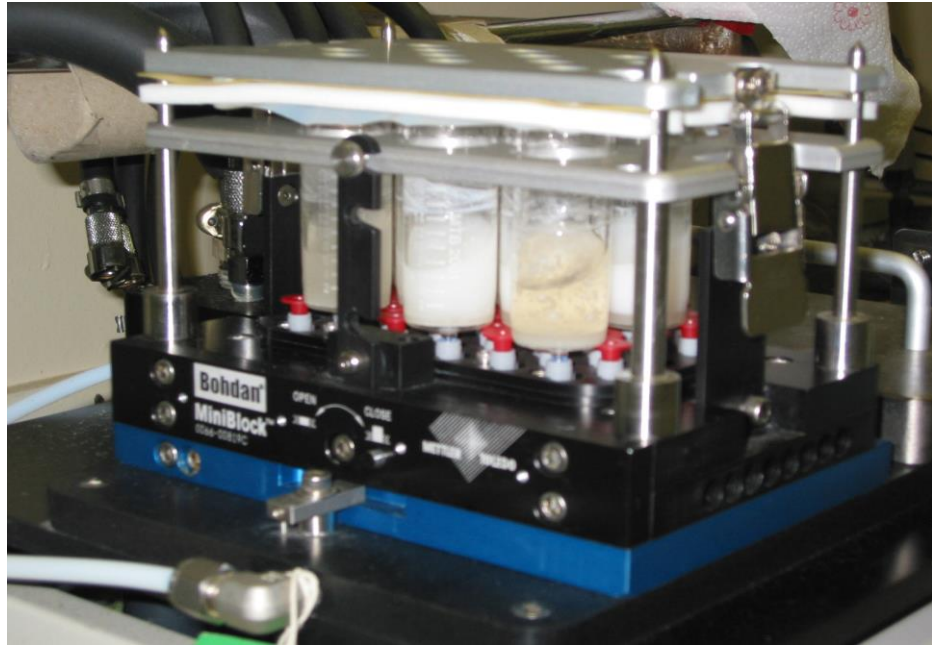
# Heterociklične spojine: struktura, lastnosti in uporaba



Diketopiperazinski kiralno solvatacijski reagenti za enostavno določanje enantiomernesestave z  $^1H$  NMR



# Stereoselektivna in ,high-throughput' sinteza (kombinatorna sinteza)



**doc. dr. Bogdan Štefane**  
**bogdan.stefane@fkkt.uni-lj.si**  
**tel: 01-24-19-264**

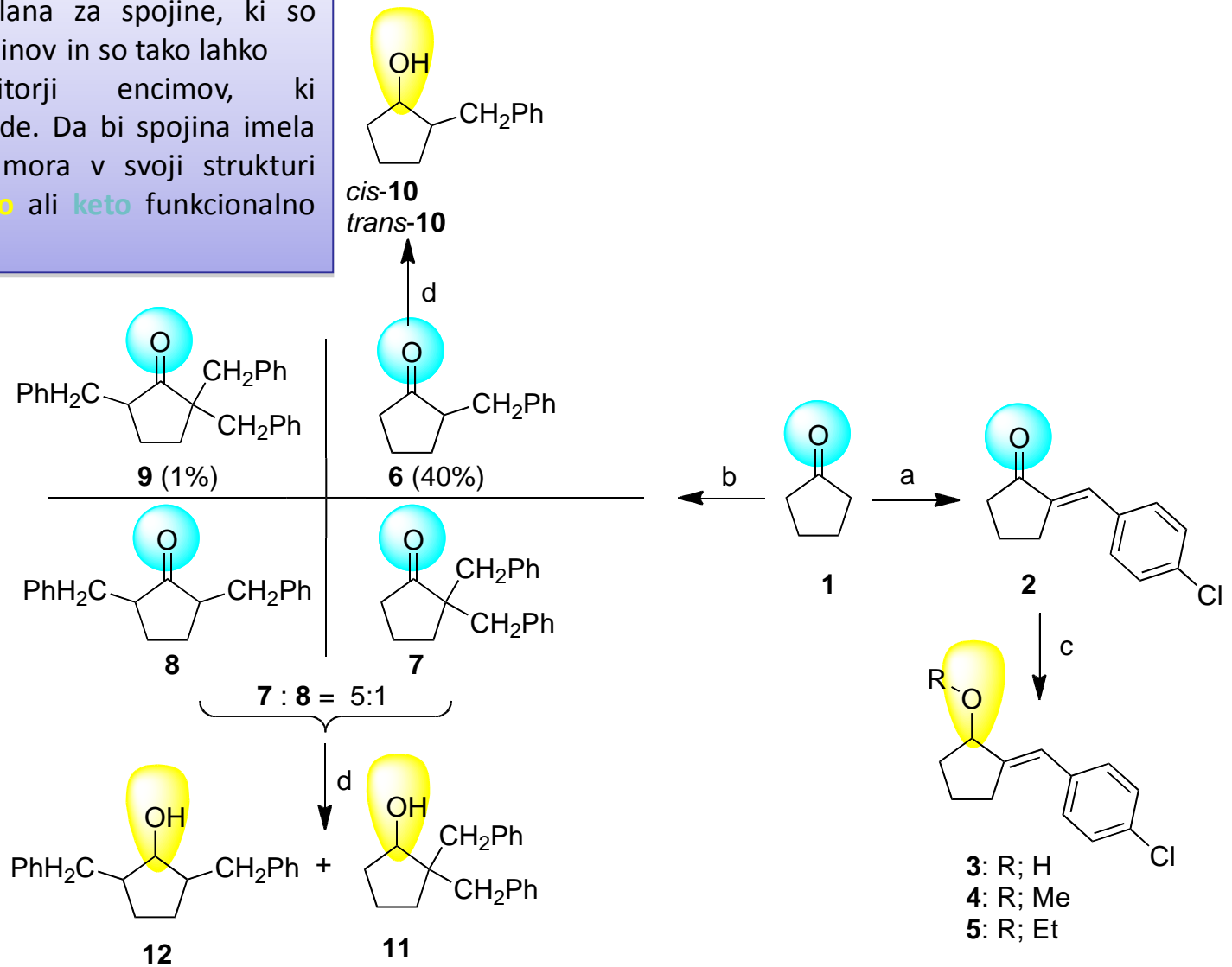


### **Sinteza nizkomolekularnih spojin kot potencialnih inhibitorjev encimov**

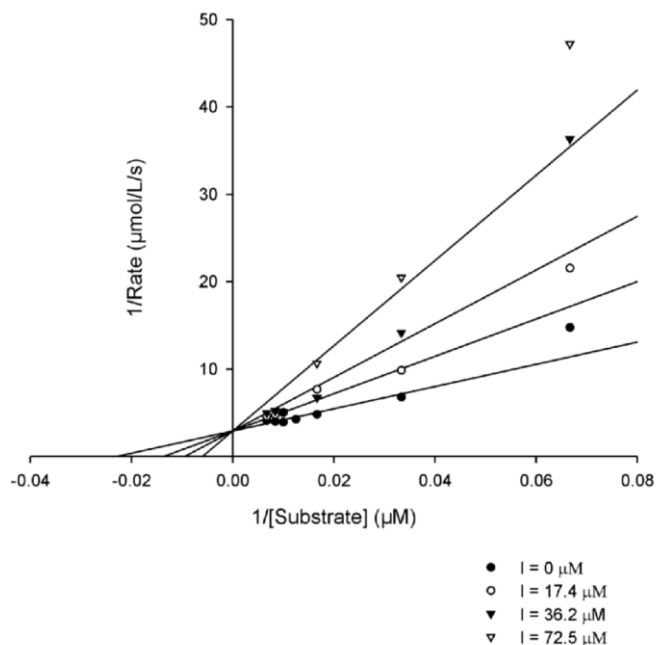
- Načrtovanje potencialnih inhibitorjev tarčnih encimov
- Sinteza in karakterizacija spojin
- Testiranje učinkovitosti inhibicije encimov (skupaj s FFA-prof.dr.S. Gobec)
- Vrednotenje aktivnosti spojin pridobljenih z encimskimi testi

## Sinteza inhibitorjev encimov AKR1C1 in AKR1C3

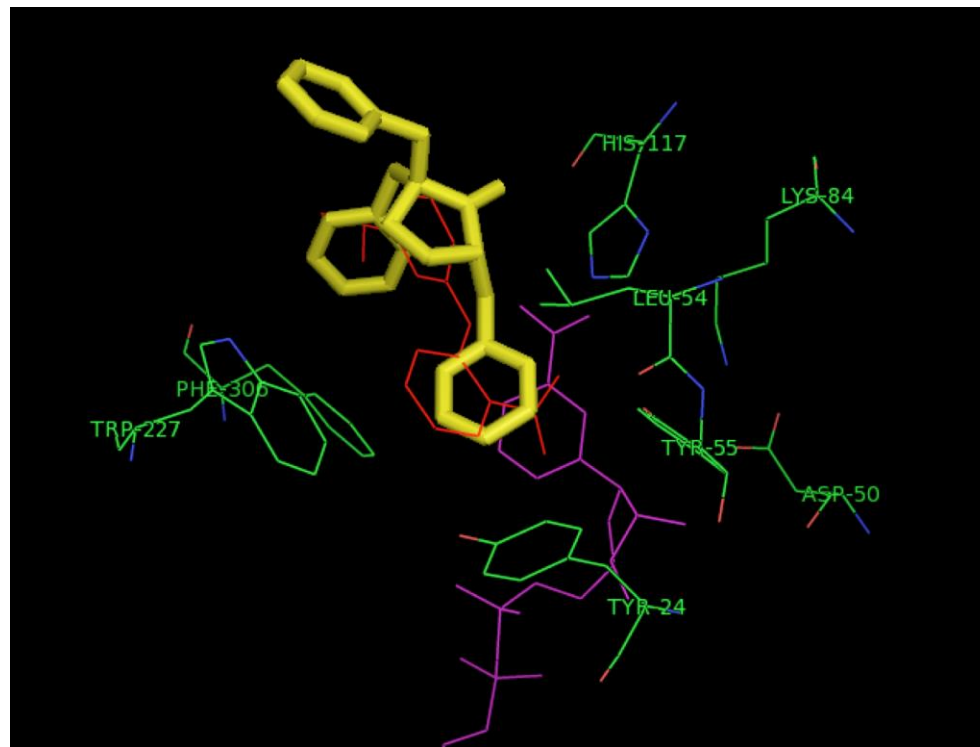
Prikaz sinteznega plana za spojine, ki so mimetiki prostaglandinov in so tako lahko potencialni inhibitorji encimov, ki metabolizirajo steroide. Da bi spojina imela inhibitory učinek, mora v svoji strukturi vsebovati **hidroksilno** ali **keto** funkcionalno skupino.



## Molekularno sidranje aktivne spojine v interakcijsko mesto encima



Kinetična analiza inhibicije encima s spojino **9**. Lineweaver-Burk predstavitev recipročnih vrednosti začetnih hitrosti encimske reakcije napram recipročnim vrednostim koncentracije aktivne spojine **9**.



Spojino **9**, ki je na encimskem testu pokazala precejšnje aktivnost smo sidrali v aktivno mesto encima in tako ugotavljali njene interakcije s tarčo.

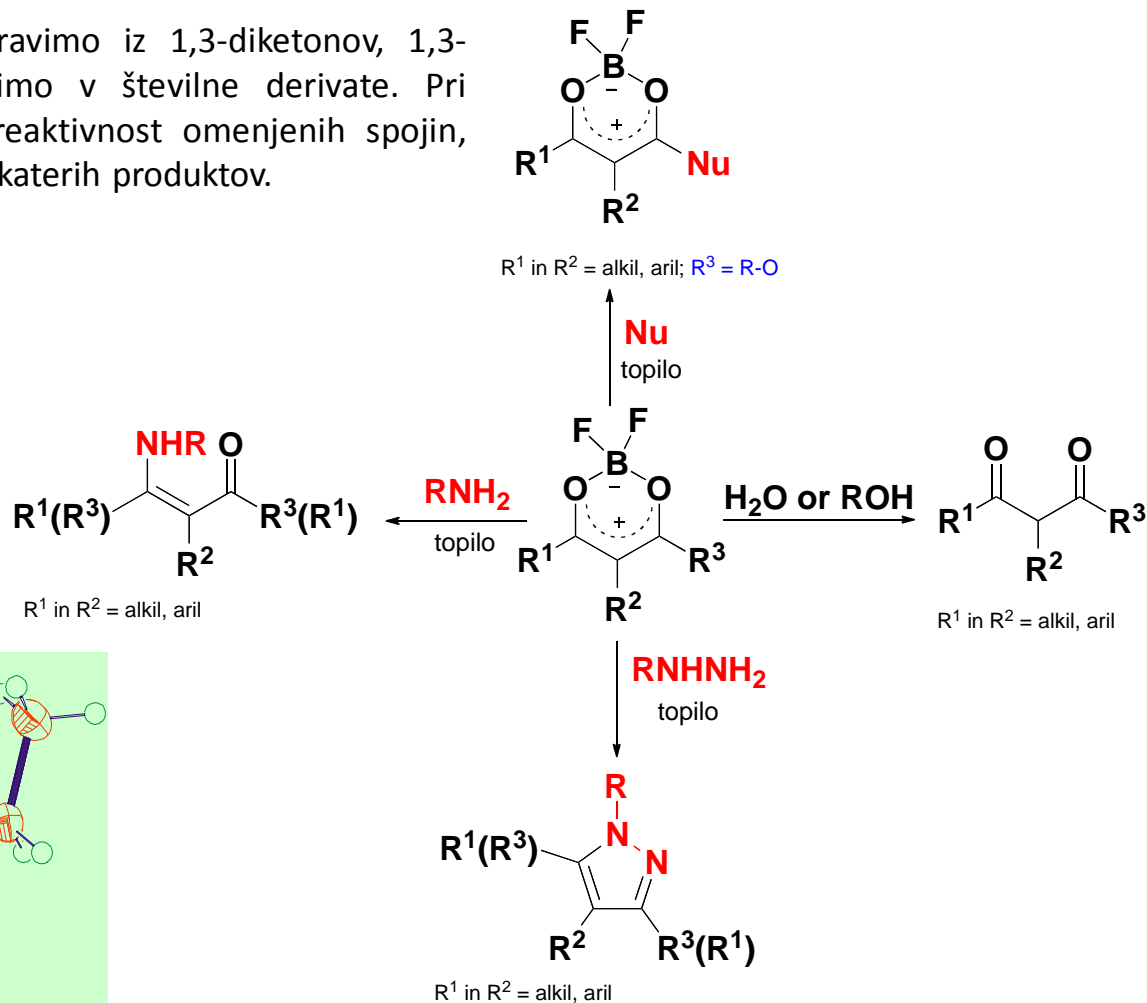
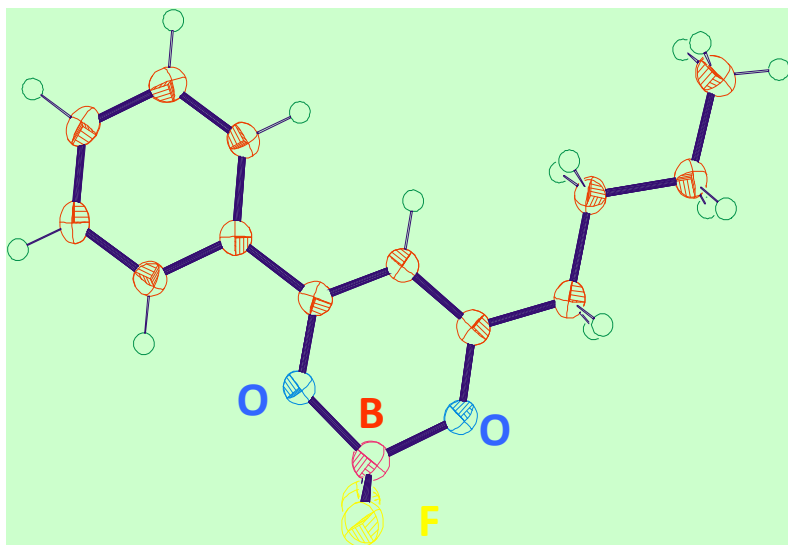
# Sinteza, transformacije in vrednotenje optičnih lastnosti difluorodioksoborovih kelatov

doc. dr. Bogdan Štefane

Borove kelate, ki jih lahko enostavno pripravimo iz 1,3-diketonov, 1,3-ketoaldehydov in ketoestrov, lahko pretvorimo v številne derivate. Pri transformacijah nas je predvsem zanimala reaktivnost omenjenih spojin, regioselektivnost reakcij in optične lastnosti nekaterih produktov.

## Določevanje strukture produktov

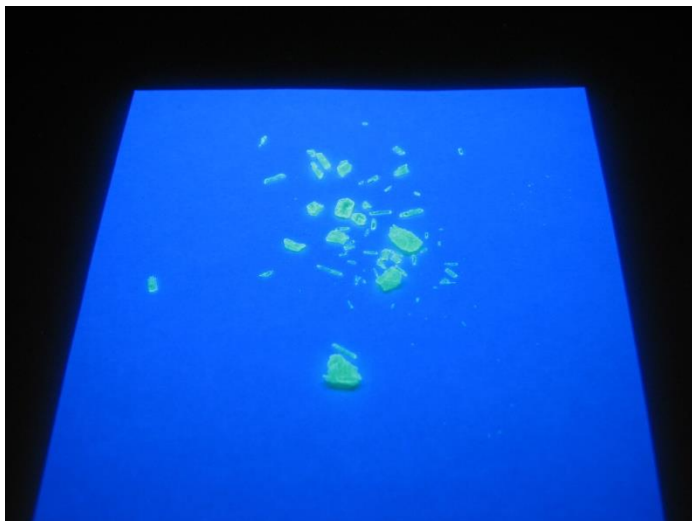
Ker so spojine tega tipa večinoma kristalinične, lahko njihovo strukturo nedvoumno potrdimo s pomočjo renske difrakcijske analize. Zgornja slika prikazuje primer strukture BF<sub>2</sub>-kelata.



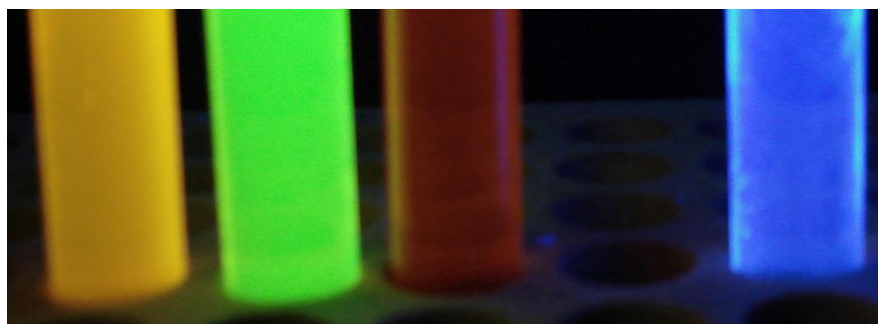
# Fluorescenčne lastnosti difluorodioksaborovih kelatov

doc. dr. Bogdan Štefane

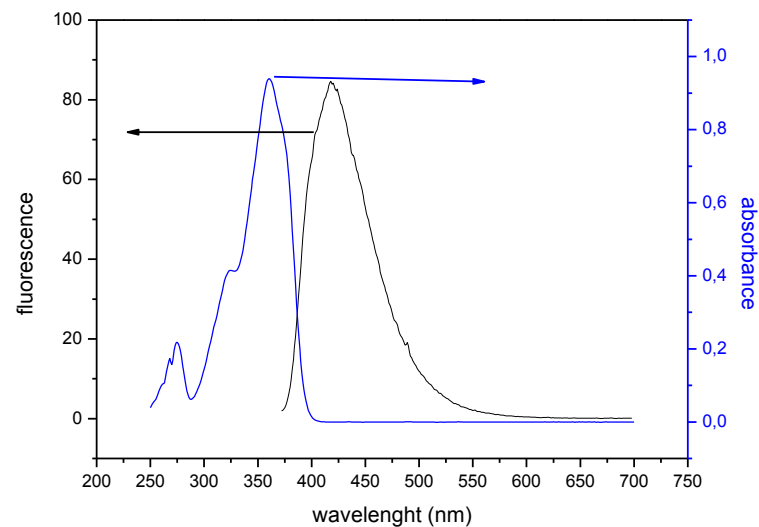
V sodelovanju z Katedro za analizno kemijo- doc. Dr. D. Kočar



Fluorescenca kristalov enega od produktov transformacije borovega kelata.



Fluorescenca spojine v različnih topilih



Primer UV-absorpcijskega in fluorescenčnega spektra  $\text{BF}_2$ -kelata.