

# DPP III Minisymposium

23. 9. 2022.

# Human Dipeptidyl Peptidase III

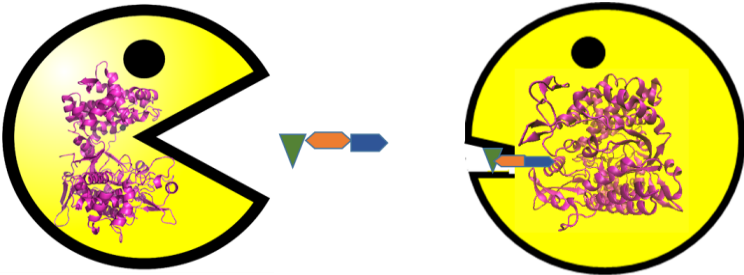
Morning session

different aspects of the action of DPP III in humans

Afternoon session

PEPTIDASE ACTIVITY OF DPP III

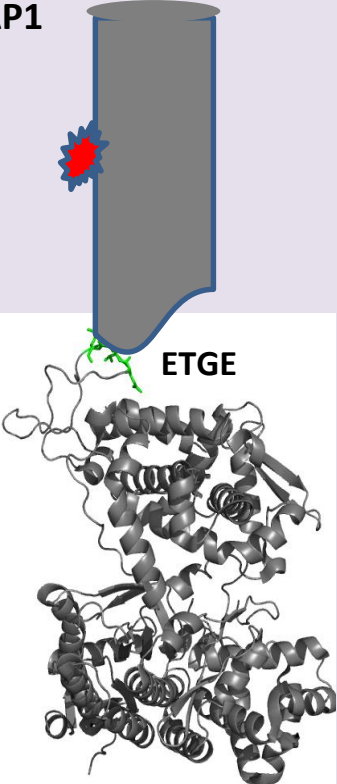
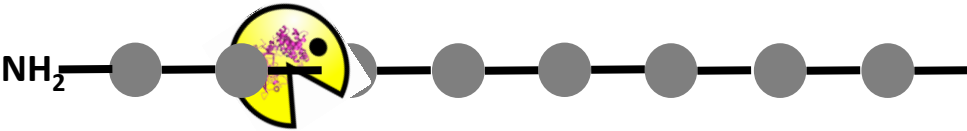
Protein-protein interaction



KEAP1

Involvement in the oxidative stress

? SH2D3C



Neuropeptides

Enzyme INHIBITORS



Metal ions

Influence on the enzyme structure and enzymatic activity. Mode of binding and mechanism of exchange of metal ions.

# BioRe-18-22 -1.9.2018 – 31.12.2020.

Tomin M and Tomić S, Oxidase or peptidase? A computational insight into a putative aflatoxin oxidase from *Armillariella tabescens*, *Proteins: Structure, Function, and Bioinformatics* (2019), 1-11 <https://doi.org/10.1002/prot.25661>

Agić D, Brkić H, Kazazić S, Tomić A, Abramić M, Aprotinin interacts with substrate-binding site of human dipeptidyl peptidase III, *Journal of Biomolecular Structure and Dynamics*, (2019), 37, <https://doi.org/10.1080/07391102.2018.1521343>

Tomić A., Horvat G., Ramek M., Agić D., Brkić H., Tomić S. New zinc ion parameters suitable for classical MD simulations of zinc metallo-peptidases. *Journal of Chemical Information and Modeling* (2019) DOI: 10.1021/acs.jcim.9b00235

Ćehić M., Suć Sajko J. Karačić Z., Piotrowski P., Šmidlehner T., Jerić I., Schmuck C., Piantanida I., Tomić S. The guanidiniocarbonylpyrrole - fluorophore conjugates as theragnostic tools for DPP III monitoring and inhibition. *Journal of biomolecular structure & dynamics* (2019)  
DOI: 10.1080/07391102.2019.1664936

Matić S, Kekez I, Tomin M, Bogár F, Šupljika F, Kazazić S, Hanić H, Jha S, Brkić H, Bourgeois B, Madl T, Gruber K, Macheroux P, Matković-Čalogović D, Matovina M & Tomić S. Binding of dipeptidyl peptidase III to the oxidative stress cell sensor Kelch-like ECH-associated protein 1 is a two-step process, *J Biomolecular Structure & Dynamics* (2020),  
DOI:10.1080/07391102.2020.1804455

Mirsada Ćehić, [doktorska disertacija](#) „Eksperimentalno i računalno istraživanje novih konjugata gvanidina s različitim fluoroforima kao liganada humane dipeptidil-peptidaze III” (2019)

# BioRe-18-22 -1.1.2021 – 31.12.2021.

Tomić A, Brkić H, **Matić Antonia**, Tomić S, Unravelling the inhibitory zinc ion binding site and the metal exchange mechanism in human DPP III, *Physical Chemistry Chemical Physics*, 2021, **59**, 3437–3453. <https://doi.org/10.1021/acs.jcim.9b00235>

Agić D, Karnaš M, Šubarić D, Lončarić M, Tomić S, Karačić Z, Bešlo D, Rastija V, Molnar M, Popović BM, Lisjak M. Coumarin Derivatives Act as Novel Inhibitors of Human Dipeptidyl Peptidase III: Combined *In Vitro* and *In Silico* Study, *Pharmaceuticals* 2021, **14**(6), 540; <https://doi.org/10.3390/ph14060540>

Blagojević B, Agić D, Teresa Serra A, Matić S, Matovina M, Bijelić S, Popović BM, An *in vitro* and *in silico* evaluation of bioactive potential of cornelian cherry (*Cornus mas* L.) extracts rich in polyphenols and iridoids, *Food Chemistry* 2021, **335**, 127619; <https://doi.org/10.1016/j.foodchem.2020.127619>

# BioRe-18-22 -1.1.2022 – 31.12.2022.

**Tomić, Antonija**; Tomić, Sanja, Demystifying DPP III Catalyzed Peptide Hydrolysis— Computational Study of the Complete Catalytic Cycle of Human DPP III Catalyzed Tynorphin Hydrolysis, *International journal of molecular sciences*, **23** (2022), 3; 1858, 24  
doi:10.3390/ijms23031858

**Matić, Sara**; Tomašić Paić, Ana; Sobočanec, Sandra; Pinterić, Marija; Pipalović, Goran; Martinčić, Monika; Matovina, Mihaela; Tomić, Sanja, Interdisciplinary study of the effects of dipeptidyl-peptidase III cancer mutations on the KEAP1-NRF2 signaling pathway. *International journal of molecular sciences*, **23** (2022), 4; 1994, 15 doi:10.3390/ijms23041994

**Karačić, Zrinka**; Šupljika, Filip; Tomić, Antonija; Brkljačić, Lidija; Tomašić Paić, Ana; Ćehić, Mirsad; Tomić, Sanja, Neuropeptides, substrates and inhibitors of human dipeptidyl peptides III, experimental and computational study - a new substrate identified. *International Journal of Biological Macromolecules*, **220** (2022); 1390-1401

**Dejan Agić**, Karnaš M, Tomić S, Komar M, Karačić Z, Rastija V, Bešlo D, Šubarić D, Molnar M, Experimental and computational evaluation of dipeptidyl peptidase III inhibitors based on quinazolinone-Schiff's bases, *Journal of Biomolecular Structure & Dynamics*, (2022) accepted

TO BE DONE AND PUBLISH:

## **Influence of Metal Di-cations on DPP III Structure and Function**

**Antonia Matic**

**Discussion On Further Studies on the Binding of Metal Di-cations to DPP III  
and Their Influence on DPP III Structure and Function**

---

**Antonija Tomić**

**Arg 669 and Arg 399 influence on substrate (ligand) stabilization**

# Morning session

- **Zrinka Karačić**
- **Antonija Tomić**
- **Dejan Agić**
  
- **Antonia Matic**

Fran Miočić-Stošić Preparation and biochemical and biophysical characterization of two proline mutant variants of human dipeptidyl peptidase III

## **Interaction of DPP III with Proteins**

### **Crystallization of the Keap1-DPP III Complex (I. Kekez)**

Interdisciplinary study of the effects of dipeptidyl-peptidase III cancer mutations on the KEAP1-NRF2 signaling pathway (S. Tomić)

### **Investigations on DPP III – SH2D3C Interactions**

(HrZZ project of M. Matovina Dipeptidyl peptidase III interaction with SH2 domain-containing protein 3C – possible link between oxidative stress response and cell migration)

**M. Matovina**  
**A. Tomašić Paić**  
**L. Barbarić**