CURRICULUM VITAE

Name: Višnja Stepanić, born Šimek

Address: Laboratory for Machine Learning and Knowledge Representation, Division of Electronics, Ruđer Bošković Institute, Bijenička 54, 10000 Zagreb

E-mail: visnja.stepanic@irb.hr

CroRIS: https://www.croris.hr/osobe/profil/6153

Web page: https://www.irb.hr/eng/About-RBI/People/Visnja-Stepanic

Google Scholar: https://scholar.google.com/citations?user=bnJkSncAAAAJ&hl=en

ResearchGate: https://www.researchgate.net/profile/Visnja_Stepanic2

ORCID: https://orcid.org/0000-0001-9518-4153

LinkedIn: https://www.linkedin.com/in/vi%C5%A1nja-stepani%C4%87-8104498/

Web of Science ResearcherID: AFW-0865-2022

Scopus Author ID: 15734295200

Expertise: discovery, design and development of compounds with biological activity; natural products; phytocompounds; medicinal chemistry; chemoinformatics; bioinformatics; working with large data sets and machine learning methods; molecular modeling; biochemistry; physical chemistry, analytical chemistry; ADME of chemicals, toxicology; nutraceuticals; functional food; work in the academic and private sector; evaluation experience

Education

2001 Ph. D., Faculty of Science University of Zagreb, Field of theoretical and computational chemistry,

1997 M. Sc., Faculty of Science, University of Zagreb

1993 B. Sc., Department of Physical Chemistry, Faculty of Science, University of Zagreb

1988 High school, School for pharmaceutical technicians, Zagreb

Affiliation

2019- present Ruđer Bošković Institute, Division of electronics, Laboratory for Computational Biology and Translational Medicine, Senior Researcher

2009-**2019** Ruđer Bošković Institute, Division of molecular medicine, Expert advisor

2006– **2008** GlaxoSmithKline Research Centre Zagreb Ltd., Principle scientist

2002 – **2006** R & D, PLIVA Int., Researcher

1998 – **2002** Ruđer Bošković Institute, Division of Organic Chemistry and Biochemistry, Research Assistant, Ph.D. Student

1994 – **1998** Ruđer Bošković Institute, Division of Physical Chemistry, Research Assistant, M.Sc. student

Participation in projects / programs

EU Projects:

1) **2024**-**2026** Enhancing capacities for technology transfer, company building and innovations in the field of ICT CapTTict (https://interreg-danube.eu/projects/capttict, www.irb.hr/capttict), Interreg Danube Region Project, **RBI coordinator, communication manager**

2) **2017**-**2022** The Scientific Centre of Excellence for Marine Bioprospecting –BioProCro, (Competitiveness and Cohesion Operational Program, European Regional Development Fund KK.01.1.1.01), **collaborator**

3) 2021 The AI4EU (The European AI on Demand Platform) Solutions Open Call 2021 for the challenge Modelling of drugs via deep learning neural network; **collaborator**

4) **2022**-**2026 Member of WG3** of COST Action CA21134 - Towards zer0 Pesticide AGRIculture : European Network for sustainability (T0P-AGRI-Network)

5) **2017**-**2021 MC Substitute** at COST Action CA16205 European Network on Understanding Gastrointestinal Absorption-related Processes

6) **2012**-**2016 MC member** of COST Action BM1203 EU-ROS

7) **2012**-**2016 MC member** of COST Action CM1106 Chemical Approaches to Targeting Drug Resistance in Cancer Stem Cells

Programs of Croatian science foundation **- collaborator*:***

1) **2023**–**2027** Analyses of interactions between organophosphorus compounds and esterases and other targets for therapy in poisoning

2) **2018-2023** Enzymatic Synthesis of Fluorinated Chiral Building Blocks EnzyFluor (IP-2018-01-4493)

3) **2014-2018** Synthesis and cytostatic evaluations of novel nitrogen heterocycles library (5596)

Programs of Ministry of Science and Education of RH:

1) **2017-2022** The Scientific Centre of Excellence for Marine Bioprospecting –BioProCro (Competitiveness and Cohesion Operational Program, European Regional Development Fund KK.01.1.1.01)

2) **2009**–**2014** Epigenetic and immunomodulatory changes in malignant head and neck tumors (098–0982464–2511)

3) **2012**–**2014** Developing methods for modeling properties of bioactive molecules and proteins (098-1770495-2919)

4) **1998**–**2001** Isotopical labeling and molecular spectroscopies (00980802)

5) **1998** Theoretical study of protonated diimide cations (Young investigator project, leader)

6) **1996**–**1998** Study of static and dynamical properties of molecules

7) **1991**–**1995** Development and application of models in chemistry

Programs in the non-academic institutes Pliva d.o.o. and GlaxoSmithKline Research Centre Zagreb Ltd:

1) **2007- 2008** Macrolides with anti-inflammatory activity, GSK Research Centre Zagreb Ltd.

2) **2006 – 2008** Pharmacokinetic behaviour of macrolides, GSK Research Centre Zagreb Ltd.

3) **2006 – 2008** Platform for generating macrolide hit molecules , GSK Research Centre Zagreb Ltd.

4) **2006 – 2008** Novel macrolide antibiotics, Research institute of Pliva d.o.o./ GSK Research Centre Zagreb Ltd.

5) **2004 – 2005** New program generating platform , Research institute of Pliva d.o.o.

6) **2002 – 2003** Novel antibiotics targets , R&D PLIVA Int.

*Additionally, participation in realization of the following projects of Ministry of Science Education and Sports of the Republic of Croatia in period **2011 - 2014**:*

1) Investigation of relationships between structure and biological activity of polyphenols, CRO-SRB project (2011-)

2) IGF2 and downstream signaling consequences in human lung cancers (335-0000000-3532)

3) Epidemiological features of systemic lupus erythematodes in Croatia (108-1081874-2419).

Prizes

2024 - Recognition of Croatian Association for Cancer Research (HDIR) for contribution to HDIR through organization of practical workshops

2022 - Recognition to the EnzyFluor project team (HrZZ IP-2018-01-4493) for the most demanding calculation using the Isabella cluster in 2021

2008 GlaxoSmithKline Exceptional Science Award (individual)

(for application of physicochemical properties on chemical class of macrolides and their global popularization in GSK)

2008 GlaxoSmithKline Recognition/Bronze Award

(for contribution to understanding of pharmacokinetic behaviour of macrolides)

2008 GlaxoSmithKline Recognition/Bronze Award

(for participation in organization of in-house meeting of computational chemists (Europa) in UK)

Publications and meeting participation (https://www.croris.hr/osobe/profil/6153**)**

Book Editing

1. **Stepanić V**, Kučerová-Chlupáčová M. Redox Active Molecules in Cancer Treatments,I SBN 978-3-0365-6731-0 (hardback); ISBN 978-3-0365-6730-3 (PDF), https://doi.org/10.3390/books978-3-0365-6730-3

2. Saso L, Gurer-Orhan H, **Stepanić V**. Modulators of Oxidative Stress: Chemical and Pharmacological Aspects, ISBN 978-3-03943-228-8 (Hbk); ISBN 978-3-03943-229-5 (PDF) https://doi.org/10.3390/books978-3-03943-229-5

3. Book of Abstracts, 10th Joint Meeting on Medicinal Chemistry 2017 / Basarić N, Namjesnik D, Perković I, **Stepanić V** (Eds). Zagreb : Croatian Chemical Society, 2017

Special journal issues – guest editor

Stepanić V, Kučerová-Chlupáčová M. Special Issue "Redox Active Molecules in Cancer Treatments" (**2021**), of Molecules (ISSN 1420-3049) belonging to the section "Medicinal Chemistry". https://www.mdpi.com/journal/molecules/special_issues/Redox_Active_Cancer

Saso L, Gurer-Orhan H, **Stepanić V**. Special Issue "Modulators of Oxidative Stress: Chemical and Pharmacological Aspects" (**2020**), of Antioxidants (ISSN 2076-3921) belonging to the section "Health Outcomes of Antioxidants and Oxidative Stress". https://www.mdpi.com/journal/antioxidants/special_issues/modulators_oxidative_stress

Book/Proceedings chapters

1. Pehar V, Oršolić D, Stepanić V.* Drug-likeness, herbicide-likeness and toxicity of herbicidal compounds – in silico analysis. Proceedings: 17th Ružička Days Today Science – Tomorrow Industry, Tomas S, Ačkar Đ. (Eds.). Osijek : Josip Juraj Strossmayer University of Osijek, Faculty of Food Technology Osijek and Croatian Society of Chemical Engineers (CSCE), 2019. 112-123. ISSN: 2459-9387
2. Parnham JM, **Stepanić V**, Tafferner N, Panek M, Verbanac D. Mild plant and dietary immunomodulators // Principles of Immunopharmacology / Parnham J. Michael ; Nijkamp P. Frans (Eds.). Basel: Birkhäuser Basel, 2018. str. 1-68.
3. **Stepanić V**, Novak Kujundžić R, Gall Trošelj K. Epigenome, Cancer Prevention and Flavonoids and Curcumin // Epigenetics and Epigenomics / Christopher J. Payne (Ed.). Rijeka: InTech, 2014. Pp. 173-209.
4. Verbanac D, Perić M, Čipčić-Paljetak H; Matijašić M, **Stepanić V**. Biologically active ingredients from food with anti-obesity properties // Obesity: Public Health Problem and Medical Challenge / Rukavina, Daniel (Ed). Rijeka : Hrvatska Akademija Znanosti i Umjetnosti, 2014. pp. 133-150. ISBN 978-953-154-282-1
5. Verbanac D, **Stepanić V***, Lučić B, Amić D, "The Must" of the Drug Discovery and Development is – Interdisciplinarity, / Bioinformatics and biological physics : proceedings of the scientific meeting / Paar, Vladimir (ur.). Zagreb, Hrvatska, 21.11.2012. : Croatian Academy of Sciences and Arts, 2013. pp. 179-189. ISBN 978-953-154-199-2

Original scientific and rewiew articles with international peer-review (IF at publishing time; IF current; journal rank at publishing time; number of citations in Web of Science)

More than 50 papers

In the last 5 years:

1. **Stepanić V,*** Hršak D, Kobetić R. The State of the Art on Chemical Databases and Libraries // Croatica chemica acta, 97 (2024), 4; P1-P12. doi: 10.5562/cca4130
2. Jurin M, Čikoš A, **Stepanić V**, Górecki M, Pescitelli G, Kontrec D, Jakas A, Dražić T, Roje M. Synthesis, Absolute Configuration, Biological Profile and Antiproliferative Activity of New 3,5-Disubstituted Hydantoins. Pharmaceuticals. 2024; 17(10):1259. https://doi.org/10.3390/ph17101259
3. Buljan A, **Stepanić V**, Čikoš A, Babić Brčić S, Bojanić K, Roje M. Total Synthesis and Biological Profiling of Putative (±)-Marinoaziridine B and (±)-N-Methyl Marinoaziridine A. *Marine Drugs*. 2024; 22(7):310. doi: 10.3390/md22070310
4. Jurin M, **Stepanić V**, Bojanić K, Vadlja D, Kontrec D, Dražić T, Roje M, Novel (±)-trans-β-lactam ureas: Synthesis, in silico and in vitro biological profiling, *Acta pharmaceutica*, 2024, 74 (1), 37-59. doi: 10.2478/acph-2024-0008
5. Pehar V, Kolić D, Zandona A, Šinko G, Katalinić M, **Stepanić V*,** Kovarik Z*. Selected herbicides screened for toxicity and analysed as inhibitors of both cholinesterases. Chem Biol Interact. 2023 Jul 1;379:110506. doi: 10.1016/j.cbi.2023.110506
6. **Stepanić V***, Kučerová-Chlupáčová M, * Review and Chemoinformatic Analysis of Ferroptosis Modulators with a Focus on Natural Plant Products. Molecules, 2023, 28 (2), 475-505. doi:10.3390/molecules28020475
7. Dokli I, Brkljača Z, Švaco P, Tang L, **Stepanić V,*** Majerić Elenkov M.* Biocatalytic approach to chiral fluoroaromatic scaffolds, Org. Biomol. Chem., 2022,20, 9734-9741. https://doi.org/10.1039/D2OB01955H
8. Milčić N**, Stepanić V**, Crnolatac I, Findrik Blažević Z, Brkljača Z, Majerić Elenkov M. Inhibitory Effect of DMSO on Halohydrin Dehalogenase: Experimental and Computational Insights into the Influence of an Organic Co-solvent on the Structural and Catalytic Properties of a Biocatalyst. Chemistry- A European Journal. 2022;28(56):e202201923. doi: 10.1002/chem.202201923, with front cover doi.org/10.1002/chem.202202869
9. Antonijević MR, Simijonović DM, Avdović EH, Ćirić A, Petrović ZD, Marković JD, **Stepanić V**, Marković ZS. Green One-Pot Synthesis of Coumarin-Hydroxybenzohydrazide Hybrids and Their Antioxidant Potency. *Antioxidants* 2021; 10(7):1106. https://doi.org/10.3390/antiox10071106

10. Oršolić D, Pehar V, Šmuc T, **Stepanić V**,* Comprehensive machine learning based study of the chemical space of herbicides, *Scientific reports* 11 (1), 1-12, doi: https://doi.org/10.1038/s41598-021-90690-w

11. Cichońska A, Ravikumar B, Allaway RJ, Wan F, Park S, Isayev O, Li S, Mason M, Lamb A, Tanoli Z, Jeon M, Kim S, Popova M, Capuzzi S, Zeng J, Dang K, Koytiger G, Kang J, Wells CI, Willson TM; IDG-DREAM Drug-Kinase Binding Prediction Challenge Consortium (Oršolić D, Lučić B, **Stepanić V**, Šmuc T), Oprea TI, Schlessinger A, Drewry DH, Stolovitzky G, Wennerberg K, Guinney J, Aittokallio T. Crowdsourced mapping of unexplored target space of kinase inhibitors. Nat Commun. 2021 Jun 3;12(1):3307. doi: 10.1038/s41467-021-23165-1.

12. Tascioglu Aliyev A, Panieri E, **Stepanić V,** Gurer-Orhan H, Saso L, Involvement of NRF2 in Breast Cancer and Possible Therapeutical Role of Polyphenols and Melatonin. *Molecules* 2021, 26, 1853. https://doi.org/10.3390/molecules26071853

13. Gelemanović A, Vidović T, **Stepanić V,** Trajković K, Identification of 37 Heterogeneous Drug Candidates for Treatment of COVID-19 via a Rational Transcriptomics-Based Drug Repurposing Approach, *Pharmaceuticals* 2021;14:87. doi: doi.org/10.3390/ph14020087

14. Amić A, Marković Z, Dimitrić Marković JM, Milenković D, **Stepanić V**. Antioxidative potential of ferulic acid phenoxyl radical. *Phytochemistry*. 2020; 170: 112218. doi:10.1016/j.phytochem.2019.112218

15. Macan Meščić A, Harej A, Cazin I, Klobučar M, **Stepanić V**, Pavelić K, Pavelić Kraljević S, Schols D, Snoeck R, Andrei G, Raić-Malić S. Antitumor and antiviral activities of 4-substituted 1,2,3-triazolyl-2,3-dibenzyl-L-ascorbic acid derivatives. Eur. J. Med. Chem. 2019;184:111739. doi:10.1016/j.ejmech.2019.111739

16. Harej A, Macan Meščić A, **Stepanić V**, Klobučar M, Pavelić K, Pavelić Kraljević S, Raić-Malić S. The Antioxidant and Antiproliferative Activities of 1,2,3-Triazolyl-L-Ascorbic Acid Derivatives. *Int. J. Mol. Sci.* 20(19) (2019) 4735. doi:10.3390/ijms20194735

17. **Stepanić V,*** Matijašić M, Horvat T, Verbanac D, Kučerová-Chlupáčová M, Saso L, Žarković N.* Antioxidant Activities of Alkyl Substituted Pyrazine Derivatives of Chalcones—In Vitro and In Silico Study. *Antioxidants*. 8(4) (2019) E90. doi: 10.3390/antiox8040090

18. Kujundžić Novak R, **Stepanić V**, Milković L, Čipak Gašparović A, Tomljanović M, Gall Trošelj K. Curcumin and its potential for systemic targeting of inflamm-aging and metabolic reprogramming in cancer. *Int J Mol Sci.* 20(5) (2019) E1180. doi: 10.3390/ijms20051180

19. **Stepanić V,*** Matić S, Amić A, Lučić B, Milenković D, Marković Z. Effects of conjugation metabolism on radical scavenging and transport properties of quercetin – *In silico* study, *J. Mol. Graph. Model*. 86 (2019) 278-285. doi: 10.1016/j.jmgm.2018.10.023

Invited lectures in the last 5 years

1. **Stepanić V,** Harnessing digital technologies to explore nature's molecules for targeted human use, 2nd European Biomedical and Veterinary Engineering Congress - BIOMEDVETMECH, Zagreb, Croatia, October **2024**
2. **Stepanić V,** Data driven drug discovery – impact of chemical libraries and AI // 7. Croatian Congress of Pharmacy with international participation, Dubrovnik, Croatia, May **2024**.
3. **Stepanić V**, Use of Chemoinformatics in Toxicology, International Symposium on Environmental and Molecular Toxicology of Chemicals, Zagreb, December **2023**, Zagreb.
4. **Stepanić V**, Brkljača Z, Majerić Elenkov M, Computational Insights into the Biocatalytic Activity of C-Type Halohydrin Dehalogenase HheC, Computational Chemistry Day, September **2023**, Zagreb.
5. **Stepanić V**, Brkljača Z, Milčić N, Crnolatac I, Findrik Blažević Z, Majerić Elenkov M, Elucidation of DMSO effects on catalytic activity of halohydrin dehalogenase HheC by molecular dynamics, Regional Biophysics Conference, Hungarian Biophysical Society, Pécs, Hungary, August **2022**.
6. **Stepanić V**, Technology driven drug discovery, 1st European Congress of Biomedical and Veterinary Engineering - BIOMEDVETMECH, Zagreb, Croatia, October **2022**
7. **Stepanić V**, Oršolić D, Šmuc T, Machine learning in chemical compound space, Mini symposium of Croatia Chemical Society, Rijeka, Croatia, July **2022**.
8. **Stepanić V**, Machine Learning in Chemistry, XIV Meeting of Young Chemical Engineers, Zagreb, 2022.
9. **Stepanić V**, (Re)purposing starts virtually by predictive machine-learning models, 27th Croatian Meeting of Chemists and Chemical Engineers, Veli Lošinj, Croatia, October **2021**.
10. **Stepanić V**, Development of phytotoxic natural molecules as complementary herbicidal agents is supported by machine learning study, 1st international conference "Food & Climate Change", October **2021**.
11. **Stepanić V**, By polyphenols against cancer?, Symposium "The First 10 Years of HDIR", Croatian Society for Cancer Research, Ruđer Bošković Institute, June 4, **2019**,.

12.**Stepanić V**, Malignant Tumors in medicinal chemistry, Regular seminar of Division of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Zagreb, April **2019**.

13.**Stepanić V,** Physicochemical properties and ADME profile of molecules – *in vitro* and *in silico* approaches, Annual meeting of Croatian Biophysical Society, Zagreb, February **2019**.

Meeting organization:

1. Member of organizing committee of annual Mini symposium of Section of medicinal and pharmaceutical chemistry of Croatian Chemical Society

2. Member of organizing committee of annual meeting Computational Chemistry Day (CCD) of Section of theoretical and computation chemistry of Croatian Chemical Society

3. Member of International organizing committee. The 12th Joint Meeting of Medicinal Chemistry (on-line), Bratislava, Slovakia, 2022.

4. Member of International organizing committee. The 11th Joint Meeting of Medicinal Chemistry, Prague, Czech Republic, 2019.

5. Member of International scientific committee and Local organizing committee. The 10th Joint Meeting of Medicinal Chemistry, Dubrovnik, June 25-28, 2017.

6. Member of a national organizing committee. HDIR-4: "From Bench to Clinic". Fourth Meeting of the Croatian Association for Cancer Research with International Participation. November 3-4, 2016, Zagreb.

7. Member of an organizing team. GSK meeting of computational chemists Europe, Stevenage, UK, 2008.

8. Member of an organizing team. The second conference of PMI project leaders (PMI, Zagreb), Hotel Sheraton Zagreb 11-12 December 2008.

Teaching in higher education

- **2016**- **2024** participation in course "Design of novel drugs", of graduate study on Faculty of Pharmacy and Biochemistry, University of Zagreb.
- **2011**–**2018** participation in course "Biologically active compounds in food", of graduate study Medical studies in Croatian on School of medicine, University of Zagreb

- **2013** – **2018** participation in course "P4 in medicine: Predictive, preventive, personalized and participatory medicine ", of graduate study Medical studies in Croatian on School of medicine, University of Zagreb
- **2012**-**2014** participation in course "IME6852Z Instrumental methods", of Specialist study of environmental health engineering on University of applied health studies, Zagreb
- **1998**–**2001** participation in courses "Molecular spectroscopy" and "Chemical kinetics" of graduate study on Faculty of natural sciences, University of Zagreb

Supervision

Dilber Ivana, The use of the AI tool AlphaFold 2 for protein structure modeling, Master's thesis, Stepanić Višnja, Nela Malatesti (Supervisors), Department of Biotechnology, University of Rijeka, 2023.

Pehar Vesna, Toxicity of selected herbicides analysed by in silico methods and by bioassays, Doctoral Thesis, Kovarik Zrinka, Stepanić, Višnja (Supervisors), Faculty of sciences, University of Zagreb, 2023.

Jagar Fran, Study of interactions between Olive compounds and tyrosine kinase HGFR/c-Met using molecular docking, Master's thesis, Stepanić Višnja, Barbarić Monika (Supervisors), Faculty of Pharmacy and Biochemistry, University of Zagreb, 2023.

Workshops

2023 - an organizer and lecturer of the workshop for the researchers and students " How to design and apply a proof-of-concept (PoC) proposal?" together with Croatian association for cancer research (HDIR), 25/5/2023

2023 - an organizer and lecturer of the workshop for the researchers and students " Why take the path of innovation and commercialisation?" together with Croatian association for cancer research (HDIR), 27/3/2023

2014 – **present** an organizer and lecturer of the workshop for the researchers and students from academic and non-academic environmentS, "Introduction into Molecular Modelling" together with Croatian association for cancer research (HDIR)

Conference/Meeting organization

1. Member of the International Scientific Committee and the Organizing Team for the Regional Biophysics Conference RBC2024, Split, 2024

2. Member of organizing committee of annual Mini symposium of Section of medicinal and pharmaceutical chemistry of Croatian Chemical Society

3. Member of organizing committee of annual meeting Computational Chemistry Day (CCD) of Section of theoretical and computation chemistry of Croatian Chemical Society

4. Member of International Scientific Committee. The 12th Joint Meeting of Medicinal Chemistry (on-line), Bratislava, Slovakia, 2022.

5. Member of International organizing committee. The 11th Joint Meeting of Medicinal Chemistry, Prague, Czech Republic, 2019.

6. Member of International scientific committee and Local organizing committee. The 10th Joint Meeting of Medicinal Chemistry, Dubrovnik, Croatia, June 25-28, 2017.

7. Member of a national organizing committee. HDIR-4: "From Bench to Clinic". Fourth Meeting of the Croatian Association for Cancer Research with International Participation. November 3-4, 2016, Zagreb.

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9. Member of an organizing team. The second conference of PMI project leaders (PMI, Zagreb), Hotel Sheraton Zagreb 11-12 December 2008.

Popularization of Science

- **2025** - Participation on the Science Festival with the topic Networks, as a lecturer, with the lecture "Chemical communication – invisible web of life"
- **2019**- Participation on the Open Day of IRB ODI2019, as a lecturer, with the lecture "The Bright and the Dark Side of Drugs".
- **2018-2019** – a supervisor at the BASF Chemgeneration – Reaching Zero experimentation workshop at the Ruđer Bošković Institute
- **2017-2019** – an educator at the ESF project "Affirmative and innovative approaches for education of talented primary school pupils and development of interdisciplinary multiannual program for the talents in STEM fields Ja raSTEM! " (Beneficiary: Primary school Lauder-Hugo Kon). My workshop enters the Croatian elementary school Curriculum.

- **2016 -2019** – a mentor of the workshop "Discovering medicines with the aid of computers" with Marko Tomin, BSc, and prof. Sanja Tomić, provided to the project Exploring Worlds of Science and Innovation‘ organized by the foundation Wissen am Werk (ZZND) and the Rudjer Boskovic Institute
- **2013**- Participation in Open Days of IRB 2013, as a guide coordinator.

Memberships

- Croatian chemical society (a member of Council for Section of Medicinal and Pharmaceutical Chemistry)
- Croatian biophysical society (a member of the Steering board)
- Croatian association for cancer research and EACR