

Dr. Robert Vianello

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Personal Data

Date & Place of Birth: 03 June 1977, Rijeka, Croatia

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Work Positions

- **Head of Laboratory**, Ruđer Bošković Institute, Zagreb, Croatia (03.2021 – present)
- **Senior Scientist**, Ruđer Bošković Institute, Zagreb, Croatia (07.2015 – present)
- **FP7-IEF Marie Curie Fellow**, National Institute of Chemistry, Ljubljana, Slovenia. Host: Dr. Janez Mavri (10.2010 – 04.2012)
- **Croatian Science Foundation Fellow**, National Institute of Chemistry, Slovenia. Host: Dr. Janez Mavri (04.2010 – 10.2010)
- **Senior Research Associate** (10.2009 – 07.2015) • **Research Associate** (06.2005 – 10.2009), Ruđer Bošković Institute, Zagreb, Croatia
- **Alexander von Humboldt Postdoctoral Fellow**, Institute of Organic Chemistry, University of Heidelberg, Germany. Host: Prof. Rolf Gleiter (01.2005 – 03.2005)
- **Senior Research Assistant** (03.2004 – 06.2005) • **Research Assistant** (12.2000 – 03.2004), Ruđer Bošković Institute, Zagreb, Croatia

Education

- **PhD in Natural Sciences**, University of Zagreb, Croatia. Thesis: "Interaction of Lewis Acids and Bases". Supervisor: Prof. Zvonimir Maksić (11.2003)
- **Dipl. Ing. in Chemistry**, Faculty of Science, University of Zagreb, Croatia. Thesis: "Proton Affinities of Some Guanidine Derivatives" (11.2000)
- **Chemistry study**, Faculty of Science, University of Zagreb, Croatia (1996–2000)
- **The Sušak High School**, Rijeka, Croatia (1992–1996)
- **Primary School**, Rijeka, Croatia (1984–1992)

Awards and Honours

- **2017 Branimir Jernej Foundation Award** – Annual award for a publication in the fields of molecular biology, neurosciences and biomedicine published in 2017 (02.2018)
- **2016 Croatian National Science Award** – Annual science award in the field on natural sciences awarded by the Croatian Parliament and the Croatian Ministry of Science and Education (12.2017)
- **Presentation of research results on the official web-site of the European Commission** (<http://www.croatia-in-the-eu.eu>) celebrating Croatia's accession to the European Union (06.2013)
- **Marie Curie Success Story**, presentation of research results in the European Commission's publication "EU FP7 People Specific Programme Success Stories Booklet" (04.2012)
- **50,000th Marie Curie Fellowship Award** – An honour given by the European Commission to 25 current FP7 Marie Curie Fellows (12.2010)
- **Promising Scientist Prize** of the Centre for the Applied Quantum Mechanics in Paris, France (09.2010)
- **2008 Award of the Croatian Academy of Sciences and Arts** for the development of scientific and artistic work (05.2008)
- **2006 Leopold Ružička Award** of the Croatian Chemical Society for young scientists (11.2007)
- **2005 Croatian National Science Award** – Annual award for junior researchers awarded by the Croatian Parliament and the Croatian Ministry of Science, Education and Sports (06.2006)
- **2004 Award by the Society of University Teachers and other Scientists in Zagreb** (12.2004)

- **2004 City of Rijeka's Public Award** – Annual award for the creative work and achievements in chemistry (04.2004)
- **1995 Award for the Achievements in Technical Culture and the Promotion of the City of Rijeka** awarded by the Society of Technical Culture and the City of Rijeka (12.1995)
- **Scholar of the City of Rijeka** (1993–2000)

Grants and Fellowships

- **Research Grant from the Croatian Science Foundation:** "Design, synthesis and computational analysis of novel optical chemical pH sensing benzazole derivatives" (2021–2025). Total financial value: 130.000 EUR (excluding salaries).
- **Commercial Research Contracts with the Pharmaceutical Company Xellia Croatia Ltd.** (2019–2022).
- **Research Grant from the Croatian Science Foundation:** "Design and synthesis of novel nitrogen-containing heterocyclic fluorophores and fluorescent anomaterials for pH and metal-ion sensing" (2015–2019). Total financial value: 130.000 EUR (excluding salaries).
- **Marie Curie Career Integration Grant:** "Computational studies of the biogenic amines of the brain for targeting neurological diseases" (FP7–PEOPLE–2012–CiG, 2013–2017). Total financial value: 100.000 EUR (excluding salaries).
- **Research Grant from the Croatian Ministry of Science, Education and Sports:** "Broensted and Lewis acids and bases in chemistry and biochemistry" (2011–2014). Total financial value: 46.000 EUR (excluding salaries).
- **Marie Curie Individual Fellowship for Career Development:** "Computational studies of proton dynamics in hydrogen bonded systems and enzymes" (FP7–PEOPLE–2009–IEF, 2010–2012) for an 18 months stay at the National Institute of Chemistry in Ljubljana (Slovenia). Total financial value: 99.127,60 EUR.
- **Stipend from the Croatian Science Foundation** for a 6 months stay at the National Institute of Chemistry in Ljubljana (Slovenia) (2010). Total financial value: 11.000 EUR.
- **Research Grant from the Unity through Knowledge Fund under the Young Researchers and Professionals Program** co-financed by the industrial partner APO Environmental Protection Services Ltd. Zagreb: "Computational prediction of the structure and catalytic activity of new organic superacids" (2008–2010). Total financial value: 35.000 EUR (excluding salaries).
- **Bilateral Croatia–Slovenia project.** Partner: Dr. Jernej Stare, National Institute of Chemistry, Ljubljana, Slovenia. (2009–2010)
- **Bilateral Croatia–Austria project.** Partner: Prof. Robert Konrat, University of Vienna, Austria. (2008–2009)
- **Alexander von Humboldt Postdoctoral Fellowship** for a 3 months stay at the University of Heidelberg (Germany) in the group of Prof. Rolf Gleiter (2005)

Selected Participation at Conferences and Events

Plenary Lectures

- ◆ "Using computers to fight neurodegenerative diseases"; **5th Symposium of Chemistry Students**; Zagreb, Croatia, 10.2018
- ◆ "Computational analysis of the catalytic activity and irreversible inhibition of monoamine oxidase for targeting neurological diseases"; **6th Central European Conference – Chemistry towards Biology**; Trieste, Italy, 09.2013

Selected Invited Lectures

- ◆ "Green, greener, in silico! The role of computational methods in chemistry and biochemistry"; **3rd ZORH Convention on the Topic of Environmental Protection in the Republic of Croatia**; Split, Croatia, 04.2022
- ◆ "*In Silico* Neuroscience"; **Opening of the Ažman's Computational Center**; National Institute of Chemistry, Slovenia, 04.2009
- ◆ "Mechanistic studies of monoamine oxidases"; **International Summer School: Multiscale Molecular Simulation for Neurological Targets**; University of Ljubljana, Slovenia, 06.2018; 08.2015
- ◆ "Computational insight into the selectivity and catalytic activity of the monoamine oxidase enzyme for targeting neurological diseases"; **1st Computational Chemistry Day**; Zagreb, Croatia, 05.2018
- ◆ "Computational insight into the catalytic activity of monoamine oxidase enzyme for targeting neurological diseases"; **10th Joint Meeting on Medicinal Chemistry**; Dubrovnik, Croatia, 06.2017
- ◆ "The selectivity and catalytic mechanism of monoamine oxidase enzymes from multi-scale computational simulations"; **Advancing the Frontiers of (Bio)Chemistry with Valence Bond Approaches**; Uppsala University, Sweden, 06.2016
- ◆ "Computational insight into the catalytic activity of monoamine oxidase for targeting neurological diseases"; **6th EuCheMS Organic Division Young Investigators Workshop**; Larnaca, Cyprus, 08.2014
- ◆ "Computer sciences and neurodegenerative diseases"; **Central Europe NeuroScience CENS Advisory Board meeting**; Belgrade, Serbia, 06.2014
- ◆ "Recent progress in understanding the catalytic activity of monoamine oxidases"; **Interdisciplinary Chemical Approaches for Neuropathology**; Valletta, Malta, 10.2013
- ◆ "Computational insight into the catalytic activity and irreversible inhibition of monoamine oxidase for targeting neurological diseases"; **12th National Conference on Biophysics**; Iasi, Romania, 06.2013

- ◆ "How are biogenic amines metabolized by monoamine oxidases?"; **Summer School: From Computational Enzymology towards Molecular Docking**; University of Ljubljana, Slovenia, 05.2013
- ◆ "Computational insight into the catalytic activity and the inhibition of monoamine oxidase B"; **15th Amine Oxidase Conference**; Toulouse, France, 07.2012
- ◆ "Computational study of vibrational properties of histamine monocation: from aqueous solution to receptors"; **Jožef Stefan Institute**; Ljubljana, Slovenia, 02.2012
- ◆ "Hydrogen bond dynamics and computational vibrational spectroscopy in aqueous solution: the case study of histamine monocation"; **XVIth International Workshop on Quantum Systems in Chemistry and Physics (QSCP-XVI)**; Kanazawa, Japan, 09.2011
- ◆ " "One group to rule them all" - polycyano organic compounds are record holding superacids"; **XVth International Workshop on Quantum Systems in Chemistry and Physics (QSCP-XV)**; University of Cambridge, England, 09.2010

Selected Lectures

- ◆ "When soft is better than hard: flexible methylene group as a useful linker in designing neutral organic superbases"; **23rd Croatian Meeting of Chemists and Chemical Engineers**; Osijek, Croatia, 04.2013
- ◆ "Computational insight into the catalytic activity and the inhibition of monoamine oxidase B"; **IRENE conference "in silico enzyme design and screening"**; Trieste, Italy, 05.2012
- ◆ "Hydrogen bond dynamics and computational vibrational spectroscopy in aqueous solution: the case study of histamine monocation"; **Ninth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2011)**; Santiago de Compostela, Spain, 07.2011

Selected Invited Popular Lectures

- ◆ "10 most important molecules of the 20th century"; **Science Festival 2012**; Rijeka, Croatia, 04.2012
- ◆ "Chemistry – Our life, our future"; **Lecture on the occasion of the 384th anniversary of the Sušak High School**; Rijeka, Croatia, 11.2011
- ◆ "From the laboratory of Maria Skłodowska Curie for a brighter future of mankind"; **Science Festival 2011**; Rijeka, Croatia, 04.2011
- ◆ "Design of new organic superacids by computational chemistry"; **Student Section of the Croatian Chemical Society**; Zagreb, Croatia, 12.2008
- ◆ "With computational chemistry towards new extra-strong acids"; **Lecture on the occasion of the 381st anniversary of the Sušak High School and the opening of a new chemistry laboratory**; Rijeka, Croatia, 11.2008

Mentorship of Postdoctoral Students

- Dr. Tana Tandarić, Ruđer Bošković Institute, Zagreb, Croatia (2022–present)
- Dr. Ema Horak, Ruđer Bošković Institute, Zagreb, Croatia (2018–2019)

Mentorship of Doctoral Students

- Lucija Hok, University of Zagreb (2019–present)
- Tana Tandarić, University of Zagreb (2016–2022). PhD Thesis: "Computational investigation of the mechanism of the irreversible inhibition of the monoamine oxidase B enzyme" (02.2021)
- Aleksandra Maršavelski, University of Zagreb (2015–2018). PhD Thesis: "Computational investigation of the catalytic activity and selectivity of amine oxidases towards histamine and *N*-methylhistamine" (07.2017)
- Nena Peran, University of Zagreb (2005–2010). PhD Thesis: "Computational study of acid–base properties of α -amino acids in water solutions" (12.2010)

Supervision of Undergraduate Students

- Dalibor Hršak, Faculty of Science, University of Zagreb. Dipl. Ing. Thesis: "Interpretation of basicity and acidity of bases of nucleic acids using triadic formula" (05.2010)
- Jelena Stojaković, Faculty of Science, University of Zagreb. Dipl. Ing. Thesis: "Proton affinities of carbenes in the gas-phase" (12.2007)
- Nena Peran, Faculty of Science, University of Zagreb. Dipl. Ing. Thesis: "Hydride affinities of unsaturated alkynes, alkenes and carbonyles – a rationalization using triadic formula" (11.2005)
- Lovorka Perić, Faculty of Science, University of Zagreb. Dipl. Ing. Thesis: "Computational design of some powerful hydride sponges" (11.2004.)

Work Experience

- ◆ Published **130 Current Contents papers** (2.811 citations, h-index = 30) and **2 book chapters**
- ◆ **Member of COST Action CA15135** "Multi-target paradigm for innovative ligand identification in the drug discovery process (MuTaLig)". Chair: Prof. Stefano Alcaro, Università Magna Graecia di Catanzaro, Italy (2016–2020)
- ◆ **Member of COST Action CM1103** "Structure-based drug design for diagnosis and treatment of neurological diseases: dissecting and modulating complex function in the monoaminergic systems of the brain". Chair: Dr. Rona Ramsay, University of St. Andrews, United Kingdom (2012–2015)
- ◆ **Guest–editor of the Special Issue** of *Croatica Chemica Acta* **2009**, *82* (1), 1–335 entitled "From Conceptual to Computational Chemistry and Back" dedicated to Prof. Zvonimir Maksić on the occasion of his 70th birthday
- ◆ **Member of Editorial boards** of *Chemistry in Industry* (from 2022), *Croatica Chemica Acta* (from 2010), *Frontiers in Chemical Biology* (from 2013), *Turkish Computational and Theoretical Chemistry* (from 2017) and *Advances in Chemistry* (2013–2017)
- ◆ **Member of the Selection Committee of the NEWFELPRO program** – new international fellowship mobility programme for experienced researchers in Croatia (from 2013)
- ◆ **Reviewer for projects** submitted to the *Estonian Science Foundation* and *Romanian Science Foundation*
- ◆ **Remote reviewer for projects** submitted to the *European Research Council* for the ERC Starting Grant and H2020-MSCA-IF-2019 call
- ◆ **Referee for papers under consideration for publication** in *Journal of Physical Chemistry*, *European Journal of Organic Chemistry*, *Journal of the American Chemical Society*, *Journal of Physical Organic Chemistry*, *Physical Chemistry Chemical Physics*, *New Journal of Chemistry*, *Chemistry – A European Journal*, *ChemPhysChem*, *ChemistrySelect*, *ACS Omega*, *Computational and Theoretical Chemistry*, *Central European Journal of Chemistry* and *Croatica Chemica Acta*
- ◆ **Member of the International Steering Committee:** "Central European Conference – Chemistry towards Biology" biennial series of conferences (from 2012)
- ◆ **Member of the Organizing Committee:** 28th Croatian meeting of chemists and chemical engineers (Rovinj, Croatia, 04.2023); Computational Chemistry Day series of conferences (3rd edition (09.2022); 2nd edition (05.2018); 1st edition (05.1027), Zagreb, Croatia); 25th Croatian meeting of chemists and chemical engineers (Poreč, Croatia, 04.2017); 5th Central European Conference – Chemistry towards Biology (Primošten, Croatia, 09.2010)
- ◆ **Chair** of the Croatian National Chapter within the Marie Curie Alumni Association (from 2014)
- ◆ **National Representative** in the "International Society for Theoretical Chemical Physics" (from 2013)

Selected Publications

1. M. Radović, L. Hok, M. Panić, M. Cvjetko Bubalo*, **R. Vianello***, M. Vinković, I. Radojčić Redovniković: "Deep eutectic solvents as a stabilising medium for NAD coenzyme: Unravelling the mechanism behind coenzyme stabilisation effect", *Green Chem.* **2022**, *24*, 7661.
2. E. Mehić, L. Hok, Q. Wang, I. Dokli, M. Svetec Miklenić, Z. Findrik Blažević, L. Tang, **R. Vianello***, M. Majerić Elenkov*: "Expanding the scope of enantioselective halohydrin dehalogenases – Group B", *Adv. Synth. Catal.* **2022**, *364*, 2576.
3. I. Boček, M. Hranjec*, **R. Vianello***: "Imidazo[4,5-*b*]pyridine derived iminocoumarins as potential pH probes: Synthesis, spectroscopic and computational studies of their protonation equilibria", *J. Mol. Liq.* **2022**, *355*, 118982.
4. L. Hok, H. Rimac, J. Mavri, **R. Vianello***: "COVID-19 infection and neurodegeneration: Computational evidence for interactions between the SARS-CoV-2 spike protein and monoamine oxidase enzymes", *Comput. Struct. Biotechnol. J.* **2022**, *20*, 1254.
5. N. Perin, L. Hok, A. Beč, L. Persoons, E. Vanstreels, D. Daelemans, **R. Vianello***, M. Hranjec*: "N-substituted benzimidazole acrylonitriles as *in vitro* tubulin polymerization inhibitors: synthesis, biological activity and computational analysis", *Eur. J. Med. Chem.* **2021**, *211*, 113003.
6. T. Tandarić, **R. Vianello***: "Computational insight into the mechanism of the irreversible inhibition of monoamine oxidase enzymes by the anti-parkinsonian propargylamine inhibitors rasagiline and selegiline", *ACS Chem. Neurosci.* **2019**, *10*, 3532.
7. A. Maršavelski, **R. Vianello***: "What a difference a methyl group makes - the selectivity of monoamine oxidase B towards histamine and N-methylhistamine", *Chem.–Eur. J.* **2017**, *23*, 2915.
8. T. Gregorić, M. Sedić*, P. Grbčić, A. Tomljenović Paravić, S. Kraljević Pavelić, M. Cetina, **R. Vianello***, S. Raić-Malić*: "Novel pyrimidine-2,4-dione-1,2,3-triazole and furo[2,3-*d*]pyrimidine-2-one-1,2,3-triazole hybrids as potential anti-cancer agents: Synthesis, computational and X-ray analysis and biological evaluation", *Eur. J. Med. Chem.* **2017**, *125*, 1247.
9. I. Despotović, **R. Vianello***: "Engineering exceptionally strong oxygen superbases with 1,8-diazanaphthalene di-N-oxides", *Chem. Commun.* **2014**, *50*, 10941.
10. Z. B. Maksić, B. Kovačević*, **R. Vianello***: "Advances in determining the absolute proton affinities of neutral organic molecules in the gas phase and their interpretation: a theoretical account", *Chem. Rev.* **2012**, *112*, 5240.