

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 with Tenure**, Ruđer Bošković Institute, Zagreb, Croatia (05.2023 – present)
- **FP7-IEF Marie Curie Fellow**, National Institute of Chemistry, Ljubljana, Slovenia. Host: Dr. Janez Mavri (10.2010 – 04.2012)
- **Senior Scientist** (07.2015 – 05.2023) • **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 (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.** (2019–2023)
- **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

- ◆ "Green, greener, *in silico!* The role of computational methods in chemistry and biochemistry"; **4th ZORH Convention on the Topic of Environmental Protection in the Republic of Croatia**; Split, Croatia, 04.2023
- ◆ "Green, greener, *in silico!* The role of computational methods in chemistry"; **1st Student Meeting on Sustainable Chemistry and Engineering (SKOKI)**; Zagreb, Croatia, 04.2023
- ◆ "Using computers to fight neurodegenerative diseases"; **5th Symposium of Chemistry Students (SISK)**; 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

- ◆ "With a little help from computer-aided drug design – new antitumor agents as tubulin polymerization inhibitors"; **10th World Conference on Physico-Chemical Methods in Drug Discovery & 6th World Conference on ADMET and DMPK**; Belgrade, Serbia, 09.2023
- ◆ "*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

- ◆ "On the shoulders of Giants"; **Science Festival 2022**; Rijeka, Croatia, 05.2022
- ◆ "10 most important molecules of the 20th century"; **Science Festival 2012**; Rijeka, Croatia, 04.2012
- ◆ "Chemistry – Our life, our future"; **Lecture for the 384th anniversary of the Sušak High School**; Rijeka, Croatia, 11.2011
- ◆ "From Maria Skłodowska Curie laboratory for a brighter future of mankind"; **Science Festival 2011**; Rijeka, Croatia, 04.2011
- ◆ "Computational design of new organic superacids"; **Student Section of the Croatian Chemical Society**; Zagreb, Croatia, 12.2008
- ◆ "With computational chemistry towards new extra-strong acids"; **Lecture for the 381st anniversary of the Sušak High School and the opening of a new chemical 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 (2018–2020)

Mentorship of Doctoral Students

- Lucija Vrban, Faculty of Science, University of Zagreb (2023–present)
- Lucija Hok, Faculty of Science, University of Zagreb (2019–2023). PhD Thesis: "Computational study on the effect of deuteration on the ligand binding to the adenosine A_{2A} receptor" (06.2023)
- Tana Tandarić, Faculty of Science, 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, Faculty of Science, 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, Faculty of Science, 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

- Aleks Logožar, Faculty of Science, University of Zagreb. Thesis: "Influence of the central donor atom on the stereochemistry of metal complexes with bis(2-pyridine-2-ylmethyl)amine and 2,2'-iminodiacetamide ligands" (09.2023)
- Lucija Vrban, Faculty of Biotechnology and Drug Development, University of Rijeka. Thesis: "Computational study of the monoamine oxidase B mechanism-based irreversible inhibitors" (09.2022)
- Dalibor Hršak, Faculty of Science, University of Zagreb. Thesis: "Interpretation of basicity and acidity of bases of nucleic acids using triadic formula" (05.2010)
- Jelena Stojaković, Faculty of Science, University of Zagreb. Thesis: "Proton affinities of carbenes in the gas-phase" (12.2007)
- Nena Peran, Faculty of Science, University of Zagreb. Thesis: "Hydride affinities of unsaturated alkynes, alkenes and carbonyles – a rationalization using triadic formula" (11.2005)
- Lovorka Perić, Faculty of Science, University of Zagreb. Thesis: "Computational design of some powerful hydride sponges" (11.2004.)

Work Experience

- ◆ Published **136 Web of Science papers** (3.250 citations, h-index = 32) 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 (together with Dr. Davor Margetić)
- ◆ **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 (4th edition (09.2023); 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)
- ◆ **Member of the Expert Panel** for the evaluation of projects submitted to the Croatian Science Foundation (from 2023; 2016–2020)
- ◆ **Member of the Steering Committee** for the management, coordination and successful implementation of the Cooperation Programme with Croatian Scientists in Diaspora "Research Cooperability" of the Croatian Science Foundation (from 2018)
- ◆ **Member of the Ethical Committee** of the Croatian Science Foundation (2018–2021)
- ◆ **Member of the Expert Committee** for the Abbvie–Croatian Croatian Science Foundation Award for young scientist in the field of pharmacy (2013–2015)
- ◆ **Member** of the Croatian Chemical Society (from 2001), Croatian Society for Theoretical and Mathematical Biology (from 2003), Croatian Society of Chemical Engineers (from 2006), Croatian Humboldt Club (from

Selected Publications (01.2024)

1. A. Beč, **R. Vianello***, M. Hranjec*: "Synthesis and spectroscopic characterization of multifunctional D- π -A benzimidazole derivatives as potential pH sensors", *Journal of Molecular Liquids* **2023**, 386, 122493.
2. L. Hok, **R. Vianello***: "Selective deuteration improves the affinity of adenosine A_{2A} receptor ligands: A computational case study with istradefylline and caffeine", *Journal of Chemical Information and Modeling* **2023**, 63, 3138–3149.
3. I. Boček, L. Hok, L. Persoons, D. Daelemans, **R. Vianello***, M. Hranjec*: "Imidazo[4,5-*b*]pyridine derived tubulin polymerization inhibitors: Design, synthesis, biological activity *in vitro* and computational analysis", *Bioorganic Chemistry* **2022**, 127, 106032.
4. 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.
5. 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", *Advanced Synthesis & Catalysis* **2022**, 364, 2576–2588, **cover page article**.
6. 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.
7. 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.
8. 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.
9. 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.
10. 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.
11. 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.
12. M. Pavlin, M. Repič, **R. Vianello***, J. Mavri*: "The chemistry of neurodegeneration: kinetic data and their implications", *Molecular Neurobiology* **2016**, 53, 3400–3415.
13. I. Despotović, **R. Vianello***: "Engineering exceptionally strong oxygen superbases with 1,8-diazanaphthalene di-*N*-oxides", *Chem. Commun.* **2014**, 50, 10941.
14. **R. Vianello***, M. Repič, J. Mavri: "How are biogenic amines metabolized by monoamine oxidases?", *European Journal of Organic Chemistry* **2012**, 7057–7065, **cover page article**.
15. 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.