

Dr. Robert Vianello

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Personal Data

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

Citizenship: Croatian

Work Positions

- 03/2016 – present **Group Leader**, Ruđer Bošković Institute, Zagreb, Croatia
- 07/2015 – present **Senior Scientist**, Ruđer Bošković Institute, Zagreb, Croatia
- 10/2010 – 04/2012 **FP7-IEF Marie Curie Fellow**, National Institute of Chemistry, Ljubljana, Slovenia. Host: Dr. Janez Mavri
- 04/2010 – 10/2010 **Croatian Science Foundation Fellow**, National Institute of Chemistry, Slovenia. Host: Dr. Janez Mavri
- 10/2009 – 07/2015 **Senior Research Associate**, Ruđer Bošković Institute, Zagreb, Croatia
- 06/2005 – 10/2009 **Research Associate**, Ruđer Bošković Institute, Zagreb, Croatia
- 01/2005 – 03/2005 **Alexander von Humboldt Postdoctoral Fellow**, Institute of Organic Chemistry, University of Heidelberg, Germany. Host: Prof. Rolf Gleiter
- 03/2004 – 06/2005 **Senior Research Assistant**, Ruđer Bošković Institute, Zagreb, Croatia
- 12/2000 – 03/2004 **Research Assistant**, Ruđer Bošković Institute, Zagreb, Croatia

Education

- 11/2003 **PhD in Natural Sciences**, University of Zagreb, Croatia. Thesis: "Interaction of Lewis Acids and Bases". Supervisor: Prof. Zvonimir Maksić
- 11/2000 **Dipl. Ing. in Chemistry**, Faculty of Science, University of Zagreb, Croatia. Thesis: "Proton Affinities of Some Guanidine Derivatives".
- 1996–2000 **Chemistry study**, Faculty of Science, University of Zagreb, Croatia
- 1992–1996 **The Sušak High School**, Rijeka, Croatia
- 1984–1992 **Primary School**, Rijeka, Croatia

Awards and Honours

- Feb 2018 **2017 Branimir Jernej Foundation Award** – Annual award for a publication in the fields of molecular biology, neurosciences and biomedicine published in 2017
- Dec 2017 **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
- Dec 2015 **2015 Ruđer Bošković Institute Director General Award** for the scientific publication with high impact factor
- Jun 2013 **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
- Dec 2012 **2012 Ruđer Bošković Institute Director General Award** for the scientific publication with high impact factor
- Apr 2012 **Marie Curie Success Story**, presentation of research results in the European Commission's publication "EU FP7 People Specific Programme Success Stories Booklet"
- Dec 2010 **50,000th Marie Curie Fellowship Award** – An honour given by the European Commission to 25 current FP7 Marie Curie Fellows
- Dec 2010 **2010 Ruđer Bošković Institute Director General Award** for high funded scientific project
- Sep 2010 **Promising Scientist Prize** of the Centre for the Applied Quantum Mechanics in Paris, France

- May 2008 **2008 Award of the Croatian Academy of Sciences and Arts** for the development of scientific and artistic work
- Nov 2007 **2006 Leopold Ružička Award** of the Croatian Chemical Society for young scientists
- Jun 2006 **2005 Croatian National Science Award** – Annual award for junior researchers awarded by the Croatian Parliament and the Croatian Ministry of Science, Education and Sports
- Dec 2004 **2004 Award by the Society of University Teachers and other Scientists in Zagreb** for the work in chemistry published in *Chem. Eur. J.* **2004**, *10*, 5751–5761
- Apr 2004 **2004 City of Rijeka's Public Award** – Annual award for the creative work and achievements in chemistry
- Dec 1995 **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
- 1993–2000 **Scholar of the City of Rijeka**

Grants and Fellowships

- 2015–2019 **Research Grant from the Croatian Science Foundation**. Total financial value: 133.000 EUR (excluding salaries).
- 2013–2017 **Marie Curie Career Integration Grant** (FP7–PEOPLE–2012–CIG call) for 48 months of reintegration phase at the Ruđer Bošković Institute in Zagreb (Croatia). Total financial value: 100.000 EUR (excluding salaries).
- 2011–2014 **Research Grant from the Croatian Ministry of Science, Education and Sports**. Total financial value: 46.000 EUR (excluding salaries).
- 2010–2012 **Marie Curie Individual Fellowship for Career Development** (FP7–PEOPLE–2009–IEF call) for an 18 months stay at the National Institute of Chemistry in Ljubljana (Slovenia). Total financial value: 99.127,60 EUR.
- 2010 **Stipend from the Croatian Science Foundation** for a 6 months stay at the National Institute of Chemistry in Ljubljana (Slovenia). Total financial value: 11.000 EUR.
- 2008–2010 **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. Total financial value: 35.000 EUR (excluding salaries).
- 2009–2010 **Bilateral Croatia–Slovenia project**. Partner: Dr. Jernej Stare, National Institute of Chemistry, Ljubljana, Slovenia.
- 2008–2009 **Bilateral Croatia–Austria project**. Partner: Prof. Robert Konrat, Max F. Perutz Laboratories, Department of Biomolecular Structural Chemistry, University of Vienna, Austria.
- 2005 **Alexander von Humboldt Postdoctoral Fellowship** for a 3 months stay at the University of Heidelberg (Germany) in the group of Prof. Rolf Gleiter

Participation at Conferences and Events

Plenary Lectures

- ♦ "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

- ♦ "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
- ♦ "Mechanistic studies of monoamine oxidases"; **International Summer School: Molecular Simulation for Neurological Targets**; University of Ljubljana, Slovenia, 08/2015
- ♦ "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
- ◆ "Computational prediction of new extremely acidic superacids awaiting experimental synthesis"; **21st Croatian Meeting of Chemists and Chemical Engineers**; Trogir, Croatia, 04/2009
- ◆ "Interpretation of the intrinsic molecular reactivity using triadic formula"; **2nd Opatija Meeting on Computational Solutions in Life Sciences**; Opatija, Croatia, 09/2007
- ◆ "Prediction of new organic superacids by computational chemistry"; **2006 Marie Curie workshop in Croatia and Serbia commemorating 150th anniversary of the birth of Nikola Tesla**; Zagreb, Belgrade, 10/2006
- ◆ "Design of neutral organic superacids"; **Institute of Organic Chemistry**, University of Heidelberg, Germany, 02/2005
- ◆ "The structure and acidity of 20 α -amino acids"; **2nd Central European Conference – Chemistry towards Biology**; Seggau, Austria, 09/2004

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
- ◆ Lectures at **COST Action CM1103 meetings** in Brussels, Belgium (02/2012); Lisbon, Portugal (04/2012); Madrid, Spain (11/2012); Smolenice, Slovakia (04/2014); Belgrade, Serbia (05/2015)

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 the 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 Postgraduate Students

<i>ongoing</i>	Tana Tandarić, University of Zagreb, in progress
<i>Jul 2017</i>	Aleksandra Maršavelski, PhD Thesis: "Computational investigation of the catalytic activity and selectivity of amine oxidases towards histamine and <i>N</i> -methylhistamine", University of Zagreb
<i>Dec 2010</i>	Nena Peran, PhD Thesis: "Computational study of acid–base properties of α -amino acids in water solutions", University of Zagreb (co-supervisor with Prof. Zvonimir Maksić)

Supervision of Undergraduate Students

<i>May 2010</i>	Dalibor Hršak, Dipl. Ing. Thesis: "Interpretation of basicity and acidity of bases of nucleic acids using triadic formula", Faculty of Science, University of Zagreb
<i>Dec 2007</i>	Jelena Stojaković, Dipl. Ing. Thesis: "Proton affinities of carbenes in the gas–phase", Faculty of Science, University of Zagreb
<i>Nov 2005</i>	Nena Peran, Dipl. Ing. Thesis: "Hydride affinities of unsaturated alkynes, alkenes and carbonyles – a rationalization using triadic formula", Faculty of Science, University of Zagreb
<i>Nov 2004</i>	Lovorka Perić, Dipl. Ing. Thesis: "Computational design of some powerful hydride sponges", Faculty of Science, University of Zagreb

Work Experience

- ◆ Published **80 scientific papers** in journals cited in the *Current Contents* database (1.500 citations, h-index = 23)
- ◆ **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 *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*
- ◆ **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*, *Chemical Physics Letters*, *ChemPhysChem*, *Physical Chemistry Chemical Physics*, *Computational and Theoretical Chemistry*, *Central European Journal of Chemistry*, *Journal of Molecular Modelling*, *Acta Chimica Slovenica* and *Croatica Chemica Acta*
- ◆ **Member of the International Steering Committee** of the "Central European Conference – Chemistry towards Biology" biennial series of conferences (from 2012)
- ◆ **Member of the Organizing Committee** of the 5th Central European Conference – Chemistry towards Biology (Primošten, Croatia, 08–11 Sep 2010) and the 25th Croatian meeting of chemists and chemical engineers (Poreč, Croatia, 19–22 Apr 2017)
- ◆ **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 Croatian Chemical Society** (from 2001), **Croatian Society of Theoretical and Mathematical Biology** (from 2003) and **Croatian Society of Chemical Engineers** (from 2006)

Selected Recent Publications

1. N. Perin, P. Roškarić, I. Sović, I. Boček, K. Starčević, M. Hranjec*, **R. Vianello***: "Amino substituted benzamide derivatives as promising antioxidant agents: A combined experimental and computational study", *Chemical Research in Toxicology* **2018**, *31*, 974–984.
2. I. Leščić Ašler, Z. Štefanić*, A. Maršavelski, **R. Vianello***, B. Kojić-Prodić: "The catalytic dyad in the SGNH hydrolase superfamily: in-depth insight into structural parameters tuning catalytic process of extracellular lipase from *Streptomyces rimosus*", *ACS Chemical Biology* **2017**, *12*, 1928–1936.
3. A. Maršavelski, **R. Vianello***: "What a difference a methyl group makes - the selectivity of monoamine oxidase B towards histamine and *N*-methylhistamine", *Chemistry – A European Journal* **2017**, *23*, 2915–2925.
4. 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*, 1247–1267.
5. **R. Vianello***, C. Domene, J. Mavri: "The use of multiscale molecular simulations in understanding a relationship between the structure and function of biological systems of the brain: The application to monoamine oxidase enzymes", *Frontiers in Neuroscience* **2016**, *10*, 327.
6. M. Pavlin, M. Repič, **R. Vianello***, J. Mavri*: "The chemistry of neurodegeneration: kinetic data and their implications", *Molecular Neurobiology* **2016**, *53*, 3400–3415.
7. D. Saftić, **R. Vianello***, B. Žinić*: "5-Triazolyluracils and their *N*¹-sulfonyl derivatives: intriguing reactivity differences in the sulfonation of triazole *N*¹-substituted and *N*¹-unsubstituted uracil molecules", *Eur. J. Org. Chem.* **2015**, *35*, 7695–7704.
8. I. Despotović, **R. Vianello***: "Engineering exceptionally strong oxygen superbases with 1,8-diazanaphthalene di-*N*-oxides", *Chem. Commun.* **2014**, *50*, 10941–10944.
9. **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**.
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", *Chemical Reviews* **2012**, *112*, 5240–5270.