

Curriculum Vitae prof. dr. Sanja Tomić,

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work experience (chronologically*)

- Date (from – until) From 2014
Institution Ruđer Bošković Institute, Division of Organic Chemistry and Biochemistry
Position Senior scientist with permanent position, head of Laboratory for Protein Biochemistry and Molecular Modelling
Work field Computational (theoretical) biophysics and biochemistry
- Date (from – until) 2013-2014
Institution Ruđer Bošković Institute, Division of Physical Chemistry
Position Senior scientist with permanent position, leads computational group in Laboratory for chemical and biological crystallography
Work field Research in the field of theoretical biophysics, biochemistry
- Date (from – until) 2008-2013
Institution Ruđer Bošković Institute, Division of Physical Chemistry
Position Senior scientist, leads computational group in Laboratory for chemical and biological crystallography
Work field Research in the field of theoretical biophysics, biochemistry
- Date (from – until) 2003-2008
Institution Ruđer Bošković Institute, Division of Physical Chemistry
Position Senior research associate
Work field Research in the field of theoretical biophysics, biochemistry
- Date (from – until) 1999-2003
Institution Ruđer Bošković Institute, Division of Physical Chemistry
Position Research associate
Work field Research in the field of theoretical biophysics, biochemistry
- Date (from – until) 1993-1999
Institution Ruđer Bošković Institute, Division of Physical Chemistry
Position Higher assistant
Work field Laboratory research, crystallography and computational chemistry
- Date (from – until) 1989-1993
Institution Ruđer Bošković Institute, Division of Physical Chemistry
Position PhD student
Work field Research in the field of crystallography and computational chemistry, assistantship in the course of general physics
- Date (from – until) 1989-1993
Institution Ruđer Bošković Institute, Division of Physical Chemistry
Position PhD student
Work field Crystallography and computational chemistry, assistantship in the course of
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general physics

Date (from – until) 1982-1986
Institution Ruđer Bošković Institute, Department of Experimental Physics
Position PhD student
Work field Research in the field of atomic and nuclear physics

Education

Qualification awarded Ph.D. in natural sciences (chemistry).
Year and institution 1993. Ruđer Bošković Institute, University of Zagreb, Croatia

Qualification awarded M.Sc. in natural sciences (nuclear physics)
Year and institution 1986. Faculty of Natural Sciences and Mathematics (Department of Physics), University of Zagreb, Croatia

Qualification awarded Engineer in physics (with diploma)
Year and institution 1982. Faculty of Natural Sciences and Mathematics (Department of Physics), University of Zagreb, Zagreb, Croatia

Training

Year 1996-1998.
Place and institution *Heidelberg, Germany, EMBL, Alexander von Humboldt fellowship*
Subject and skills covered *Computational molecular biophysics and chemistry*

Year 1991.
Place and institution *Utrecht, The Netherlands, Rijkuniversiteit, Laboratory of Crystal and Structural Chemistry, NUFFIC fellowship*
Subject and skills covered *Crystallography and molecular modelling*

Languages

MOTHER TONGUE Croatian

FOREIGN LANGUAGES

English fluent

German basic

PUBLICATIONS

Author of 6 book chapters and 95 research papers published in international journals and 5 educational publications. Citations: > 1100 (WoS).

Projects since 2003

Coordinator

2002. – 2004. bilateral project with Germany (R.C. Wade), 'Vorhersagen zur Selectivität, Regulierung und Inhibition von Enzymen durch COMBINE Analyse',

2002. – 2003. bilateral project with Austria (M. Ramek), 'Combined *ab initio*, molecular mechanics, molecular dynamics and QSAR approach to plant hormone auxins'.

2004. – 2005. bilateral project with Austria (M. Ramek), 'Combined application of quantum mechanics and molecular mechanics methods in study of molecules important in biology and biotechnology'.

2005. – 2006. bilateral project with Slovenia (D. Janežič) 'Computational simulations of protein structure and dynamics'.

2007. – 2008. bilateral project with Slovenia (D. Janežič) 'Study of protein structure and dynamics by computational methods '.

'Proučavanje strukture i dinamike proteina računalnim metodama'.

2008. – 2010. bilateral project with Austria (Grit Daniele Stragaz), 'Reactivity of metal centres in proteins - theoretical study '.

2009 – 2010. bilateral project with Slovenia (Milan Hodošček), 'Theoretical study of reactivity of metal centers in proteins'

2007 – 2013. MZOŠ project 'Computational study of bio-macromolecules and development of new algorithms' (098-1191344-2860)

2012 – 2015 'Alexander von Humboldt, Research Group Linkage' programm: 'Study of plant enzymes from metallopeptidase families M20 and M49'

2014 – 2017 HRZZ project: 'Flexibility, activity and structure correlations in the dipeptidyl peptidase III family' (01.07.2014-30.06.2017)

2016 – 2017 Bilateral project with Austria (Karl Gruber, TU, Graz), 'An Interdisciplinary Study on Atypical Dipeptidyl Peptidases III (DPPs III) Structure and Dynamics '.

2018 – 2022 HRZZ project: 'Biological relevance of dipeptidyl peptidase III and its impact on human health' (IP-2018-01-2936)

Participant

2007. – 2009. Work package leader at the FP6 project 'Reinforcement of the Centre for Computational Solutions in the Life Sciences' (coordinator David Smith)

2011.–2012. Cogito bilateral project with France (coordinator M. Hranjec)

2010. QCM-2010-2-0027, bilateral project with Spain (coordinator M. Perez Gonzalez, University of Barcelona)

2013-2016: FP7-REGPOT-2012-2013-1 'Enhancement of the Innovation Potential in SEE through new Molecular Solutions in Research and Development' (EUR 4,738,978).

Invited lectures at international conferences and on internationally recognized scientific institutions since 2005.

Regional Biophysics Meeting 2005, 16.-20. 03. 2005. Terme Zreče, Slovenia, '*Computer modelling of complex bio-systems*' ,

Third Humboldt Conference on Computational Chemistry', 1.-5. 09. 2006., Varna, Bulgaria, '*Study of protein specificity and selectivity by computational methods*' ,

Humboldt Conference on Noncovalent Interactions', 15.-17. 11. 2007., Vršac, Srbija, '*Non covalent interactions in protein complexes*' ,

29. 11, 2007. SISSA (Scuola Internaz. Superiore di Studi Avanzati), Trst, Italy (invitation of Prof. P. Carloni) '*Macromolecules and their complexes, structure, dynamics, reactions*'.

2008 Summer School 15.–17. 12. 2011. Institute for Theoretical Studies, Heidelberg, Germany, '*Metallo enzymes: Insights into Ligand Binding and Protein Dynamics*'.

3.–7. 9. 2012, Regional Biophysical Conference, Kladovo, Srbija, '*Molecular modeling of nucleic acid - small molecule interactions*'.

24.10.2013. Croatian Academy of Science, Zagreb, Croatia, '*Nobel prize in Chemistry 2013*'

13. - 21. 05. 2014. Karolinska Institutu, Huddinge, Sweden, '*A few stories about metal ions in biomacromolecules*'

23.07.2014. MOLECULAR MODELLING WORKSHOP '*Comparative modeling of proteins and MD simulations*'

09. 10. 2014. Chatolic University of Chile, Chemical Faculty, Santiago de Chile, '*Metaloenzymes*'

Faculty for Natural Sciences and Mathematics, University of Zagreb, 12.05.2015.

'*Flexible molecules - how to determine the bioactive conformation?*'

23.01.2015, TU-Graz, DPP III Minisymposium, '*Zn coordination in the active site of DPP III, substrate binding and long-range conformational motion – a new exhaustive study*'

24. 09. 2015 Karolinska Institutu, Huddinge, Sweden, 'Long range fluctuations of human DPP III – influence of ligand binding'

Regional Biophysics Conference 25-28 08 2016, Trieste, Italy

'Understanding substrate recognition and function of human dipeptidyl peptidase III'

10. 02. 2017, TU-Graz, DPP III Minisymposium, 'Understanding hDPP III,

Mechanism – an aid in rationalization of the mutants (in)activity'

12. 05. 2018., Chemistry Day, PMF, University of Zagreb, 'Computational studies as an aid to the experiments in revealing the secrets of biomacromolecules'.

18-23.06.2018. Math/Chem/Comp 2018, Dubrovnik, 'Computer Aided Design of Biomacromolecular Systems' - Workshop.

Lectures at international conferences since 2005.

16th CRO-SLO CRYST MEETING, 13.–17. 06 2007. Petričani, Croatia, 'Divalent metal cations in proteins: abundance, coordination, function',

4th Central European Symposium on Theoretical Chemistry, 22.–27. 09. 2007. Litschau, Austria, 'The protein-protein interactions- molecular modelling study'.

13th Hellenic Symposium on Medicinal Chemistry, 12.–16. 03. 2008. Athens, Greece, 'Towards understanding enantio-selective enzyme catalysed chemical transformation of pro-drugs'

ESF-EMBO symposium PROTEIN DESIGN and Evolution for Biocatalysis, 25.–30. 10. 2008., Sant Fellu de Guixols, Spain, 'Combined 3D QSAR and QM/MM Study of the Burkholderia cepacia Lipase Enantioselectivity'

WATOC 2011, 17.–22. 7. 2011., Santiago de Compostelo, Spain, 'Step Forward in Understanding Mechanism of Non-heme Fe²⁺ Dependent Dioxygenase Dke1 Catalysis'.

20 Years of Croatian Crystallographic Association 25.01.2012. Croatian Academy of Science 'In Silico Enzyme Design and Screening' meeting, 7.–9. 5. 2012., Trst, Italy, 'Molecular dynamics based studies on human DPP III revealed determinants for its broad substrate selectivity'

6th Central European Conference "Chemistry towards Biology", 10.-13.09.2013, Trieste, Italy, 'Elucidation of metal – binding sites in proteins' i s posterom 'understanding transport of iron cation in acetylacetone dioxygenase from Acinetobacter johnsoii',

International Conference on Biochemistry and Molecular Biology, 26-29.04.2016, Venice, Italy, 'Influence of ligands and protein binding to structure and flexibility of human dipeptidyl peptidase III'

Organizational skills and competences since 2005.

Organizer of 4 international conferences and program organizer of International School of Biophysics:

1st South Eastern European Workshop on Practical Approaches to Computational Biology, Opatija, Croatia, 1 - 4, 09. 2005.

The 2nd Opatija Meeting on Computational Solutions in the Life Sciences, Opatija, Croatia, 4 -9 09. 2007.

The 3rd Adriatic Meeting On Computational Solutions in the Life Sciences, Primošten, Croatia, 1 - 5 09. 2009.

5th Central European Conference - Chemistry towards Biology, Primošten, Croatia, 8 - 11 09. 2010.

11th Greta Pifat-Mrzljak International School of Biophysics: Biomacromolecular complexes and assemblies, Primošten, Croatia, 30.09 - 09.10.2012.

DPP III Minisymposium, Zagreb March 21st 2016.

Reviewer in more than 10 international journals, like *J. Chem. Inf Mod.*, *J. Comp. Aid. Mol. Design*, *J. Mol. Catalysis B, Enzymatic*, *J Mol. Structure, Proteins*, *Croatica Chem. Acta*, *J.*

Inor. Biochem, Trends Biotech., BBA Newsletter, Protein Eng. Des. Selection, Int. J of Quant. Chem., FEBS, BMC Struct. Biol.,...

Awards

1991-1992. NUFFIC fellowship, Rijkuniversiteit, Utrecht, Netherland

1996-1998 Alexander von Humboldt research fellowship

2012. Ruđer Bošković Institute award for scientific publication

Academic Teaching

Since 2013 titular professor at University of Rijeka

Since 2011 titular professor at University of Zagreb

Practical exercises in physics (1986/87), exercises in physics (1988-1990), exercises in biophysics (1994/95) University of Zagreb

Since 2003. Lecturer of the new subject ('Molecular modeling of biomacromolecules') at Postgraduate study in biophysics (University of Zagreb)

Current classes

"Biomacromolecules Crystallography and Modeling" (Luić, Tomić,) Faculty of Natural Sciences and Mathematics, at University of Zagreb, Graduate study, "Molecular modelling of biomacromolecules" (Faculty of Natural Sciences and Mathematics, at University of Zagreb, University of Split and University of Osijek, PhD studies in Biochemistry & Biophysics, "Computational Chemistry" at University of Rijeka, Department for Biotechnology, Doctorate study)

Mentorship of doctoral dissertations - defended

Branimir Bertoša, University of Zagreb, 2008.

Krešimir Šikić, University of Zagreb, 2008.

Dejan Agić, (comentor with dr. sc. M. Abramić) University of Zagreb 2012.

Hrvoje Brkić, University of Zagreb, 2014.

Marina Grabar Branilović, University of Zagreb, 2014.

Antonija Tomić, University of Zagreb, 2015.

Marko Tomin, University of Zagreb, 2018.

Mentorship of doctoral dissertations – current

Mirsada Čehić (comentor with Ivo Piantanida), University of Zagreb

Sara Matić, University of Zagreb

Mario Gundić, University of Zagreb

Mentor of four diploma students (Igor Ceilinger, Mijo Šimunović, Ivan Dokmanić, Nora Tir, Ivana Čavka)

Commissions, committees, boards and work groups

Member of the scientific panel for Natural sciences of the Croatian Ministry of Science (2014-2016)

President of Croatian Biophysical society, 2010-2013.

Member of the international QSAR society, EBSA, Croatian Physical society, Croatian Chemical Society, Croatian Crystallographic Society, member of the Central European Conference 'Chemistry Towards Biology' Steering committee (2010, 2013, 2014), member of the Regional Biophysical meeting Steering committee (2014), member of Croatian Humboldt club.