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[Bibliography \(COBISS\)](#)

Mathematical or computer modeling of natural phenomena, and chemistry in particular, challenged many great spirits. Let us see what [big shots](#) think about it.

Currently I am head of the Laboratory for Biocomputing and Bioinformatics at the National Institute of Chemistry. Our research is oriented toward understanding the systems of biological interest on molecular level. In particular we are interested in chemical reactions in solution and enzymes, hydrogen bonding, nuclear quantum effects, transport phenomena and receptor triggering. Drug design, chemical reactions relevant for carcinogenesis and computational support of pharmacology are direct applications. Currently design of novel girase inhibitors and complexation of oral diabetics are ongoing projects in the direction of drug design. Bioinformatics is a complementary direction of research in our laboratory. Computer simulation is the main research tool used in our laboratory. In addition, we are using vibrational spectroscopy, NMR spectroscopy, surface plasmonic resonance. Synthesis and testing of novel compounds is in collaboration with the Faculty of Pharmacy, University of Ljubljana. Pharmacological research is done in collaboration with the Institute of Pharmacology and Experimental Toxicology, Faculty of Medicine, University of Ljubljana.

Education

- B.Sci., 1987, Faculty of Chemistry, University of Ljubljana, Slovenia
- M.Sci., 1989, Ab-initio Calculations of Intramolecular Hydrogen Bonding and Proton Potentials in Hydrogen Malonate, Faculty of Chemistry, University of Ljubljana.
- Ph.D., 1992, Computer Simulations of Molecular Interactions in Biological Systems, University of Ljubljana.

Positions

- 1987- National Institute of Chemistry, Ljubljana, Slovenia
- 1989 spent four months in the group of Prof. Herman J.C. Berendsen and Prof. Wilfred F. van Gunsteren, Department of Biophysical Chemistry, University of Groningen, The Netherlands.
- 1991-1992 spent five months in the group of Prof. Herman J.C. Berendsen in Groningen.
- May, June 1993 joined the group of Prof. Hans Vogel, Department of Biochemistry, University of Calgary, Canada.
- November 1993- November 1995 joined the group of Prof. Herman J.C. Berendsen in Groningen.
- December 1995, joined the group of Prof. Hans Vogel, Department of Biochemistry, University of Calgary, Canada.
- October-December 2003, Visiting professor, Department of Molecular Physics, University of Franche-Comte, Besancon, France.
- September-November 2004, Fulbright Scholar with Arieh Warshel, Department of Chemistry, University of Southern California, Los Angeles.
- January 1996 - , Researcher at the National Institute of Chemistry, Ljubljana, Slovenia.

Teaching

- Undergraduate course: Chemical Dynamics, 1995 University of Groningen, the Netherlands
- Summer School, Training Course on Molecular Modeling and Computer Assisted Combinatorial Chemistry, organized by ICS-UNIDO, Trieste, Italy, one week every year 1998-.
- Graduate course: Computer Aided Drug Design, Faculty of Pharmacy, University of Ljubljana, Slovenia 2003-present.

Other Professional Activities

- Meeting of Decision Makers from Academia, Chemical and Pharmaceutical Industry on the Relevance of Combinatorial Chemistry and Molecular Modeling, June 26-27, 2000, Bled, Slovenia (organizer together with Prof. S. Miertus)
- Training Course on Molecular Modeling and Computer Assisted Combinatorial Chemistry, June 28-July 2, 2000, Ljubljana, Slovenia (organizer together with Prof. S. Miertus)
- Workshop, Statistical Mechanics, August 27 - September 2, 2000, Bled Slovenia, (organizer together with Prof. B. Borštnik)

Honors

- Long Term Human Frontier Science Program Fellowship 1993-1995.
- Fulbright Scholarship, University of Southern California, September-November 2004
- Lecture at the Gordon Research Conference Isotopes in Biological and Chemical Sciences, Ventura, CA, 2/2