

**prof. RNDr. Jaroslav Koča, DrSc.**  
CEITEC, Scientific Director for Life Sciences

### **Education**

1993 - D. Sc. (DrSc.) - Masaryk University, Brno (Chemistry)  
1983 - Ph. D. (CSc.) - Komensky University, Bratislava, Slovakia (Chemistry)  
1979 - M.S. (RNDr.) - Purkyně University, Brno (Mathematics and Chemistry)

### **Employment**

1995 - Full Professor  
1988 - 1995 : Associate Professor  
1983 - 1988 : Assistant Professor  
Faculty member in Undergraduate and Graduate Program in Organic, Mathematical and Computer Assisted Chemistry, Education in Chemistry, Information Technology in Chemistry, Modeling in Biochemistry and Environmental Science, Chemoinformatics and Bioinformatics, 22 Diplom-students, 25 PhD students.

### **Research interests**

Mathematical and computer assisted chemistry and biochemistry, computer assisted molecular modeling of biologically interesting chemical species, information technology in chemistry and biochemistry. Last years mainly conformational search, molecular docking and molecular dynamics simulations on peptides, proteins, oligonucleotides, carbohydrates, and their complexes. Methods for analysis conformational potential energy surfaces and energy landscapes of chemical reactions using molecular mechanics and quantum chemistry techniques.

### **Publications**

6 monographs, 1 textbook, over 120 journal full text papers, several computer programs and program systems ; WOS citations > 900 (autocitations excluded), H-index: 24

### **Management experience**

One year (1994/95) Head of Chemistry Department, Fac Sci (approx. 70 employees]. In 1996, he established and become a head (1996-2000) of Laboratory of Biomolecular Structure and Dynamics (about 25 people), yearly budget of about 0.2 mil. EURO. In 2001, he founded National Centre for Biomolecular Research and became director (up to now, these days about 100 people), yearly budget more than 3 mil. EURO. Principal investigator of several national and international grants, one of the most successful in FP7 is the project POSTBIOMIN, budget over 1 mil. EURO.

### **Further university and academic service:**

- Czech representative in Program Committee "Ideas" of 7th FP (2006- )
- Pool of Experts to evaluate scientific proposals, European Commission FP6, FP7, Brussels (2004-)
- Member of national D.Sc. defense boards in organic chemistry and physical chemistry
- Member of Scientific Boards: Masaryk University (MU) (1998-9, 2006- ), Faculty of Science MU (1997-9, 2003- ), Faculty of Informatics MU (1995- )
- Member of national commission that is taking decisions about accreditation of university curricula in Chemistry (2000- )
- Member of Doctoral Study Boards: organic chemistry, physical chemistry, biochemistry, biophysics, biomolecular chemistry; State examination commissions on undergraduate or doctoral level-chairman: education in chemistry, biomolecular chemistry
- Board of Directors, Czech Chemical Society (2001-); National committee of the Czech Chemical Society (2001- ); Chairman of the Brno branch of the Czech Chemical Society (1997 - )

### Faculty development

2002-2003 (CERMAV Grenoble, France – 6 months visiting professor (VP)), 1999-00 (Pacific Northwest National Laboratory, Richland, WA, USA - 1 year VP), 1998 (Univ. Grenoble, France – 3 months VP), 1996 (Univ. Athens, Greece - 2 months VP), 1993 (Univ. Nantes, France – 4 months VP), 1993 (Univ. of Tennessee, Knoxville, USA – 2 months visiting researcher (VR)), 1992 (Univ. Trondheim, Norway - 1 month VR), 1991 (Univ. Rennes, France - 1 month - teaching doctoral course), 1991 (Univ. Trondheim, Norway - 3 months VP), 1988-90 (Univ. Trondheim, Norway - 2 years NTNF postdoctoral fellow), 1985 (Institute of Cybernetics and Information Processes, Berlin, Germany - 1 month – research stay).

### Selected publications

- [1] Koca J.: Potential Energy Hypersurface and Molecular Flexibility. *J.Mol.Struct.* 291, 255-269 (1993)
- [2] Koca J., Perez S., Imberty A.: Conformational Analysis and Flexibility of Carbohydrates using the CICADA approach with MM3. *J.Comput.Chem.* 16, 296-310 (1995)
- [3] Stefl R., Koca J.: Unrestrained Molecular Dynamics Simulations of d(AT5)2 Duplex in Aqueous Solution: Hydration and Sodium Ions Binding in the Minor Groove. *J. Am. Chem. Soc.* 122, 5025-5033 (2000)
- [4] Koca J., Zhan Ch-G., Rittenhouse R.C., Ornstein R.: Mobility of the Active Site bound Paraoxon and Sarin in Zinc-Phosphotriesterase by Molecular Dynamics Simulation and Quantum Chemical Calculation. *J. Am. Chem. Soc.* 123, 817-826 (2001).
- [5] Kulhanek P., Schlag E.W., Koca J.: A Novel Mechanism of Proton Transfer in Protonated Peptides. *J. Am. Chem. Soc.* 125, 13678-13679 (2003)
- [6] Koca J., Zhan, Ch-G., Rittenhouse R., Ornstein R.: Coordination Number of Zinc Ions in the Phosphotriesterase Active Site by Molecular Dynamics and Quantum Mechanics. *J. Comput. Chem.* 24, 368-378 (2003)
- [7] Petrek, M., Otyepka, M., Banas, P., Kosinova, P., Koca, J., Damborsky, J.: CAVER: A New Tool to Explore Routes from Protein Clefts, Pockets and Cavities. *BMC Bioinformatics* 7, 316-324 (2006)
- [8] Otyepka M., Bartova I., Kriz Z., Koca J.: Different Mechanisms of CDK5 and CDK2 Activation as Revealed by CDK5/P25 and CDK2/CYCLIN A Dynamics . *J. Biol. Chem.* 281, 7271-7281 (2006)
- [9] Prokop M., Adam J., Kriz Z., Wimmerova M., Koca J.: TRITON: a graphical tool for ligand-binding protein engineering. *Bioinformatics* 24, 1955-1956 (2008)
- [10] Jirouskova Z., Svobodova Varekova R., Vanek J., Koca J.: Electronegativity Equalization Method: Parameterization and Validation for Organic Molecules using the Merz- Kollman-Singh Charge Distribution Scheme. *J. Comput. Chem.* 30, 1174-1178 (2009)