Born 13.02.67 in Medias/Romania

Married, 1 child

Degrees

1985-1990: Degree in Chemical Engineering – Chemical Engineering Dept. of the 'Babes-Bolyai' University, Cluj-Napoca, Romania.

1992-1993: Master of Science in Organic and Macromolecular Chemistry – Université des Sciences et Technologies de Lille.

1993-1996: Ph.D. in Molecular Modeling: 'Continuum Solvent Models and their Application in Virtual Screening for Inhibitors of Trypanothione Reductase' - Université des Sciences et Technologies de Lille (26.11.1996).

2004-2005: 'Habilitation a Diriger des Recherches' - Université des Sciences et Technologies de Lille (specific French degree – Habilitation as research superviser of Ph.D. students)

Professional Activity

1990-1992: Teaching Assistant of the Organic Chemistry Dept. of the 'Babes-Bolyai' University, Cluj-Napoca, Romania.

1993-1996: Research Assistant in Molecular Modeling, within the frame of a Joint European Laboratory involving the Pasteur Institute of Lille (URA 1309, headed by Prof. André Tartar), and the Free University of Brussels (UCMB, Shoshana Wodak & Daniel van Belle).

1996-1997: Scientist at the Pasteur Institute of Lille

1997-2003: Director (worldwide) of the Molecular Modeling department of the Drug Discovery company CEREP.

2003-present: CNRS Principal Scientist – UMR8525 "Structure and Chemistry of Biomolecules", affiliated to the Laboratoire d'Infochimie, UMR 7177, Université Louis Pasteur Strasbourg since **2007**.

Awards

1985: Gold Medal & Prize for Theoretical Chemistry at the International Chemistry Olympiad, Bratislava, Slovakia.

Expertise

1. Fundamental Molecular Modeling:

- Modeling algorithms: design, programming and applications – molecular mechanics and dynamics, conformational sampling methodology, optimization procedures.

- Continuum solvent models: development of original approaches based on simplified solutions of the Poisson differential equation

- Site-ligand interaction modeling and Docking procedures: development of original approaches based on hybrid evolutionary strategies and their application at the computational screening of putative enzyme inhibitors.

2. Chemoinformatics and High Throughput Modeling in Drug Design:

- Author of original “High Throughput” modeling procedures dedicated to rational drug discovery in a robotized Combinatorial Chemistry-based context. These involved techniques for real-time generation and exploiting of molecular databases featuring full-blown multiconformational models of several tenths of millions of combinatorial compounds.

- Design and validation of novel three-dimensional and topological molecular descriptors and molecular similarity metrics (fuzzy logics-based fingerprint matching and pharmacophore-driven molecular overlay procedures). Design of Activity Profile prediction tools based on an original generalization of the definition of the “Neighborhood Behavior” concept.

- Development of linear and non-linear data mining techniques based on massively parallel evolutionary descriptor selection approaches.

- Development and critical assessment of novel linear and non-linear (neural nets, partition trees) Quantitative Structure-Activity Relationships. Author of successful predictive

models of Caco2 apparent permeability, human oral absorption of drugs, cytochrome CYP2D6 inhibition propensity, cyclooxygenase-II binding affinity, and others.

- Application of the modeling tools in various drug discovery projects, most of them in direct collaboration with major pharmaceutical companies partners of Cerep (Bristol-Myers Squibb, Sanofi-Aventis, Fournier, Servier…)

3. Informatics

- Expert user of Accelrys software (InsightII, Cerius2 and its SDK) and good knowledge of other packages – Tripos, Brugel, X-PLOR, MOE. Good knowledge of chemical database tools – Catalyst, ISIS/Base, ISIS/Host, JChem

- Programming in Fortran, Pascal, Basic, java, C-shell, awk, perl, HTML. Grid computing skills.

- Author and developer of an integrated web-driven suite of tools including automated 2D->3D conversion, pharmacophore-based "fuzzy" querying of large 3D databases of up to 10^8 compounds, activity profile prediction, automated mining for Structure-Activity relationships and application of the herein obtained mathematical models ofr "in silico" property predictions.

- Unix network management (NFS & NIS)

4. Teaching of Organic Chemistry & Chemoinformatics

- Undergraduate & graduate level teaching

- Ph.D. student supervision

5. Project Management:

- Worldwide (Rueil-Malmaison, France and Redmond, WA) management of the modeling team of Cerep (5 persons).

- Involvement in more than a dozen of drug discovery projects, in direct collaboration with major player of the pharmaceutical industry