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Education

- 2002 Ph.D. in Natural Sciences, Swiss Federal Institute of Technology (ETH), Zurich, Switzerland
- 1998 M.S. in Biochemical Engineering, Institute of Chemical Technology, Prague, Czech Republic
- 1996 B.S., Licence de Biochimie, Université Joseph Fourier, Grenoble, France

Awards and Fellowships

- 2003 BAYER Award for Excellence in Computational Chemistry, Germany
- 2003 Arpida AG Fellowship, Munchenstein, Switzerland
- 2000 Certificate in Advanced English, University of Cambridge, UK, Int. Examination
- 1998 HLAVKA Award, for the best thesis in applied biochemistry, Czech Republic
- 1997 SVOC Award, Institute of Chemical Technology, Prague, Czech Republic

Research Experience

2004 – 2007 Postgraduate Fellow

Harvard University, Harvard Medical School, Radiology Department, Boston, USA

2007 – present Advisors: Alun G. Jones, Ph.D., Mahmood Ashfaq, Ph.D.

2004 – 2007 Advisors: Amin I. Kassis, Ph.D., Lakshmanan K. Iyer, Ph.D.

- Modeled Sigma-1 and -2 GPCR receptors and their ligand-based pharmacophores (QSAR)
- Developed datamining strategy to explore literature, genome and microarray data to identify suitable targets within the functional protein network (omics, systems biology)
- Analyzed structures of cancer-related targets, performed homology modeling
- Designed and docked small prodrugs suitable for cancer imaging and therapy (drug design)
- Designed pharmacophore-based combinatorial libraries of drug-like compounds (screening)

2003 – 2004 Postgraduate Fellow

Arpida AG, Basel and Department of Chemistry and Applied Biosciences, ETH Zurich, Switzerland

Advisors: Dr. Sorana Greiveldinger-Poenaru, Dr. Dieter Gillessen, Prof. Gerd Folkers

- Applied docking of Iclaprim derivatives (currently drug in clinical phase III trials)
- Performed structure-comparative analysis of specie-dependent target proteins of Iclaprim
- Built a modeling center for medicinal chemists within the company

1998 – 2002 Graduate Research Fellow

Department of Chemistry and Applied Biosciences, ETH Zurich, Switzerland

Advisor: Prof. Gerd Folkers, Thesis title: "Current Problems in Molecular Docking"

- Spearheaded research in virtual screening
- Designed automatic generator of tautomers and established calculation of tautomeric stabilities
- Developed methodology for multiple binding mode analysis of weakly binding ligands
- Improved virtual screening by considering crystal water molecules in simulations

References upon request.

Experience and Skills

Molecular Modeling

- Homology modeling: MOE, Accelrys InsightII, Tripos Sybyl, BLAST, Swiss-Model
- Molecular dynamic simulation and minimization: AMBER, Swiss-Model, Gromos, MM2, MOPAC
- Protein-based docking and virtual screening: AutoDock, DOCK, FlexX, Gold, SLIDE; developed docking including cofactors, metal ions, waters, tautomers
- Active site analysis and energy probing: GRID, Dowser
- *De novo* design: LUDI, AlleGrow, MOE pharmacophore analysis

Computational Chemistry

- Chemical databanking: MDL ISISBase, Beilstein, CSD, PubChem, ChemBank
- Combinatorial chemistry design: MOE QuaSAR, CAVEAT
- QSAR: ComFa, VolSurf, SYBYL, similarity search, drug-likeness filtering, ADMET properties
- QM/MM: Gaussian, MOPAC, small-molecule parameterization, calculation of tautomeric stabilities
- Designed automatic generator of tautomers AGENT

Bioinformatics and Systems Biology

- Omics: NCBI Entrez, Ensembl, Gene Ontology, UniProt, InterPro, PDB, David, iHOP
- Pathway knowledge databases: Ingenuity Pathway Analysis, LSGraph, Cytoscape
- Gene microarrays: Oncomine, Bioconductor, R, GeneXPress
- Scripting in UNIX shell, Sybyl SPL, MOE SVL, Perl, R, use of scripts in C

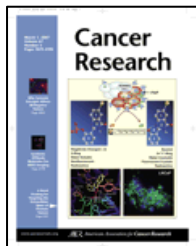
Experimental Biological Chemistry

- CD, ITC, MS, NMR measurements
- Protein expression and purification, PCR, bacteriophage-transfection methods
- Enzymatic activity, enzyme kinetics assays including radioligands, solubility of compounds

Additional Information

- Professional activity: Organizing committee of 3 international meetings; Webmaster
- Talks: Was invited to over 10 international talks, including 2 at ACS National Meetings
- Languages: Fluent in English, French, German, Czech (mother tongue), good in Italian, Russian
- Memberships: International Society of Computational Biology, American Chemical Society

Selected Publications



Journal cover page: Pospisil P, Wang K, Al Aowad AF, Iyer LK, Adelstein SJ, Kassis AI. Computational modeling and experimental evaluation of a novel prodrug for targeting the extracellular space of prostate tumor. *Cancer Res* 2007;67:5.

Research-highlight article: Pospisil P, Iyer LK, Adelstein SJ, Kassis AI. A combined approach to data mining of textual and structured data to identify cancer-related targets. *BMC Bioinformatics* 2006;7:354.

- de Graaf C, Pospisil P, Pos W, Folkers G, Vermeulen NPE. Binding mode prediction of cytochrome P450 and thymidine kinase protein–ligand complexes by consideration of water and rescoring in automated docking. *J Med Chem* 2005;48:2308-18.
- Pospisil P, Ballmer P, Scapozza L, Folkers G. Tautomerism in computer-aided drug design. *J Recept Signal Transduct* 2003;23:361-71.
- Pospisil P, Pilger BD et al, and Folkers G. Synthesis, kinetics, and molecular docking of novel 9-(2-hydroxypropyl)purine nucleoside analogs as ligands of herpesviral thymidine kinases. *Helv Chim Acta* 2002;85:3237-50.
- Pospisil P, Kuoni T, Scapozza L, Folkers G. Methodology and problems of protein-ligand docking: case study of dihydroorotate dehydrogenase, thymidine kinase, and phosphodiesterase 4. *J Recept Signal Transduct* 2002; 22:141-54.

Totally 14 publications. Two manuscripts in preparation.