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Assistant Professor - Chemoinformatics

Professional and training periods

1996 **Training period at université de Lille 1 on falling drops frequency from stalactites.** *Development of experimental devices, data treatments.* (1 month)

1996 **Training period at Institut d'Astrophysique de Paris on a vulgarisation article on green ray phenomenon.** *bibliographic search, redaction.* (1 month)

1998 **Training period at the Institute for Space Science and Astrophysics of Kent about impacts in granular medias.** *Development of experimental devices, data treatment, modelization of the problem, bibliographic search, redaction of a report in english.* (5 months)

1999 **Training period at Institut d'Astrophysique de Paris on a photographic study of the chromospheric Bright Points.** *Realization of a device for digitalization of astronomic observations films, digital image treatment, data analysis, redaction of a report.* (3 months)

1999-2002 **PhD. at Centre de Recherche Paul Pascal under the direction of J. Elezgaray. and Y.H. Sanejouand.** *Development of a a dynamics model for biomolecules, of numerical differential equation solving methods, of force field evaluation, development of statistical corrections (generalized Langevin equation), test and validation of methods, analysis and programming in the source code of the molecular dynamics software CHARMM, use of the software, use of parallel computers.* (3 years)

2003-2004 **Marie-Curie fellowship, at Università degli studi di Milano, Dipartimento di Chimica Organica e Industriale, Pr. A. Bernardi's group. Development on Glycidic Scaffolds of a molecular library of GM1 ganglioside mimics, for cure of Cholera symptoms.** *Collaborations in the Glycidic Scaffolds European research network, molecular dynamics,Monte Carlo simulations, docking, free energy calculations, principal component analysis, participation to development of a C++ code for theoretical calculations of 2D NOE experiments, data analysis, validation and test of methods, management and use of Linux-Irix computer and of an IBM cluster, responsibility of a graduated student, Italian language learning.* (18 months)

2004-2006 **European funding, at Université Louis Pasteur de Strasbourg, Faculté de Pharmacie, Laboratoire de Pharmacochimie de la Communication Cellulaire, UMR7081, groupe du Dr. D. Rognan. Design and docking of compound library targeted on GPCRs.** *Collaborations in the European consortium on GPCRs, sequence alignement, homology modeling, molecular mechanics, Monte Carlo simulations, docking, free energy calculations, principal component analysis, virtual screening, data analysis, compound classification and databases, pharmacophoric search, interaction finger prints, docking of fragment, methods validation and testing.* (2 years)

2006-now **Assitant professeur at Université de Strasbourg** *Teaching, QSAR, Molecular Descriptors, Data Mining, Applicability Domain, Chemography, Drug Design, Ionic Liquids, Development of chemoinformatics toolbox in Object Pascal, Web CGI development.*

Computer skills

- UNIX, HP-UX, Linux, Irix, Windows, Mac
- Fortran77/90/95, C/C++, Pascal, Tcl/Tk, Python, Perl, awk/sed, Object Pascal, Maple, Matlab
- Accelrys inc., Tripos inc., Schrodinger inc., OpenEye inc., Chemaxon inc., InteLigand, BioSolveIT, ClassPharmer, CHARMM, Amber, Gromacs, Gaussian, Gamess, Spartan, Autodock, LigBuilder

Language Knowledge

French	native
English	fluent
Italian	fluent
Russian	fair

Hobbies

Traveling (Europe,USA,Russia), violin, cinema, sport (basket, bicycle), video games

Education

1993-1994 French secondary school diploma

1994-1996 DEUG in Science of Materials at université de Lille 1

1996-1997 Licence of Physics at université de Lille 1, distinction Good

1997-1998 Maitrise (equivalent to a M. sc) of Physics at université de Lille 1

1998-1999 DEA (one year degree required before doctoral studies) of Theoretical Physics (Paris VI, Paris VII, E.N.S., Polytechnique)

1999-2002 PhD: "Modeling large scale dynamics of proteins"

References

These persons are familiar with my professional qualifications and my personality:

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Phd Thesis

The dynamics of proteins is dominated by slow and large movements involving a large number of atoms. These movements are responsible for the transitions between two very different forms of the same protein. It was shown that those movements could be described by a small number of degrees of liberty. These were well described by a small sub-ensemble of normal modes of the proteins. In this thesis are presented some bids to realize from a complete molecular model of proteins, a model reduced to those large scale movements. The importance of the fast movements is shown. Those are reintroduced in the model by two means: first a scaling factor is applied to the parameters of the bonded interactions of the original force field and second, a stochastic term called Generalized Langevin term, is introduced. The thesis explains how to obtain the parameters of this new model. A derived approach is also presented, in which the protein is decomposed in several blocks each being described with the model previously developed. At last, some examples of efficient calculation of the non bonded interactions are presented using the characteristics of the new model.

Bibliography

Coupling overall rotations with modal dynamics, Elezgaray J; Marcou G; Sanejouand Y-H, *Theor. Chem. Acc.*, 2001, 106, 62-68

Exploring the natural conformational changes of the C-terminal domain of calmodulin, Elezgaray J; Marcou G; Sanejouand Y-H, *Physical Review E*, 2002, 66

Modeling large scale dynamics of proteins, PhD. thesis, Marcou G, Université de Bordeaux 1, 2002

Synthesis, conformational studies and mannosidase stability of a mimic of 1,2-mannobioside., Mari S; Posteri H; Marcou G; Potenza D; Micheli F; Cañada FJ; Jiménez-Barbero JJ; Bernardi A, *Eur. J. Org. Chem.*, 2004, 5119-5125

Synthesis and conformational analysis of galactose-derived bicyclic scaffolds., Mari S; Cañada FJ; Jiménez-Barbero JJ; Bernardi A; Marcou G; Motto I; Velter I; Nicotra F; La Ferla B, *Eur. J. Org. Chem.*, 2006, 2925-2933

Optimizing fragment and scaffold docking by use of molecular interaction fingerprints Marcou G; Rognan D, *JCIM*, 47(1), 195-207, 2007

First round of a focused library of cholera toxin inhibitors Podlipnik C; Velter I; La Ferla B; Marcou G; Belvisi L; Nicotra F; Bernardi A, *Carbohydrate Research*, 342(12-13), 1651-1660, 2007

Hot-spots-guided receptor-based pharmacophores (HS-Pharm): A knowledge-based approach to identify ligand-anchoring atoms in protein cavities and prioritize structure-based pharmacophores Barillari C; Marcou G; Rognan D, *JCIM*, 48(7), 1396-1410, 2008

Computer-aided design of new metal binders Varnek A; Fourches D; Kireeva N; Klimchuk O; Marcou G; Tsivadze A; Solov'ev V, *Radiochim. Acta*, 96 (8), 505-511, 2008

ISIDA - Platform for virtual screening based on fragment and pharmacophoric descriptors Varnek A; Fourches D; Horvath D; Klimchuk O; Gaudin C; Vayer P; Solov'ev V; Hoonakker F; Tetko IV; Marcou G, *Curr. Comput. Aided Drug Des.*, 4(3), 191-198, 2008

Predicting the Predictability: A Unified Approach to the Applicability Domain Problem of QSAR Models Horvath D; Marcou G; Varnek A, *JCIM*, 49(7), 1762-1776, 2009

Inductive Transfer of Knowledge: Application of Multi-Task Learning and Feature Net Approaches to Model Tissue-Air Partition Coefficients Varnek A; Gaudin C; Marcou G; Baskin II; Pandey AK; Tetko IV, *JCIM*, 49(1), 133-144, 2009

Applicability Domains for Classification Problems: Benchmarking of Distance to Models for Ames Mutagenicity Set Sushko I; Novotarskyi S; Korner R; Pandey AK; Cherkasov A; Lo JZ; Gramatica P; Hansen K; Schroeter T; Muller KR; Xi LL; Liu HX; Yao XJ; Oberg T; Hormozdiari F; Dao PH; Sahinalp C; Todeschini R; Polishchuk P; Artemenko A; Kuz'min V; Martin TM; Young DM; Fourches D; Muratov E; Tropsha A; Baskin I; Horvath D; Marcou G; Muller C; Varnek A; Prokopenko VV; Tetko IV, *JCIM*, 50(12), 2094-2111, 2010

ISIDA Property-Labelled Fragment Descriptors Ruggiu F; Marcou G; Varnek A; Horavath D; *Mol. Inf.*, 29(12), 855-868, 2010

In Silico Design of New Ionic Liquids Based on Quantitative Structure-Property Relationship Models of Ionic Liquid Viscosity Billard I; Marcou G; Ouadi A; Varnek A, *J. Phys. Chem. B*, 115(1), 93-98, 2011

Local neighborhood behavior in a combinatorial library context Horvath D; Koch C; Schneider G; Marcou G; Varnek A, *J. Comp. Aided Mol. Des.*, 25(3), 237-252, 2011

Online chemical modeling environment (OCHEM): web platform for data storage, model development and publishing of chemical information Sushko I; Novotarskyi S; Körner R; Pandey A; Rupp M; Teetz W; Brandmaier S; Abdelaziz A; Prokopenko VV; Tanchuk VY; Todeschini R; Varnek A; Marcou G; Ertl P; Potemkin V; Grishina M; Gasteiger J; Schwab C; Baskin II; Palyulin VA; Radchenko EV; Welsh WJ; Kholodovych V; Chekmarev D; Cherkasov A; Aires-de-Sousa J; Zhang Q-Y; Bender A; Nigsch F; Patiny L; Williams A; Tkachenko V; Tetko IV, *J. Comp. Aided Mol. Des.*, 25(6), 533-554, 2011

Quantitative Structure-Property Relationship (QSPR) Modeling of Normal Boiling Point Temperature and Composition of Binary Azeotropes Solov'ev V; Oprisiu I; Marcou G; Varnek A, *Ind. & Eng. Chem. Res.*, 50(24), 14162-14167, 2011

Stability constants of complexes of Zn2+, Cd2+, and Hg2+ with organic ligands: QSPR consensus modeling and design of new metal binders Solov'ev V; Sukhno I; Buzko V; Polushin A; Marcou G; Tsivadze A; Varnek A, *J. Incl. Phen. Macrocyc. Chem.*, 72(3-4), 309-321, 2012

Generative Topographic Mapping (GTM): Universal Tool for Data Visualization, Structure-Activity Modeling and Dataset Comparison Kireeva N; Baskin II; Gaspar HA; Horvath D; Marcou G; Varnek A, *Mol. Inf.*, 31(3-4), 301-312, 2012

QSPR Approach to Predict Nonadditive Properties of Mixtures. Application to Bubble Point Temperatures of Binary Mixtures of Liquids Oprisiu I; Varlamova E; Muratov E; Artemenko A; Marcou G; Polishchuk P; Kuz'min V; Varnek A, *Mol. Inf.*, 31(6-7), 491-502, 2012

Interpretability of SAR/QSAR Models of any Complexity by Atomic Contributions Marcou G; Horvath D; Solov'ev V; Arrault A; Vayer P; Varnek A, *Mol. Inf.*, 31(9), 639-642, 2012

Mining Chemical Reactions Using Neighborhood Behavior and Condensed Graphs of Reactions Approaches De Luca A; Horvath D; Marcou G; Solov'ev V; Varnek A, *JCIM*, 52(9), 2325-2338, 2012

Using self-organizing maps to accelerate similarity search Bonachera F; Marcou G; Kireeva N; Varnek A; Horvath D, *Bioorg. & Med. Chem.*, 20(18), 5396-5409, 2012

Complexation of Mn2+, Fe2+, Y3+, La3+, Pb2+, and UO22+ with Organic Ligands: QSPR Ensemble Modeling of Stability Constants Solov'ev V; Marcou G; Tsivadze A; Varnek A, *Ind. & Eng. Chem. Res.*, 51(41), 13482-13489, 2012

Models for Identification of Erroneous Atom-to-Atom Mapping of Reactions Performed by Automated Algorithms Muller C; Marcou G; Horvath D; Aires-de-Sousa J; Varnek A, *JCIM*, 52(12), 3116-3122, 2012

Publicly available models to predict normal boiling point of organic compounds Oprisiu I; Marcou G; Horvath D; Brunel B; Rivollet F; Varnek A, *Themochim. Acta*, 553, 60-67, 2013

Predicting Ligand Binding Modes from Neural Networks Trained on Protein-Ligand Interaction Fingerprints Chupakhin V; Marcou G; Baskin I; Varnek A; Rognan D, *JCIM*, 53(4), 763-772, 2013

Do Not Hesitate to Use Tversky-and Other Hints for Successful Active Analogue Searches with Feature Count Descriptors Horvath D; Marcou G; Varnek A *JCIM*, 53(7), 1543-1562, 2013

Generative Topographic Mapping-Based Classification Models and Their Applicability Domain: Application to the Biopharmaceutics Drug Disposition Classification System (BDDCS) Gaspar H; Marcou G; Horvath D; Arault A; Lozano S; Vayer P; Varnek A, *JCIM*, 53(12), 3318-3325, 2013

Quantitative Structure-Property Relationship Modeling: A Valuable Support in High-Throughput Screening Quality Control Ruggiu F; Gizzi P; Galzi J-L; Hibert M; Haiech J; Baskin I; Horvath D; Marcou G; Varnek A, *Anal. Chem.*, 86(5), 2510-2520, 2014

The use of three-dimensional similarity in assessing the risk of cross-reactivity between carbamazepine and psychotropic drugs Le Louarn E; Barbaud A; Trechot P; Marcou G; Lepoittevin J-P, *Eur. J. Clin. Pharmacol.*, 70(4), 495-498, 2014

Using Chemoinformatics Tools from R Marcou G; Baskin II, *in* Data Mining in Drug Discovery, *Edited by* Hoffmann R D; Gohier A; Pospisil P, **Wiley-VCH**, 179-208, 2014

Computational chemogenomics: Is it more than inductive transfer? Brown J B; Okuno Y; Marcou G; Varnek A; Horvath D, *JCAMD*, 28(6), 597-618, 2014

Individual Hydrogen-Bond Strength QSPR Modelling with ISIDA Local Descriptors: a Step Towards Polyfunctional Molecules Ruggiu F; Solov'ev V; Marcou G; Horvath D; Graton J; Le Questel J-Y; Varnek A, *Mol. Inf.*, 33(6-7), 477-487, 2014

Simple Ligand-Receptor Interaction Descriptor (SILIRID) for alignment-free binding site comparison Chupakhin V; Marcou G; Gaspar H; Varnek A *Comput. Struct. Biotechnol. J.*, 10, 33-37, 2014

Design of a General-Purpose European Compound Screening Library for EU-OPENSCREEN Horvath D; Lisurek M; Rupp B; Kühne R; Specker E; von Kries J; Rognan D; Andersson CD; Almqvist F; Elofsson M; Enqvist P-A; Gustavsson A-L; Remez N; Mestres J; Marcou G; Varnek A; Hibert M; Quintana J; Frank R, *Chem. Med. Chem.*, in press, 2014

Teaching

Master de Chimie Spécialité Chemoinformatique et Modélisation, Mathematics

Master de Chimie Spécialité Chemoinformatique et Modélisation, Statistics

Master de Chimie Spécialité Chemoinformatique et Modélisation, Data Mining

Master de Chimie Spécialité Chemoinformatique et Modélisation, Drug Design

Master de Chimie Spécialité Chemoinformatique et Modélisation, Chemoinformatics

Ecole de Chimie, Polymères et Matériaux Informatics

Ecole de Chimie, Polymères et Matériaux Statistics

Licence de Chimie-Biologie Molecular structures

Formation Continue Introduction to Chemoinformatics

Responsabilities

co-director of the Master de Chimie, Spécialité Chemoinformatique (double diploma with Kazan Federal University, Russia) and joint master with Paris-Diderot, In Silico Drug Design.

Organisation and promotion of the Chemoinformatics Strasbourg Summer School (CS3) (2008-2010-2012-2014).

Management of IT resources and web sites.

Strasbourg, October 7, 2014