Fiorella Ruggiu, PhD — Curriculum Vitae

Driving license B and car owner

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Professional goals:

Chemoinformatician, Modeller, Software developer

Education – *PhD in Chemistry, specialisation Chemoinformatics*

2010-2014 PhD in Chemistry, specialisation in chemoinformatics (Strasbourg University, France). Title: *"Property-enriched fragment descriptors for adaptive QSAR"* Supervisors: Dr. D. Horvath, Pr. A Varnek (Laboratory of Chemoinformatics) Referees: Pr. J. Aires de Sousa (Lisbon University), Pr. O. Taboureau (Paris Diderot U.) Jury members: Dr. P. Ertl (Novartis), Dr E. Kellenberger (Strasbourg University).
Research subject: *Development of ISIDA fragment descriptors and their use in QSAR modelling of hydrophobicity (LogP & CHI), acidity (pK_a), hydrogen bonding (pK_{BHX}), hERG channel inhibition, GPCRs and Proteases binding affinities.*

2008-2010 Master in Chemistry, specialisation in chemoinformatics, Strasbourg University (France) with first class honours (mention "Très bien").

2006-2008 Bachelor in Chemistry, Strasbourg University (France) with distinction (mention "Assez bien").

2004-2006 "Classes préparatoires" in physics and chemistry, Ecole Nationale Supérieure de Chimie de Lille (France).

2001-2004 International Baccalaureate, Schule Schloss Salem (Überlingen, Germany), with trilingual diploma in English, French and German, obtained with 39 points (out of 45).

1992-2001 European School of Munich, Germany.

Publications

- F. Ruggiu, G. Marcou, A. Varnek, D. Horvath, "*ISIDA Property-labelled Fragment descriptors*", *Mol Inf,* 29(12), p. 855–868, 2010.
- F. Ruggiu, P. Gizzi, J.-L. Galzi, M. Hibert, J. Haiech, I. Baskin, D. Horvath, G. Marcou, A. Varnek, *"Quantitative Structure–Property Relationship Modeling: A Valuable Support in High-Throughput Screening Quality Control*", *Anal Chem*, 86(5), p. 2510-2520, 2014.
- F. Ruggiu, V. Solov'ev, G. Marcou, D. Horvath, J. Graton, J.-Y. Le Questel, A. Varnek, "*Individual hydrogen bond strength QSPR modelling with ISIDA local descriptors : a step towards polyfunctional molecules*", *Mol Inf,* 33, p. 477-487, 2014.
- S. Brandmaier, W. Peijnenburg, M.K. Durjava, B. Kolar, P. Gramatica, E. Papa, B. Bhhatarai, S. Kovarich, S. Cassani, M. Rahmberg, T. Öberg, N. Jeliazkova, L. Golsteijn, M. Comber, L. Charochkina, S. Novotarskyi, I. Sushko, A. Abdelaziz, E. D'Onofrio, P. Kunwar, F. Ruggiu and I.V. Tetko, "*The QSPR-THESAURUS: The Online Platform of the CADASTER Project*", *ATLA*, 42, p. 1–12, 2014.

Professional background and experience

2013 **Japan Society for the Promotion of Science Postdoctoral Fellowship**, Department of Systems Bioscience for Drug Discovery, Graduate School of Pharmaceutical Sciences, Kyoto University (Japan) for 4 months.
Research subject: *Chemogenomics modelling of GPCRs using SVM and ISIDA descriptors, visualisation of chemical space via the similarity matrix and support vectors.*

2010-2013 **Teaching & internships supervision of master students**, Laboratory of Chemoinformatics, Strasbourg University (France). Tutorial chemistry and computational chemistry practical classes. Elaborated practical classes subjects. Supervision of computational chemistry projects for master students related to my PhD.

2010 **Master Internship in chemoinformatics**, Laboratory of Chemoinformatics, Strasbourg University (France) for 6 months under the supervision of D. Horvath.
Research subject: *Development of ISIDA fragment descriptors and their use in QSAR.*

2009 **Internship in chemoinformatics**, Institute for Bioinformatics and Systems Biology, Helmholtz Zentrum Muenchen (Germany) for 2 months under the supervision of I. Tetko.
Research subject: *QSAR modelling of toxicity using the ochem plateform*.

2008 **Summer job as waitress in Japan**, Hotel Ambiento, Tateshina (Japan) for 2 months.

IT skills

Environments: Linux (Mageia, Debian, Fedora, Ubuntu), Windows
Programming languages: C/C++, Java, Free Pascal, HTML/PHP
Scripting languages: bash, tcsh, perl, python, R
Database: SQL
Chemoinformatics Soft.: ChemAxon, ChemOffice, ISIDA, Spartan, LigandScout, MOE , ochem, Conquest
Others: Latex, Microsoft Office, Gimp, EndNote, JabRef

Languages

French – *native speaker*, English – *nearly native speaker (High school in English)*

German – *nearly native speaker (lived 18 years in Germany)*, Italian – *moderate,* Japanese – *basic*

Interests

Travelling, running, biking, hiking, handicrafts (DIY, knitting, jewellery making, etc.)

References (these people are familiar with my work)

Dr. Dragos Horvath, *senior scientist at the CNRS (French National Centre for Scientific Research),* Laboratory of Chemoinformatics, University of Strasbourg (France)

e-mail: dhorvath@unistra.fr telephone: +33 3 68 85 13 21

Dr. Gilles Marcou, *associated professor of the University of Strasbourg*, Laboratory of Chemoinformatics, University of Strasbourg (France)

e-mail: g.marcou@unistra.fr telephone: +33 3 68 85 13 04

Dr. Peter Ertl, *leading scientist in the Chemoinformatics department at Novartis Institutes for Biomedical Research,* Novartis (Switzerland)

e-mail: peter.ertl@novartis.com telephone : +41 61 32 40 685