Francesca Grisoni

about
Female, Italian
26-02-1988
francesca.grisoni@unimib.it

expertise
molecular descriptors
chemometrics
QSAR modelling
multivariate analysis

technical skills
regression, classification
clustering, programming
data visualization
database curation

languages
Italian ★★★★★
English ★★★★☆
German ★★★☆☆

programming
MATLAB, advanced
python, intermediate
R, beginner
html scripting, beginner

software
KNIME, LaTeX, Dragon
RDKit, VEGA, CDK, SPSS
QSAR Toolbox, EPI Suite

Interests
molecular descriptors
drug discovery/design
(eco)toxicology
natural products
machine learning

education

2013-2016 **Ph.D. in Environmental Sciences**
University of Milano-Bicocca
Thesis: *"In silico assessment of aquatic bioaccumulation: advances from chemometrics and QSAR modelling"*
Supervisor: Prof. R. Todeschini
Referees: Prof. Dr. J. Kirchmair, Prof. Dr. O. Nicolotti, Prof. Dr. A. Finizio

2010–2012 **M.Sc. in Sciences and Technologies for Environment and Landscape**
University of Milano-Bicocca, 110/110 *cum laude*
Thesis: *"Study of variable selection methods and regression methods for the development of QSAR models on environmental and toxicological endpoints"*
Supervisor: Prof. R. Todeschini

2007–2009 **B.Sc. Environmental Sciences and Technologies**
University of Milano-Bicocca, 110/110 *cum laude*
Supervisor: Dr. B. Delmonte

experience

since 1 2017 **University of Milano Bicocca - Postdoc researcher** Milano, Italy
- Project: "*Improved molecular representation for natural-product inspired de novo design*"

Dec 2016 **ETH Zurich - Research Fellow** Zurich, Switzerland
- Project: "*Development of novel holistic molecular descriptors for drug discovery and design*" (Prof. Dr. G. Schneider).

08-11 2016 **University of Milano-Bicocca - Research Fellow** Milano, Italy
- Project: "*Development of novel chemometric approaches to assess the bioaccumulation of chemicals in aquatic environment*". (Prof. R. Todeschini)

04-07 2016 **SmartStat Milano - Data Scientist** Milano, Italy
- Machine learning for user-tailored web advertising

01-12 2016 **Bracco Imaging Italia - Biostatistical consultant** Colleretto Giacosa, Italy
Bracco Pharma group, Bio Industry Park, Colleretto Giacosa, Italy.
- Biostatistical analysis of *in vivo* safety and biodistribution studies

07–09 2015 **U.S. EPA - Guest PhD student** RTP, U.S.A.
National Center of Computational Toxicology, Research Triangle Park, NC, United States (Dr. R. Judson)
- Project: "*Integrating pharmacokinetics into the assessment of bioaccumulation potential in humans*".

06–08 2014 **ETH Zurich - Guest PhD student** Zurich, Switzerland
Institute of Pharmaceutical Sciences, CADD Group (Prof. Dr. G. Schneider)
- Project: "*Similarity searching in virtual compound libraries*".

publications

F. Grisoni, V. Consonni, R. Todeschini.
Impact of molecular descriptors on computational models.
In *Computational Chemogenomics*, Methods in Molecular Biology, Springer. (In press)

F. Grisoni, D. Reker, P. Schneider, L. Friedrich, V. Consonni, R. Todeschini, A. Koeberle, O. Werz, G. Schneider
Matrix-based molecular descriptors for prospective virtual compound screening
Molecular Informatics, 36, 1-7 (2017)

R. Todeschini, D. Ballabio, F. Grisoni
Beware of unreliable Q^2! A comparative study of regression metrics for predictivity assessment of QSAR models
Journal of Chemical Information and Modeling, 56(10), 1905-191 (2016)

R. Todeschini, D. Ballabio, V. Consonni, F. Grisoni
A new concept of higher-order similarity and the role of distance/similarity measures in local classification methods
Chemometrics and Intelligent Laboratory Systems 157, 50–57 (2016)

S. Nembri, F. Grisoni, V. Consonni, R. Todeschini
In silico prediction of Cytochrome P450-drug interaction: QSAR models for CYP3A4 and CYP2C9
International Journal of Molecular Sciences 17(6), 914 (2016)

F. Grisoni, V. Consonni, M. Vighi, S. Villa, R Todeschini
Expert QSAR system for predicting the bioconcentration factor under the REACH regulation
Environmental Research 148, 507-512 (2016)

M. Cassotti, F. Grisoni, S.Nembri, R.Todeschini
Application of the Weighted Power-Weakness Ratio (wPWR) as a Fusion Rule in Ligand–Based Virtual Screening.
MATCH Commun. Math. Comput. Chem. 76, 359-376 (2016)

F. Grisoni, V. Consonni, M. Vighi, S. Villa, R. Todeschini
Investigating the mechanisms of bioconcentration through QSAR classification trees
Environment International 88, 198–205 (2016)

K. Mansouri, A. Abdelaziz, A. Rybacka, A. Roncaglioni, A. Tropsha, A. Varnek, A. Zakharov, A. Worth, A. Richard, C.M. Grulke, D. Trisciuzzi, D. Fourches, D. Horvath, E. Benfenati, E. Muratov, E. B. Wedebye, F. Grisoni, G.F. Mangiatordi, G.M. Incisivo, H. Hong, H.W. Ng, I.V. Tetko, I. Balabin, J. Kancherla, J. Shen, J. Burton, M. Nicklaus, M. Cassotti, N.G. Nikolov, O. Nicolotti, P.L. Andersson, Q. Zang, R. Politi, R.D. Beger, R. Todeschini, R. Huang, S. Farag, S.A. Rosenberg, S. Slavov, X. Hu, R.S. Judson
CERAPP: Collaborative Estrogen Receptor Activity Prediction Project
Environmental Health Perspectives 124(7), 1023-1033 (2016)

F. Grisoni, V. Consonni, S. Nembri, R. Todeschini
How to weight Hasse matrices and reduce incomparabilities
Chemometrics and Intelligent Laboratory Systems 147, 95–104 (2015)

R. Todeschini, F. Grisoni, S. Nembri
Weighted power–weakness ratio for multi-criteria decision making
Chemometrics and Intelligent Laboratory Systems 146, 329–336 (2015)

F. Grisoni, V. Consonni, S. Villa, M. Vighi, R. Todeschini
QSAR models for bioconcentration: Is the increase in the complexity justified by more accurate predictions?
Chemosphere 127, 171–179 (2015)

F. Grisoni, M. Cassotti, R. Todeschini
Reshaped Sequential Replacement for variable selection in QSPR: comparison with other reference methods
Journal of Chemometrics 28, 249–259 (2014)

M. Cassotti, F. Grisoni, R. Todeschini
Sequential Replacement algorithm: An efficient approach to variable selection
Chemometrics and Intelligent Laboratory Systems 133, 136–148 (2014)

presentations, posters and lectures

online course F. Grisoni (2017). *"Machine learning for chemoinformatics: an introduction"*. Marie Curie ITN - BigChem Project, 17/05/2017.

co-chariperson A. Focks, M. Vighi, F. Grisoni, A. Barsi. Society of Environmental Toxicology and Chemistry (SETAC) Europe Meeting. Session: "*Predictive models in ecotoxicology: bridging the gap between scientific progress and regulatory applicability*". Brussels (BE), 10/05/2017.

oral communication F. Grisoni, M. Vighi, V. Consonni, S. Villa, R. Todeschini (2017). *"Towards more interpretable QSARs: Lessons Learned from Aquatic Bioaccumulation Models"*. SETAC Europe, Brussels (BE), 10/05/2017.

oral communication F. Grisoni (2017). *"From molecules to molecular descriptors: tips and tricks for real-world applications"*. Marie Curie ITN - BigChem Spring School, Barcelona (SP), 21/04/2017.

frontal lectures. Lectures on the topics of molecular descriptors, QSAR and applications. Course "Methods in Drug Design" (Prof. Dr. G. Schneider). ETH Zurich, Institute of Pharmaceutical Sciences, Zurich (SW) 23-24/02/2017.

poster F. Grisoni, S. Nembri, V. Consonni, D. Ballabio, R. Todeschini (2016). *"Exploiting the potential of molecular descriptors through data-fusion strategies: A case study on Cytochrome P450."* 21st EuroQSAR, Verona (IT)

poster R. Todeschini, D. Ballabio, F. Grisoni (2016). *Beware of Unreliable Q^2! A comparative study of Regression Metrics for predictivity assessment of QSAR models* 21st EuroQSAR, Verona (IT)

poster A. Herrera, F. Grisoni, D. Ballabio, R. Todeschini, N. Navas, C. Cardell, C. (2016). *Preliminary studies of ultraviolet radiation over time in paint mock-ups.* 2nd International Conference on Innovation in Art Research and Technology (inArt 2016), Ghent (BE).

frontal lectures. Teaching assistant in the chemometrics course (Prof. R. Todeschini). Lectures on molecular descriptors; assistant in the practical course. University of Milano-Bicocca, Dept. of Earth and Env. Sciences, M.Sc. in Chemical Sciences, 2015.

poster F. Grisoni, V. Consonni, S. Nembri, R. Todeschini (2015). *"How to weight Hasse matrices and reduce incomparabilities"*. Analytical Chem. Congress of SCI, Trieste (IT)

oral communication F. Grisoni, M. Cassotti, R. Todeschini (2015). *"Reshaped Sequential Replacement for variable selection"*. Italian Chemometrics Workshop, Rome (IT)

poster F. Grisoni, V. Consonni, S. Villa, M. Vighi, R. Todeschini (2014). *"QSAR models for bioconcentration: is the increase in the complexity balanced by better predictions?"* QSAR 2014, Istituto di Ricerche Farmacologiche Mario Negri, Milan (IT)

poster F. Grisoni, M. Cassotti, R. Todeschini (2012). *Comparison of variable selection methods*. Strasbourg Summer School on Chemoinformatics. Strasbourg (FR).