Alberto Manganaro

Birth place: Città di Castello (PG), Italy
Sex: Male
Nationality: Italian
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Education

Apr 2006 — University of Milano Statale – Polo di Crema
Degree in Computer Science
Final grade: 110/110 cum laude
Degree thesis: *"Metodologie chemiometriche per lo studio di matrici di correlazione di grandi dimensioni e costruzione del corrispondente codice in MATLAB"* (*"Chemometric methodologies for studying wide correlation matrices and development of corresponding code in MATLAB"*) performed at Milano Chemometrics and QSAR Research Group, Milano - Bicocca University.

Professional experiences

Feb 2012 - now — Founder of the consultancy company Kode s.r.l (www.kode-solutions.net).

Nov 2008 - now — Partner of the Laboratory of Environmental Chemistry and Toxicology led by prof. Emilio Benfenati at Istituto di Ricerche Farmacologiche "Mario Negri", Milano. Research work is mainly related to the development of in-silico models for toxicological endpoints required by the REACH regulation.

Apr 2006 - now — Member of the Milano Chemometrics and QSAR Research Group (michem.disat.unimib.it/chm) led by prof. Roberto Todeschini, at university of Milano - Bicocca. Research work is mainly related to multivariate statistical analysis and statistical software development.

Scientific consultant for Talete srl (www.talete.mi.it): chemometrics consulting and collaboration in the development of software for multivariate analysis.

Sep - Dec 2002 — Temporary teacher of Computer Science in high school "Istituto Tecnico Industriale Statale A. Volta", Lodi.

1999 - 2002 — Partner of Eidos SAP s.r.l. (industrial and environmental risk assessment): development of web-based application and standalone software, office IT technician.

Software development and IT related activities

Developer of the open-source application **ToxRead** (http://www.toxgate.eu/). ToxRead is an open-source free platform that allows interactive read-across analysis of chemicals.

Co-developer of the commercial software **DRAGON version 7**. DRAGON is the most spread software for the calculation of molecular descriptors. New version includes full GUI and shell environment both for Windows and Linux operative systems.

Developer of **istChemFeat** application under ANTARES EU project (freely available on www.kode-solutions.net) for the analysis of chemical features in molecules dataset.

Developer of **istMolBase** (freely available on www.kode-solutions.net), application for visualizing and managing a dataset of molecules based on the VEGA libraries.

Developer of the **KNIME** node for Dragon. The node allows to execute the commercial software Dragon inside the KNIME analytics platform.

Co-developer of the commercial software **dProperties**. dProperties calculates several physicochemical properties and drug-like indices.

Developer of the open-source application **VEGA** platform (http://www.vega-qsar.eu). VEGA is an open-source free platform that implements several QSAR models, especially aimed to the use for the REACH regulation.

Co-developer of the commercial software **DRAGON version 6**. DRAGON is the most spread software for the calculation of molecular descriptors. New version includes full GUI and shell environment both for Windows and Linux operative systems.

Developer of software modules for the **CAESAR – Computer Assisted Evaluation of industrial chemical Substances According to Regulation** project (www.caesar-project.eu). CAESAR is an EC funded project which is specifically dedicated to develop QSAR models for the REACH legislation.

Co-developer of the online free database **MOLE db** (Molecular Descriptors Database). The database is intended as a research and teaching tool and allows to search for a specific group of molecules and analyse the corresponding values of molecular descriptors.

Co-developer of scientific application **DART – Decision Analysis by Ranking Techniques**. DART is a software package for multicriteria decision making, based on several partial and total ranking algorithm, including Hasse Diagrams. DART is downloadable for free at European Chemicals Bureau website (ecb.jrc.it).

Information Technology skills

- Known programming languages and development tools: Java, C/C++, Visual Basic, Object Oriented Pascal (Delphi/Lazarus), SQL, MATLAB, R;
- Expertise with tools for data mining and analytics: KNIME, Weka, Statistica
- Knowledge of networking authoring and development technologies: HTML, XML, PHP, ASP, JQuery, AngularJS, D3.js, MySQL Server, Apache webserver;
- Experiences with: Linux , Windows , management of small networks, system administration.

Fields of interest

Chemometrics, QSAR, Software Development and Infomation Technology, In-Silico methods as alternative to animal-testing, Multicriteria Decision Making strategies, Applied Statistics.

Publications

Papers on peer-reviewed international journals

27. "A new structure-activity relationship (SAR) model for predicting drug-induced liver injury, based on statistical and expert-based structural alerts"
F. Pizzo, A. Lombardo, A. Manganaro, E. Benfenati
Frontiers in Pharmacology (2016), vol. 7

26. "Integrated in silico strategy for PBT assessment and prioritization under REACH"
F. Pizzo, A. Lombardo, A. Manganaro, C.I. Cappelli, M.I. Petoumenou, F. Albanese, A. Roncaglioni, M. Brandt, E. Benfenati
Environmental Research (2016) vol. 151, 478–492

25. "Integrating in silico models to enhance predictivity for developmental toxicity"
M. Marzo, S. Kulkarni, A. Manganaro, A. Roncaglioni, S. Wu, T.S. Barton-Maclaren, C. Lester, E. Benfenati
Toxicology (2016), vol. 370, 127-137

24. " A knowledge-based expert rule system for predicting mutagenicity (Ames test) of aromatic amines and azo compounds"
D. Gadaleta, S. Manganelli, A. Manganaro, N. Porta, E. Benfenati
Toxicology (2016), vol. 370, 20-30

23. "New quantitative structure–activity relationship models improve predictability of Ames mutagenicity for aromatic azo compounds"
S. Manganelli, E. Benfenati, A. Manganaro, S. Kulkarni, T.S. Barton-Maclaren, M. Honma
Toxicological Sciences (2016)

22. "Results of a round-robin exercise on read-across"
E. Benfenati, M. Belli, T. Borges, E. Casimiro, J. Cester, A. Fernandez, G. Gini, M. Honma, M. Kinzl, R. Knauf, A. Manganaro, E. Mombelli, M.I. Petoumenou, M. Paparella, P. Paris, G. Raitano
SAR and QSAR in Environmental Research (2016), 1-14

21. "A new integrated in silico strategy for the assessment and prioritization of persistence of chemicals under REACH"
F. Pizzo, A. Lombardo, M. Brandt, A. Manganaro, E. Benfenati
Environment International (2016), vol. 88, 250-260

20. "New clues on carcinogenicity-related substructures derived from mining two large datasets of chemical compounds"
A. Golbamaki, E. Benfenati, N. Golbamaki, A. Manganaro, E. Merdivan, A. Roncaglioni, G. Gini
Journal of Environmental Science and Health (2016), Part C, 00-00, Just accepted

19. "Predicting persistence in the sediment compartment with a new automatic software based on the k-Nearest Neighbor (k-NN) algorithm"
A. Manganaro, F. Pizzo, A. Lombardo, A. Pogliaghi, E. Benfenati
Chemosphere (2016), vol. 144, 1624-1630

18. "Hierarchical rules for read-across and in silico models of mutagenicity"
E. Benfenati, S. Manganelli, S. Giordano, G. Raitano, A. Manganaro
Journal of Environmental Science and Health (2015), accepted paper

17. "Comparison of in silico tools for evaluating rat oral acute toxicity"
R. Gonella Diaza, S. Manganelli, A. Esposito, A. Roncaglioni, A. Manganaro, E. Benfenati
SAR and QSAR in Environmental Research (2015), vol. 26 issue 1, 1-27

16. "ToxRead: A tool to assist in read across and its use to assess mutagenicity of chemicals"
G. Gini , A.M. Franchi , A. Manganaro , A. Golbamaki , E. Benfenati
SAR and QSAR in Environmental Research (2014), vol. 25 issue 12, 999-1011

15. "A generalizable definition of chemical similarity for read-across"
M. Floris, A. Manganaro, O. Nicolotti, R. Medda, G. F. Mangiatordi, E. Benfenati
Journal of Cheminformatics (2014), vol. 6, 39

14. "A new in silico classification model for ready biodegradability, based on molecular fragments"
A. Lombardo, F. Pizzo, E. Benfenati, A. Manganaro, T. Ferrari, G. Gini
Chemosphere (2014), vol. 108, 10-16

13. "Automatic knowledge extraction from chemical structures: the case of mutagenicity prediction"
T. Ferrari, D. Cattaneo, G. Gini, N. Golbamaki Bakhtyari, A. Manganaro, E. Benfenati
SAR and QSAR in Environmental Research (2013), vol. 24 issue 5, 365-83

12. "VEGA-QSAR: AI Inside a Platform for Predictive Toxicology"
E. Benfenati, A. Manganaro, G. Gini
PAI, CEUR Workshop proceedings (2013), vol. 1107

11. "In silico models for predicting ready biodegradability under REACH: a comparative study"
F. Pizzo, A. Lombardo, A. Manganaro, E. Benfenati
Science of The Total Environment (2013), vol. 463-464, 161-8

10. "Using toxicological evidence from QSAR Models in practice"
E. Benfenati, S. Pardoe, T. Martin, R Gonella Diaza, A. Lombardo, A. Manganaro, A. Gissi
Altex (2013), vol. 30 issue 1, 19-40

9. "CORAL software: QSAR for anticancer agents"
E. Benfenati, A. A. Toropov, A. P. Toropova, A. Manganaro, R. Gonella Diaza
Chemical Biology and Drug Design (2011), vol. 77 issue 6, 471-476

8. "CAESAR models for developmental toxicity"
A. Cassano, A. Manganaro, T. Martin, D. Young, N. Piclin, M. Pintore, D. Bigoni, E. Benfenati
Chemistry Central Journal (2010), vol. 4, suppl. 1, art. no. S4

7. "QSAR modelling of the toxicity to Tetrahymena pyriformis by balance of correlations"
A. A. Toropov, A. P. Toropova, E. Benfenati, A. Manganaro
Molecular Diversity (2010), vol. 14 issue 4, 821-827

6. "QSAR modelling of carcinogenicity by balance of correlations"
A. A. Toropov, A. P. Toropova, E. Benfenati, A. Manganaro
Molecular Diversity (2009), vol. 13 issue 3, 367-373

5. "QSPR modeling of enthalpies of formation for organometallic compounds by SMART-based optimal descriptors"
A. A. Toropov, A. P. Toropova, E. Benfenati, A. Manganaro
Journal of Computational Chemistry (2009), vol. 30 issue 15, 2576-258

4. "Canonical Measure of Correlation (CMC) and Canonical Measure of Distance (CMD) between sets of data. Part 2. Variable reduction"
V. Consonni, D. Ballabio, A. Manganaro, A. Mauri, R. Todeschini
Analytica Chimica Acta (2009), 648, 45-51

3. "Canonical Measure of Correlation (CMC) and Canonical Measure of Distance (CMD) between sets of data. Part 1. Theory and simple chemometric applications"
R. Todeschini, D. Ballabio, V. Consonni, A. Manganaro, A. Mauri
Analytica Chimica Acta (2009), 648, 52-59

2. "Introduction to MOLE DB - on-line Molecular Descriptors Database"
D. Ballabio, A. Manganaro, V. Consonni, A. Mauri, R. Todeschini
MATCH, communications in mathematical and in computer chemistry (2009), 62, 199-207

1. "Peptides multivariate characterisation using a molecular descriptor based approach"
A. Mauri, D. Ballabio, V. Consonni, A. Manganaro, R. Todeschini
MATCH, communications in mathematical and in computer chemistry (2008), 60, 671-690

Book chapters

1. "The DART (Decision Analysis by Ranking Techniques) software"
A. Manganaro, D. Ballabio, V. Consonni, A. Mauri, M. Pavan, R. Todeschini
in "Ranking methods", R. Todeschini and M. Pavan (ED), Elsevier, 2008

Other papers

3. "Animal abuse and human abuse. Partners in crime"
F. Sorcinelli, A. Manganaro, M. Tettamanti
Italian Journal of Criminology (2014), 6.4: 225-233.

2. "Evaluation of multivariate classification and variable selection for the distinction of cachaca and rum samples"
R. Todeschini, D. Ballabio, C. Rojas, A. Manganaro, A. Mauri, V. Consonni, P. Tripaldi
Alimentos, Ciencia e Ingenieria (2007), 16, 113-115

1. "CFA interpolation testbench"
A. Manganaro, P. Brambati, P. Benzi
Note del Polo, Dipartimento di Tecnologie dell'Informazione – Università degli Studi di Milano, 008 (February 2003)

Oral presentation, lectures and teaching

13. "How to use the free in silico tools of PROSIL"
Prosil final workshop, Milano (Italy), 21 september 2016

12. "Short course on VEGA"
QSAR 2014, Milano (Italy), 17 and 19 June 2014

11. "New software to support read across, based on multiple profilers"
G. Gini, A. M. Franchi, A. Manganaro, A. Golbamaki, E. Benfenati
QSAR 2014, Milano (Italy), 19 June 2014

10. "Applicability domain for mutagenicity models: an a priori approach, based on chemical classes"
R. Gonella Diaza, G. Raitano, A. Manganaro, E. Benfenati
QSAR 2014, Milano (Italy), 17 June 2014

9. "How to build a QSAR model"
ECO summer school, Verona (Italy), 11 June 2012

8. "VEGA software"
Italian Chemometric Workshop, Pavia (Italy), 22 May 2012

7. "The VEGA platform: an open-source tool for the prediction of eco-toxicological endpoints"
Università di Milano-Bicocca, Milano (Italy), 27 October 2011

6. "Chemiometria e modellistica QSAR: metodi in silico per ridurre l'utilizzo di animali"
Training course: Colture cellulari: i metodi alternativi, Genova (Italy), 24 September 2010

5. "Metodologie in silico per ridurre e/o sostituire l'utilizzo di animali"
Training course: Sperimentazione animale: aspetti etici, normativi, scientifici, pratici e di sicurezza, Genova (Italy), 14 April 2010

4. "DART – Decision Analysis by Ranking Techniques"
MATH/CHEM/COMP 2008 Conference, Verbania (Italy), 10–13 June 2008

3. "MOLE DB – Molecular Descriptors online database"
Italian Chemometric Workshop, Pisa (Italy), 14-15 May 2008

2. "DART – Decision Analysis by Ranking Techniques"
Italian Chemometric Workshop, Pisa (Italy), 14-15 May 2008

1. "Analisi di correlazione di descrittori molecolari su grandi insiemi di dati"
Italian Chemometric Workshop, Modena (Italy), 15-16 February 2007