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Biography

Paola Gramatica is Full Professor of Environmental Chemistry, ex- Associate Professor of Organic Chemistry, at the University of Insubria (Varese-Italy). She has been the head of QSAR and Environmental Chemistry Research Unit at the Department of Structural and Functional Biology (DBSF) since 1995.

She graduated in Pure Chemistry in 1972 at the University of Milan, where she carried out research devoted to the biosynthesis, structural elucidation, synthesis, and biotransformation of organic natural products in the Department of Organic and Industrial Chemistry. She became an Associate Professor of Organic Chemistry in 1987 and Full Professor of Environmental Chemistry in 2005.

Since 1994 she has been working on QSAR and chemometric methods' applications to environmentally relevant organic compounds. She was scientifically responsible in 2 EU-Projects. She is author of about one hundred papers in international journals, peer reviewed.

She is member of the Directive Council of SETAC-Italian Branch, of the Editorial Board of Chemosphere and of SAR & QSAR in Environmental Research and referee of many scientific journals in environmental field. She is working as QSAR expert for the European Joint Research Centre (Ispra) and for OECD (Organization for Economic Cooperation and Development) in the validation of QSAR models for regulatory acceptance in the new policy of chemicals (REACH).

Research interests

The principal research interests are in the development of QSAR models by applying chemometric methods of regression and classification and holistic theoretical descriptors of the molecular structure of chemicals. The developed QSAR models are applied for the prediction of physico-chemical properties and biological activities of environmental pollutants (PAHs, PCBs, pesticides, aromatic and aliphatic organic compounds, etc.). Some applications of these studies deal with tropospheric oxidations of Volatile Organic Compounds (VOCs), Persistent Organic Pollutants (POPs) long-range transport and persistence, biodegradability, pesticide partition properties, aquatic toxicity and mixture toxicity (EU Projects PREDICT and BEAM), mutagenicity and Bioconcentration Factor modelling. The main field of research interest is relative to Persistent Bioaccumulative and Toxic (PBTs) chemicals. An important aspect of the research is the proposal of methods for the validation of QSAR models.

Teaching experience and appointments

The teaching activity is devoted to various courses related to the environmental pollution for Biology (Environmental Pollution and Ecotoxicology) and Engineering degrees, in particular: Environmental Chemistry I and II, Risk Assessment, Environmental Legislation and Certification, Analytical Chemistry and Chemometrics, in addition to the course of Organic Chemistry for Biology, Biotechnology and Analysis and Protection of Natural Resources. Paola Gramatica is Coordinator of Environmental Pollution and Ecotoxicology courses for the Degrees in Biology (undergraduate and graduate) and she represents the School of Sciences (Varese) in the International Relations Commission of the University of Insubria.

Representative publications

- 1) P.Gramatica, F.Villa and E.Papa
Statistically validated QSARs based on theoretical descriptors for the modelling of the aquatic toxicity of organic chemicals in Pimephales promelas (Fathead Minnow).
J. Chem. Inf. Model. 45,1256-1266. 2005
- 2) P.Gramatica and E. Papa
An update of the BCF QSAR model based on theoretical molecular descriptors.
QSAR & Combinatorial Science 24, 953-960, 2005
- 3) E.Papa, F.Battaini and P.Gramatica
Ranking of Esters' Aquatic Toxicity modelled by QSAR
Chemosphere 2005, Vol 58/5 pp 559-570.
- 4) P. Gramatica, E. Papa and F. Battaini
Ranking and classification of non-ionic organic pesticides for environmental distribution: a QSAR approach
Int. J. Environ. Anal. Chem. 84 (1-3): 65-74, 2004
- 5) E. Papa, S. Castiglioni, P. Gramatica, V. Dukhovny , O. Kayumov and D. Calamari
Screening the leaching tendency of pesticides applied in Amu Darya Basin (Uzbekistan)
Water Research , 38, 2004, 3485-3494.
- 6) P.Gramatica, P.Pilutti and E.Papa
Validated QSAR Prediction of OH Tropospheric degradability: splitting into training-test set and consensus modeling
J.Chem. Inf. Comp.Sci.. 44, 2004, 1794-1802.
- 7) P. Gramatica, P.Pilutti and E. Papa
A Tool for the Assessment of VOC Degradability by Tropospheric Oxidants Starting from Chemical Structure
Atm. Env 2004, 38(36), 6167-6175
- 8) P. Gramatica, F. Battaini and E. Papa
QSAR prediction of physico-chemical properties of esters
Fresenius Environmental Bulletin13, 2004, 1258-1262.

- 9) P. Gramatica, E. Papa and S. Pozzi
Prediction of POP environmental Persistence and Long Range Transport by QSAR and Chemometric Approaches
Fresenius Environmental Bulletin 13, 2004, 1204-1209.
- 10) A. Tropsha*, P. Gramatica*, and V. K. Gombar*
The Importance of Being Earnest: Validation is the Absolute Essential for Successful Application and Interpretation of QSPR Models
QSAR & Combinatorial Science., 22, 2003, 69-77.
- 11) P. Gramatica, P. Pilutti and E. Papa
QSAR Prediction of Ozone Tropospheric Degradation
QSAR & Combinatorial Science, 22, 2003, 364-373.
- 12) P. Gramatica and E. Papa
QSAR Modeling of Bioconcentration Factor by Theoretical Molecular Descriptors
QSAR & Combinatorial Science, 22, 2003, 374-385.
- 13) P. Gramatica, V. Consonni and M. Pavan
Prediction of Aromatic Amines Mutagenicity from Theoretical Molecular Descriptors
SAR & QSAR Env Res., 14, 2003, 237-250.
- 14) Paola Gramatica, Pamela Pilutti and Ester Papa
Predicting the NO₃ Tropospheric Degradability of Organic Pollutants by Theoretical Molecular Descriptors
Atm. Environ., 37 (22) , 2003, 3115-3124.
- 15) L. Eriksson, J. Jaworska, A. Worth, M. Cronin, R.M McDowell and P. Gramatica
Methods for reliability, uncertainty assessment, and applicability evaluations of regression based and classification QSARs
Envir. Health Perspectives, 111 (10): 1361-1375 AUG 2003
- 16) Backhaus, T., Altenburger, R., Arrhenius, ., Blanck, H., Faust, M., Finizio, A., Gramatica, P., Grothe, M., Junghans, M., Meyer, W., Pavan, M., Porspring, T., Scholze, M., Todeschini, R., Vighi, M., Walter, H.. and Grimme, L.H.
The BEAM-project: prediction and assessment of mixture toxicities in the aquatic environment.
Continental Shelf Research 23 (17-19): 2003, 1757-1769,
- 17) M.Vighi, R. Altenburger, A. Arrhenius, T.Backhaus, W.Bodeker, H.Blanck, F.Consolaro M.Faust, A.Finizio, K.Froehner, P.Gramatica, L.H.Grimme, F.Gronvall, V.Hamer, M.Scholze and H.Walter
Water quality objectives for mixtures of toxic chemicals: problems and perspectives.
Ecotox. and Environ. Safety, 54, 2003, 139-150.
- 18) P. Gramatica, S.Pozzi, V.Consonni and A. Di Guardo
Classification of environmental pollutants for global mobility potential

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19) P. Gramatica and A. Di Guardo
Screening of pesticides for environmental partitioning tendency
Chemosphere , 47, (2002), 947-956.

20) P. Gramatica, A.Santagostino, E. Bolzacchini and B. Rindone
Atmospheric monitoring toxicology and QSAR modelling of nitrophenols
Fresenius Environ. Bull. 11, (2002) , 757-762.

21) P. Gramatica, P. Pilutti and E. Papa
Ranking of Volatile Organic Compounds for Tropospheric Degradability by
Oxidants: a QSPR Approach.
SAR & QSAR Env Res., 13, 2002, 743-753.

22) P.Gramatica, M.Corradi and V.Consonni
Modelling and prediction of soil sorption coefficients of non-ionic organic pesticides
by different sets of molecular descriptors. Chemosphere, 41 (5) (2000) 763-777.

23) P.Gramatica, M.Vighi, F.Consolaro, R.Todeschini, A.Finizio and M.Faust
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toxicological mode of action.
Chemosphere, 42 (2001), 873-883.

24) P.Gramatica, F.Consolaro and S.Pozzi
QSAR approach to POPs screening for atmospheric persistence. Chemosphere,
(2001) 43/4-7, 655-664.

25) M.Vighi, P.Gramatica, F.Consolaro and R.Todeschini
QSAR and chemometric approaches for setting water quality objectives for
dangerous chemicals.
Ecotox and Environ Safety, 49, (2001)206-220.

26) P.Gramatica, V.Consonni and R.Todeschini
QSAR Study of the Tropospheric Degradation of Organic Compounds
Chemosphere, 38 (1999), 1371-1378.

27) P.Gramatica, N.Navas and R.Todeschini
Classification of organic solvents and modelling of their physico-chemical
properties by chemometric methods using different sets of molecular descriptors.
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28) E.Bolzacchini, V.Consonni, P.Gramatica, S.Meinardi, M.Orlandi, B.Rindone
and R.Todeschini
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Characterization and use of B-lactam and B-Lactam Metabolite Poly-L-Lysines
which Recognize Human IgE Antibodies. Bioconjugate Chemistry, 10 (3) (1999)
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29) P.Gramatica, N.Navas and R.Todeschini
3D-modelling and prediction by WHIM descriptors. Part 9. Chromatographic
relative retention time and physico-chemical properties of polychlorinated
biphenyls (PCBs).
Chemom. Intell. Lab. Sys., 40 (1998) 53-63

30) R.Todeschini and P.Gramatica
New 3D-molecular descriptors: the WHIM theory and QSAR applications.
In 3D-QSAR in Drug Design, Vol.2 (Ed.H.Kubinyi, G.Folkers and Y.C.Martin),
KLUWER/ESCOM, (1998), 355-380.