

## CV of PAOLA GRAMATICA

Paola Gramatica is full professor of Environmental Chemistry at Insubria University (Varese, Italy), Delegate of the Rector for International Relationships. She was Director of the Structural and Functional Biology Department (DBSF) of Insubria Univ. in 2007-2010.

She is leader of the QSAR Research Unit in Environmental Chemistry and Ecotoxicology (since 1997), now in the Department of Theoretical and Applied Sciences (DiSTA).

She is author of more than 150 scientific papers on ISI international journals (about 7000 citations and h index= 38 in Web of Science, about 10000 citations and h= 44 in Google Scholar, February 2017), four chapters on her researches in scientific books and more than 300 presentations to meetings (some invited plenary conference), mainly in applications of QSAR (Quantitative Structure - Activity Relationships) models to environmental chemicals topics. The QSARINS software is the main outcome of the last 20 years of experience in validated QSAR modeling.

PG is included in the list of Top Italian Scientists.

### **EDUCATION**

Graduation in Pure Chemistry (Organic Natural Compounds) cum laude - 1972, University of Milan.

### **EMPLOYMENT**

#### ***-Full Professor of Environmental Chemistry and Cultural Heritage***

Department of Theoretical and Applied Sciences (Environmental and Natural Sciences courses) – **2012- present**

Faculty of Sciences (Biology, Biotechnology, Natural Sciences and Environmental Engineer courses) Insubria University- **2005-2012**

#### ***-Associate Professor of Organic Chemistry 1995 –2005***

Faculty of Sciences (Biology, Biotechnology, Natural Sciences courses) Insubria University

#### ***-Researcher in Organic Chemistry 1981- 1995***

Department of Organic and Industrial Chemistry, Milano University (winner of Associate Professor competition in **1987**).

#### ***-Research Contractor in Organic Chemistry 1975-1981***

Department of Organic Chemistry, Milano University

#### ***-Fellowship (Lincoln Nat. Acad. and MIUR) 1972-1975***

Natural Organic Chemistry Institute, Milano University

### **Professional Qualifications and Associations:**

- Member of the Italian Chemical Society (SCI)
- Member of the Managing Board of the Interdivisional Group of Green Chemistry (SCI) (2006-2009, 2016-2018)

- Member of the Managing Board of the Environmental and Cultural Heritage Div. of SCI (2006-2009)
- Member of the Society of Environmental Toxicology and Chemistry (SETAC).
- Member of the Directive of the SETAC-Italian Branch
- Member of the Cheminformatics and QSAR Society
- Member of the Mediterranean Scientific Association of Environmental Protection (MESAEP)
- Member of the OECD Expert Group on Quantitative Structure-Activity Relationships (QSARs) (2002-2006)

### **Membership of Editorial Boards:**

- Molecular Informatics
- Sustainable Chemistry and Pharmacy
- Chemical Processes and Materials
- The Open Applied Informatics Journal (TOAINFOJ)
- SAR and QSAR in Environmental Research (2002-2011)
- Chemosphere (2005-2007)
- Guest Editor of Environmental Science and Pollution Research 2006 (Special Issue and Sections in memory of Prof. Davide Calamari)
- Referee of many (more than 50) international scientific journals in environmental field and chemical application of computer science (cheminformatics).
- Referee of scientific project proposals for different countries.
- Scientific responsible or Workpackage leader in 3 EU-Projects (FP4- PREDICT, FP5-BEAM and FP7-CADASTER).

### **Research interests:**

At the University of Milan PG carried out researches on the biosynthesis, structural elucidation, synthesis, and biotransformation of organic natural products in the Department of Organic and Industrial Chemistry till 1994.

Her present research field in University of Insubria, where she is leading the QSAR Research Unit in Environmental Chemistry and Ecotoxicology, is on QSAR modelling of organic environmental pollutants. Different classes of organic compounds (POPs, PBTs, PAHs, Pesticides, EDs, etc.) have been studied by chemometric/QSAR approaches to highlight the relationship between molecular structure and various physico-chemical and analytical properties or biological activities, such as persistence, biodegradability, toxicity, mutagenicity, endocrine disruption properties, etc.

Applications of these studies deal with tropospheric oxidations of Volatile Organic Compounds (VOCs), Persistent Organic Pollutants (POPs) long-range transport and

persistence, pesticide partition properties, mutagenicity/carcinogenicity of PAHs/PACs, Bioconcentration Factor (BCF) and Endocrine Disruptors Chemicals (EDCs) modeling. The main field of interest is relative to Persistent Bioaccumulative and Toxic (PBTs) chemicals. Last group of chemicals, studied for their environmental concern as emerging pollutants, are pharmaceuticals and personal care products (PPCPs). An important aspect of the research is the proposal of methods for the validation of QSAR models: the papers on QSAR validations have thousands of citations in the literature.

Her group has been involved in two EU Projects (FP4-PREDICT and FP5-BEAM) on aquatic toxicity and mixture toxicity. She was leader of a Workpackage on QSAR modeling in the EU-FP7 Project CADASTER for REACH and in a PRIN project for PBT and ED modelling also for REACH. Paola Gramatica has worked as QSAR expert for the European Joint Research Centre (Ispra) and was a selected member of the OECD Task Force of QSAR Experts for the definition of the OECD principles for QSAR validation for regulation applicability. PG has many international collaborations (in EU, but also in China, USA, Canada and India).

### **Teaching experience and appointments**

The teaching activity, in the past on Organic Chemistry courses, is now devoted to courses on Environmental Chemistry and Basis of Chemometrics for Environmental Sciences, Biology and Engineering for Environmental and Work Safety degrees. Paola Gramatica was Coordinator of Environmental Pollution and Ecotoxicology curricula for the Degrees in Biology (Bachelor and Master). She is Professor in the Chemistry and Environmental Science PhD degree and in the Specialization School for Assessment and Management of Chemical Risk.