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Biography

Dr. Ester Papa was born in Varese (Italy) in 1977. She graduated cum Laude in Biology in 2001 at the University of Insubria (Varese, Italy) with a thesis entitled "Environmental fate of persistent organic pollutants: a QSAR approach". In 2005, at the same university, she completed her PhD-thesis entitled "QSAR approach to Persistent, Bioaccumulable, and Toxic (PBT) organic pollutants, sources of biodiversity stress", obtaining a PhD in "Analysis, Protection and Management of Biodiversity".

She was a Post-Doctoral fellow at the University of Insubria, (2005-2008) on the project entitled "QSAR modelling of toxicity, physico-chemical properties and environmental behaviour of organic pollutants adsorbed to air particulate matter". Since January 2009 she is Assistant Professor of Environmental Chemistry (CHIM/12) at the University of Insubria of Varese (Italy); her research activity takes place at the department of Structural and Functional Biology of - QSAR Research Unit in Environmental Chemistry and Ecotoxicology.

Dr. Papa is involved in national and international research projects (PRIN project, 2008-2010; FP7 project CADASTER, 2009-2012).

She is a member of the Society of Environmental Toxicology and Chemistry (SETAC) and of the Italian Chemistry Society (SCI) since 2001 and she is a referee for the Journal of Pharmaceutical and Biomedical Analysis, Analytical and Bioanalytical Chemistry, Analytica Chimica Acta, Ecotoxicology and Environmental Safety, Journal of Molecular Graphics and Modelling, Environmental Science and Technology.

Qualifications and awards

2001. Degree in Biological Sciences from the University of Insubria (Varese)

2005. PhD in "Analysis, Protection and Management of Biodiversity" from the University of Insubria (Varese).

During her PhD studies she spent a total of six months working at the John Moores University (Liverpool, UK), in the QSAR and Modelling Group under the supervision of Dr. Mark T.D. Cronin, and at the Umeå University (Umeå, Sweden), in the Miljöökemi research unit under the supervision of Dr. Patrik Andersson.

She received the best poster presentation award at the 10th EuChEMS-DCE International Conference in Rimini (2005) with a poster entitled: "Organic pollutant uptake and bioconcentration in vegetation".

Research interests

During her current research she applies QSAR (Quantitative Structure-Activity Relationships) and multivariate analysis to different topics related to environmental pollution such as:

- The environmental partitioning of pesticides
- Atmospheric reactivity of Volatile Organic Compounds (VOCs)
- Environmental fate of Persistent Organic Pollutants (POPs)
- Bioconcentration of organic pollutants in aquatic organisms
- Toxicity of organic pollutants to aquatic organisms
- Screening and prioritization of Persistent, Bioaccumulative and Toxic compounds (PBTs) and POPs for regulatory purposes
- Environmental fate of pharmaceuticals and endocrine disruptors

Teaching experience and appointments

Since her graduation she supervised students, first level and second level Degree in Biological Sciences, and she took part in teaching activities with seminars for the Environmental Chemistry, and the Risk assessment courses and lectures for the Ecotoxicology course (University of Insubria, Varese)

During aa. 2007/2008 and aa. 2008/2009 (first semester) Dr. Ester Papa officially worked at the University of Insubria (Varese) as contract professor. She taught courses “Ecotoxicology (mod. B – 2CFU)”, “Applied Ecotoxicology (Mod. A – 1 CFU)” and “Chemical Risk Assessment (2 CFU)” to the students of the first level (bachelor) and second level (master) Degree in Biological Sciences.

Since January 2009 she also teaches “Chemometrics” (Mod. B of the course “Environmental chemistry and Chemometrics”– 3 CFU)” to the students of the second level Degree in Biological Sciences

Representative publications

1. P. Gramatica, P. Pilutti and E. Papa. Ranking of Volatile Organic Compounds for Tropospheric Degradability by Oxidants: a QSPR Approach. *SAR QSAR Environ. Res.*, 13, **2002**, 743-753.
2. P. Gramatica, P. Pilutti and E. Papa. QSAR Prediction of Ozone Tropospheric Degradation. *QSAR & Combinatorial Science*, 22, **2003**, 364-373.
3. P. Gramatica and E. Papa. QSAR Modeling of Bioconcentration Factor by Theoretical Molecular Descriptors *QSAR & Combinatorial Science*, 22, **2003**, 374-385.
4. P. Gramatica, P. Pilutti and E. Papa. Predicting the NO₃ Tropospheric Degradability of Organic Pollutants by Theoretical Molecular Descriptors. *Atmospheric Environment.*, 37 (22), **2003**, 3115-3124.
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. *Journal of Chemical Information and Computer Sciences*, 44, **2004**, 1794-1802.
7. 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.

8. E. Papa, F. Battaini and P. Gramatica. Ranking of Esters' Aquatic Toxicity modelled by QSAR. *Chemosphere* **2005**, Vol 58/5, 559-570.
9. P. Gramatica and E. Papa. An update of the BCF QSAR model based on theoretical molecular descriptors. *QSAR and Combinatorial Science*, **24**, **2005**, 953-960.
10. E. Papa, F. Villa and P. Gramatica. Statistically validated QSARs, based on theoretical descriptors, for modeling aquatic toxicity of organic chemicals in Pimephales promelas (Fathead Minnow), *Journal of Chemical Information and Modeling*, **45**, **2005**, 1256-1266.
11. H. Liu, E. Papa, P. Gramatica. QSAR Prediction of Estrogen Activity for a Large Set of Diverse Chemicals under the Guidance of OECD Principles. *Chemical Research in Toxicology*, **2006**, **19**, 1540-1548.
12. P. Gramatica, F. Battaini, E. Giani, E. Papa, RJA Jones, D. Preatoni, RM Cenci. Analysis of mosses and soils for quantifying heavy metal concentrations in Sicily: A multivariate and spatial analytical approach. *Environmental Science and Pollution Research*, **2006**, **13**, **1**, 28-36
13. S. Banfi, E. Caruso, L. Buccafurni, R. Murano, E. Monti, M. Gariboldi, E. Papa, P. Gramatica. Comparison between 5,10,15,20-tetraaryl- and 5,15-diarylporphyrins as photosensitizers: Synthesis, photodynamic activity, and quantitative structure-activity relationship modeling, *Journal of Medicinal Chemistry*, **2006**, **49**, **11**, 3293-3304
14. H. Liu, E. Papa, Walker J, P. Gramatica. In silico Screening of Estrogen-Like Chemicals Based on Different Nonlinear Classification Models, *Journal of Molecular Graphics and Modelling*, **2007**, **26**, 135-144.
15. P. Gramatica, E. Papa. Screening and ranking of POPs for Global Half-Life: QSAR approaches for prioritisation based on molecular structure, *Environmental Science and Technology*, **2007**, **41**, 2833-2839.
16. E. Papa, J. Fick, R. Lindberg, M. Johansson, P. Gramatica, P. L. Andersson. Multivariate chemical mapping of antibiotics and identification of structurally representative Substances. *Environmental Science and Technology*, **2007**, **41**, 1653-1661.
17. P. Gramatica, E. Giani, E. Papa. Statistical external validation and consensus modeling: A QSPR case study for Koc prediction *Journal of Molecular Graphics and Modelling* **2007**, **25**, 755-766.
18. E. Papa, J. Dearden, P. Gramatica. Linear QSAR regression models for the prediction of bioconcentration factors by physicochemical properties and structural theoretical molecular descriptors. *Chemosphere*, **2007**, **67**, 351-358.
19. P. Gramatica, P. Pilutti, E. Papa. Approaches for externally validated QSAR modeling of Nitrated Polycyclic Aromatic Hydrocarbon mutagenicity *SAR QSAR Environ. Res.*, **2007**, Vol. 18 (1-2), 169-178.
20. P. Gramatica, E. Papa, A. Marrochi, L. Minuti, A. Taticchi. QSAR Modelling of PAH Mutagenicity by Classification Methods based on Holistic Theoretical Molecular Descriptors, *Ecotoxicology and Environmental Safety*, **2007**, **66**, 353-361.
21. H. Liu, E. Papa, P. Gramatica. Evaluation and QSAR modeling on multiple endpoints of estrogen activity based on different bioassays, *Chemosphere*. **2008**, **70**, 1889-97.
22. H. Zhu, A. Tropsha, D. Fourches, A. Varnek, E. Papa, P. Gramatica, T.

- Öberg, P. Dao, A. Cherkasov, I. Tetko. Combinational QSAR Modeling of Chemical Toxicants Tested against *Tetrahymena pyriformis*, *Journal of Chemical Information and Modeling*, **2008**, 48, 766-784.
23. IV. Tetko. I. Sushko, AK Pandey H. Zhu, A. Tropsha, E. Papa, T. Öberg, R. Todeschini, D. Fourches, A. Varnek, Critical assessment of QSAR models of environmental toxicity against *Tetrahymena pyriformis*: Focusing on applicability domain and overfitting by variable selection *Journal of Chemical Information and Modeling*, **2008**, 48, 1733-1746.
24. E. Papa, P. Pilutti, P. Gramatica. Prediction of PAH mutagenicity in human cells by QSAR classification, *SAR QSAR Environ. Res.*, **2008**, 19, 115-127.
25. E. Papa, P. Gramatica. Screening of persistent organic pollutants by QSPR classification models: a comparative study *Journal of Molecular Graphics and Modelling*, **2008**, 27, 59-65.
26. E. Papa, P. Gramatica. Externally validated QSPR modelling of VOC tropospheric oxidation by NO₃ radicals *SAR QSAR Environ. Res.*, **2008**, Vol. 19 (7-8), 655-668