Dr. Ana Maldonado

Researcher in Chemoinformatics

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I am a senior scientist at the Solvay Laboratory of the Future (LOF), currently as a visitor researcher at the University of Amsterdam where I collaborate with a multidisciplinary team to address industrial problems applying chemometrics and modeling.

I love to make ideas happen by building projects and bringing people together. My strengths are good network abilities, an enthusiastic and open mind, and a love for multidisciplinary approaches. I have experience on structuring and management of new projects, from defining the ideas to raising the necessary funds. I also have broad experience on (chemical) data management, data valorization, predictive modeling and writing of research deliverables (reports, publications and patents).

PROFESSIONAL EXPERIENCE

since 2009 Senior scientist at Solvay. Visitor researcher at HCSC. *LOF Bordeaux (FR) and UvA HIMS, Amsterdam (NL)*

Key responsibilities turn around assisting our GBU clients in their predictive modeling and chemometric needs to address a wide range of molecular discovery and optimization projects of industrial interest. A dozen of projects and few years later, I have gain experience in areas as diverse as photovoltaic chemistry, surfactant and solvent formulation, catalysis and eco-toxicology.

2007- 2009 Post-doctoral researcher. Joint project UvA - Rhodia. "Rational Design and synthesis of new and efficient hydrocyanations catalysts". *UvA HIMS, Amsterdam (NL)*

As a researcher within the Heterogeneous Catalysis and Sustainable Chemistry (HCSC) group I collaborated with a board of industrial experts at Rhodia. Using virtual molecular design and predictive modeling engines we found new hydrocyanation catalysts for the production of butiadene a key compound for the Nylon 6,6 production. Results lead to a patent and three publications.

2002-2006 PhD in Theoretical and Computational Chemistry. *ITODYS Laboratory (CNRS, UMR 7086), University Paris 7-Denis Diderot (FR)*

During my PhD at the University Paris 7-Denis Diderot, I designed and implemented a virtual screening tool called MolDiA (Molecular Diversity Analysis). This is one of the only structure-based approaches that use customizable weights on molecular descriptors to compute similarity and diversity measures of given datasets. Applications include the development of QSAR models, fast identification of potential lead compounds and optimal library design. Results lead to four publications.

2002-2005 Physical Chemistry teacher. *Sainte Clotilde High School, Paris (FR)*

During my PhD at the University Paris 7-Denis Diderot, I decided to give Physical Chemistry lessons to high school kids as a way to support myself and gain insights in French culture and language. This was a real challenge that allowed me to dramatically improve my French within months and enriched my experience as a student in France.

1998-2001 Assistant professor for Chemistry, Mathematics and Physical Chemistry. *USB, Caracas (VZLA)*

EDUCATION AND COURSES

Jan 2009 Tutorial: Understanding Molecular Simulations,
UvA, Amsterdam (NL)

Nov 2008 MATLAB based Optimization Techniques, Statistical Methods in MATLAB,
Euston Conference Center, London (UK)

Sept 2006 PhD degree in Theoretical and Computational Chemistry, obtained with honors.
ITODYS Laboratory (CNRS, UMR 7086), University Paris 7-Denis Diderot (FR)

Mai 2002 Chemistry degree, (B.Sc and M. Sc), obtained with honors.
University Simon Bolívar (USB), Caracas (VZLA)

SKILLS AND ATTRIBUTES

● **Relational:** Aptitude to work in multidisciplinary teams. Social, collaborative and enthusiastic. Organized and structured but flexible and dynamic. High capacity to adapt to changes. Independent without detachment of the surrounding. Solution oriented. Creative and idealistic.

● **Scientific:** Broad experience on management, analysis and mining of data. Expertise on predictive modeling, descriptor analysis and QSAR/QSPR model construction and validation, as well as, on the design and generation of virtual databases. Experience in the use and implementation of Semantic Web Technologies (XML, RDF, CML) in a chemical framework. Skilled in writing of research deliverables (reports, publications and patents).

Good knowledge of programming languages (C, C++, Visual Basic, Visual Studio, Latex), chemometric and statistical tools (MatLab, MathCad, S-Plus, Minitab, ISIS-Draw, Hyperchem, ChemSketch, ChemWindow, ChemAxon, Codessa, etc.).

● **Human:** Support non-governmental organizations which fight for children rights and health in the word. Experience as volunteer in different humanitarian projects (Venezuela and Thailand). Hobbies include swimming, traveling, gardening, reading, and more recently sailing and snowboarding.

● **Foreign languages:** Spanish (natural language), French and English (bilingual), Italian and Dutch (goods notions), Chinese and Grec (notions).

PUBLICATIONS

1. Zea Strassberger, Maurice Mooijman, Eelco Ruijter, Albert H. Alberts, Ana G. Maldonado, Romano Orru, Gadi Rothenberg. Finding furfural hydrogenation catalysts via predictive modeling. Adv. Synt. Cat. 352(13): 2201-2210 (2010)

2. Ana. G. Maldonado, Gadi Rothenberg. Predictive modeling in homogeneous catalysis: a tutorial. Chem. Soc. Rev. 39: 1891-1902 (2010).

3. Ana. G. Maldonado, Gadi Rothenberg. Predictive modelling in catalysis – from dream to reality. Chem. Eng. Proc. June (2009).

4. Ana G. Maldonado, Jos A. Hageman, Sergio Mastroianni, Gadi Rothenberg. Backbone Diversity Analysis in Catalyst Design. Adv. Synth. Cat. Adv. Synth. Catal. 351: 387-396 (2009).

5. Carles Bo, Manuel Urbano Cuadrado, Jorge Carbó and Ana G. Maldonado. New Quantum Mechanics-Based Three-Dimensional Molecular Descriptors for Use in QSSR Approaches: Application to Asymmetric Catalysis J. Chem. Inf. Model.47(6): 2228-2234 (2007).

6. Ana G. Maldonado, Jean-Pierre Doucet, Michel Petitjean and Bo-Tao Fan. MolDiA: A Novel Molecular Diversity Analysis Tool. Part 1: Principles and Architecture. J. Chem. Inf. Model.47(6): 2197-2207 (2007).

7. Ana G. Maldonado, Michel Petitjean, Jean-Pierre Doucet, Annick Panaye and Bo Tao Fan. MolDIA: XML based system of molecular diversity analysis towards virtual screening and QSPR. SAR and QSAR in Environmental Research 17(1): 11-23 (2006).

8. Ana G. Maldonado, Michel Petitjean, Jean-Pierre Doucet and Bo Tao Fan. Molecular Similarity and Diversity: Concepts and Applications. Review article, Molecular Diversity, 10(1): 39-79 (2006).

9. Ana G. Maldonado, Using XML for Structuring the Chemical Information: Towards a Chemical Knowledge Representation. Long paper published by MDPI. Online Edition ISBN 3-906980-17-0 (2005).

10. Ana G. Maldonado and J.L.Paz, Study of the solvent stochastic effects in a strongly driven two level system in Four Wave Mixing spectroscopy .Short paper published by the International Society for Optical Engineering (SPIE). Ed. Proceeding SPIE, 4419: 34-37 (2001).

PATENTS

1. S. Mastronianni, P. Pringle, A. Maldonado, G. Rothenberg, I. Mikhel. March 24th (2011) Organophosphorus compounds, catalytic systems including said compounds, and hydrocyanation method using said catalytic systems. Patent No.: WO/2011/032835. PCT/EP2010/062755.

2. F. Decampo, G. Mignani, B. Pavageau, A. Maldonado. Avril 20th (2012) Accepteurs quinones pour application photovoltaique. Patent depot R12045.

More Information available at http://www.agmaldonado.com
References available upon request