Welcome to Marrero's Home Page

Prof. Yovani Marrero Ponce BSc, MSc, PhD

Professor of Pharmacology, Biochemistry, Organic and Medicinal Chemistry

Drug Discovery and Molecular Design, Chem-Bio-Informatic, Chemometric, Molecular Modelling, Computational and Theoretical Chemistry Specialist

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QUALIFICATIONS

Bachelor of Science (B.Sc): Pharmaceutical Sciences, Central University of Las Villas, Santa Clara, Villa Clara, Cuba, 7/01.

Golden Award for Academia Results, 7/01.

Master of Science (M.Sc): Biochemistry, Medical University "Dr. Serafin Ruiz de Zarate Ruiz", Santa Clara, Villa Clara, Cuba. 1/02-2/04.

Philosophical Doctor (Ph.D): Chemical Sciences, Havana University, Havana City, Cuba. 7/05.

EXPERTISE AND CURRENT WORK INTERESTS

Teaching main interests: My current teaching interests include the organic, bioorganic, pharmaceutical and medicinal chemistry as well as "rational" drug design. More recently, I am also interested in the teaching of the molecular pharmacology and biochemistry.

Research main interests: My current research interests are in the area of drug discovery, specifically the development of new computational methods for chem-bio-informatics investigations. In this sense, I'm also interested in the development of novel molecular and macromolecular (proteins and nucleic acids) descriptors for using in the development of QSPR/QSAR, "rational" (computer-aided) drug design, characterization of molecular similarity, computational (virtual and *in silico*) screening, proteins and nucleic acids classification, macromolecule-drug interactions, folding degree description, and early pharmacokinetics and toxicity prediction. More recently, I am also interested in comparative modelling, and docking and scoring. These research areas (plus QSAR/QSPR) are powerful when used individually, but their true power is exploited when they are used together to provide a complete story of the interaction of a ligand with its receptor.

Some Recent Publication…

Marrero-Ponce, Y.; *et al.* 3D-Chiral Quadratic Indices of the "Molecular Pseudograph's Atom Adjacency Matrix" and their Application to Central Chirality Codification: Classification of ACE Inhibitors and Prediction of σ-Receptor Antagonist Activities. *Bioorg. Med. Chem.* **2004,** *12*, 5331-5342.

Marrero-Ponce, Y. Linear Indices of the "Molecular Pseudograph's Atom Adjacency Matrix": Definition, Significance Interpretation and Application to QSAR Analysis of Flavone Derivatives as HIV-1 Integrase Inhibitors. *J. Chem. Inf. Comput. Sci*. **2004**, *44*, 2010-2026.

Marrero-Ponce, Y.; *et al. TOMOCOMD-CARDD*, a Novel Approach for Computer-Aided "Rational" Drug Design: I. Theoretical and Experimental Assessment of a Promising Method for Computational Screening and *in silico* Design of New Anthelmintic Compounds. *J. Comput. Aided Mol. Des.* **2004**, *18*, 615-633.

Marrero-Ponce, Y.; *et al.* Protein Linear Indices of the "Macromolecular Pseudograph's α-Carbon Atom Adjacency Matrix" in Bioinformatics. Part 1. Prediction of Protein Stability Effects of a Complete Set of Alanine Substitutions in Arc Repressor. *Bioorg. Med. Chem.* **2005**, *13*, 3003-3015.

Marrero-Ponce, Y.; *et al.* Ligand-Based Virtual Screening and *in silico* Design of New Antimalarial Compounds Using Non-Stochastic and Stochastic Total and Atom-type Quadratic Maps. *J. Chem. Inf. Comput. Sci*. **2005**, *45*, 1082-1100.

Marrero-Ponce, Y.; *et al.* A Computer-Based Approach to the Rational Discovery of New Antitrichomonas Drugs by Atom-Type Linear Indices. *Current Drug Discovery Technologies.* **2005**, *2*, 245-265.

Marrero-Ponce, Y.; *et al.* Non-Stochastic and Stochastic Linear Indices of the Molecular Pseudograph's Atom Adjacency Matrix: A Novel Approach for Computational *–in silico-* Screening and "Rational" Selection of New Lead Antibacterial Agents. *J. Mol. Mod.* **2006**, *12*, 255-271.