Welcome to Castillo's Home Page

Prof. Juan Alberto Castillo Garit BSc,

Professor of Toxycology, 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.

EXPERTISE AND CURRENT WORK INTERESTS

Teaching main interests: My current teaching interests include general toxicology and ecotoxicology. I am also interested in the organic, bioorganic, pharmaceutical and medicinal chemistry as well as "rational" drug design.

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, I am also interested in ecotoxicological predictions. 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.; **Castillo-Garit, J. A.**; Olazabal, E.; *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, 615-634.*

Marrero-Ponce, Y.; **Castillo-Garit, J. A.**; Torrens, F. *et al*. Atom, Atom-Type, and Total Linear Indices of the "Molecular Pseudograph's Atom Adjacency Matrix": Application to QSPR/QSAR Studies of Organic Compounds**.** *Molecules.* **2004**, *9,* 1100-1123.

Marrero-Ponce, Y.; **Castillo-Garit, J. A.**; Olazabal, E.; *et al.* **A**tom, Atom-Type and Total Molecular Linear Indices as a Promising Approach for Bioorganic & Medicinal Chemistry: Theoretical and Experimental Assessment of a Novel Method for Virtual Screening and Rational Design of New Lead Anthelmintic. *Bioorg. Med. Chem*. **2005**, *13*, 1005-1020.

Marrero-Ponce, Y., Medina, R., **Castillo-Garit, J.A.**., *et al.* Protein linear indices of the 'macromolecular pseudograph 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., **Castillo-Garit, J.A.** & Nodarse, D. Linear indices of the 'macromolecular graph's nucleotides adjacency matrix' as a promising approach for bioinformatics studies. Part1: Prediction of paromomycin's affinity constant with HIV-1 Ψ-RNA packaging region. *Bioorg. Med. Chem*. **2005**, *13*, 3397-3404.

Marrero-Ponce, Y. & **Castillo-Garit, J. A.** 3D-chiral atom, atom-type, molecular linear indices and their applications to central chirality codification. *J. Comput. Aided Mol. Des*. **2005,** *19*, 369-383.

Castillo-Garit, J. A., Marrero-Ponce, Y. & Torrens, F. Atom-based 3D-chiral quadratic indices. Part 2: Prediction of the corticosteroid-binding globulin binding affinity of the 31 benchmark steroids data set. *Bioorg. Med. Chem*. **2006**, *14*, 2398-2408.