Welcome to Gerardo's Home Page

Prof. Gerardo Maikel Casañola Martin, BSc.
Professor of Organic, Inorganic and Analytical 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): Chemistry, Central University of Las Villas, Santa Clara, Villa Clara, Cuba, 7/03.

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.

Research main interests: My current research interests are in the area of drug discovery, specifically the identification through computational methods of novel inhibitors of the enzyme tyrosinase as well as virtual screening studies to select new more potent, effective, and selective compounds with such activity, which could become in leads or drug-like compounds. Tyrosinase is a enzyme widely distributed in the phylogenetic scale, and is involve in melanogenesis processes in human beings, browning in vegetables and plants; and encapsulation, sclerotization and wound healing in insects, for that reason, inhibitors of the enzyme could have many uses and potential applications in the treatment of hyperpigmentation and skin disorders, in food additives and as alternative to control of insects pests. 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.

Some Recent Publication…

Casañola-Martín, G. M.; Khan, M. T. H.; Marrero-Ponce, Y.; Ather, A.; Sultankhodzhaev, M. N.; Torrens, F. New tyrosinase inhibitors selected by atomic linear indices-based classification models. *Bioorg. Med. Chem. Lett.* 2006, *16*, 324-330.

Marrero-Ponce, Y.; Khan, M. T. H.; **Casañola-Martín, G. M**.; Ather, A.; Sultankhodzhaev, M. N.; Torrens, F. Atom-based 2D Quadratic Indices in Drug Discovery of Novel Tyrosinase Inhibitors. Result of in silico Studies Supported by Experimental Results. *QSAR. Comb. Sci.* Accepted for publication

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