Welcome

Prof. Maykel Cruz Monteagudo BSc

Professor of Toxicology

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

Mailing Address

Applied Chemistry Research Center and Unit of Computer-Aided Molecular "*Biosilico*" Discovery and Bioinformatic Research (**CAMD-BIR Unit**), Faculty of Chemistry-Pharmacy & Department of Drug Design, Chemical Bioactive Center. Central University of Las Villas, Santa Clara, 54830, Villa Clara, Cuba.

Contact Information

Fax: 53-42-281130 (Cuba), Phone: 53-42-281510 (Cuba), and *e*-mails: **gmailkelcm@yahoo.es**

QUALIFICATIONS

Bachelor of Science (B.Sc): Pharmaceutical Sciences, Central University of Las Villas, Santa Clara, Villa Clara, Cuba, 7/03.

Golden Award for Academia Results, 7/03.

EXPERTISE AND CURRENT WORK INTERESTS

Teaching main interests: My current teaching interests include the toxicological sciences, 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 approaches for chem-bio-informatics investigations in the field of early pharmacokinetics and toxicity prediction. In this sense, I'm also interested in the application of computational methods (including multivariate statistical techniques, as well as Artificial Intelligence techniques) for using in the development of QSPR/QSAR, "rational" drug design, characterization of molecular similarity, computational (virtual and *in silico*) screening and proteins and nucleic acids classification.

Some Recent Publication…

- Humberto Gonzáles-Díaz, Ornella Gia, Eugenio Uriarte, Ivan Hernádez, Ronal Ramos, Mayrelis Chaviano, Santiago Seijo, Juan A. Castillo, Lázaro Morales, Lourdes Santana, Delali Akpaloo, Enrique Molina, **Maikel Cruz**, Luis A. Torres, Miguel A. Cabrera. Markovian chemicals "in silico" design (MARCH-INSIDE), a promising approach for computer-aided molecular design I: discovery of anticancer compounds. *Journal of Molecular Modelling*, **2003**, *9*, 395-407.
- Humberto González-Díaz, **Maykel Cruz-Monteagudo**, Reinaldo Molina, Esvieta Tenorio and Eugenio Uriarte. Predicting multiple drugs side effects with a general drug-target interaction thermodynamic Markov model. *Bioorganic & Medicinal Chemistry*. **2005**, *13*, 1119-1129.
- Humberto González-Díaz, **Maykel Cruz-Monteagudo**, Dolores Viña, Lourdes Santana, Eugenio Uriarte and Erik De Clercq. QSAR for anti-RNA-virus activity, synthesis, and assay of anti-RSV carbonucleosides given an unify representation of spectral moments, quadratic, and topologic indices. *Bioorganic & Medicinal Chemistry Letters*. **2005**, *15*, 1651-1657.
- **Maykel Cruz-Monteagudo**, Humberto González-Díaz. Unified drug–target interaction thermodynamic Markov model using stochastic entropies to predict multiple drugs side effects. *European Journal of Medicinal Chemistry*. **2005**, *40*, 1030-1041.