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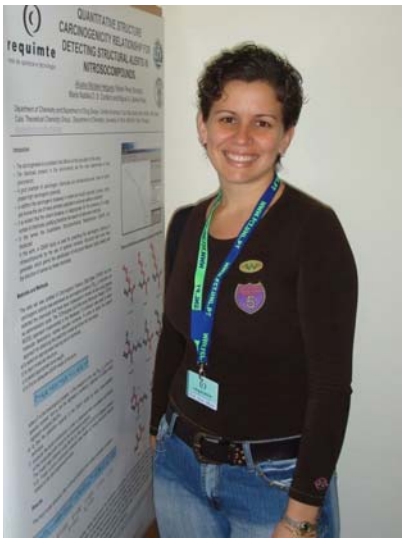

Prof. Aliuska Morales Helguera, BSc.
Professor of General Chemistry, Physical–Chemistry and Chemical Toxicology.
Drug Discovery and Molecular Design, Chemometric, Molecular Modelling, Computational and Theoretical Chemistry Specialist.
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QUALIFICATIONS
Bachelor of Science (B.Sc): Chemistry 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 the Physical–Chemistry, Statistics, toxicological and medicinal chemistry as well as "rational" drug design.

Research main interests: My current research interests are in the area of safer drug design, specifically the development of new computational methods for prediction of carcinogenic activity. In this sense, I'm also interested in the application of novel molecular descriptors for using in the development of QSAR/QTAR, "rational" (computer-aided) drug design, characterization of molecular similarity, computational (virtual and *in silico*) screening, as well as the obtaining of rules that can be used for identify structural alerts and thus these can be implemented into expert system. More recently, I am also interested in molecular modelling of biological reaction mechanisms associate to the carcinogenic phenomenon, using molecular simulations.

Some Recent Publication…

Morales AH, González MP, Rieumont JB. TOPS-MODE approach to predict mutagenicity in dental monomers. *Polymer* 2004, 45, 2045-2050.
González MP, Morales AH, Molina RR, García JF. A topological sub-structural approach of the mutagenic activity in dental monomers.1. Aromatic epoxides. *Polymer* 2004, 45, 2773-2779.
González MP, Dias LC, Morales AH. A topological sub-structural approach to the mutagenic activity in dental monomers. 2. Cycloaliphatic epoxides. *Polymer*. 2004, 15, 5353-5359.
Morales AH, Cabrera MA, Combes RD, González MP. The Prediction of Carcinogenicity from Molecular Structure. *Current Computer-Aided Drug Design*, 2005, 1, 65-72.
Morales AH, Cabrera MA, González MP, Molina RR, González HD. A Topological Sub-structural Approach Applied to the Computational. Prediction of Rodent Carcinogenicity, *Bioorganic & Medicinal Chemistry*, 2005, 13, 2477-2488.
González MP, Morales AH, Cabrera MA, Quantitative structure–activity relationship to predict toxicological properties of benzene derivative compounds. *Bioorganic & Medicinal Chemistry*, 2005, 13, 1775-1781.
Morales AH, Cabrera MA, Combes RD, González, MP. Quantitative structure activity relationship for the computational prediction of nitrocompounds carcinogenicity. *Toxicology*. 2006, 220, 51 – 62.
Morales AH. Duchowicz PR. Cabrera MA. Castro EA. Cordeiro N. González MP. Application of the replacement method as a novel variable selection strategy in QSAR. 1. Carcinogenic potential. *Chemometrics and Intelligent Laboratory Systems* 2006, 81, 180–187.
Morales AH. Cabrera MA, González MP. A Radial Distribution Function approach to predict rodent carcinogenicity. *Journal of Molecular Modeling* 2006, 19, 1-12.