

List of Publications...

RESEARCH PAPERS

[Only published, in print and accepted papers are listed]

Published Papers

Marrero-Ponce, Y. Total and Local Quadratic Indices of the Molecular Pseudograph's Atom Adjacency Matrix: Applications to the Prediction of Physical Properties of Organic Compounds. *Molecules*. **2003**, 8, 687-726.

Marrero-Ponce, Y.; Cabrera, M., A.; Romero, V.; Ofori, E.; Montero, L. A. Total and Local Quadratic Indices of the "Molecular Pseudograph's Atom Adjacency Matrix". Application to Prediction of Caco-2 Permeability of Drugs. *Int. J. Mol. Sci.* **2003**, 4, 512-536.

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Marrero-Ponce, Y.; González-Díaz, H.; Romero-Zaldivar, V.; Torrens, F.; Castro, E. A. 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.

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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.

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- Marrero-Ponce, Y.; Medina, R.; Castro, E. A.; de Armas, R.; González, H.; Romero, V.; Torrens, F. Protein Quadratic Indices of the “Macromolecular Pseudograph’s α -Carbon Atom Adjacency Matrix”. 1. Prediction of Arc Repressor Alanine-mutant’s Stability. *Molecules*. **2004**, *9*, 1124–1147.
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Accepted Papers

- Marrero-Ponce, Y.; Torrens, F. Bond-Based Global and Local (Bond and Bond-Type) Quadratic Indices and Their Applications to Computer-Aided Molecular Design. 1.

- QSPR Studies of Octane Isomers. *J. Comput. Aided Mol. Des.* Accepted for publication.
- Marrero-Ponce, Y.; Khan, M. T. H.; Casañola-Martin, G. M.; Ather, A.; Sultankhodzhaev, M. N.; Torrens, F. Atom-Based 2D Quadratic Indices in Drug Discovery of Novel Tyrosinase Inhibitors. Results of *in silico* Studies Supported by Experimental Results. *QSAR Comb. Sci.* Accepted for publication.
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- Marrero-Ponce, Y.; Torrens, F., Torres, L. Novel 2D TOMOCOMD-CARDD Descriptors: Atom-based Stochastic and non-Stochastic Bilinear Indices and their QSPR Applications. *Molecules.* Submitted for publication.

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