Poster Presentation

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Drug-Design QSARs based on QTAIM Electron Localization/Delocalization Indices

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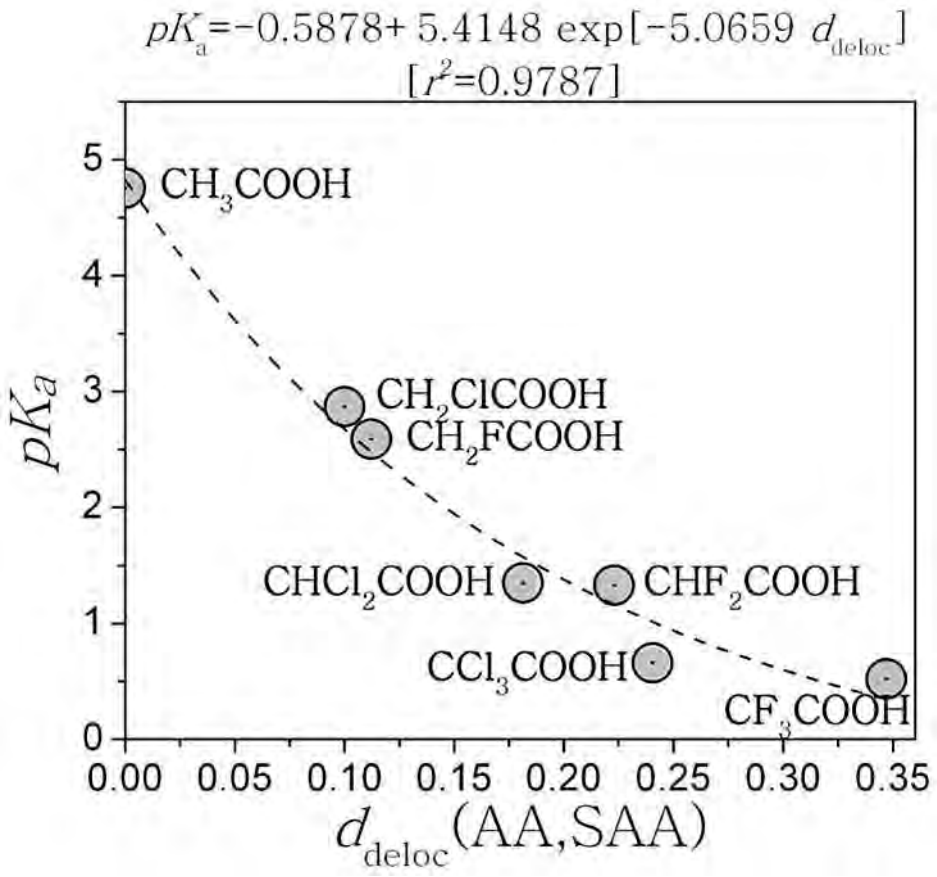
Following the lead of chemical graph-theoretical connectivity matrices, electron localization/delocalization matrices (LDMs) and their matrix-invariants derived forms will be introduced and shown to provide a faithfully encoding of the properties of the molecules by comparing with experiment. The matrix elements of an LDM are obtained from Bader's quantum theory of atoms in molecules (QTAIM) whereby the diagonal elements are the localization indices and the off diagonal elements are 1/2 of the delocalization indices. The sum of any row or column is the total electron population of a given atom while the sum of all sums is, of course, the total number of electrons in the molecule (N). The matrix is, thus, rich with electronic (and structural) information, implicitly and explicitly, and is conceivably useful in generating quantitative molecular descriptors for structure-to-activity relationship studies (QSAR). This talk will briefly review the uses and concepts of molecular electron density descriptors with emphasis on this new class of descriptors as a novel, possibly promising, possibility.

[1] *C. F. Matta; "Invited Review: Modeling of Biophysical Properties and Biological Activity From the Characteristics of the Molecular Electron Density Distribution and those of Electron Localization and Delocalization"; Journal of Computational Chemistry, S,* ***[2]*** *C. F. Matta, A. A. Arabi; "Electron-density descriptors as predictors in quantitative structureactivity/property relationships and drug design"; Future Medicinal Chemistry 3, 969-994 (2011).,* ***[3]*** *C. F. Matta (Ed.); Quantum Biochemistry: Electronic Structure and Biological Activity; Wiley-VCH: Weinheim (2010).*



Keywords: Drug design, Quantitative Structure-to-Activity Relationship (QSAR), Electron localization and delocalization