

## Kohonen network study of aromatic compounds based on electronic and nonelectronic structure descriptors.

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### Autorzy

Jarosław Panek

Aneta Jezierska

Marjan Vračko

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### Streszczenie

Atoms in Molecules (AIM) and Electron Localization Function (ELF) methodologies were applied to describe the electronic structure of 88 aromatic compounds. The analyzed database contains molecules substituted by nucleophilic and electrophilic groups which are responsible for electron density distribution in the molecule and further for its reactivity. Radial Distribution Function (RDF), Weighted Holistic Invariant Molecular (WHIM), Three-Dimensional Molecule Representation of Structures based on Electron Diffraction (3D- MoRSE) and Geometry, Topology and Atom-Weights Assembly (GETAWAY) descriptors were taken into account describing the structures of the analyzed molecules. According to generated descriptor space the classification of the molecules has been subsequently performed using unsupervised learning strategy and Kohonen network. The final step of descriptor space testing was supervised learning of Counter-Propagation Artificial Neural Network (CPANN) using n-octanol/water partition coefficient (logP), dipole moment (DM) and molecular refractivity (MR) as target values.

### Adres publiczny

<http://dx.doi.org/10.1021/ci049752t>

### Strona internetowa wydawcy

<https://www.acs.org/content/acs/en.html>