

A Novel Approach to Geometric Fingerprinting and a Comparative Study of Its Application to 3D-QSAR Modelling

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Abstract

In collaboration with the Computer-Chemie-Centrum of the University of Erlangen-Nuernberg in Germany, Avantium has developed a new method to capture geometric information contained in a molecular structure using fingerprinting technology. The newly developed fingerprinting algorithm, which is coded in the software application Fingal, is capable of describing both the topological and geometric characteristics of a molecule. Fingal is extremely fast and the resulting fingerprints are high in information content. It has a wide applicability in indexing, geometric (sub)structure screening, conformer similarity searching and it can be used as a descriptor generation method in predictive modeling. In a recent publication, the good performance of Fingal was demonstrated in a comparative QSAR study using other descriptor types and structures.

For the full article please see <http://www3.interscience.wiley.com/cgi-bin/abstract/109931645/ABSTRACT>

