Abstract

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Uniquely discriminating molecular structures using novel eigenvalue-based descriptors

In this article, we explore novel spectra-based descriptors to discriminate molecular graphs. As known, classical structure descriptors based on the eigenvalues of the underlying adjacency matrix are often insufficient since there exist a large number of isospectral graphs. Briefly recall that the spectrum is the set of eigenvalues of the characteristic polynomial.

To tackle the problem, we propose five families of novel descriptors based on the eigenvalues of certain molecular matrices representing chemical structures. Note that in this paper, we only consider the underlying skeleton of a molecular graph. Because it is crucial to study the discrimination power (often called degeneracy) by not merely using synthetic (isomeric) structures, we apply the novel measures to both real and synthetic molecular graphs. Also, we use ten different types of molecular matrices to calculate the novel descriptors and determine correlations between them.

It turns out that the novel descriptors possess high discrimination power when being applied to appropriate molecular matrices. Evidently, the study also reveals that special kinds of matrices capture structural information of the molecular graphs more meaningfully than others, particularly the adjacency matrix which turned out often to be insufficient to develop molecular descriptors.