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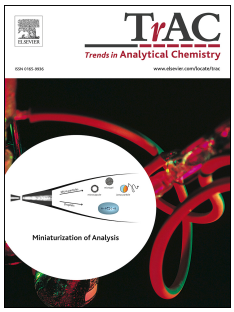

Chemical image moments and their applications

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Abstract

The extraction of chemical information in samples is essential to analytical modeling. In this contribution, the applications of several image moments on the analyses of chemical signals are introduced, including the quantitative analysis of multiple target components in mixture and the qualitative analysis of samples based on the chemical spectra obtained from HPLC coupled with photodiode array detector, LC-MS, Fluorescence, Terahertz, NMR or NIR analytical instruments. As the extension, chemical image moment approach has also been used in the prediction of protein phosphorylation sites as well as quantitative structure-activity relationship (QSAR) researches. The obtained satisfactory results indicate that the proposed approach is a convenient way to effectively extract target information and could reduce the difficulty of analytical experiments and improve the analytical speed, accuracy and reliability. Our study presents the specific charm of chemical image moments and provides novel insight into analytical chemistry.

Keywords: Chemical image; Moment; Chemometrics; Analytical chemistry; Data mining

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