Abstract

In
Encyclopedia of Spectroscopy and Spectrometry,
Lindon J.C., Tranter G.E., Koppenaal D., Eds.; 2nd edition,
Academic Press - Elsevier, Waltham, MA, USA, p. 392-403 (2010).

Varmuza K.:

Computer methods in mass spectrometry for chemical structure assignment

Mass spectra of chemical compounds have a high information content. This article describes computer-assisted methods for extracting information about chemical structures from low-resolution mass spectra. Comparison of the measured spectrum with the spectra of a database (library search) is the most used approach for the identification of unknowns. Different similarity criteria of mass spectra as well as strategies for the evaluation of hitlists are discussed. Mass spectra interpretation based on characteristic peaks (key ions) is critically reported. The method of mass spectra classification (recognition of substructures) has interesting capabilities for a systematic structure elucidation.

This article is restricted to electron impact mass spectra of organic compounds and focuses on methods rather than on currently available software products or databases.

This article covers methods and applications that were current in the mid-1990s. However, a short update describing some more recent developments together with some literature sources has been included at the end of this article.

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Varmuza K.:
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Chemical structure information from mass spectrometry.