

PW3 Progress in the development of the NIST/NIH/EPA mass spectral library

Anzor Mikaia and Stephen E. Stein

National Institute of Standards and Technology, Gaithersburg, MD 20899-8320, USA

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Procedures for database evaluation are described.

A series of progressively refined stages of analysis of data for the evaluation of the NIST/NIH/EPA mass spectral library will be described. The stages include: (a) preliminary evaluation of new data, (b) discovery of inconsistencies between formula, molecular weight and structure, (c) detection of significant differences between the spectra of a compound obtained from various sources, (d) a thorough manual evaluation of data involving examination of spectral data along with the scrutiny of the compound identity information (e) comparison to the spectra of related compounds, such as analogs, isomers and derivatives, and (f) the selection of the best from the choice of multiple spectra for a compound.

The established priorities for spectra of compounds to be acquired and the requirements for measured spectra will be discussed.