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Design and implementation of mass spectrometer database

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Mass spectrometer, as a type of beam instrument, is capable of measuring and analyzing the mass and charge of different molecules and ions in a sample, thus identifying the type of particles. Mass spectrometer database software is an important part of mass spectrometer, which can realize the function of storing, managing, sharing and analyzing mass spectrometer data. Therefore, the establishment and improvement of specialized mass spectrometry databases and library retrieval techniques can facilitate the rapid identification and confirmation of compounds, providing a more efficient and accurate solution for substance detection. In this paper, a comprehensive mass spectrometry database management system is designed and implemented to simplify the user operation process from the collection, storage and management of mass spectrometry data to the querying, matching and analyzing of the data, providing a fast and accurate solution to meet the needs of scientific research on mass spectrometry data. The software uses Python for the implementation of core algorithms, builds a database based on MySQL and collects mass spectrometry data to fill in the database, and finally uses PyQt to design and implement a friendly and beautiful graphical user interface. With this software, unknown compounds in the samples can be identified and their possible structures and properties can be recognized, which provides a strong support for their application fields.

Footnotes

Funding Agency

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Yes

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