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Structural Elucidation from Mass Spectra

マススペクトルからの構造予測

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Identification of metabolites from spectra is a major task in metabolomics. Formal identification requires that both mass spectra and chromatographic retention of a metabolite in question perfectly match with those of a standard compound, necessitating the preparation of an in-house library of standard compounds. This setup is, however, too expensive for ordinary research groups. To reduce the experimental cost we have been developing MassBank, a spectral database of standard compounds. The system is collaboratively developed and maintained, and data are distributed among multiple servers. In this talk I explain the relationship between molecular structure and spectra and introduce the basic identification scheme in metabolomics. Then the relationship between molecular class and partial match is discussed. I will also mention the software platform under development as the next-generation
of MassBank system.

Keywords: mass spectrometry, molecular structure, fragmentation