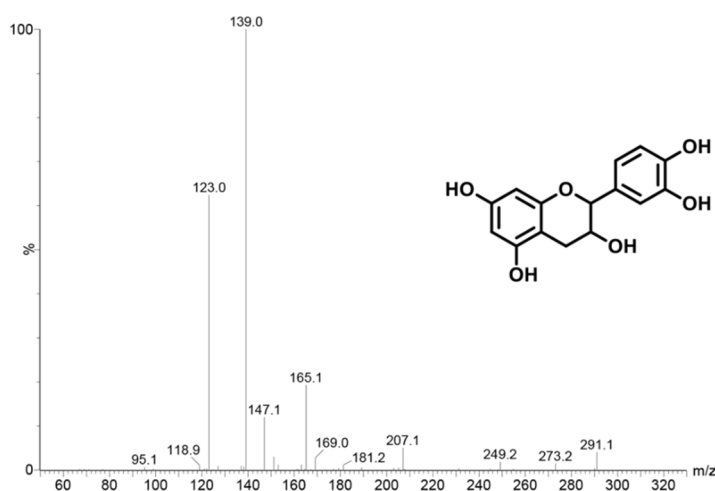


## Summary

# Tandem Mass Spectrum Database

Over the past 20 years, the development of the electrospray ionization technology has led to an increase in the use of LCMS/MS for chemical analysis. It is frequently used to evaluate natural products (NPs) from marine and terrestrial habitats, including the microorganisms, plants, animals, and humans. Thus, determining the identity of a metabolite and natural product characterization are critical for understanding biological processes, finding bioactive hit, and developing new medicinal compounds. Tandem mass spectrometry (MS/MS) has been shown to be a high-throughput and sensitive method for the identification of organic compounds. As a result, the concept of development of mass spectral libraries evolved. For volatile compounds, a GC/MS analysis, followed by library searching, has long been an accepted way of making identifications of organic compounds in complex mixtures. However, identification of non-volatile compounds through LCMS/MS is still a challenging task for chemist due to the limitations of *in-silico* mass spectral libraries. Thus, there is a need to develop an experimental tandem mass spectrum database for the scientific and academic community.



On the basis of above facts CSIR-CDRI, Lucknow developed a indigenous prototype of Tandem Mass Spectrum library of natural products to explore chemical diversity of Indian flora using LCMS/MS. The present creation ([www.tmsdatabase.org](http://www.tmsdatabase.org)) provides mass spectrometry based methodologies to identify the

natural compounds in complex mixture and herbal extracts.

**Design and capabilities of MS/MS database:** National and international collaborators/contributors can contribute in database at same platform. Scientific updates on biological activity of individual compound is available on [www.tmsdatabase.org](http://www.tmsdatabase.org) (for biologist interest). Number of library can be created for different class of compounds i.e. alkaloids, terpenoids, steroids, amino acids etc.

Contact Us: Dr. Sanjeev Kanojija,  
E-mail: [sanjeev\\_kanojija@cdri.res.in](mailto:sanjeev_kanojija@cdri.res.in)