SnaPeaks

Mass Spectrometry Platform for **Natural Product Analysis**

SnaPeaks

Platform for tandem mass spectrometry (MS/MS) of Natural Products

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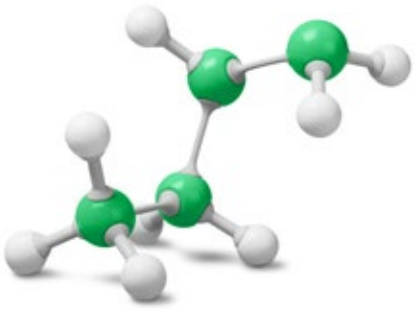
ChemEssen

Overcome the lack of data on mass spectrometry for natural products

MS/MS Spectral Database of Natural Products



Technology Status

- The database of natural products has already been built and contains about 300,000 natural product information, but it only has information on the molecular structure and origin of natural products.
- There is very little MS/MS mass spectrometry data for natural products.
- There are very few data on the physical properties and physiological activity of natural products.

Current Issues

- Analyzing the unknown extracts of a natural substances through a mass spectrometer is limited due to lack of MS/MS spectral library.
- It is difficult to analyze physical properties and physiological activity without knowing what the active ingredients of potent natural products are.
- After all, there are many difficulties in commercializing active components by extracting natural products.

Development Goals

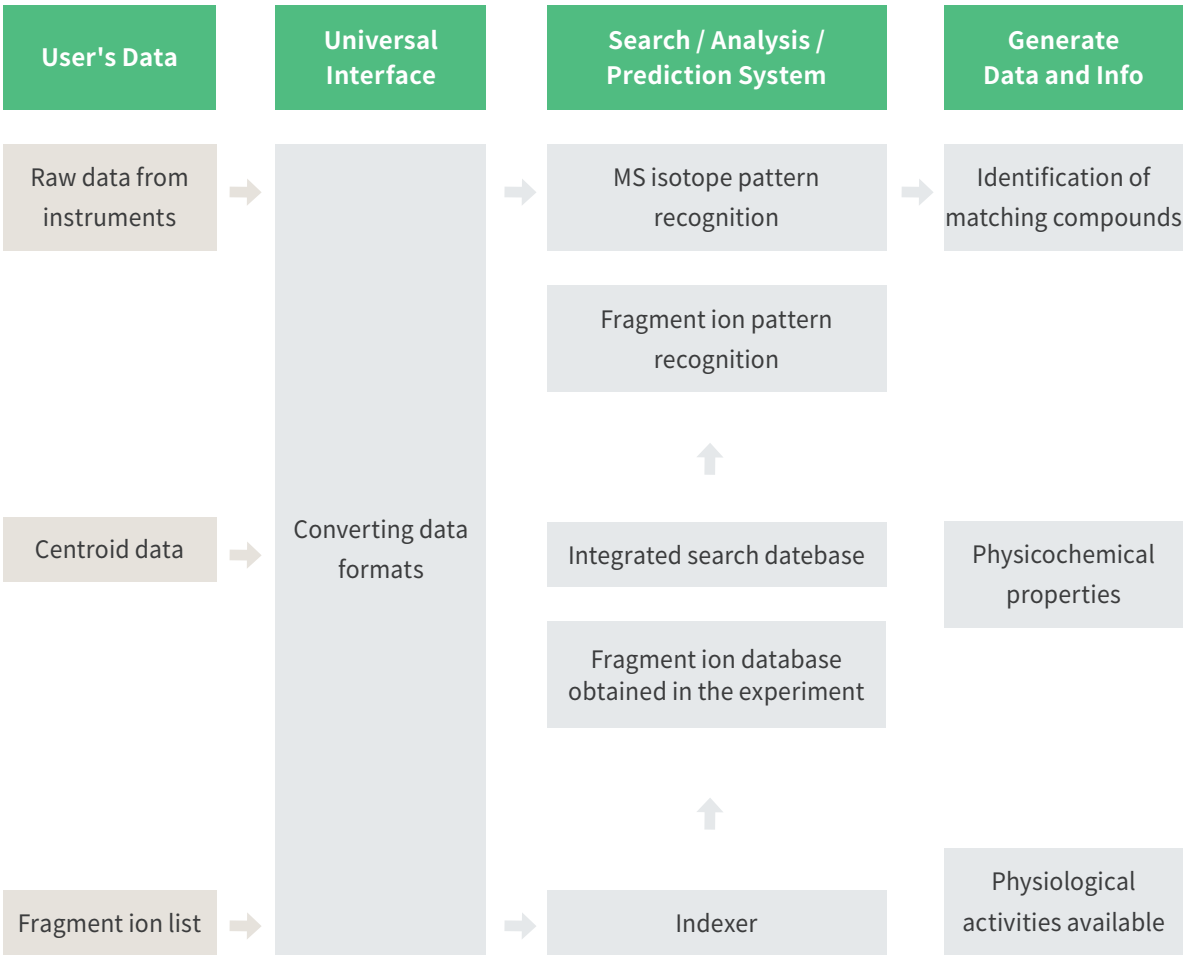
- Get tandem mass spectrometry (MS/MS) data for natural products.
- Identify the active components from the database that contains the tandem mass spectrometry (MS/MS) library.

Product Overview

Product Name : SnaPeaks

Detailed Product Features

- Search MS/MS spectrum using chemical name, formula, or chemical identifier.
- Analyze the structure and characteristic information of active ingredients with spectral data obtaining from a mass spectrometer.



Identify the active components of natural products

- Areas where secondary metabolite analysis of natural products can be applied;

Cosmetics

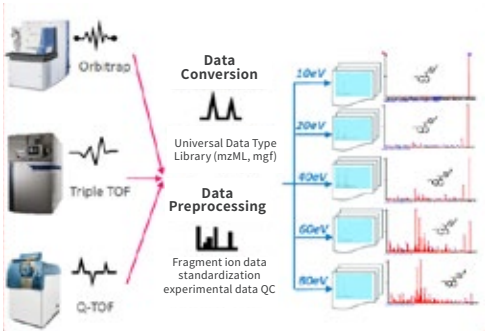
Medicine

Functional Food

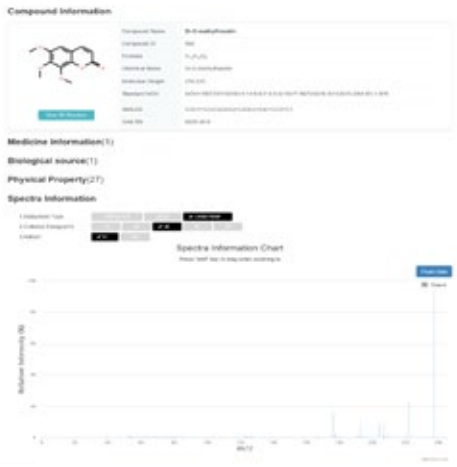
- You can identify the active components of natural products used in various industries and confirm property information.
- By providing medicinal herbs information containing active ingredients, you can broaden the range of natural products to be extracted.

Experience search system and MS/MS libraries based on **high-end mass spectrometer**

Secondary metabolite fragment ion DB



Development of MS/MS search algorithm and commercialization



Technology to analyze the components of natural extracts

- Standard samples were measured with a high resolution mass spectrometer.
- Includes MS/MS spectra in the library obtained at various energy levels.
- Verified through the chemical structures and AI algorithms.

Library and database to identify the components

- Built and expanded MS/MS spectral libraries based on Electrospray Ionization (ESI) for natural products.
- Explored the vast MS/MS spectrum obtained from three different instruments.
- Supports various file formats of user measurement data for convenience.

Improved UI & UX

- Search by compound name, formula, chemical identifier, or spectrum.
- Provides basic, physical property, and medicine herbs information of compounds.

Product Specification

More extensive data and better search performance

Number of natural compounds	**2,600+ ea**
Number of fragment ion	**70,000+ ea**
Applicable MS equipment	**More than 6 equipments**
number of energy referenced for pattern recognition	**3 ea**
Speed of search engine	**17,000 spectra/sec**
Performance of search engine*	**97%**
Instrument Type	**TripleTOF / Q-TOF / Orbitrap**
Ionization method	**ElectroSpray Ionization (ESI)**
Fragmentation Method	**Collision Induced Dissociation (CID)** **Higher Energy Collisional Dissociation (HCD)**
Adduct Ion	**$[M+H]^+$ / $[M+Na]^+$**

** The above specifications are the third year goal of project funded by the Ministry of Commerce, Industry and Energy. Currently in the third year.*

** Performance evaluation on search engine is based on MassBank method.*
Accuracy = (True positive + True negative) / (True positive + True negative + False positive + False negative)
It is considered positive that the target compound is within the top 10 of the matching compounds.

How To Use

Easily and quickly search the desired spectrum data.

① Access www.snapeaks.com

www.snapeaks.com

② Text Search

1. Search by chemical name, formula, or chemical identifier.
2. Select a matching compound from the result list and move to the detailed page.

Search a compound

Or, MS/MS Spectrum Search

1. Upload a MS/MS Spectrum file
2. Check the input spectrum and search
3. Find spectrum matching with the input spectrum

ChemEssen offers new solutions through the fusion of **chemical science** and **information technology**.

SnaPeaks was jointly developed by Korea Basic Science Institute, Bioinformatics and Molecular Design Research Center, BioSpectrum, and ChemEssen.

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