

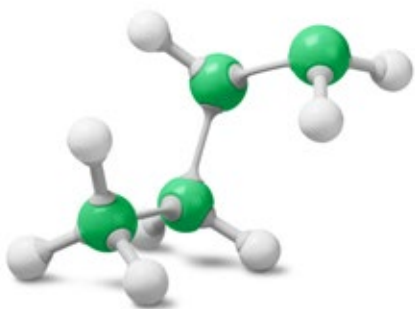
Mass Spectrometry Platform for **Natural Product Analysis**

SnaPeaks

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

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.

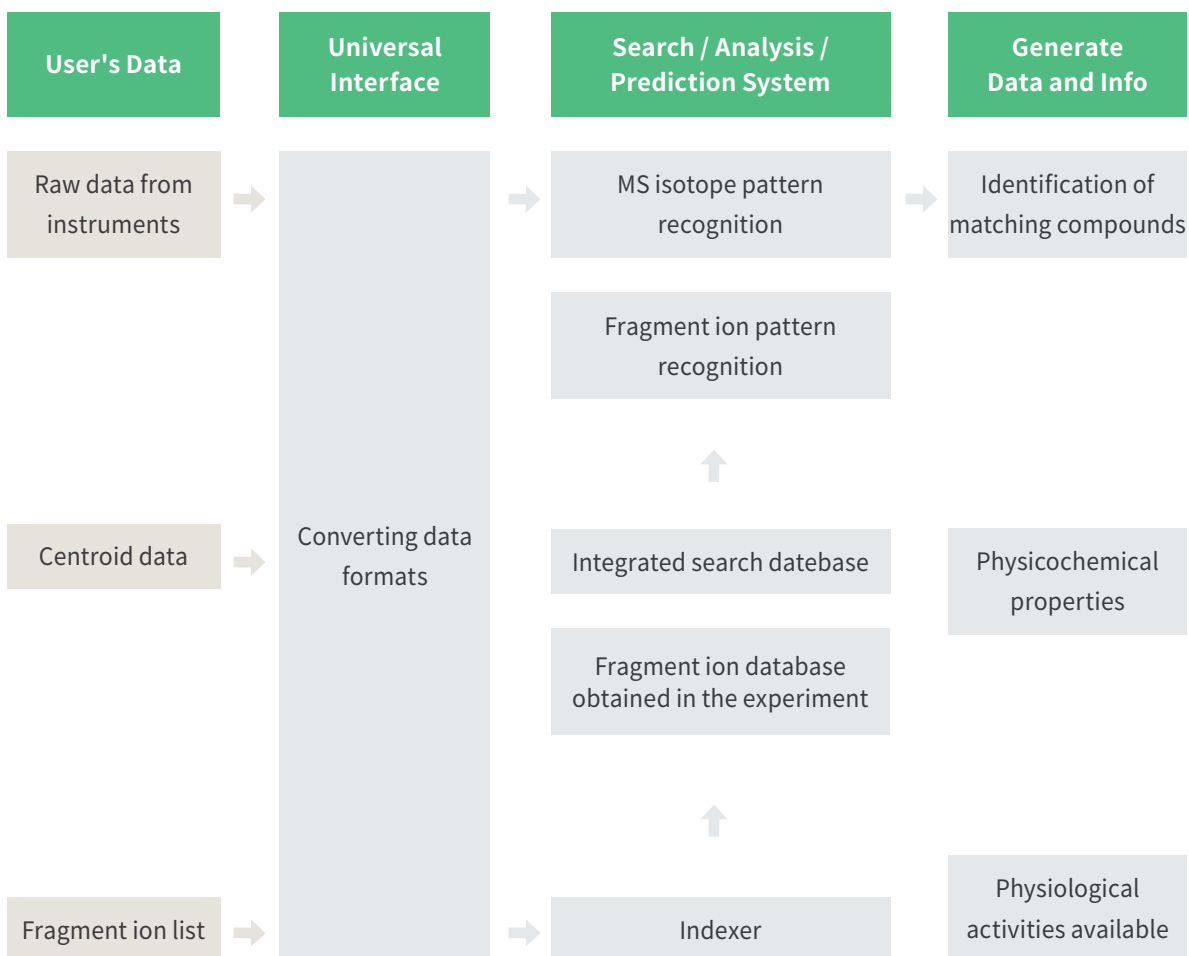
Product Overview

Product Name :



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.



Product Applications

Identify the active components of natural products

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

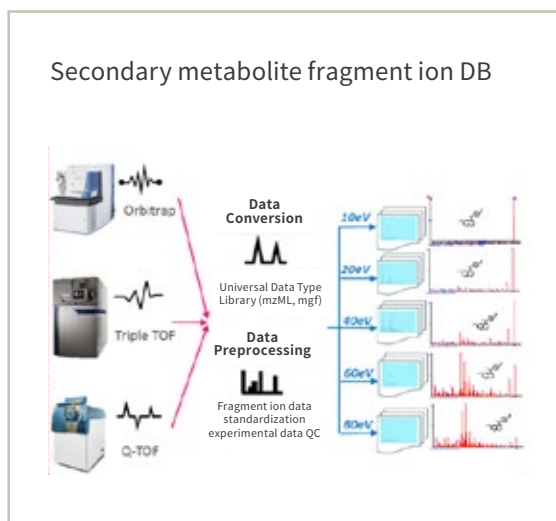


- You can identify the active components of natural products used in various industries and confirm property information.
- By providing medicinal herbs information containing active ingredients, you can broaden the range of natural products to be extracted.



Product Features

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

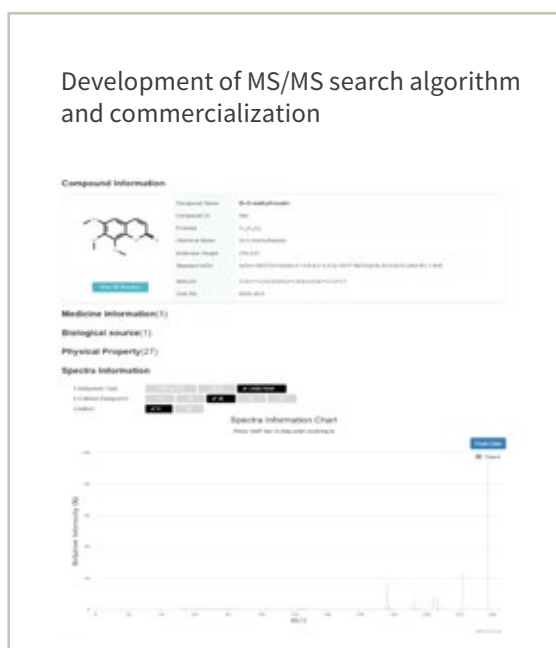


Technology to analyze the components of natural extracts

- 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



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

②

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.

Website www.snapeaks.com

Address 1408, AceHighTechCity 2-Cha, 25 Seonyu-ro 13-gil, Yeongdeungpo-gu, Seoul 07282 Republic of Korea.

Tel +82 . 2 . 3143 . 5933

Fax +82 . 2 . 3143 . 5920

email staff@chemessen.com