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NMR databases for identifying the metabolites

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In all living organisms, enzyme-catalyzed metabolic reactions result in the formation of metabolites. These metabolites are essential for the growth and survival of organisms, for example, blood glucose levels in mammals [1]. Identifying these metabolites is crucial in developing a new potential therapeutic agent. NMR-based metabolite detection is very effective to overcome the challenges of metabolite identification. Different steps in the identification of these metabolites in humans, animals, plants, and other sources are illustrated in **Fig.1.**

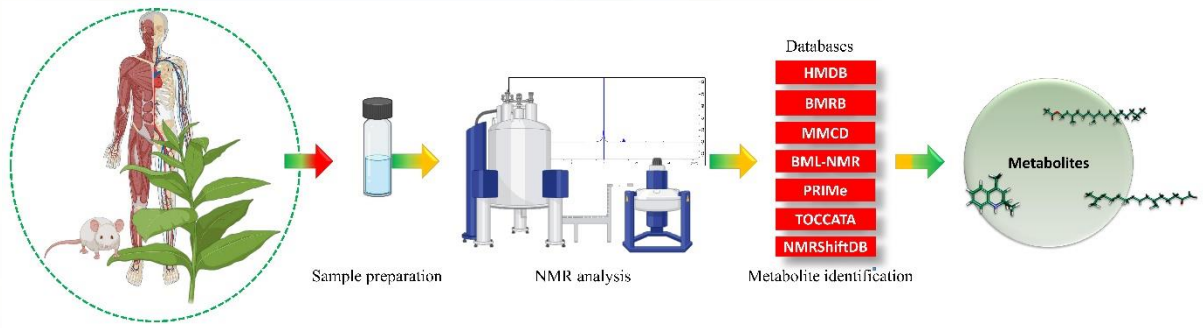

Fig.1 Identification & characterization of metabolite

Some commonly available NMR metabolite databases are;

1. Human Metabolome Database (HMDB).

HMDB(https://hmdb.ca/spectra/nmr_one_d_search/new) is a free database providing detailed information regarding human metabolites. Chemical, molecular biology, biochemical, and clinical information are available with HMDB. This database is associated with other databases such as KEGG, GenBank, DrugBank, T3DB, PubChem,MetaCyc, ChEBI, PDB, UniProt, SMPDB, and FooDB. Supporters of HMDB are the Canadian Institutes of Health Research, the Metabolomics Innovation Centre (TMIC), andthe Canada Foundation for Innovation (CFI) [2].

2. Biological Magnetic Resonance Bank (BMRB).

BMRB(https://bmrb.io/)is a repository containing experimental data from nuclear magnetic resonance (NMR) spectroscopy studies of biological molecules such as peptides, proteins, nucleic acids, carbohydrates, and their complexes. BMRB collects and archives NMR data,

including spectral data, derived constraints (distance and dihedral angle restraints), and structural coordinates for biological macromolecules. The BMRB provides three-dimensional structures and dynamics of macromolecules. This database helps scientists analyze biological systems structure, dynamics, and chemistry and assists the development of the biomolecular NMR spectroscopy area [3].

3. Madison-Qingdao Metabolomics Consortium Database (MMCD)

MMCD is a collaborative effort between researchers in Madison, USA, and Qingdao, China, to advance metabolomics research. It contains primary and secondary metabolites, xenobiotics, metabolic pathways, and biological information. MMCD also contains details of >20,000 metabolites and other biologically important small molecules. This database contains an efficient and flexible query system with search engines for text, structure, mass, and NMR details. NMR-based identification of metabolites uses one-dimensional (1D) and two-dimensional (2D) NMR methods, like 2D-^{1}H-13C HSQC (Heteronuclear single quantum coherence). National Magnetic Resonance Facility at Madison provides support to MMCD [4].

4. Birmingham Metabolite Library (BML-NMR).

BML-NMR(https://www.bml-nmr.org/) database is specialized for identifying and characterizing metabolites by NMR spectroscopy. BML-NMR houses a collection of NMR spectra obtained from various metabolites, which are crucial for comparing and identifying metabolites in experimental samples based on their chemical shifts and characteristic peaks. BML-NMR contains 1D and 2D J-resolved NMR spectra of 208 metabolites [5].

5. Platform for RIKEN Metabolomics via SpinAssign (PRIMe).

PRIMe(https://prime.psc.riken.jp/) is an integrated database and analysis platform RIKEN (the Institute of Physical and Chemical Research in Japan) developed to support metabolomics research. PRIMe integrates various types of metabolomics data, including metabolite profiles, metabolic pathways, and associated biological information. It supports both experimental data and computational predictions. The PRIMe website helps in the statistical analysis, pathway enrichment analysis, and tools for comparative analysis of metabolite profiles from different samples [6].

6. TOSCY Customized Carbon Trace Archive (TOCCATA).

TOCCATA is a specialized database developed for ^{13}C NMR spectroscopy. It functions as a repository for curated ^{13}CNMR spectral data, which helps in the identification and characterization of a diverse range of organic compounds. These spectra serve as reference data for researchers and analysts conducting structural elucidation and compound identification using ^{13}CNMR spectroscopy[7].

7. NMRShiftDB

NMRShiftDB(https://nmrshiftdb.nmr.uni-koeln.de/) is a database specifically focused on nuclear magnetic resonance (NMR) spectroscopy data for organic compounds. It provides information about chemical shifts observed in NMR spectra, which are crucial for the identification and structural elucidation of organic molecules. NMRShiftDB contains curated

NMR spectra, including proton (^{1}HNMR) and carbon-13 (^{13}CNMR) and organic compound's chemical shift values [8].

8. MetaboLights.

MetaboLights is a widely used and comprehensive metabolomics database (https://www.ebi.ac.uk/metabolights/) managed and supported by the European Bioinformatics Institute (EMBL-EBI). It serves as a centralized repository for metabolomics experimental data and associated metadata. It contains data from nuclear magnetic resonance (NMR) spectroscopy, mass spectrometry (MS), and chromatography techniques. Metabo Lights adheres to community standards and guidelines for metabolomics data deposition, ensuring data interoperability and facilitating data reuse and integration with other bioinformatics resources [9].

In conclusion, NMR-based metabolite identification is a powerful tool in scientific research, particularly useful in metabolomics and drug discovery. It can provide accurate structural information and quantitative data necessary for understanding the metabolism and pathway associated with health and disease. Metabolite databases also help in developing new therapeutic strategies targeting metabolic pathways.

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