Metabolomics Resources:

1. Metabolomics Databases

1. LC-MS Databases (Liquid Chromatography-Mass Spectrometry): LC-MS research data for download can be accessed done through various repositories and databases where researchers often deposit their datasets for public access. Some prominent sources include:
    1. Metabolomics Workbench: Provides a vast collection of metabolomics data, including LC-MS datasets, along with associated metadata and experimental details.
    2. MetaboLights: A repository for metabolomics experiments, it houses a wide range of datasets, including LC-MS data, and offers tools for visualization and analysis.
    3. MassIVE (Mass Spectrometry Interactive Virtual Environment): Focuses on MS data, offering access to high-quality datasets including LC-MS, proteomics, and other omics datasets.
    4. GNPS (Global Natural Products Social Molecular Networking): Particularly useful for natural product research, it hosts LC-MS datasets and enables molecular networking to explore chemical diversity.
    5. PRIDE Archive: While primarily for proteomics data, it also includes some metabolomics datasets, including LC-MS data.
    6. European Bioinformatics Institute (EBI) Metabolomics: Offers access to metabolomics datasets, including LC-MS data, along with analysis tools and resources.
    7. DataCite: An open repository that aggregates datasets from various disciplines. You can search for specific LC-MS datasets within its collection.
    8. BMRB (Biological Magnetic Resonance Bank): A repository for NMR spectroscopy data related to biomolecules.
    9. MetaboLights: A repository for metabolomics data, including LC-MS datasets related to metabolomics research.
    10. Human Metabolome Database (HMDB): Contains metabolomic data, including NMR spectra, for human tissues and biofluids.
    11. SpectraBank: A repository for various spectroscopic data, including NMR

spectra.

12. NMRShiftDB: A database specifically focused on organic structures and their NMR spectra.
13. CCPN (Collaborative Computational Project for NMR): Offers tools, software, and access to NMR data.
14. Chemical Shift Repository (CSR): Provides a platform for storing and sharing chemical shift data.
15. Cambridge Structural Database (CSD): Contains a vast collection of small molecule crystal structures, some of which may include associated NMR data.
16. Spectral Database for Organic Compounds (SDBS): Contains NMR, IR, MS, and Raman spectra for various organic compounds.
17. ACD/NMR Predictors: Offers software for NMR prediction and includes access to a database of predicted spectra.

2. NMR Databases
    1. BMRB (Biological Magnetic Resonance Bank): A repository for NMR spectroscopy data related to biomolecules.
    2. MetaboLights: While primarily for metabolomics data, it also hosts NMR datasets related to metabolomics research.
    3. HMDB (Human Metabolome Database): Contains metabolomic data, including NMR spectra, for human tissues and biofluids.
    4. SpectraBank: A repository for various spectroscopic data, including NMR spectra.
    5. NMRShiftDB: A database specifically focused on organic structures and their NMR spectra.
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1. Metabolomics Books

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