Metabolomics Resources in the Biological Magnetic Resonance Data Bank (BMRB)

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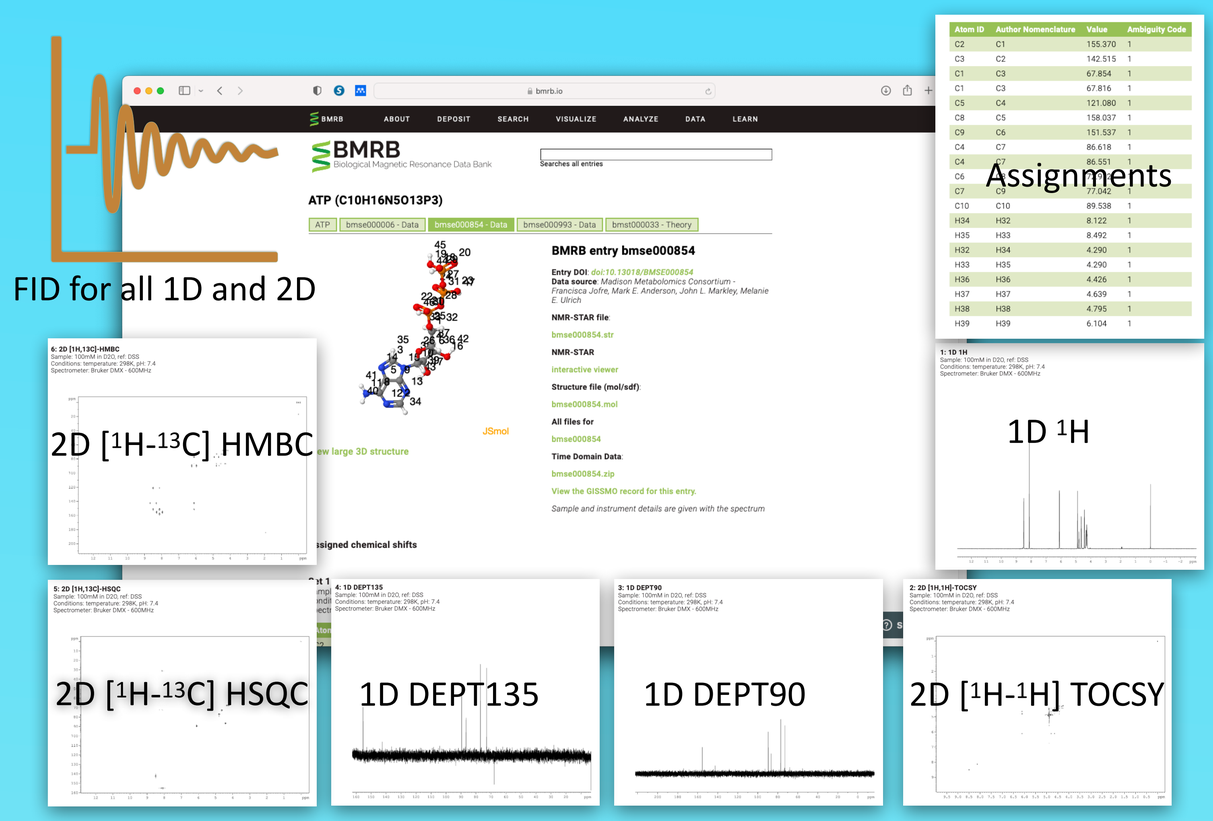
BMRB small molecules library (https://bmrb.io/metabolomics/)

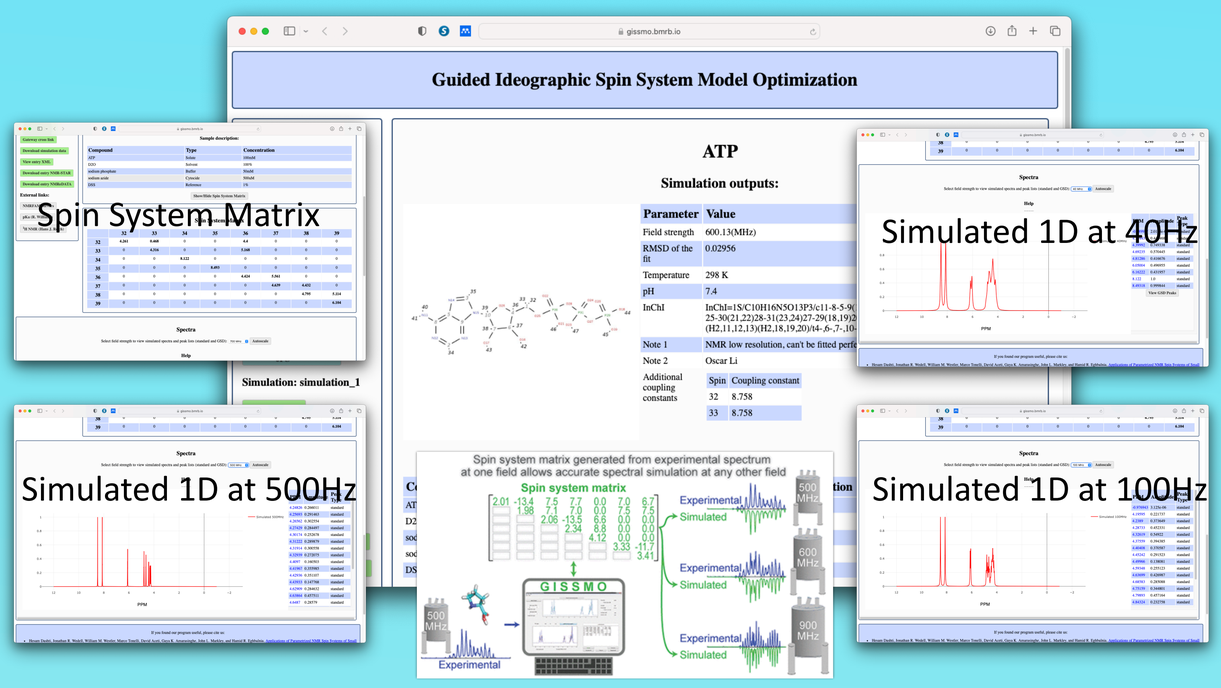
BMRB[1] provides curated set of reference NMR spectroscopic data for more than 1000 metabolites measured using a standardized experimental protocol

Each reference data set consists of
- Chemical shift assignments
- Sufficient time domain data (FID) from a set of 1D and 2D experiments to analyze the molecule

This library could be used to analyze and identify molecules in bio-fluids and other metabolite mixtures. Peak lists of 1D and 2D experiments can be searched across the database through web interface or using BMRB-API



GISSMO Library (https://gissmo.bmrb.io/)



Guided Ideographic Spin System Model Optimization[2,3] (GISSMO) enables the efficient calculation and refinement of spin system matrices(chemical shift and coupling constants against experimental 1D-^{1}H spectra of small molecules.

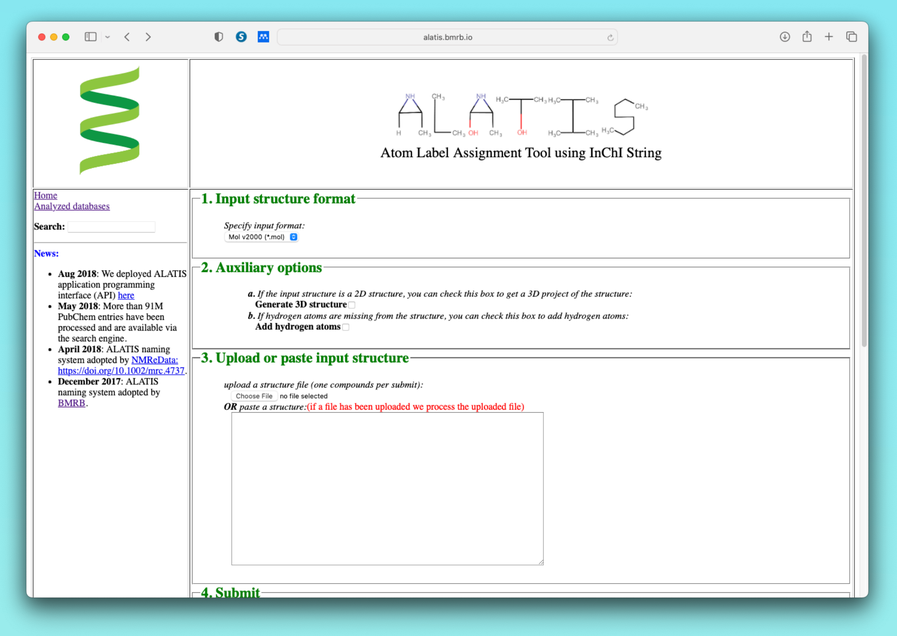
GISSMO library includes
- Library of over 1000 parameterized small molecules
- Spin system matrix for every molecule
- Recalculated 1D spectra at various field strengths (40Hz to 1.3GHz) and peak lists at each field strength

ALATIS Library (https://alatis.bmrb.io/)

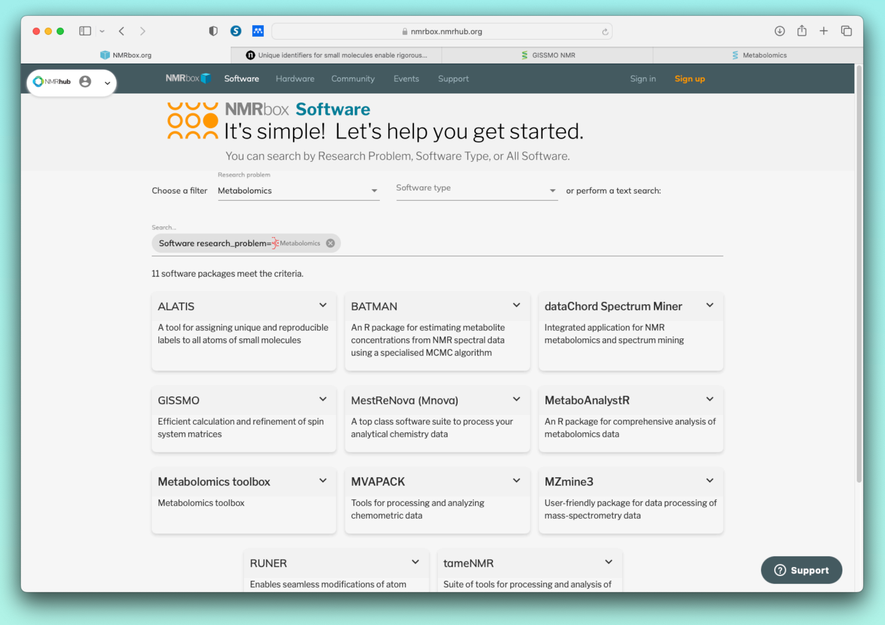
Atom Label Assignment Tool Using InChI String[4] (ALATIS) creates unique InChI identifiers for small molecules through rigorous labeling of their atoms including protons.This numbering system helps to identify molecules across different databases guaranteeing uniqueness of labels at the atomic level.

ALATIS library includes
- Unique InChI strings for molecules from various databases like BMRB, PubChem, HMDB and RCSB-PDB Ligand-Exp
- Cross-links from PDB entries to BMRB, HMDB and PubChem[5]

BMRB follows ALATIS numbering system in its small molecules database.



NMRbox: Software and Computing resource (https://nmrbox.nmrhub.org/)



NMRbox[6] is a resource for biomolecular NMR software. It provides tools for finding the software you need along with documentation and tutorials for getting the most out of the software. NMRbox services are available via cloud-based virtual machines and is available free for academic users.

In addition to **ALATIS** and **GISSMO**, NMRbox provides other ready to use computing resource along with various preinstalled software tools like, **BATMAN, dataChord Spectrum Miner, MestReNova(Nova). MetaboAnalystR, Metabolomcis toolbox, MVPACK, MZmine3, RUNER, tameNMR** and **MATLAB**.

NMRHhub is an umbrella organization which grants access to data collection infrastructure (Network of Advanced NMR: NAN), analysis platform (NMRbox), data resource (BMRB) as well as Non-uniform sampling and reconstruction project (NUScon) through single portal.

PDF version of this poster

NMRhub.org

NMRbox NUScon NAN BMRB

1. Jeffrey C Hoch et al., *Nucleic Acids Research*, Volume 51, Issue D1, 6 January 2023, Pages D368–D376,
2. Hesam Dashti et al., Analytical Chemistry 2018 90,18, 10646-10649
3. Hesam Dashti et al., Analytical Chemistry. 2017 89, 22, 12201–12208
4. Hesam Dashti et al., Sci Data 4, 170073 (2017)
5. Hesam Dashti et al., Sci Data 6, 190023 (2019)
6. Jeffrey C Hoch et al.., Biophysical Journal, 112: 1529-1534, 2017.