

## BMRB small molecules library

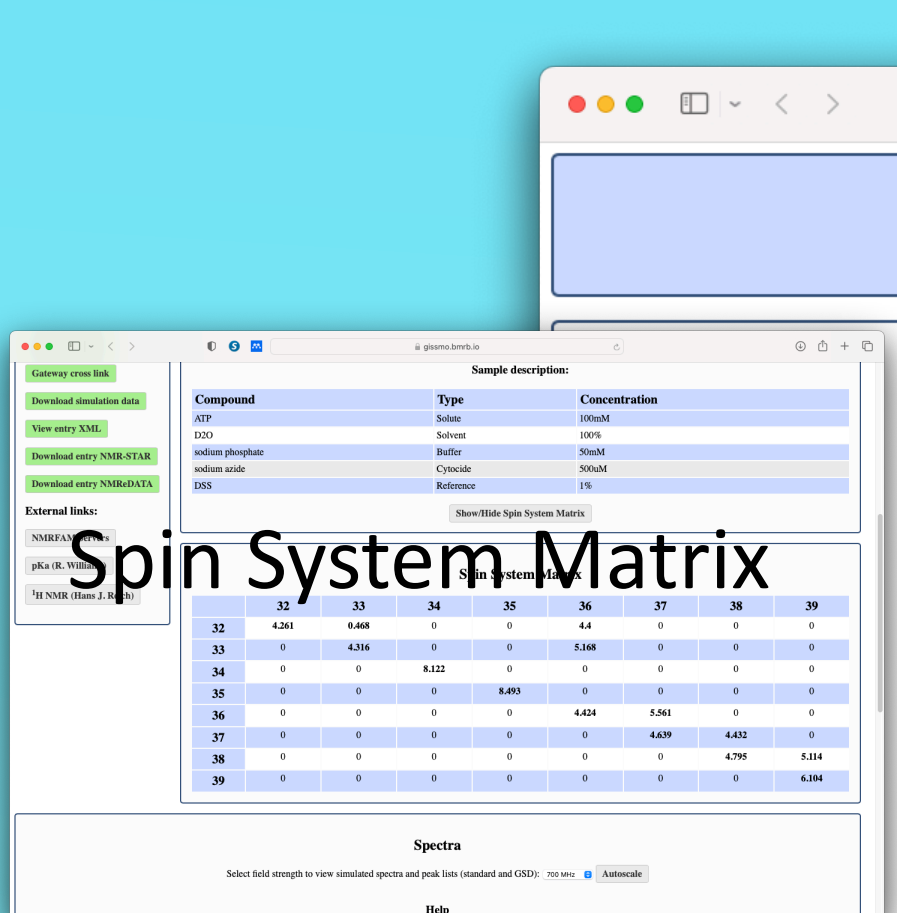
(<https://bmrbl.io/metabolomics/>)

BMRB<sup>1</sup> provides curated set of reference NMR spectroscopic data for more than 1000 metabolites measured using a standardized experimental protocol

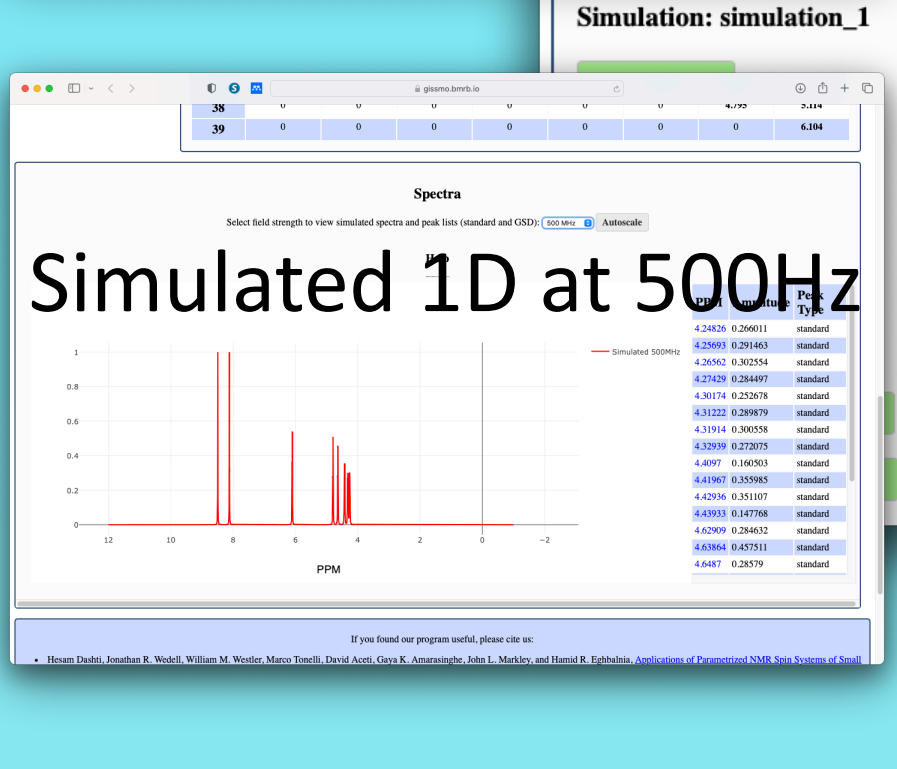
Each reference data set consists of

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

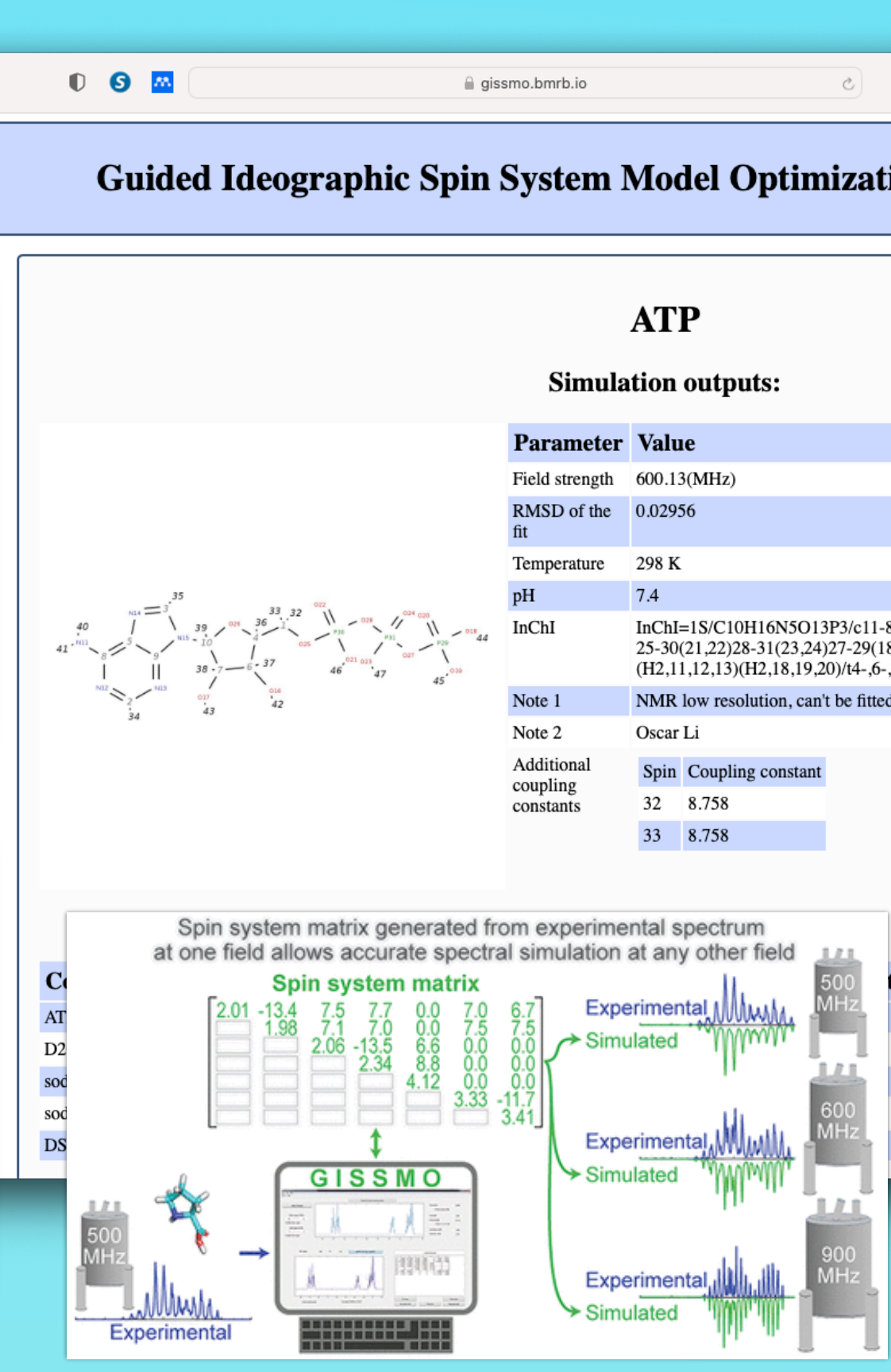
This library could be used to analyze and identify molecules in bio-fluids and other metabolite mixtures. Peak lists of 1D and 2D experiments can be searched across the database through web interface or using BMRB-API



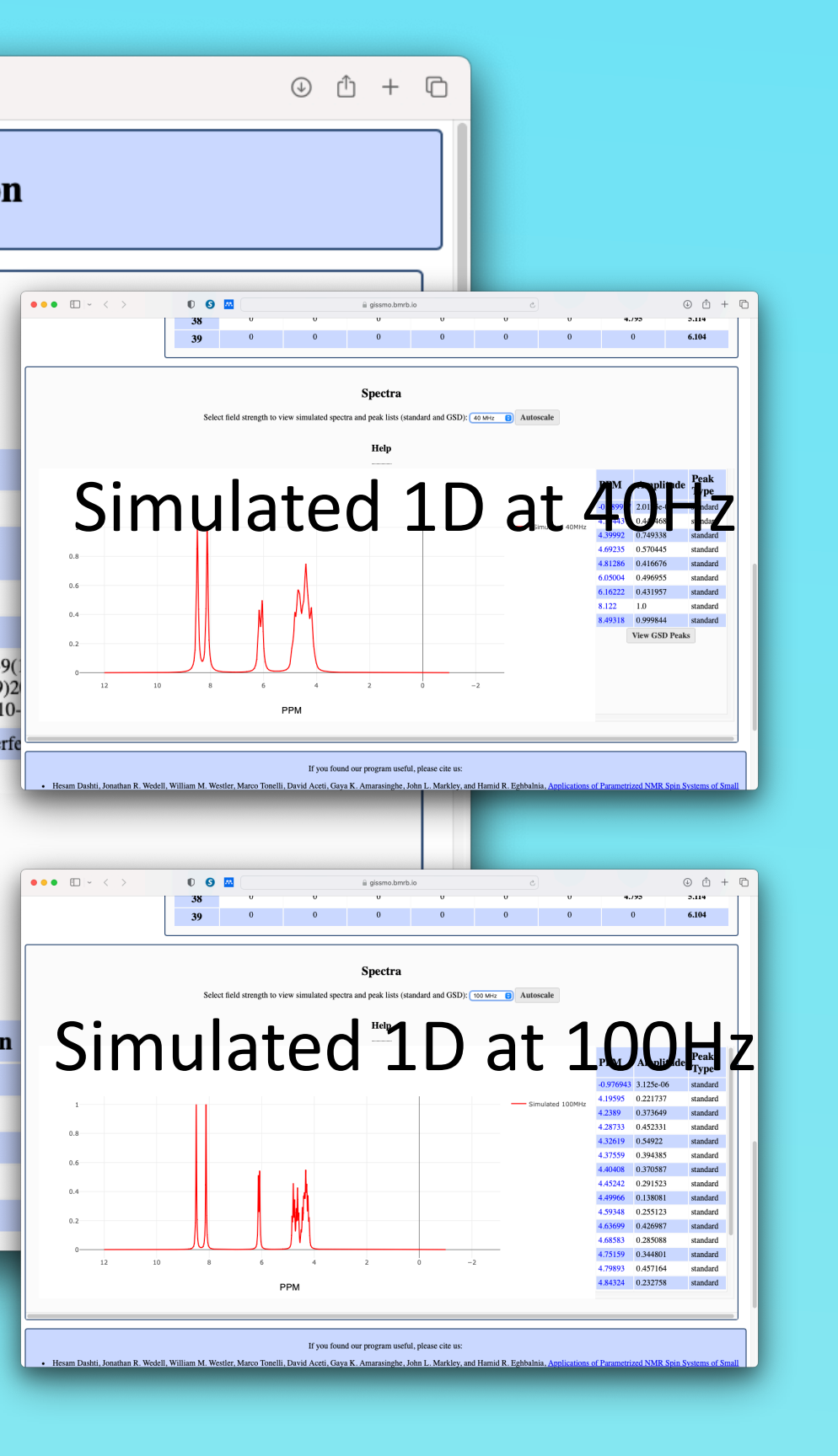
Spin System Matrix



Simulated 1D at 500Hz



Guided Ideographic Spin System Model Optimization



ATP Simulation outputs:

Parameter Value

Field strength 600.13 MHz

RMSD of the fit 0.02956

Temperature 298 K

pH 7.4

InChI InChI=1SC10H16NSO13P3c11-8-5-9-25-30(2,2,2)3-11(2,3,4)7-20(14,15,16)(12,11,12,13)H2,18,19,20(14-16,7-10)

Note 1 NMR low resolution, can't be fitted perfectly


Note 2 Ocar-Li

Note 3 Spin coupling constants

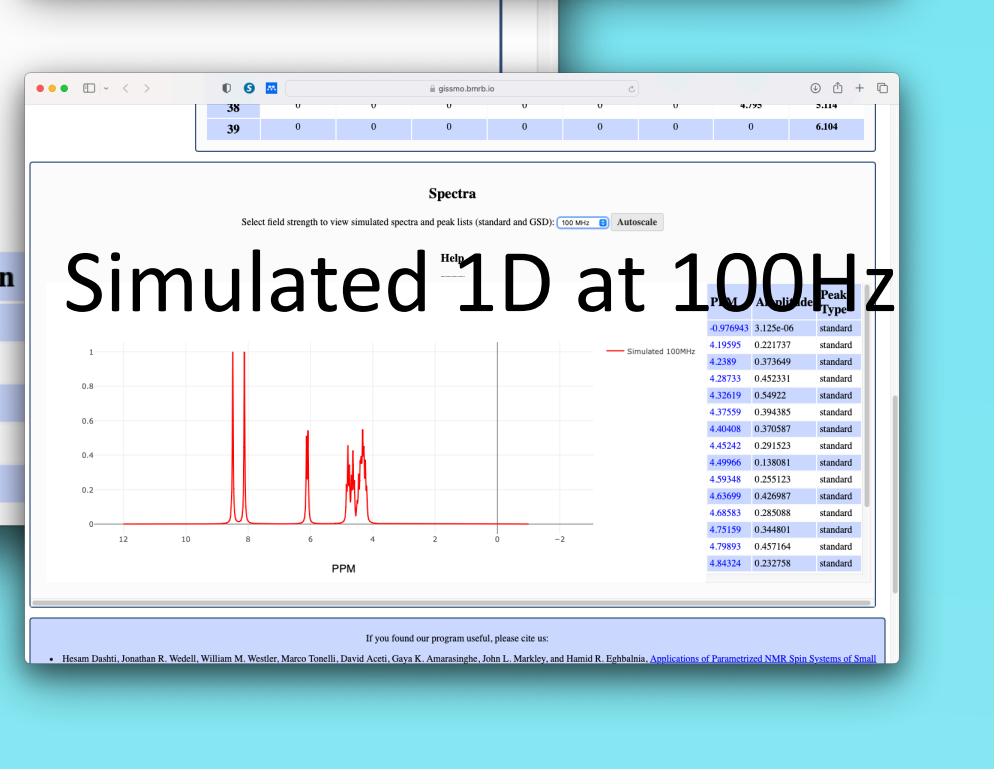
Additional coupling constants

32 8.758

33 8.758



Simulated 1D at 40Hz



Simulated 1D at 100Hz

## ALATIS Library

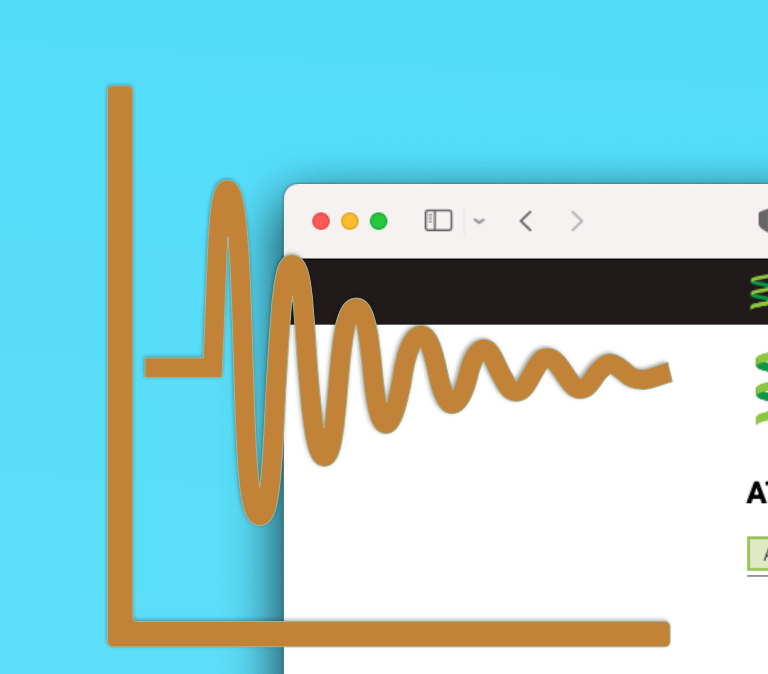
(<https://alatis.bmrbl.io/>)

Atom Label Assignment Tool Using InChI String<sup>4</sup> (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.

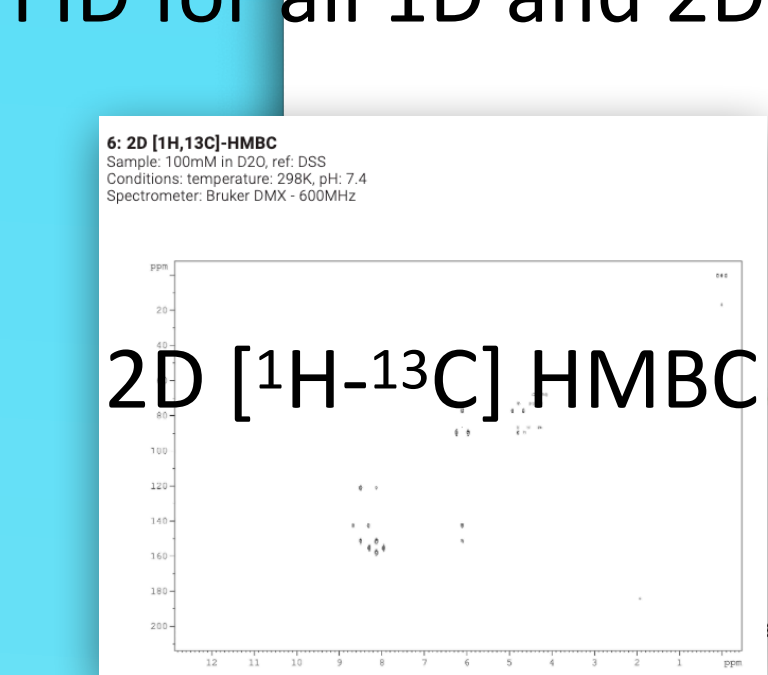
ALATIS library includes

- 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<sup>5</sup>

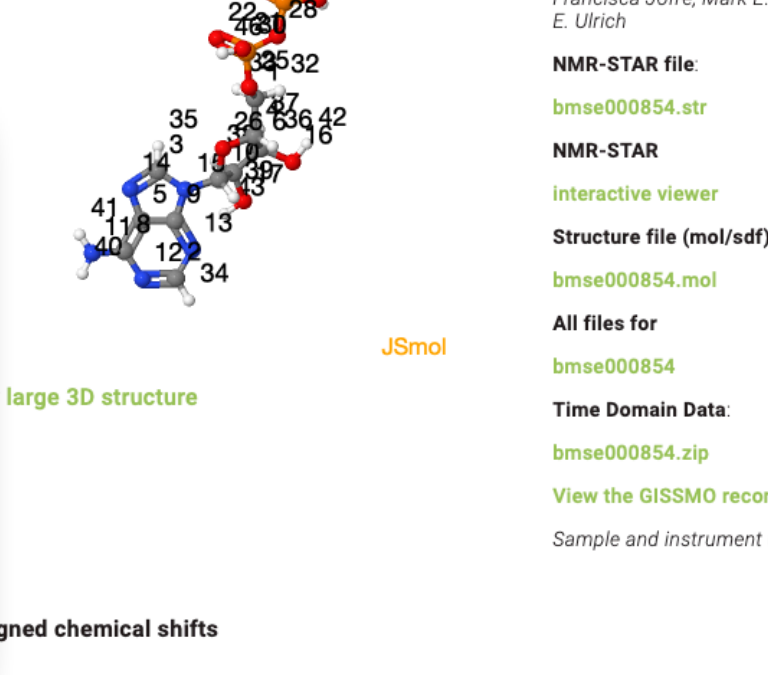
BMRB follows ALATIS numbering system in its small molecules database.



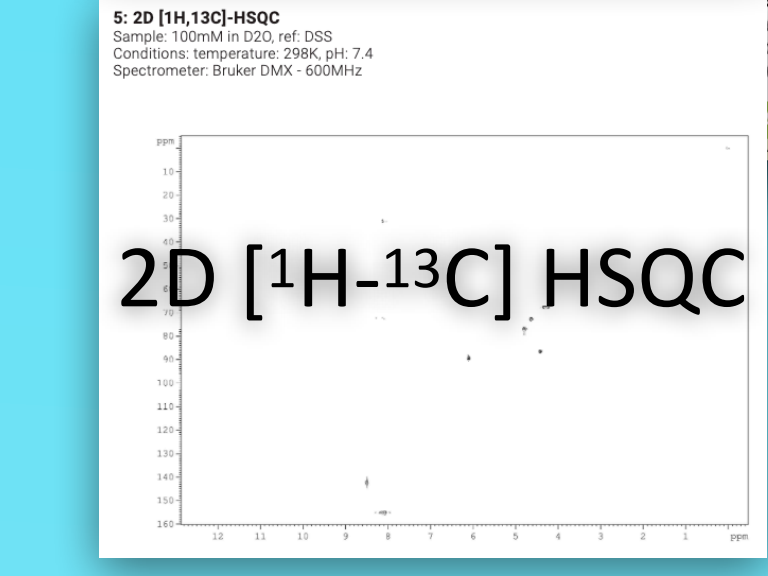
FID for all 1D and 2D



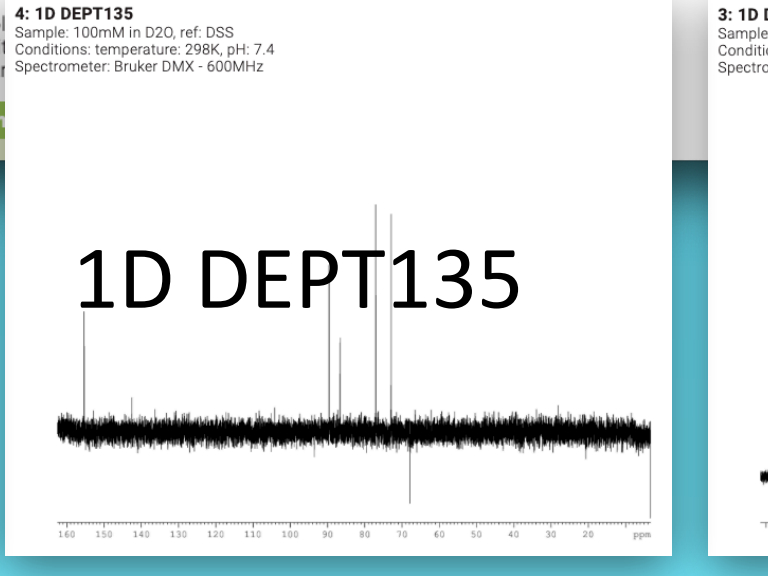
2D [1H-13C] HMBC



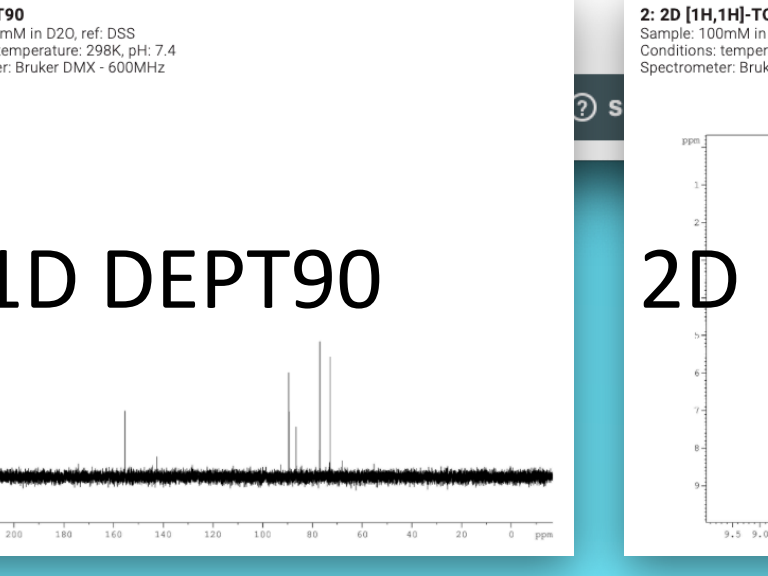
1D 1H



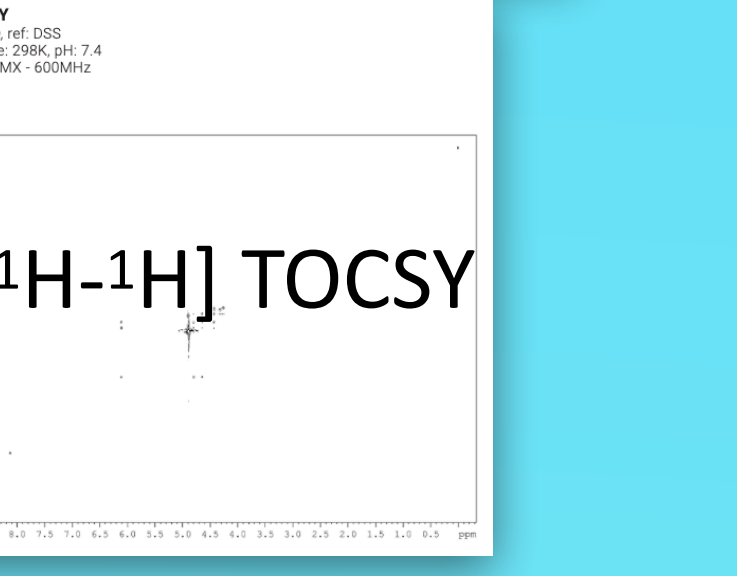
2D [1H-13C] HSQC



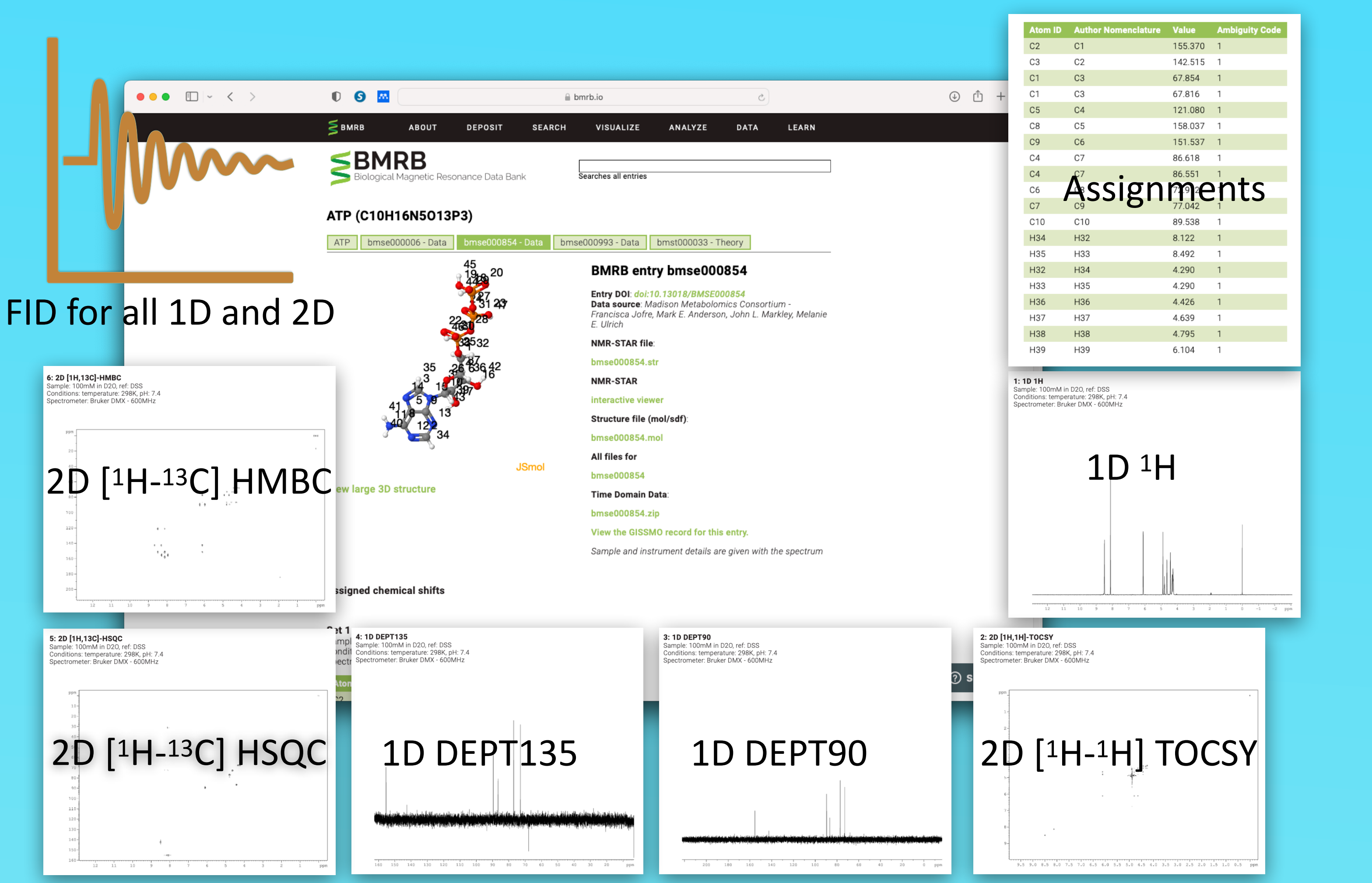
1D DEPT135



1D DEPT90



2D [1H-1H] TOCSY



BMRB entry bmrbl000854

Entry DOI: doi:10.13011/bmrbl000854

Data source: Metabolite Metabolomics Consortium

Reference: John, Mark E. Anderson, John L. Markley, Melanie E. Ulrich

NMR-STAR file: bmrbl000854.star

NMR STAR: bmrbl000854.star

Structure file (mol/sdf): bmrbl000854.mol

All files for bmrbl000854

Time Domain Data: bmrbl000854.f2

View the GISSMO record for this entry.

Sample and instrument details are given with the spectrum

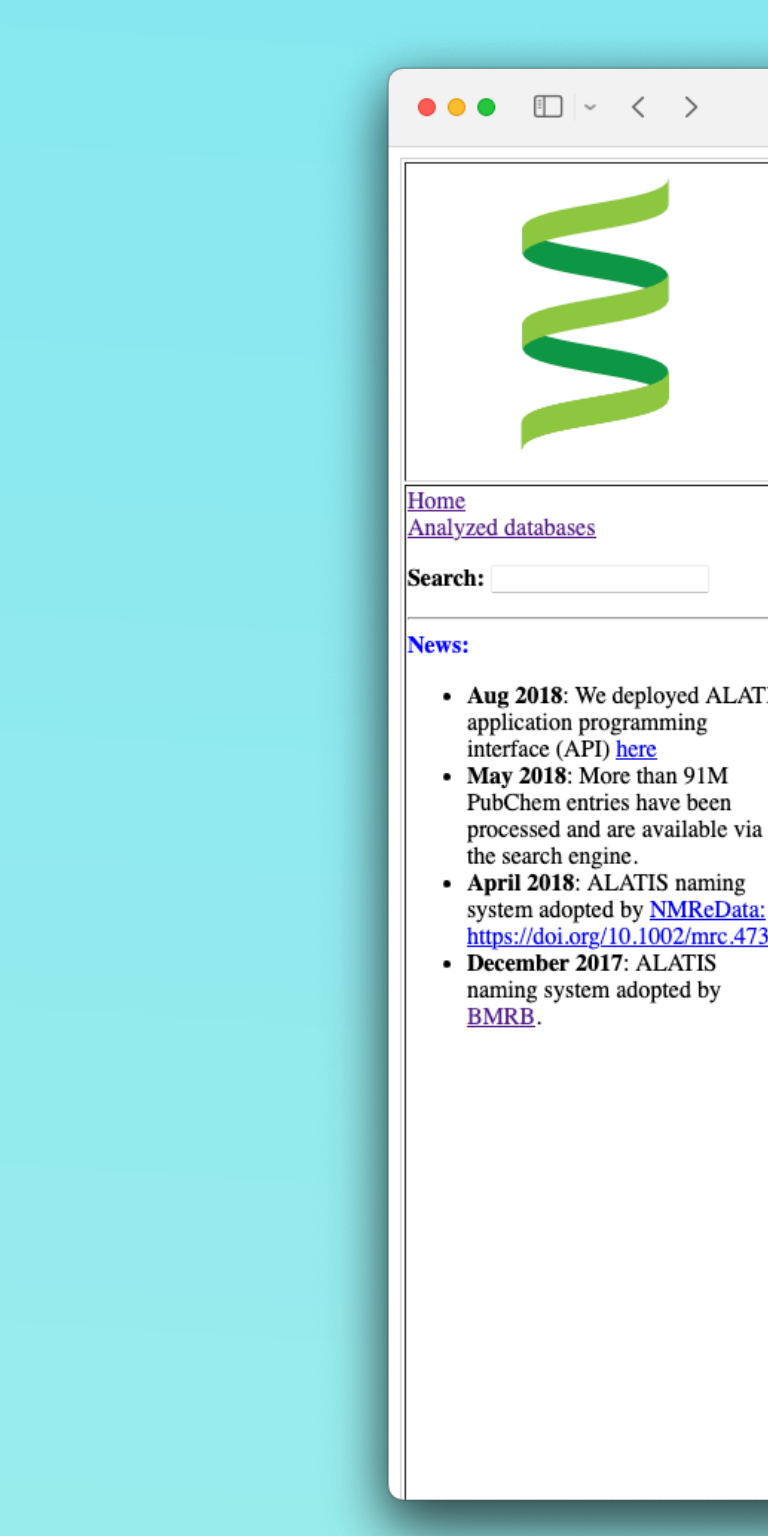
## GISSMO Library

(<https://gissmo.bmrbl.io/>)

Guided Ideographic Spin System Model Optimization<sup>2,3</sup> (GISSMO) enables the efficient calculation and refinement of spin system matrices (chemical shift and coupling constants) against experimental 1D-1H 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

Atom Label Assignment Tool using InChI String

1. Input structure format

Specify input format:

Search:

News:

- Aug 2018: We deployed ALATIS application programming interface (API) [here](#)
- May 2018: More than 91M PubChem entries have been processed and are available via the search engine.
- April 2018: ALATIS naming system adopted by NMRDataBank <https://doi.org/10.1002/nmr.4717>
- December 2017: ALATIS naming system adopted by BMRB

2. Auxiliary options

a. If the input structure is a 2D structure, you can check this box to get a 3D project of the structure: ☐ Generate 3D structure

b. If hydrogen atoms are missing from the structure, you can check this box to add hydrogen atoms: ☐ Add hydrogen atoms

3. Upload or paste input structure

upload a structure file (one compound per submit):

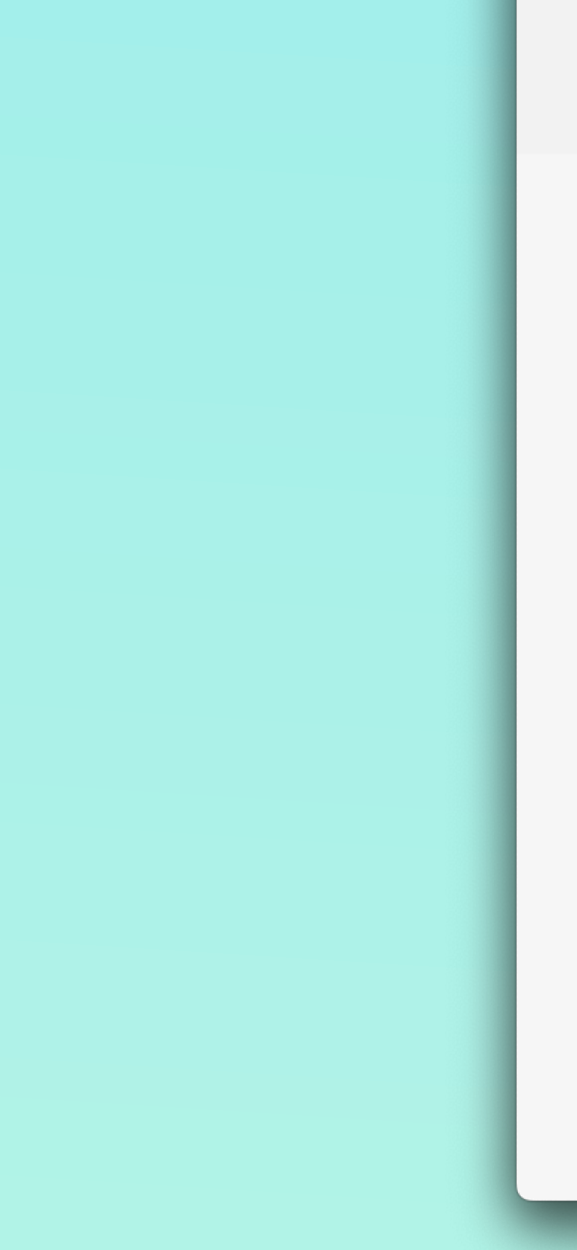
Choose File: no file selected

OR paste a structure (if a file has been uploaded we process the uploaded file)

4. Submit

## NMRbox: Software and Computing resource

(<https://nmrbox.nmrhub.org/>)



NMRbox Software

It's simple! Let's help you get started.

You can search by Research Problem, Software Type, or All Software.

Research problem: Choose a filter: Metabolomics Software type: or perform a text search:

Software research problem: Metabolomics

11 software packages meet the criteria.

ALATIS

A tool for assigning unique and reproducible labels to all atoms of small molecules

BATMAN

An R package for estimating metabolite concentrations from NMR spectral data using a specialized MCMC algorithm

dataChord Spectrum Miner

Integrated application for NMR metabolomics and spectrum mining

GISSMO

Efficient calculation and refinement of spin system matrices

MestReNova (Mnova)

A top class software suite to process your analytical chemistry data

MetaboAnalystR

An R package for comprehensive analysis of metabolomics data

Metabolomics toolbox

Metabolomics toolbox

MVAPACK

Tools for processing and analyzing chemometric data

MZmine3

User-friendly package for data processing of mass-spectrometry data

RUNER

Enables seamless modifications of atom

tomeNMR

Suite of tools for processing and analysis of

Support

NMRbox<sup>6</sup> 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**, **Metabolomics toolbox**, **MVAPACK**, **MZmine3**, **RUNER**, **tameNMR** and **MATLAB**.

NMRHub 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.

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.