

## BMRB small molecules library

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

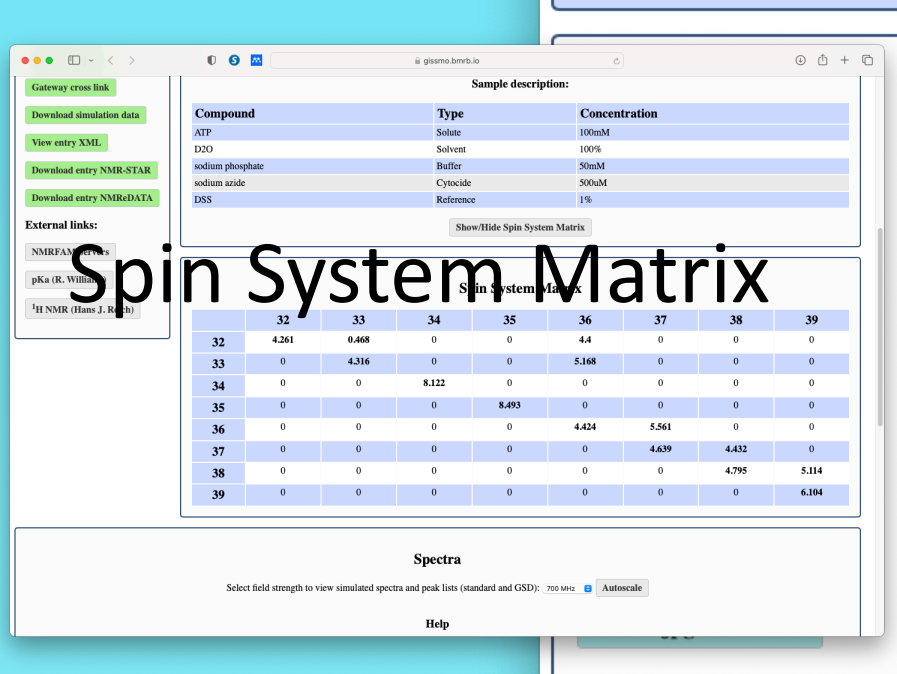
### Assignments

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

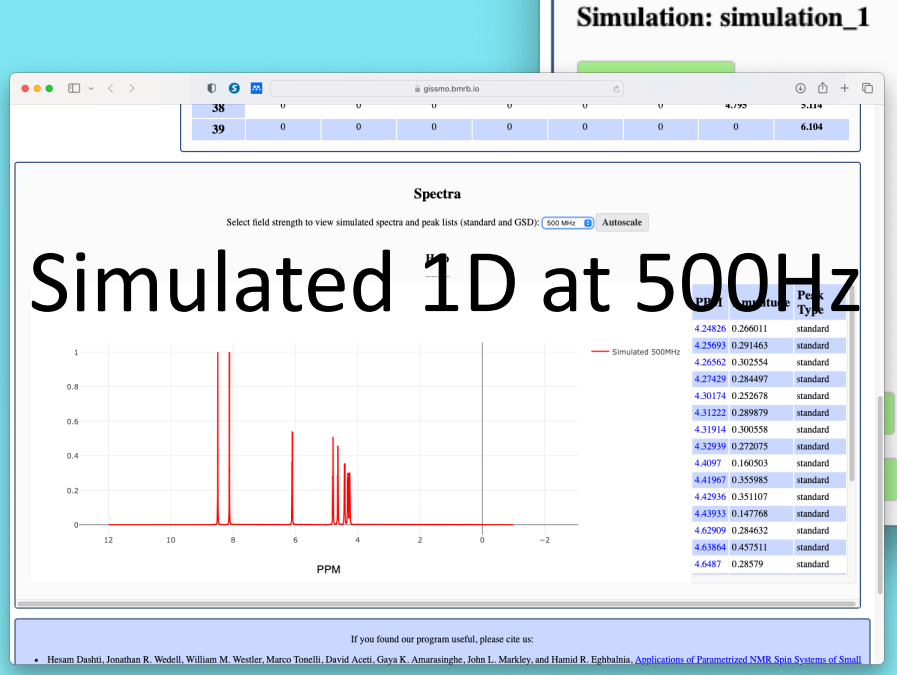
- Each reference data set consists of
- Chemical shift assignments
  - Sufficient time domain data (FID) from a set of 1D and 2D experiments to analyze the molecule

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



Simulation: simulation\_1


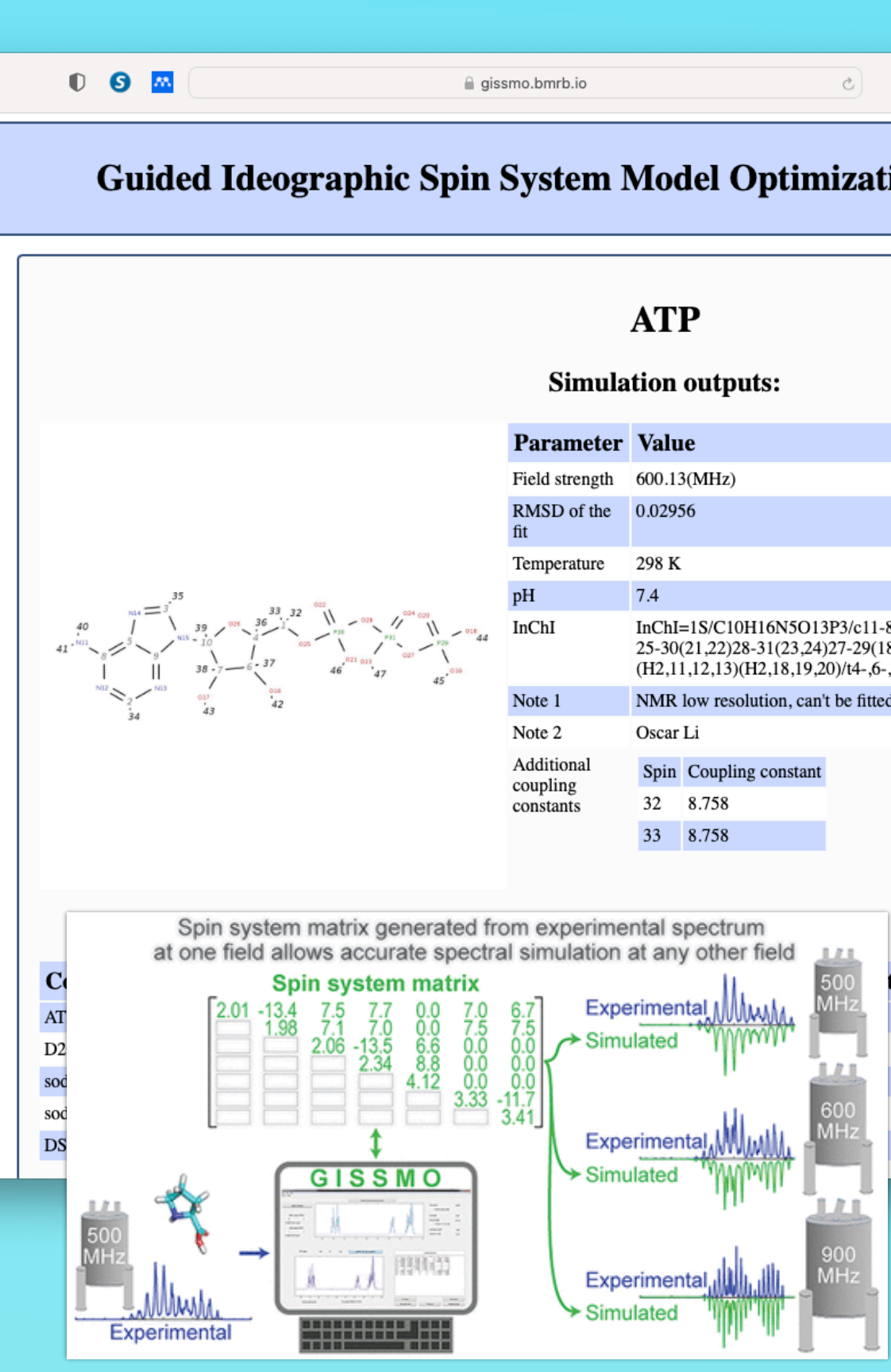


### Guided Ideographic Spin System Model Optimization

ATP

Simulation outputs:

Parameter	Value
Field strength	600.13MHz
RMSD of the fit	0.02956
Temperature	298 K
pH	7.4
InChI	InChI=1SC10H16N5O13P3
Note 1	NMR low resolution, can't be fitted perfectly
Note 2	Oscar Li
Additional coupling constants	Spin Coupling constant: 22, 8.758, 33, 8.758



## ALATIS Library

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

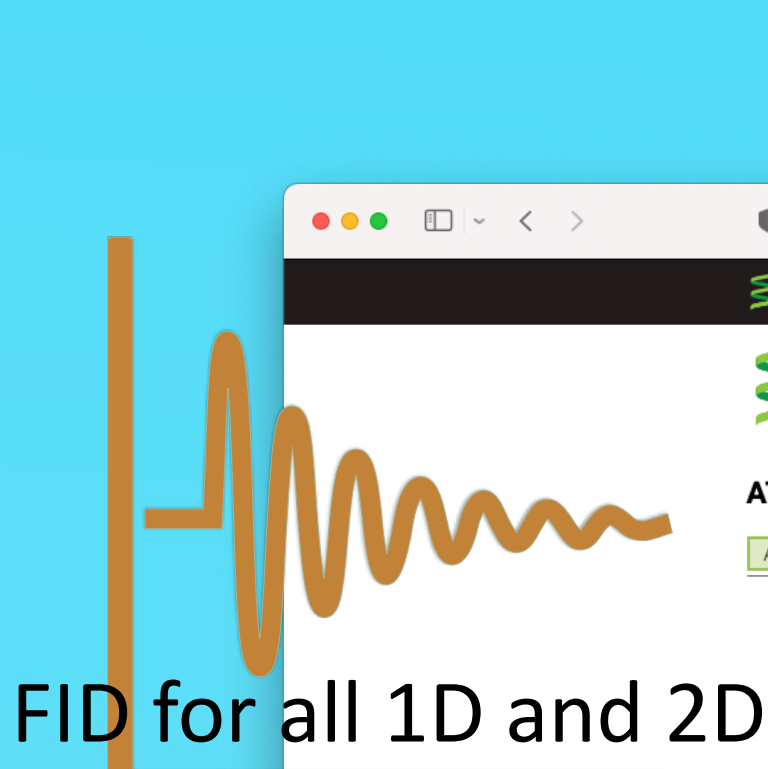
### Assignments

Atom Label Assignment Tool Using InChI String<sup>3</sup> (ALATIS) creates unique InChI identifiers for small molecules through rigorous labeling of their atoms. This numbering system helps to identify molecules across different databases and flawlessly compare the properties of their individual atoms

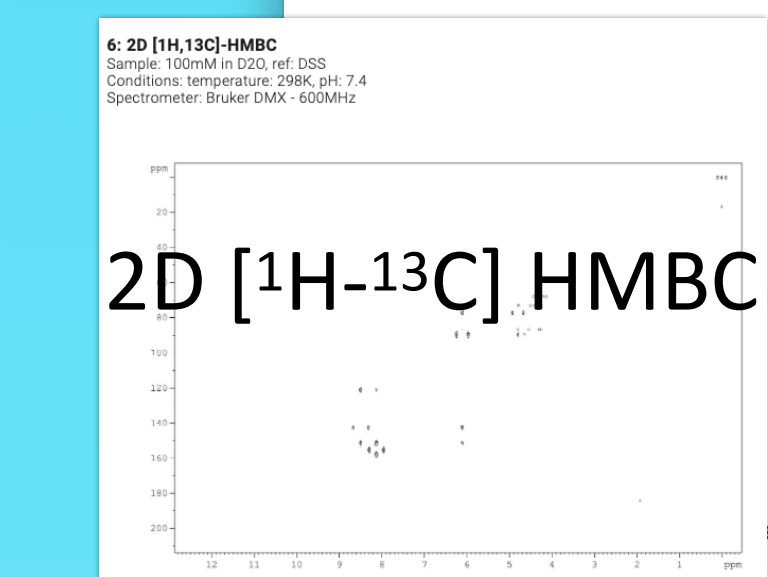
- ALATIS library includes
- Unique InChI strings for molecules from various databases like BMRB, PubChem, HMDB and RCSB-PDB Ligand-Exp
  - Cross-links from PDB entries to BMRB, HMDB and PubChem

BMRB follows ALATIS numbering system in its small molecules database.


### FID for all 1D and 2D



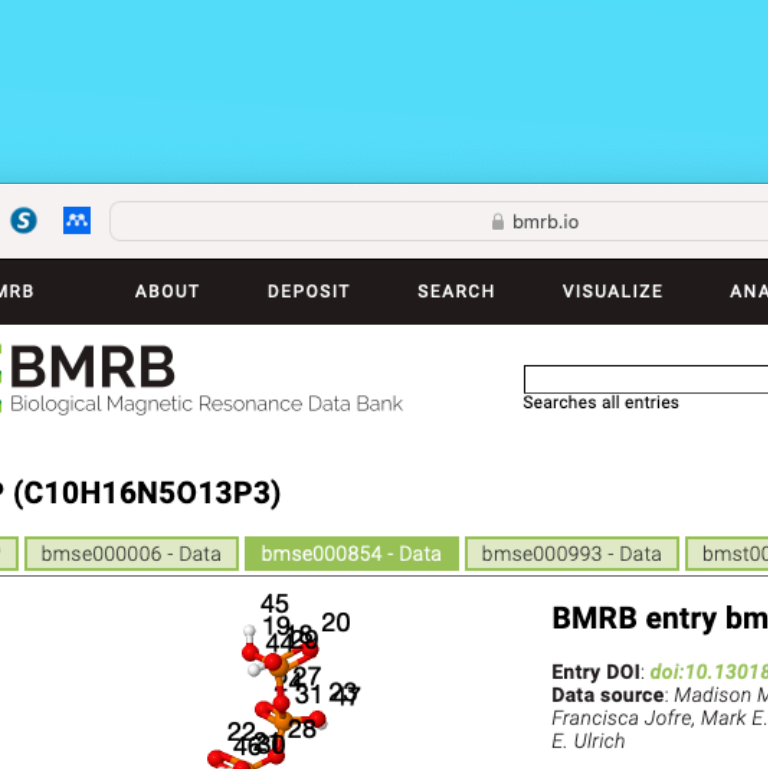
### 2D [1H-13C] HMBC



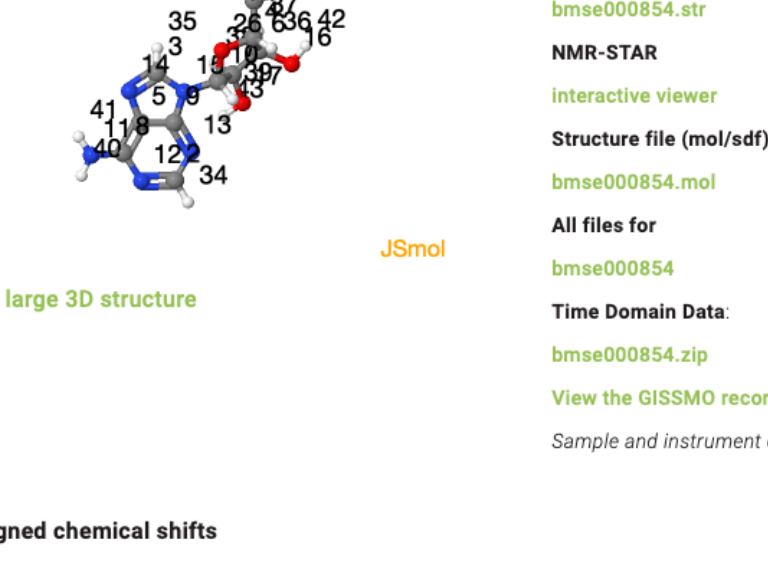
### 2D [1H-13C] HSQC



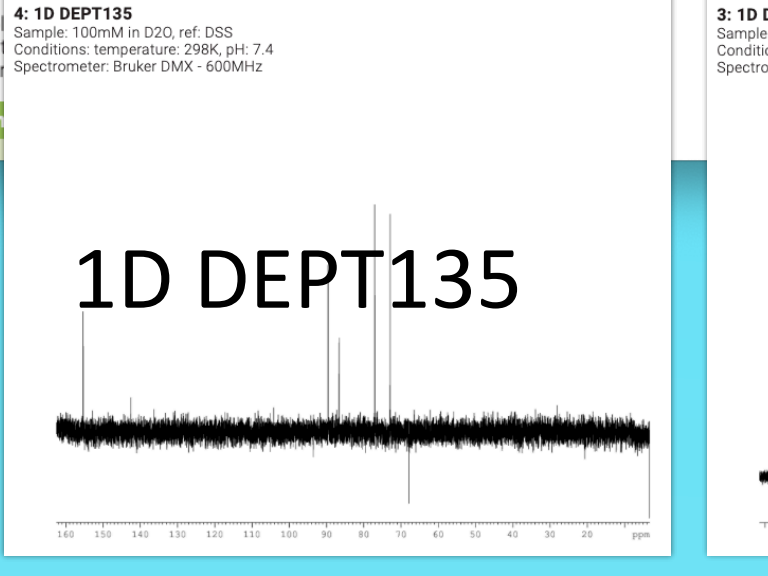
### 1D DEPT135



### 1D DEPT90



### 2D [1H-1H] TOCSY



## GISSMO Library

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

### Assignments

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

- GISSMO library includes
- Library of over 1000 parameterized small molecules
  - Spin system matrix for every molecule
  - Simulated 1D spectra at various field strength (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:

2. Auxiliary options

3. Upload or paste input structure

4. Submit

## NMRbox: Software and Computing resource

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

### Assignments

### NMRbox Software

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

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

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

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

NMRbox<sup>4</sup> is a resource for biomolecular NMR software. It provides tools for finding the software you need, documentation and tutorials for getting the most out of the software, and cloud-based virtual machines for executing the software. NMRbox is available free for academic use.

NMRbox provides ready to use computing resource along with various preinstalled software tools like **ALATIS**, **BATMAN**, **dataChord Spectrum Miner**, **GISSMO**, **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) and 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., *Sci Data* 4, 170073 (2017)
4. Jeffrey C Hoch et al., *Biophysical Journal*, 112: 1529-1534, 2017.