# The BMRB archive of Protein, Nucleic Acid and Metabolite NMR Data



Biological Magnetic Resonance Data Bank (BMRB:

https://bmrb.io ) serves the biomolecular NMR

community by supporting a curated archive of

primary and derived data and metadata linked to

scientific investigations under the "FAIR Principles"

(Findable, Accessible, Interoperable, and Reusable)<sup>1</sup>.

BMRB is a member and a core archive of the

Worldwide Protein Data Bank (wwPDB: https://

www.wwpdb.org), which collects the coordinate data

along with assigned chemical shifts and restraints

from NMR structural studies through the OneDep

(https://deposit.wwpdb.org) deposition system. NMR

data from other studies are collected by the

BMRBdep (https://deposit.bmrb.io) deposition

system. BMRB's goal is to empower scientists in

their analysis of the structure, dynamics, and

chemistry of biological systems and to support

further developments in the field of biomolecular

NMR-STAR data model

The NMR-STAR<sup>2</sup> is the official data format of

BMRB and the deposition and archival format of

NMR Spectroscopic data at the wwPDB. It is a Self-

defining Text Archive and Retrieval (STAR) format

with controlled vocabularies(tags) defined by the

NMR-STAR dictionary. The NMR-STAR data model

supports all kinds of NMR data, metadata and

≶BMRB ABOUT DEPOSIT SEARCH VISUALIZE ANALYZE DATA LEARN

theoretical coupling constants

other data types

chem shift reference O

spectral peak list

assembly supercategory O chem shift anisotropy

NMR experiments used to derive these data -

Systematic chemical shift offsets

Atom chem shift 0

Click here to view a graphical representation.

Show tags without values Download

NMR structure of the murine DLC2 (deleted in liver cancer -2) SAM

NMR spectroscopy.

derived data.

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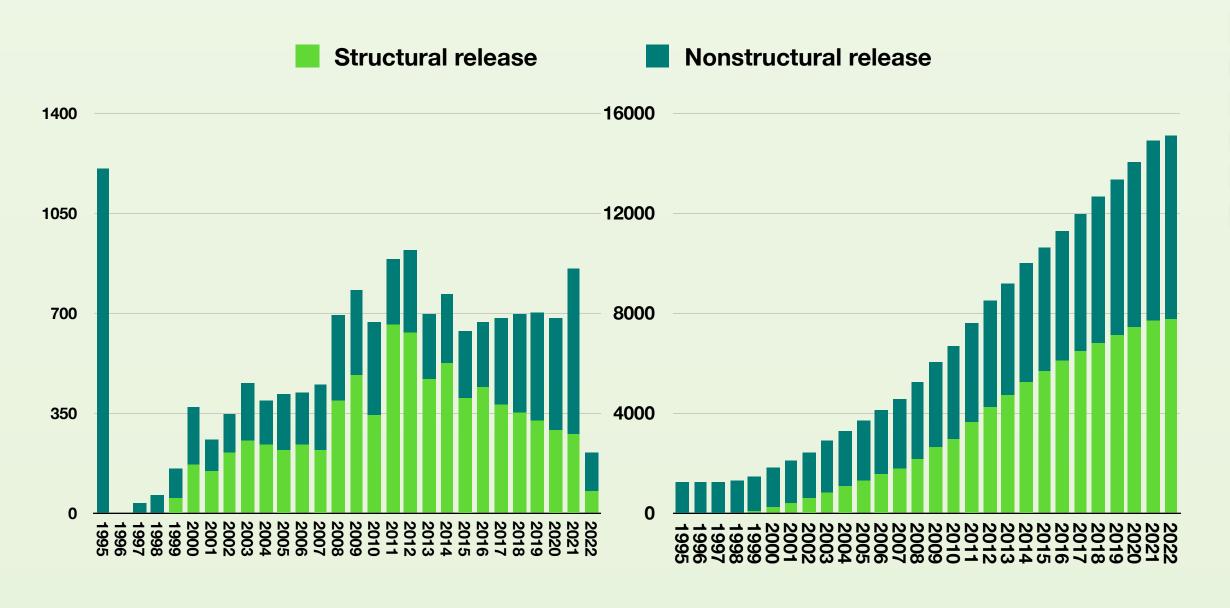
data\_undefined □ save\_entry\_information \_Entry.Sf\_category Kumaran Baskaran, Jonathan R. Wedell, Hongyang Yao, Dimitri Maziuk Hamid R. Eghbalnia, Michael M. Gryk, Colin W. Wilburn, and Jeffrey C. Hoch

> Department of Molecular Biology and Biophysics, UConn Health, 263 Farmington Avenue, Farmington, CT 06030, USA



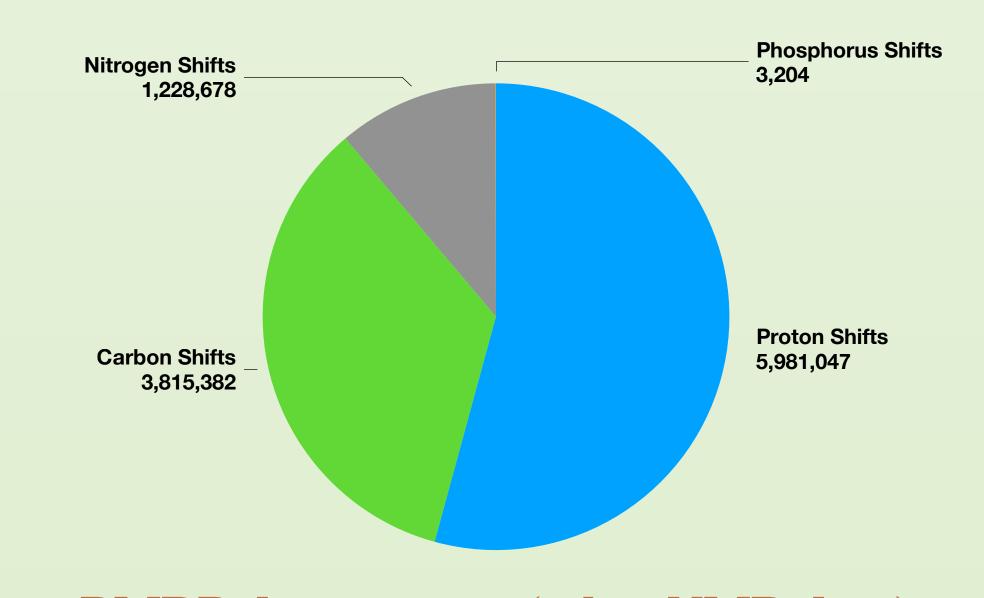
### BMRB growth statistics

The bar graph shows the growth of the BMRB archive. As of April 2022, BMRB holds 15083 entries with 7759 entries having corresponding

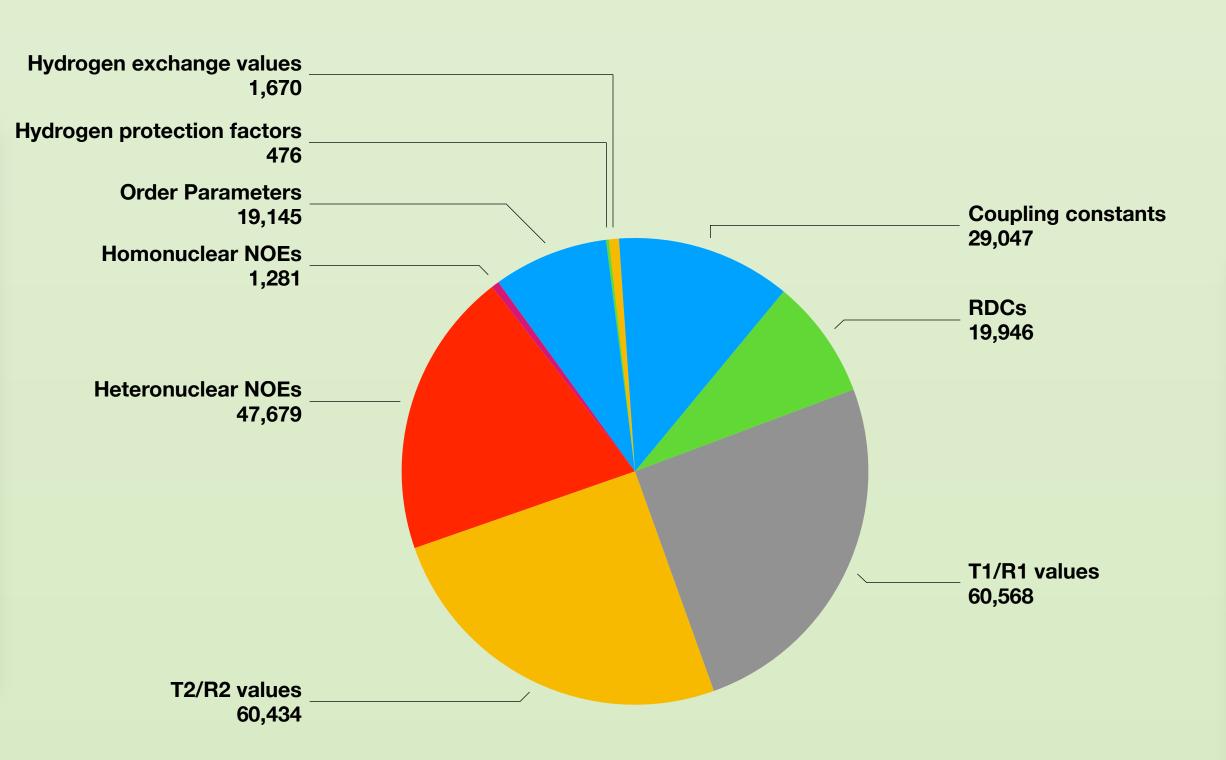


#### BMRB data content (chemical shifts)

As of April 2022, BMRB holds over 10 million chemical shifts from 14156 protein, 548 DNA and 532 RNA entries. In addition to the chemical shift data, other NMR data also available at the BMRB



BMRB data content (other NMR data)



coordinate data in the PDB and 7324 NMR entries.

**BMRB** 

### **BMRB Software resouce**

## BMRB GitHub: <a href="https://github.com/bmrb-io">https://github.com/bmrb-io</a>

Data access

ind data using the instant

search or advance search

Access through web

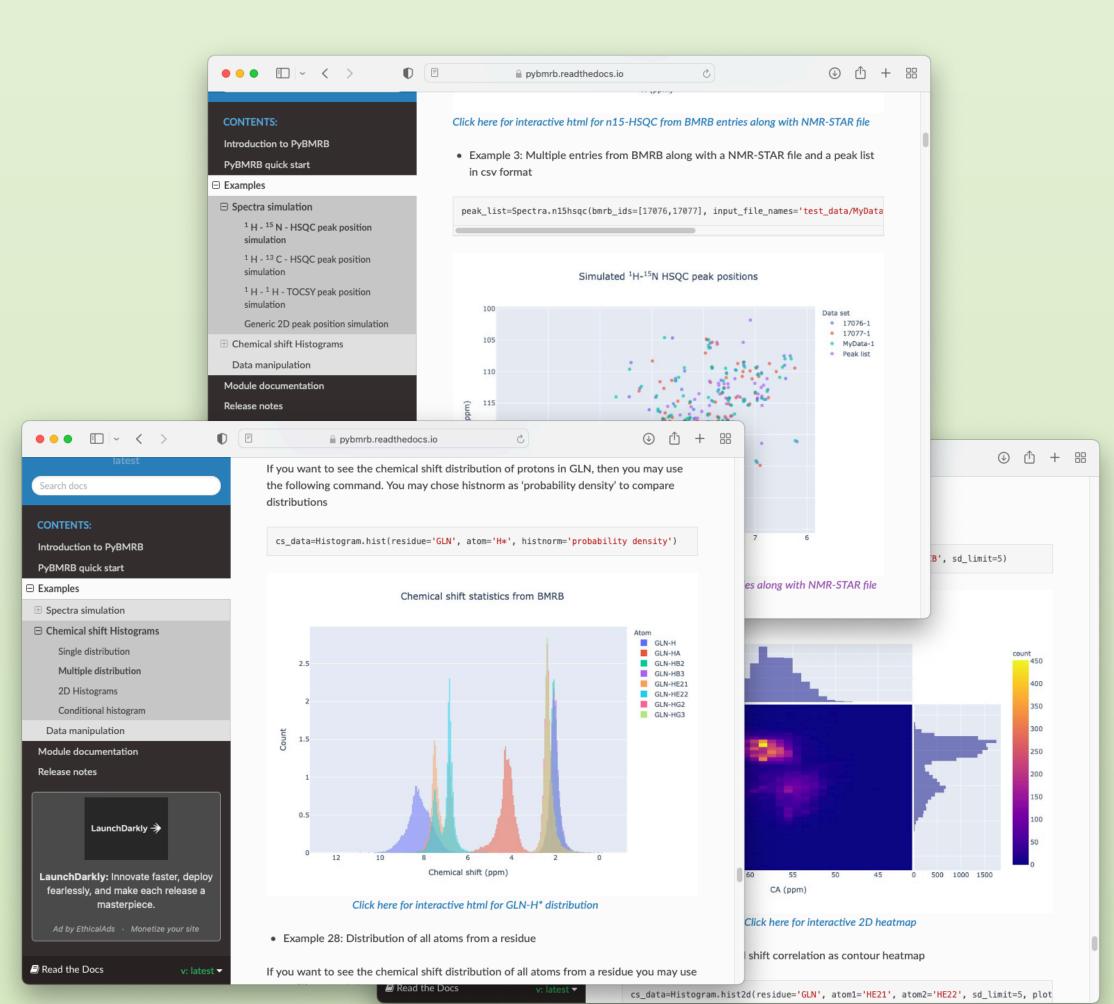
browser or BMRB API

of PyNMRSTAR

- BMRB API : provides machine to machine access to BMRB data base
- PyNMRSTAR : Python NMR-STAR parser
- PyBMRB: BMRB data visualization tools in Python
- RBMRB: BMRB data visualization tools in R

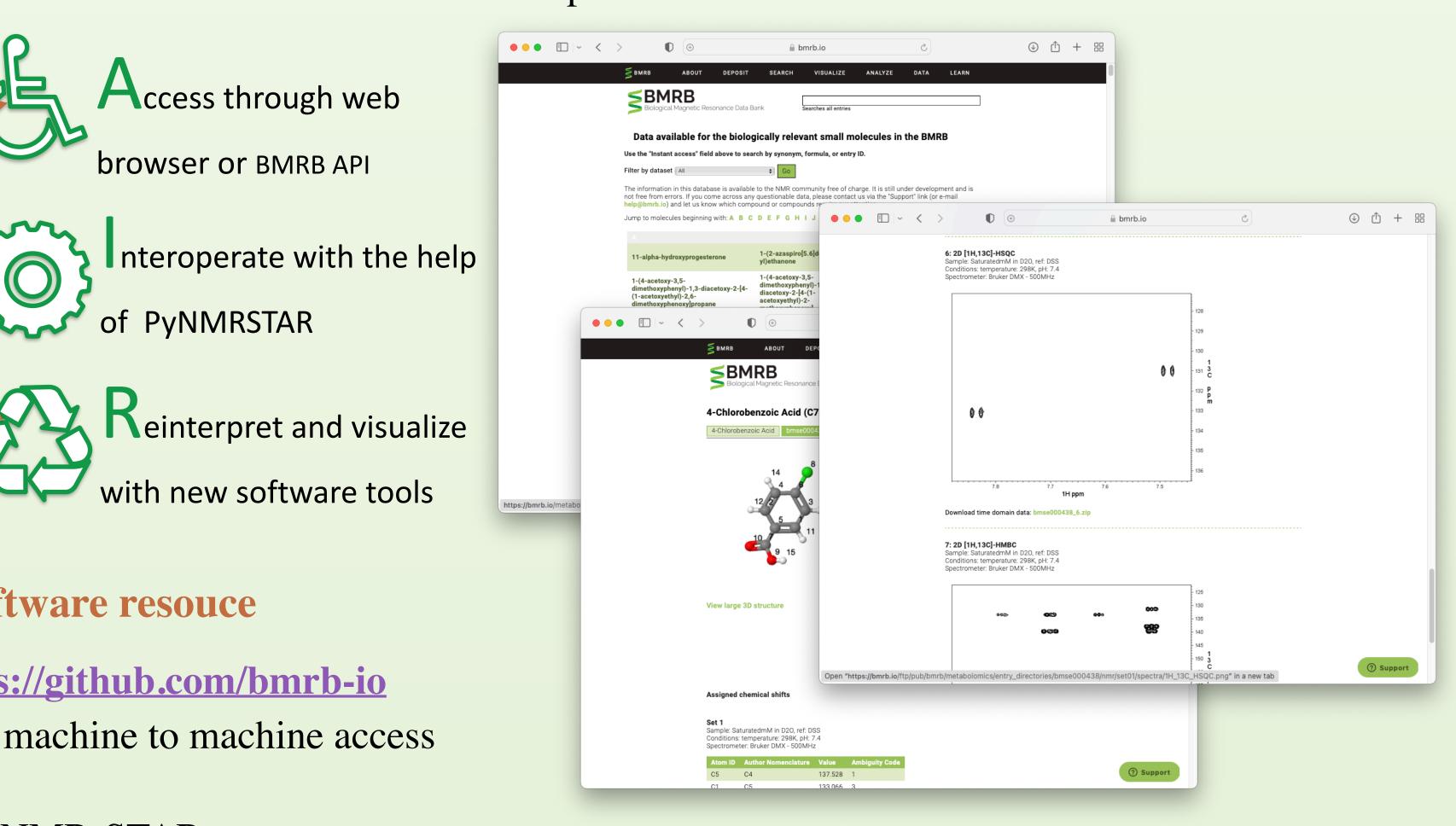
#### BMRB data visualization

Chemical shift histograms and simulated HSQCs can be generated using PyBMRB or RBMRB.



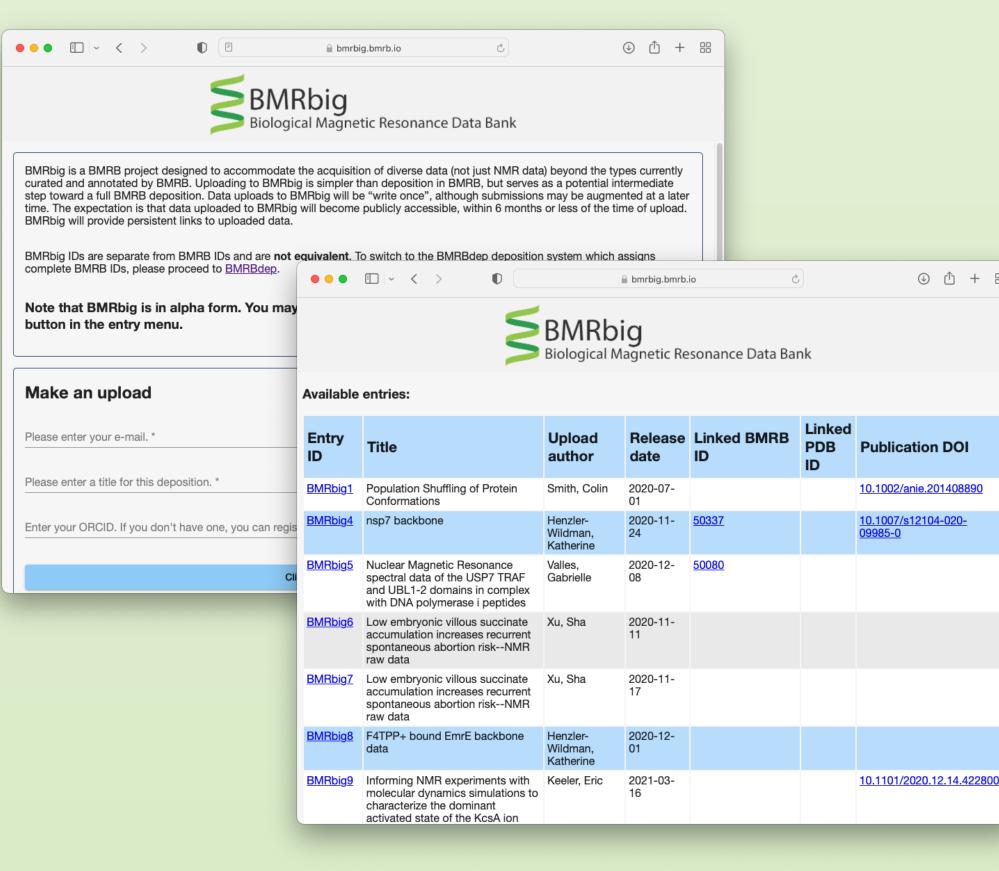
#### Small molecules library

BMRB maintains a library of carefully curated NMR spectroscopic data of over 1000 biologically important small molecules.



#### **BMRBig**

BMRbig is a BMRB project designed to accommodate the acquisition of diverse data (not just NMR data) beyond the types currently curated and annotated by BMRB. Uploading to BMRbig is simpler than deposition in BMRB, but serves as a potential intermediate step toward a full BMRB deposition. Data uploads to BMRbig will be "write once", although submissions may be augmented at a later time



- 1. Wilkinson, M. D.; et al. Scientific data 2016, 3, 160018.
- 2. Ulrich, E. L.; et al. J. Biomol. NMR 2019, 73 (1-2), 5.

