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

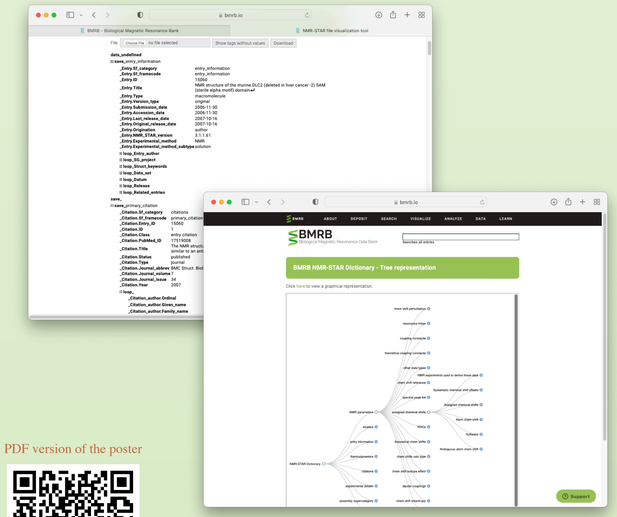
Kumaran Baskaran, Jonathan R. Wedell, Hongyang Yao, Dimitri Maziuk Hamid R. Eghbalnia, Michael M. Gryk, Colin W. Wilburn, and Jeffrey C. Hoch

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

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)[1]. 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 spectroscopy.

NMR-STAR data model

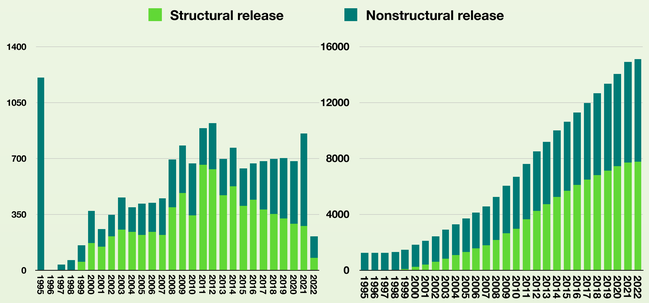
The NMR-STAR[2] is the official data format of BMRB and the deposition and archival format of NMR Spectroscopic data at the wwPDB. It is a Self-defining Text Archive and Retrieval (STAR) format with controlled vocabularies(tags) defined by the NMR-STAR dictionary. The NMR-STAR data model supports all kinds of NMR data, metadata and derived data.



PDF version of the poster

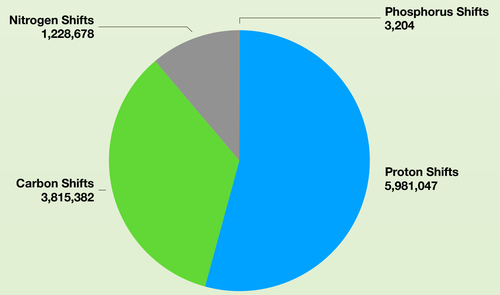
BMRB growth statistics

The bar graph shows the growth of the BMRB archive. As of April 2022, BMRB holds 15083 entries with 7759 entries having corresponding coordinate data in the PDB and 7324 NMR entries.

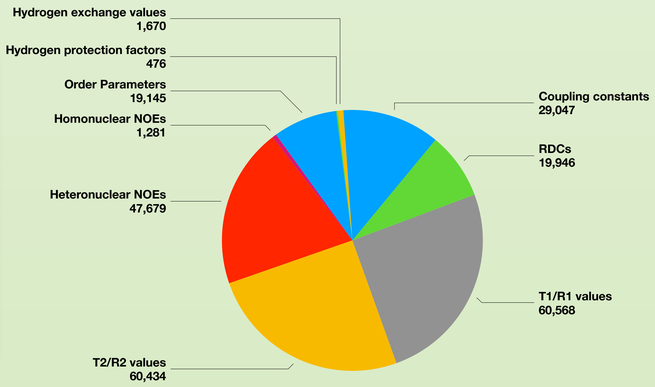


BMRB data content (chemical shifts)

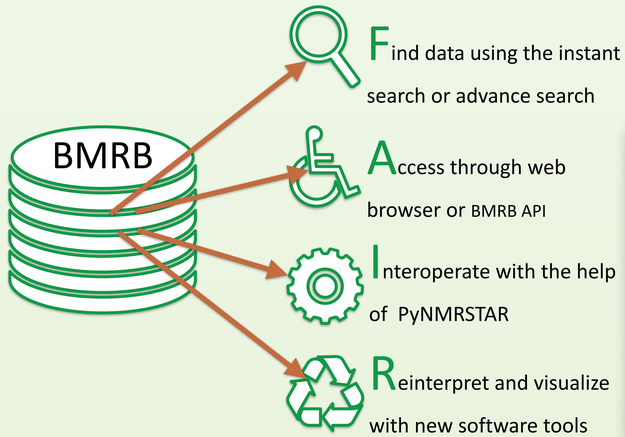
As of April 2022, BMRB holds over 10 million chemical shifts from 14156 protein, 548 DNA and 532 RNA entries. In addition to the chemical shift data, other NMR data also available at the BMRB



BMRB data content (other NMR data)



Data access



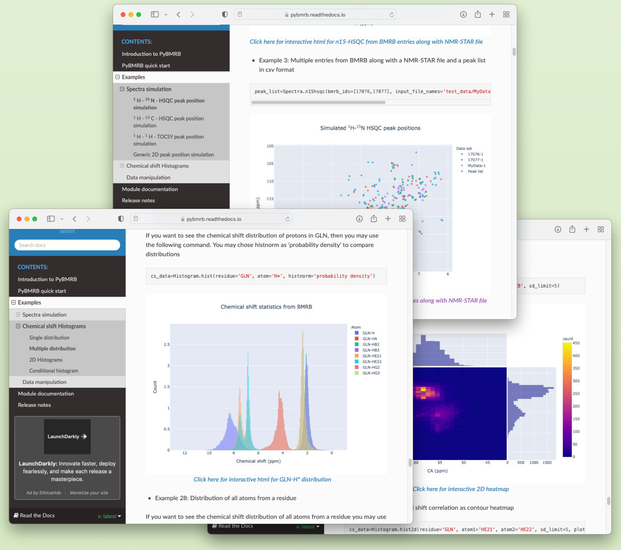
BMRB Software resouce

BMRB GitHub: https://github.com/bmrb-io

- 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

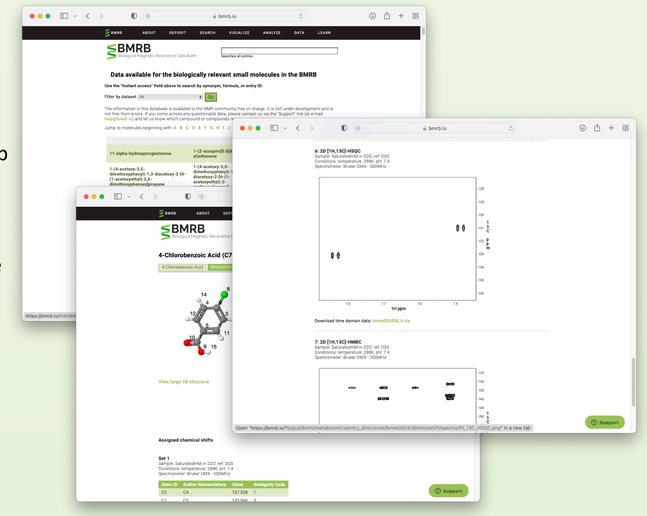
BMRB data visualization

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



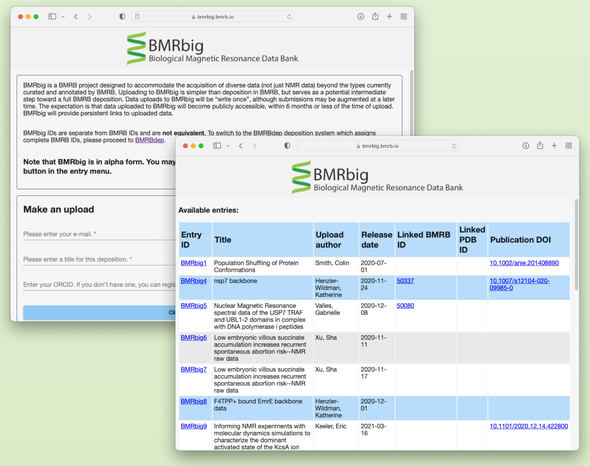
Small molecules library

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.*