PyBMRB: Data visualization tool for BigMagResBank

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Abstract

The Biological Magnetic Resonance Data Bank (BioMagResBank or BMRB https://bmrb.io), founded in 1988, is the international, open archive for data generated by Nuclear Magnetic Resonance (NMR) spectroscopy of biological systems. NMR spectroscopy is unique among biophysical approaches in its ability to provide a broad range of atomic and higher-level information relevant to the structural, dynamic, and chemical properties of biological macromolecules, as well as report on metabolite and natural product concentrations in complex mixtures and their chemical structures. NMR-STAR is the official data format of BMRB and BMRB provides python parser (PyN- MRSTAR https://github.com/uwbmrb/PyNMRSTAR), a data visualization tool (PyBMRB https://github.com/uwbmrb/PyBMRB) and an Application Program Interface (API) (BMRB-API https://github.com/uwbmrb/BMRB-API) to access the BMRB archive. PyBMRB displays the chemical shifts data in each entry as a simulated NMR spectrum and to generates database-wide chemical shift his- tograms of different atom types in proteins and nucleic acids. PyBMRB provides access to BMRB data through the API and generates portable and interactive visualizations as a single html file. It also supports data visualization workflows using Jupyter Notebooks, which can be both easily created and shared.

No need to download and parse the data from BMRB for data visualization. PyBMRB does it for you.

Features:

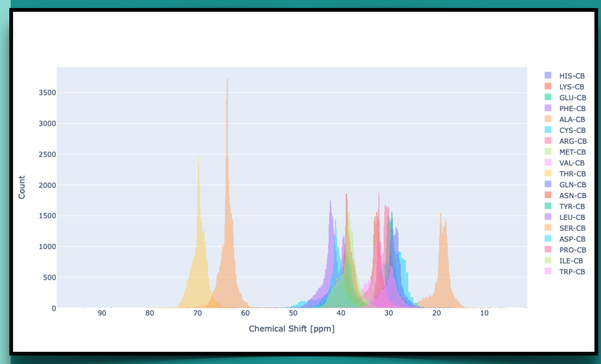
- Plot HSQC peak positions for any BMRB entry
- Compare list of BMRB entries as NMR spectra
- Compare your data with one or more BMRB entries
- Chemical shift histograms from BMRB database
- Interactive graphics as stand alone html

```
> n15hsqc(bmrbid=[17074,17076],
filename='my_data.str',groupbyresidue=True)
```

Please scan the QR code for the digital copy of this poster

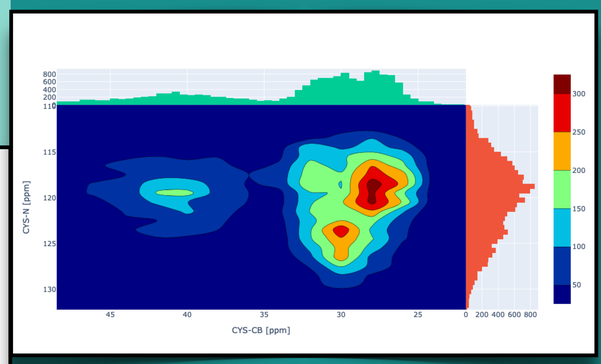
Sample visualizations

Chemical shift histogram of CB atoms from BMRB database



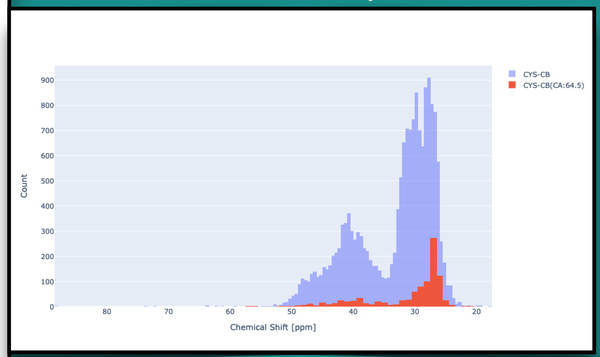
>h.hist(atom='CB')

Chemical shift correlation of Cysteine CB and N



>h.hist2s(residue='CYS', atom='CB')

Chemical shift correlation of Cysteine CB and N



>h.conditional_hist(residue='CYS', atom='CB', atomlist=['CA'], cslist=[64.5])

BMRB is constantly working to improve the PyBMRB visual- ization tool. The next update aims to include simulation of more NMR experiment types and include visualization options for other data types such as distance and dihedral-angle restraints that are present in the BMRB database.

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