Data Production

MD: Calculate correlation functions

Selection Object

All MD analyses start with specifying the atoms/bonds of interest
Same object as in data below
Define selections (.select_bond)
Bond selections (.sel1, .sel2)
Vectors, positions (.v,.pos)
Trajectory management (.traj)
Default labels (.label)

Basic Processing

pyDR.md2data

ROMANCE (frames)

Frame Object (pyDR.Frames.FrameObj)

All MD analyses start with specifying the atoms/bonds of interest
Define bond frame (.tensor_frame)
Define reference frames (.new_frame)
Send to data object (.frames2data)
Send to iRED (CC) object (.frames2ired)

Cross-correlation (iRED)

iRED Object (pyDR.iRED)

Calculates reorientational modes (rank 1/2), converts to data
Send to data object (.ired2data)

NMR: Load from file

pyDR.IO.readNMR
Text file with experimental parameters and data

Via data fitting

(source) Data Object

Same as data object below. Produces a new data object via fitting or optimization (.fit,.opt2dist)

Data Storage/Visualization

Project Object

Data container
Provides quick access to a large data set, sorted via various parameters.
Allows efficient batch processing and efficient-storage and reloading

Batch processing
Detector optimization (.detect)
Batch fitting (.fit,.opt2dist)

Display
Plot management (.plot,.plot_obj,.current_plot,.fig)
ChimeraX manager (.chimera)

Data indexing:
[0] single index
[[0,3,4]] selection
[1:5:2] slicing
['no_opt'] keywords
['p6.+N15'] RegEx

Storage:
Saves data, including data reduction (.save)
Manages data reloading (minimize time/memory/drive space)

Data Object

Data: Relaxation rates / Correlation functions (.R)
Standard deviation (.Rstd)
Order Parameters + standard deviation (.S2,.S2std)

Fits: Source data (.src_data)
Fitted data (.Rc, .S2c)
Statistical parameters (.chi2,.chi2red,.AIC,.AICc)

Display: Plot data+sensitivity (.plot)
Plot fit quality (.plot_fit)
Display in chimeraX (.chimera)
Display in NGL view (.nglview)

Fitting: Fit data using detectors (.fit)
Optimize fit to a distribution (.opt2dist)

Metadata: Data title (.title)
Labels (.label)
Sensitivity parameters (.info)
Descriptive data history (.details)

Selection Object (.select)

Locations in PDB corresponding to data
(len(data.select)=len(data))
Define selections (.select_bond)
Bond selections (.sel1, .sel2)
Display selections (.repr_sel)
Default labels (.label)

Source Information Object (.source)

Organizes data, talks to Project object
File locations (.filename,.original_file, .topo, etc.)
Processing info (.status,.n_det,.additional_info)
Title constructor (.title)

Sensitivity Object (.sens)

Defines data sensitivity vs. correlation time
(can be a detector object)
Correlation time (.z,.tc)
Sensitivity (.rhoz)
Parameters (.info)
Plotting (.plot_rhoz)
Send to detector (.detect)

Detector Object (.detect)

Determines fitting for data object
(child class of sensitivity class)
Same as sense (.z,.tc,rhoz,.info,.plot_rhoz)
Detector setup (.r_auto, .r_target, .r_no_opt)