

# 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

## Data Storage/Visualization

### Project Object

#### Data container

Provides quick access to a large data set, sorted via various parameters.  
Allows efficient batch processing, 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)

#### 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 (.Detector)

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)

#### 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)

## 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)