1 Data structures

The code is based on physical objects.

The information that describes a solution (compounds, concentrations, and solvents) are stored in a Solution object.

Since a well can be modified at different times throughout an experiment, the states of that well are saved in action objects that contain the time the action was performed and the Solution object describing the state of that well.

A well's action objects are stored in an actionList object.

A well object contains an actionList as well as the well's location, path to it's data file, as well as a matrix or data frame that holds the data. Other functions such as data smoothers or splines specific to that well may also be stored in a well object.

A wellList object holds multiple well objects.

2 Loading or generating well data and annotations

2.1 Create well list from CSV annotation file

A wellList object may be generated from an annotation file. This is easiest to explain by example.

2.2 Create well list programatically