

NMRLipids databank structure

<https://github.com/NMRLipids/Databank>

Raw simulation data

Publicly available, e.g., in Zenodo



Databank builder

(Python code: **AddData.py**)

Indexes publicly available **simulation data**
based on information given by contributor



Experimental data

(git repository with yaml and data files)

Indexed experimental data (**Data/experiments**)



Quality evaluator

(Python code: **searchDATABANK.py**, **QualityEvaluation.py**)

Connects experimental and simulation
Datasets and calculates quality measures



NMRLipids Databank

(git repository with yaml files)

Indexed information on simulation data (**Data/Simulations**)
and quality evaluation (**Data/QualityEvaluation**)



Databank analyzers

(Jupyter notebooks, Python codes)

Pulls the data from databank
to perform analyses



Results

(git repository with yaml and data files)

Results from the databank can
Be indexed as the databank
(for example *Data/DENSITIES*)