

Data

/Leiden

/SWRI

...

genXSxxx.R

Takes the original data and interpolates them to fixed-grid resolution.

Generated

/Leiden

/0.1nm

/1 nm

/SWRI

/0.1nm

/1nm

...

1_gather.R

Generates a set of data managing priorities (ex. Leiden for XS, SWRI for BR, Plessis for CH4 BR...)

Cross-sections

/0.1nm

/1 nm

...

2_genSamples.R

Generates random samples for XS and BR and store them in ChemDBPublic

ChemDBPublic

/PhotoProcs

/0.1nm

/1 nm