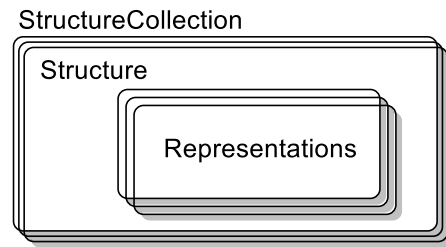


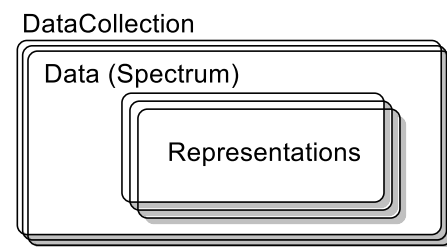
Thinking about data object models

(this is not the presentation, just ideas)

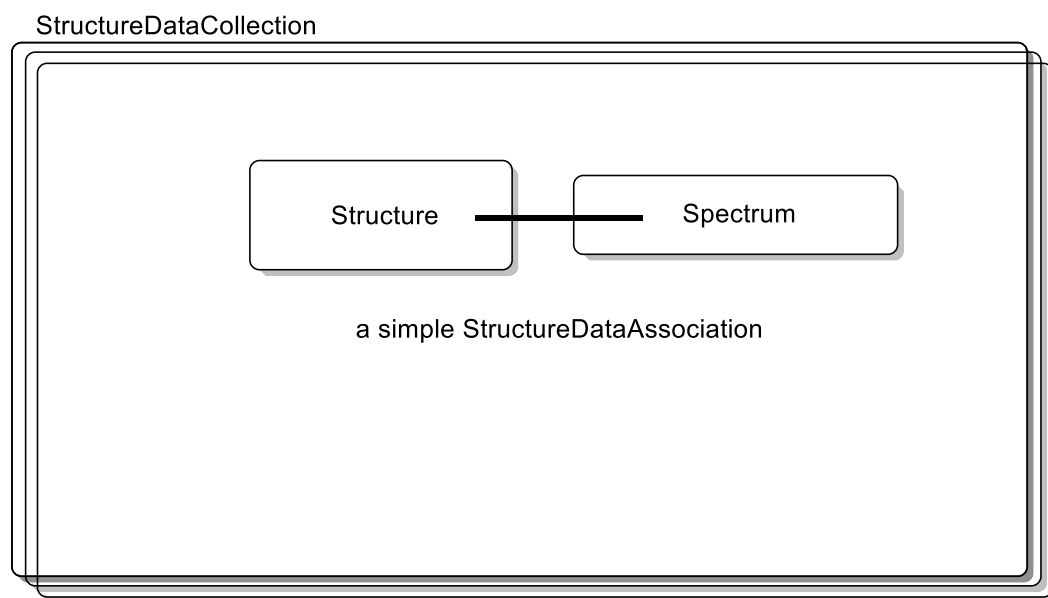
a collection of structures without associated data



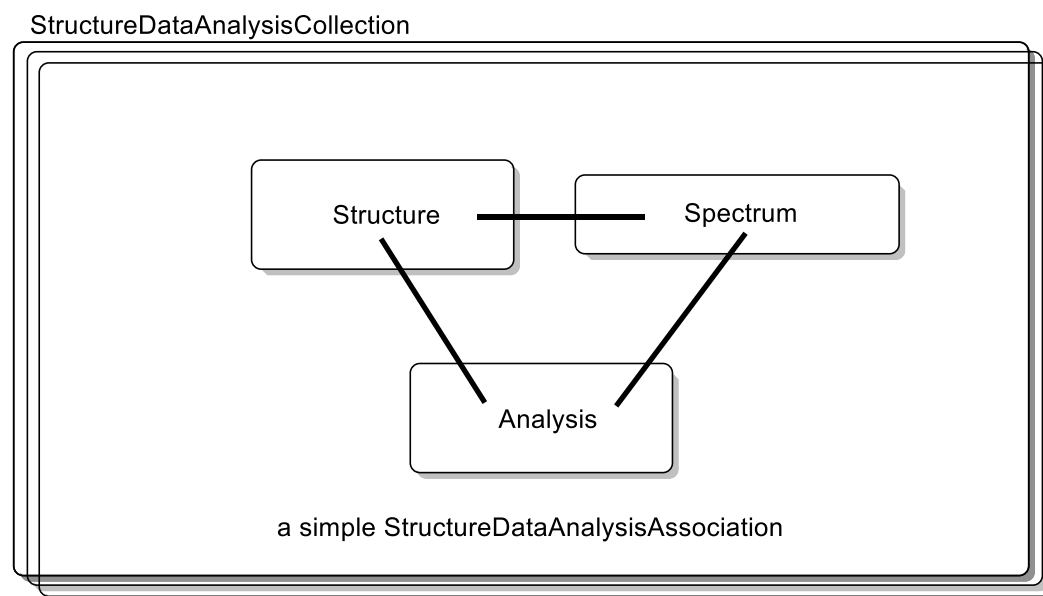
a collection of spectra – just a pile of spectra, no structures!



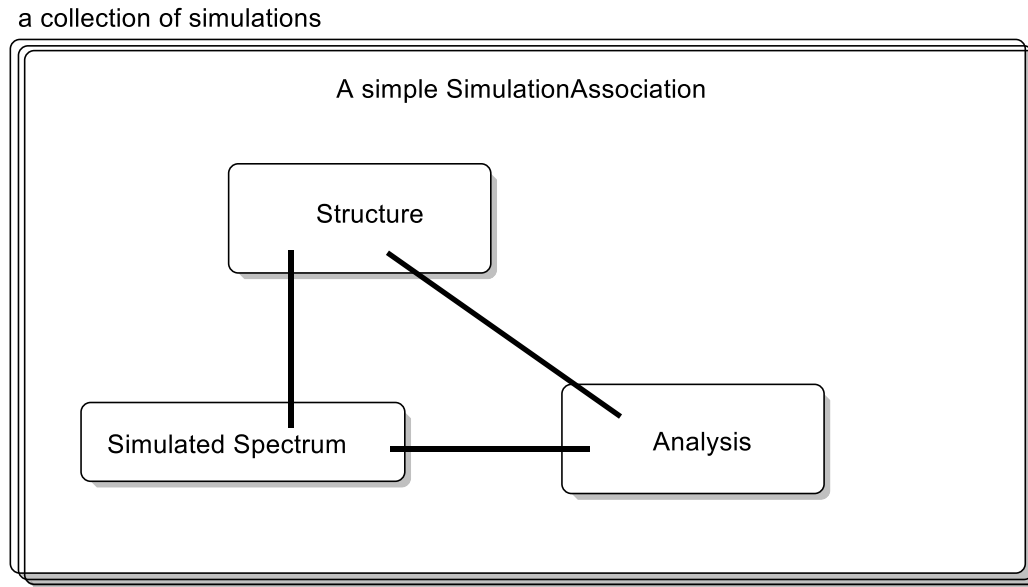
a collection of structures and their associated spectra



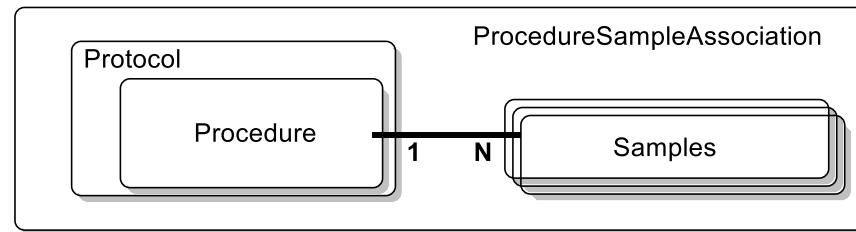
a collection of structure-spectrum analyses



a collection of simulations

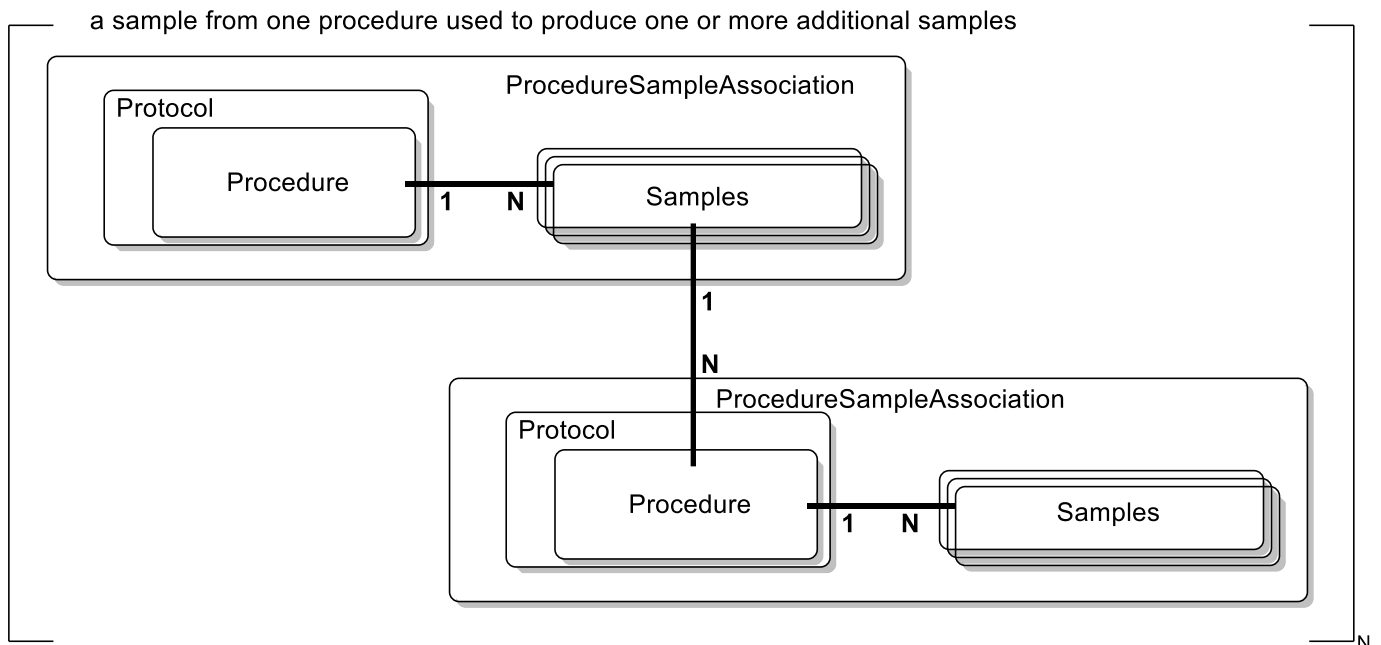


a procedure based on a protocol producing multiple samples

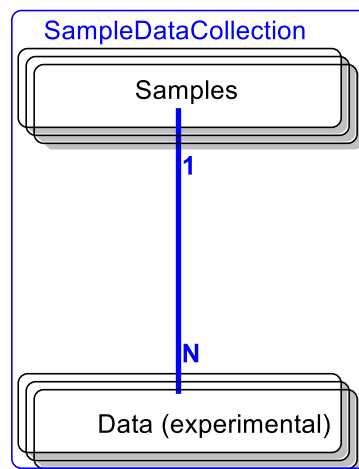


a sample from one
procedure used to produce
one or more additional
samples

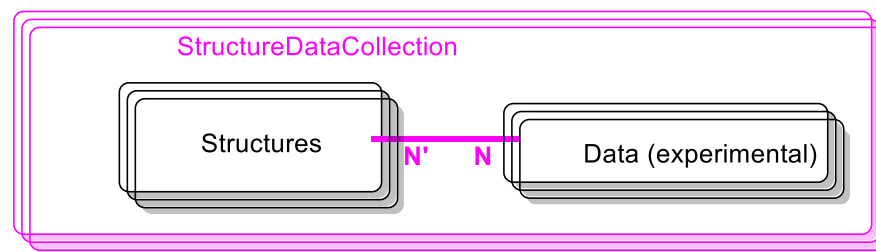
(think “carrying out a
reaction” and “taking nmr
samples”)



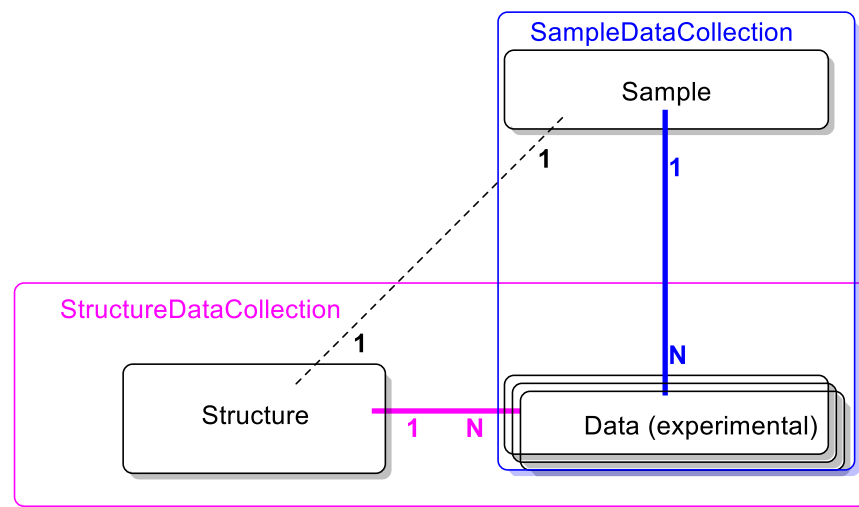
a collection of samples and their associated spectra



a collection of structures with their associated spectra



Inferring the structure of a compound based on a sample's spectra.



The full enterprise.

All of which (or any part
of which) can be
described using an IUPAC
FAIRSpec Finding Aid

