How is data organized in the LIMS?

The LIMS system utilizes several data model constructs in order to generate any experimental data entry. However, there are four (4) data models that are of most significance: chemical, material, experimental data, and well plate. A simplified schematic is shown in Fig 1.

Fig 1. Schematic illustrating the connections between the data models.

Chemical

Chemicals are the simplest classification in the LIMS and represent the lowest level of data complexity. Any and all chemical species belong to the Chemical data model. Each chemical is assigned a distinct category, such as: monomer, polymer, solvent, catalyst, additional reagent (e.g. surfactants), and so on. The list of chemical categories can be expanded at any time, in accordance with user recommendations and BioPACIFIC MIP needs.
Not all fields in the Chemical model are required for user entry; in fact, many of them are optional. Basic information, such as names, formulas, molecular weights, and categories, are required.

Material

Materials are the next level of data complexity. Materials are defined as any and all substances comprised of or using other substances, e.g. small molecules and monomers synthesized in a reaction using Chemicals, polymers, and so forth.

Composites

Composites are the last classification, representing chemical species of the highest compositional complexity. In the LIMS, composites represent complex macromolecular structures compromised of two (2) or more polymers. This is not directly analogous to the concept of composites in materials science, but a loose mental association is not entirely off-base.

Experimental Data: Connecting the models

Each experimental data entry relates back to information concerning the components, polymers, and/or composites used in the sample to which the data applies. This means that each time a piece of data is submitted to the LIMS (e.g. a mass spectrum), information about the component(s), polymer(s), and/or composite in that sample is **required** by the system. This information is then used to piece together the experimental data entry, which also captures information about the instrumentation used, when it was used, the data category, and other information.

Additionally, each experimental data entry requires an experimental identifier (experiment ID). The experiment ID is analogous to a serial number for the given sample and should be attached to each piece of experimental data in which that sample was used.

The workflow would proceed as follows:

- 1) synthesize your sample and generate an experiment ID (from either the electronic lab notebook, ELN, or from the LIMS metadata tool)
- 2) characterize your sample (e.g. via SAXS/WAXS) and submit the data under that experiment ID
- 3) repeat (2) for however many characterization types you perform on that sample