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 (i.e. reagents and products in a synthetic protocol) 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, is required.

Material

Materials are the next level of data complexity. Materials are defined as any and all Chemicals involved in its synthesis. The real identity of the Material, then, is the intended or primary product species.

Key information contained in the Material model include a common name, unique identifier (coming from the corresponding ELN page), synthetic mechanism, and reagent and product chemical species information.

Experimental Data

Each experimental data entry relates back to information concerning the Materials (and, thus, Chemicals) 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 Material is **required** by the system. Thankfully, the ELN helps simplify data entry.

Information about Chemicals and Materials is imported into the LIMS through the ELN, via the Import & Upload Data Wizard (Fig 2). All information found in Reagent and Product tables in the ELN gets parsed by the LIMS, and the ELN's unique identifier is also retrieved to link data between the two systems and build the corresponding Chemical and Material data structures within the LIMS database.

Fig 2. Highlight of Import & Upload Data in LIMS navigation menu.

After the user makes this connection between the ELN and LIMS in the Import Wizard, the LIMS will ask a series of short questions before arriving at a data upload screen. More about this process will be described in the Tutorial page.