ELN Page Annotations

Page Annotations are a unique feature of the ELN (Fig 1). These annotations come in the form of various modules, located at the top of any given ELN page, that collect information about different processes. This information helps to annotate the page about details such as: chemical reagent and product information for a synthesis; biological protocols used in a synthetic biology experiment; descriptions for the contents of well plates; and so on. This information remains linked to the ELN page, is stored in the LIMS for programmatic access, and is shared via page snapshots.



Fig 1. Page annotation menu. From left to right: Chemical synthesis, Biological information, Well plates, Chemspeed annotation tools, Symphony X Peptide Synthesizer, small angle X-ray scattering (SAXS), chemical Structure Editor, Flow Chemistry, and Tecan SPARK (BNL).

Chemical Synthesis

Basic information about the chemical reagents used and products produced in an experiment are recorded in the Chemical Annotation module (Fig 2). This information is used to populate Chemical data entries in the LIMS database and provides a simple, historical account of the reagent quantities and product yields in the synthesis.



Fig 2. Reagent and product tables in the ELN's Chemical Annotation module. Rows can be added/removed as needed by the user inputting values to the table.

Biology Annotations

Biological page annotations (Fig 3) are meant to capture the wealth of information available in conducting synthetic biology experiments. In this annotation tool, users can add, view, and edit information regarding organisms, nucleotides, plasmids, and protocols utilized in their synthetic biology experiments.



Fig 3. Biological annotation panel. These annotations capture information about organisms, nucleotides, plasmids, and various protocols applicable to synthetic biology experiments.

Well Plates

Well plate annotations (Fig 4) in the ELN come in two different forms: **chemical** and **biological**. Depending on the plate choice you specify, you will walk through a process for capturing formulation information (chemical) or well-by-well culture information (biological). Once saved, the plate is given a unique ID and a QR code, and is made available in a visual display with your other well plates. Plates can then be edited or removed from your ELN page.



Fig 4. Plate annotation panel. Users first specify a plate type (chemistry or biology) and then follow the prompts. Biological plates have another layer of detail, allowing well-by-well annotation and file uploads. Once a well plate is created, it shows in the list with other plates, along with their QR codes.

Note for Microrheology and Optics11 Indenter Users: If you are using either of these instruments, or another instrument with a program that asks for your well plate serial number before going forward, please note that you can find that number above the QR code of your well plate, as shown in Fig 5.



Fig 5. Individual well plate. The blue circle indicates the universal unique identifier (UUID) used to represent the serial number of the plate. This is the number embedded in the QR code, and is the number expected by access-granting scripts that ask for the well plate serial number.

Chemspeed

The Chemspeed annotation module is designed to facilitate and streamline experimental access to the Chemspeed instrument. The module provides a mechanism for designating a Chemspeed experiment (Fig 6), with parameters including temperature and atmospheric conditions alongside the employed polymerization scheme. Once the Chemspeed experiment is registered, you can add chemicals (Figs 7, 8, 9) to the stock solutions table and assign volumes for each reaction in each reaction vessel (Fig 10). You may then download stock reagent files for the Chemspeed instrument by clicking the Download Text File button. Note: double-check the file for accuracy and make sure you save your table before doing so to prevent data loss, as there is no auto-save functionality for these tables.



Fig 6. Chemspeed experiment registration. Allows you to name and provide input parameters for your Chemspeed experiment, including: polymerization mechanism, temperature, time, and atmosphere.



Fig 7. Chemspeed add/search for stock chemicals. This feature allows you to search for chemicals in the BioPACIFIC MIP LIMS based on common name, chemical formula, or SMILES string. Additionally, this search is expanded beyond the LIMS to return results from the public chemical database found at PubChem.



Fig 8. Chemspeed add chemical to LIMS. You may add chemicals directly to the LIMS by clicking the Add New Chemical button, which will result in the window shown here. You must upload a representative structure image file and input some basic parameters. Upon save, the chemical is registered in the LIMS and added to the Stocks table.



Fig 9. Chemspeed add chemical from PubChem. Allows you to add the chemical returned from PubChem to the LIMS database in addition to your stocks table. A few values are requested which cannot be retrieved from PubChem, including density. Successful addition adds the chosen chemical to the LIMS database for future reference.



Fig 10. Chemspeed stocks table. Displays all chemicals added to the stocks table with a thumbnail image of their structure. Each row of the stocks table represents a reaction in a reaction vessel. Volumes are then added and must follow any limitations imposed by the instrument. Consult with your project scientist for more details about volume limitations for viscous and non-viscous materials.

Symphony

The Symphony module is designed to greatly simplify the provision of Symphony data files to your ELN page(s). Data from the Symphony X Peptide Synthesizer is automatically transmitted to the BioPACIFIC MIP LIMS, where it is then parsed and registered into the database and made available to the ELN through simple search and point-and-click addition of your Symphony methods files (Fig 11). Each attached Symphony methods collection is displayed as an information card (Fig 12). Clicking on the individual files associated with the method (e.g., an amino acid file or program file) displays a table with all of the values belonging to the original file (Fig 13).



Fig 11. Symphony module. Displays the search results of querying the system for Symphony methods files. These methods can be linked to your ELN page simply by clicking the button.



Fig 12. Symphony module file cards. Displays the attached/linked Symphony methods files.



Fig 13. Symphony module file card file view. Displays the parsed methods file/file dependent's information in tabular format.

SAXS

This module provides a mechanism to link and view data from the small angle X-ray scattering (SAXS) instrument at BioPACIFIC MIP. It works similarly to the Symphony, in that there's a retrieval/data search window (Fig 14) from which you may link data files to your ELN page.



Fig 14. SAXS retrieval/data search window. This functions identically to the Symphony workflow, but displays different information, such as a (post-processed) image thumbnail preview.

Upon linking, you can then further preview your SAXS data by browsing the various SAXS data cards (Fig 15). These cards provide an expanded thumbnail image of the scattering pattern (which is a post-processed image) and a plot trace of I vs q from the raw text files. You may download the original *.tiff image and *.txt files by clicking their respective links.



Fig 15. Display of attached (linked) SAXS file cards. These cards provide a larger version of the search thumbnail image preview and also give you an interactive plot by which to perform a cursory examination of the raw data (I vs q, with error bars).

Structures

The Structures annotation module of the ELN provides users with a chemical structure editor (Fig 16) that has many of the functionalities found in ChemDraw, including the ability to load/read ChemDraw files. The editor leverages the open-source chemical structure tool known as Ketcher. Users can generate both chemical and biological structures (e.g. proteins, genes, nucleotide sequences, etc) in this editor via the Molecules and Macromolecules editor modes, respectively.

Fig 16. Structure annotation module. Users can generate, save, export, and load molecule and macromolecule structures.

Structures can be stored in the ELN page and/or exported out as image files (or other formats, where permitted). Saved structures appear as cards, which can be loaded back into the editor. The structures themselves are stored as JSON objects, making them useful candidates for feeding into AI/ML models!

Flow

This section will be written at a later date.

Tecan SPARK (BNL)

The Tecan SPARK is a UV-Vis spectrophotometer designed to analyze well plates. It is housed in the Biological Nanostructures Laboratory in CNSI at UCSB. This module, as shown in Fig 17, serves to link BioPACIFIC MIP-related data from the Tecan SPARK to their corresponding ELN pages. It functions similarly to the other retrieval-and-link modules (Symphony, SAXS), but offers little in the way of additional features at this time.

Fig 17. Tecan SPARK ELN annotation module. This module allows users to link their Tecan SPARK data from the BNL to their ELN pages.

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