



Use Case 1: Requesting Work from a CRO: Compound Synthesis and Related Sample Data Management

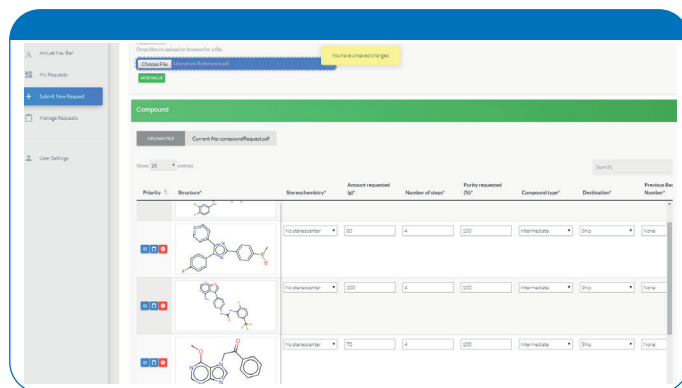
How to Effectively Manage Work Request Management, Compounds and Related Sample Data Between CRO and Pharma Company

Provide a better collaboration platform for working with CRO network. Eliminate multiple tools and a series of systems that require CROs to work in multiple systems to load data

- Increase Efficiency
 - Streamline overall workflow processes to provide a single solution for the receipt of new compounds
- Effective Project Management
 - Enable internal scientists to understand both the status of the work being performed as well as view the experiments executed by the CRO in near real time

The CRO request manager (or scientists) will receive a notification of the new request within the home page of the system and via email. The request will either be placed into a new notebook or project. The CRO scientists can then review the proposed synthesis and place the compounds directly into the ELN for execution.

Upon receiving the list of compounds, the work can be distributed to the CRO scientists or if allowed they can view all the requested compounds. The requests can mask company fields and present the CRO with alternative values (Reg ID v. sample ID). The request can include mandatory fields that the CRO needs to fill in to complete the request.



Priority	Structure	Reagent/substrate	Amount requested (g)	Number of uses	Purity requested (ppm)	Concentration	Distribution	Product Reference
High	<chem>C1=CC=C(C=C1)C(=O)O</chem>	100	10	100	Intermediate	100	100	100
High	<chem>C1=CC=C(C=C1)C(=O)O</chem>	100	10	100	Intermediate	100	100	100
High	<chem>C1=CC=C(C=C1)C(=O)O</chem>	100	10	100	Intermediate	100	100	100

Figure 1. Compound Order and Fulfillment solution after SD file upload

The CRO scientists will execute their experiment in the Arxspan ELN. The ELN is a full-featured Chemistry notebook for the execution of compound synthesis. The web-based platform provided support for both ChemDraw and Marvin JS with stoichiometry support. Reaction planning and execution allow for calculation of compound properties, yield, % yield based on the actual amounts used.

Figure 2. Compound Order and Fulfillment solution CRO view of Project or Table of Contents

Figure 3. Chemistry experiment within the Arxspan ELN.

Next steps and copying of experiments allow reaction genealogy to be tracked from first experiment to final product.

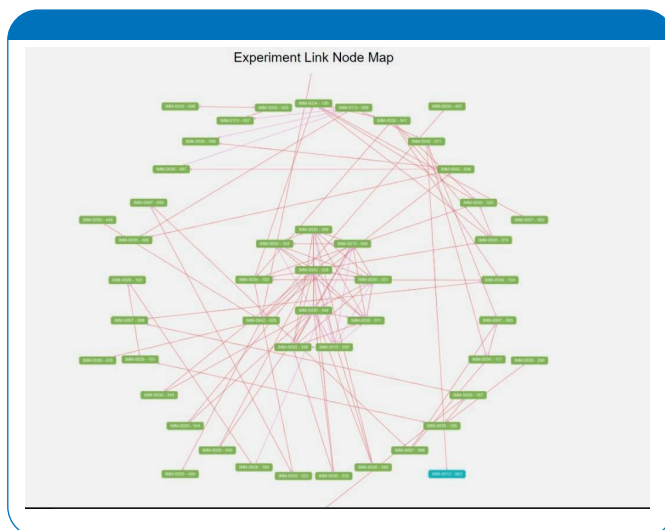


Figure 4. Automatic Linking of experiments in The Arxspan ELN

The experiments captured in the Arxspan ELN can allow internal scientists to be notified when new experiments have been created. Experiments can be placed into projects allowing work to be automatically categorized by project. The CRO's access can be limited to "write only" allowing them to contribute to a project but limiting their view of data to the experiments they create.

Figure 5. Arxspan ELN Project view for write only collaborator

Utilizing the Arxspan platform, internal scientists can track and review the proposed synthetic pathways prior to execution or review the experimental work upon completion of an experiment.

Experiment Name	Status	Type	Creator	Date Created (EDT)
AP-1009-002	saved	Chemistry	Jeff Carter	10/3/2018 4:32:41 PM
AP-1017-005	saved	Biology	Joe Demo	10/3/2018 4:26:32 PM
AP-1017-006	saved	Biology	Joe Demo	10/3/2018 4:30:05 PM
AP-1017-007	saved	Biology	Joe Demo	10/3/2018 4:35:59 PM
Landmark Title by Limiting Dilution Colony Counting				
AP-1017-020	saved	Chemistry	Joe Demo	10/4/2018 6:02:54 PM
AP-1017-011	saved	Chemistry	Joe Demo	10/4/2018 6:08:43 PM
AP-1017-023	saved	Biology	Joe Demo	10/4/2018 6:20:06 PM
AP-1017-013	created	Biology	Joe Demo	10/4/2018 6:22:27 PM
AP-1020-001	saved	Biology	Evelin Schrodinger	10/3/2018 4:40:10 PM
AP-1019-003	saved	Biology	Jeff Carter	10/3/2018 5:48:28 PM

Showing 1 to 10 of 25 entries

Figure 6. Arxspan ELN Project view for full access user

When the final production is synthesized, The Arxspan platform enables registration of the compound via an integrated workflow. This step allows for compound to be registered as synthesized instead of “binning compounds” into an SD file for data transfer. The ability to load individual compounds allows for real time correction of issues with the compound submission, eliminating delays between submission and correction.

The screenshot shows a chemical reaction with a highlighted product. Below the reaction is a registration form with the following fields:

Overview	Conditions	Equivalents	Measured Mass
Product	14-(2-hydroxyethyl)-2	1	73 mg
Molecular Weight	141.15	Theoretical Mass	73.076
Molecular Formula	C ₁₀ H ₁₁ N	Theoretical Moles	1.000
Reg ID	RegID	Yield	84.2 %
	Purity	Inventory Items	Inventory

Figure 7. Highlighted links to either register a compound or place a compound into inventory within Arxspan

The System can be configured to prompt the user for information including purity, amount to register, etc. The system also prompts the user to include files like NMR and Mass Spec etc. to ensure all data is included in the registration event.

The screenshot shows the manual registration workflow. On the left, a chemical structure is displayed. On the right, a form titled "Structure Already Exists: AT-0226" contains the following fields:

- Scientist: --NONE--
- Purity %: []
- Appearance: []
- Submitted Amount*: []
- Amt. Units*: --NONE--
- Color: []
- Batch Comment: []
- Barcode: []

Figure 8. Workflow to manually register a compound

Once the compound passes the validation rules in the Arxspan platform, batch ID is placed back in to the ELN experiment. The system places the sample into Inventory and a barcode ID generated for the container (vial, bottle, etc..).

The screenshot shows the completed registration workflow. Below the chemical reaction is a registration form with the following fields:

Overview	Conditions	Equivalents	Measured Mass
Product	1-(2-chloro-3-methoxy-5-(2,4-dimethylpyridin-2-yl)-6-(1-tert-butyl-2-hydroxyethyl)-1H-imidazole-4-yl)ethan-1-ol	1	73 mg
Molecular Weight	438.536	Theoretical Mass	73.076
Molecular Formula	C ₂₃ H ₃₀ ClNO ₃	Theoretical Moles	1.000
Reg ID	AT-0226-19	Yield	84.2 %
	Purity	Inventory Items	Inventory

Figure 9. Completed Registration with Registration or Sample ID

Alternatively, the system provides the means to allow for batch loading a series of compounds associated in a request.

In this workflow, a scientist or coordinator can log into a web-page to register a set of compounds. The system provides a means of requiring specific company metadata and allows an SD File to be loaded. The file can be loaded with a pre-configured upload template or the fields can be mapped at the time of loading.

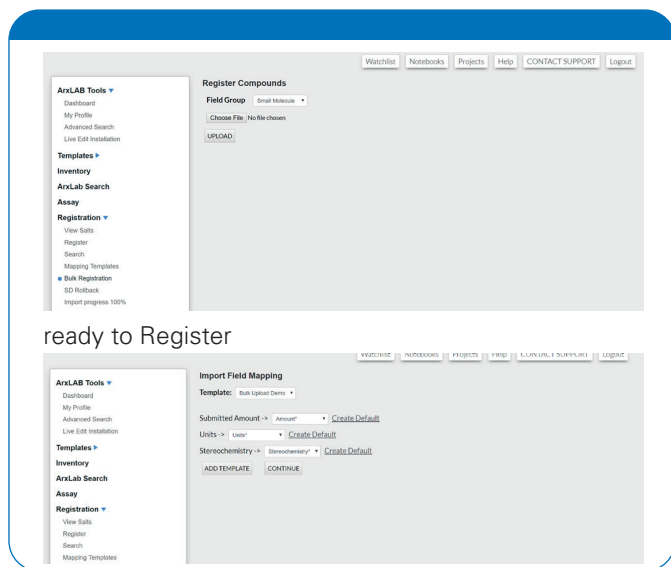


Figure 10. Bulk Registration Landing Page

When the file is read into the system, error checking is performed against internally-set rules, and the scientists receive a list of errors associated with the file. Once these are corrected, the structures are published to EDB. EDB system then performs final validation, uniqueness checking and publishes a final Registration or batch ID (sample). Arxspan then receives the registration IDs and publishes them back into our system.

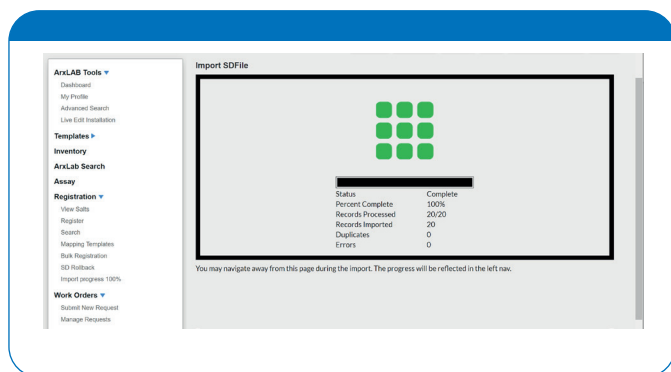


Figure 11. Completion of a Successful Registration

Utilizing Registration for the creation of data validation rules Management of the registration workflow is configured to meet a company's business needs. The system allows for custom fields to be created with rules on both data type (string, number, date, file, etc..) format and range of acceptable values. One or several different forms can be configured to meet the specific requirements need for each CRO.

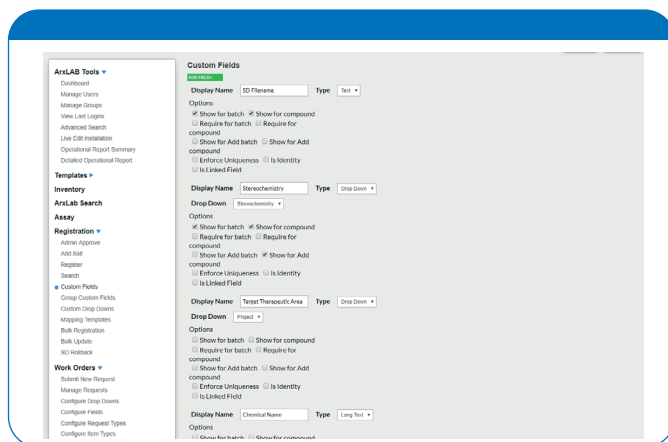


Figure 12. Custom field in Arxspan's ELN

In addition to custom fields, Arxspan provides the ability to salt and solvate strips as part of the registration workflow. The system allows for salts and solvates to be loaded into the registration system and as a compound is registered, it is removed allowing the base form to be registered.

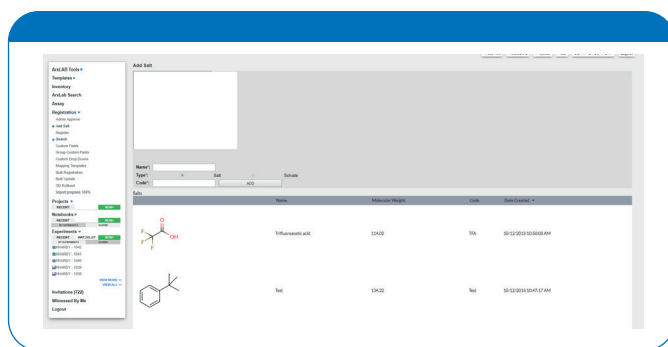


Figure 13. Salt and Solvates table in Arxspan Registration

Read our related use cases:

- Use Case 2: How to Custom Order Compounds from a CRO: Request and Shipping Management
- Use Case 3: Receiving Compounds from a CRO
- Use Case 4: Storing Experimental Pharmacological Data in an Assay System
- Use Case 5: Managing experimental results data from CRO
- Use Case 6: Simplifying the Administration of your enterprise systems



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