

Project Lighthouse

Automated Synthesis User Experience

A close-up photograph of a person's head and shoulders, wearing a white lab coat, looking down at a silver MacBook Air laptop. The laptop screen displays a user interface for a software called "Project Lighthouse". The interface shows a workflow titled "Projects > Fun Synthesis Times > New Synthesis" with steps: Reaction Type, Set Destiny, Reaction Setup, Validation, Materials Sourcing, and Review. The "Reaction Setup" step is currently active. It asks to "Specify Your Reaction Parameters" and notes that materials need to be provided directly or sourced commercially. The "REACTION TYPE" is set to "Amide Coupling" and the "DESIRED MASS" is "14 g". Below this, a "Reaction List" section shows three entries under "REACTION GROUP". Each entry consists of two chemical structures (amine and carboxylic acid), a "Set Conditions" button, a product structure, a "LEAD TIME" of "3 days", and a "CONFIDENCE" percentage (98%, 89%, and 75% respectively). There is also a "Reaction Inspector" button. At the bottom of the list, there is an "Upload A Compound List" button. The laptop is a MacBook Air, as indicated by the text at the bottom of the screen.

Synthesis Management

Project Page

Quick access to pressing tasks.

The multiple syntheses a Chemist might have running at once are listed on this page.

I'm pretty easily distracted so I often work on a few things at once."
- Lilly Medicinal Chemist and ASL User

The screenshot displays the 'Project Page' of the Synthesis Management system. At the top, there's a navigation bar with 'Projects > Fun Synthesis Times' and a 'New Synthesis' button. A green arrow points to the 'New Synthesis' button with the text 'Click to launch new synthesis.' Below the navigation, there's a section titled 'Your Input Is Needed' with a checkbox for 'Ship your samples for the following synthesis: My Other Cool Reaction Library' and a 'Mark as Shipped' button. To the right, there's a 'Route Modified' log for 'Super Sulfonamide' with details: Submitted by Todd de Collo on December 8th, 2018; Started: 12/10/18 at 9:02 AM; Incubation was extended at a higher temperature. A red arrow points to this log with the text 'Syntheses with changes since last login,'. Further down, there's a 'Completed' log for 'Urea Fo' Rea' with details: Submitted by Rick and Marty on December 8th, 2018; COMPLETED: 12/10/18 at 10:04 PM; The target mass of all desired products was successfully synthesized. A red arrow points to this log with the same text. On the left side, there's a 'Syntheses' section with a 'Waiting For Building Blocks' dropdown. It lists 'My Cool Reaction Library' (Amide Coupling, r1234abcd5678efgh, Submitted by Todd de Collo on December 12th, 2018) and 'What Even Is A Mide?' (Amide Coupling, r1234abcd5678efgh, Submitted by Alex Hadik on December 12th, 2018). Both entries show a status of 'Waiting for shipping information to be provided.' and 'Waiting for capacity to become available for automated synthesis.' respectively. A red arrow points to the 'Syntheses' section with the text 'Comprehensive list of all syntheses in project. Searchable and organized by category.' At the bottom, there's an 'In Progress' section with a single entry: 'Let's Make Some Chemicals!' (Suzuki Coupling), which is also waiting for shipping information. A search bar at the top right says 'Search by Synthesis ID, Name, Creator or Date'.

Launching A New Synthesis

Global Reaction Settings

Track progress through launch experience.

Name the reaction and optionally provide an ELN number for future reference.

Select the desired reaction type.

Indicate if the product of this synthesis will be a final compound, or an intermediate.

transpictic

Projects > Fun Synthesis Times > New Synthesis

Reaction Type Set Destination Reaction Setup Materials Sourcing Review

Let's set some basic info for your reaction.
You'll set up the details of your reaction later on.

Name your synthesis and define how it will be used.
You will refer back to your synthesis using this name. ELN Number
How will your final compound be used?

Nifty Synthesis Library 851925 Intermediate Final Product

What kind of reaction would you like to run?

Amide Coupling

$R_1-NH_2 + HO-C(=O)R_2$

Buchwald Coupling

$R-C_6H_4-X + H_2N-R_2$

Suzuki Coupling

$R-B(OH)_2 + X-R_2$

Sulfonamide Formation

$R_1-NH_2 + Cl-S(=O)(=O)R_2$

Urea Formation

$R_1-NH_2 + C(=O)-NH-R_2$

REACTION TYPE ELN Number TARGET MASS REACTIONS EST. COMPLETION EST. COST

Previous Next

Proceed to next step.

Launching A New Synthesis

Destinations for Synthesized Product

Projects > Fun Synthesis Times > New Synthesis

Reaction Type Set Destination Reaction Setup Materials Sourcing Review

By default, a **Store Purified Product** destination is set. Change the destination type with the dropdown.

Non-configurable details are shown to the right.

Set the destination parameters.

Add a new destination from dropdown.

Set Destinations For Your Final Product

Your synthesis requires materials to be provided directly, as well as sourced commercially.

Store Purified Product ▾

AMOUNT: 4 mmol

Configuration

TEMPERATURE: 4 °C

FACILITY: L2S2

FORM: DMSO Stock

Details

VIAL: 3x A1 vials

SOLVENT: DMSO

CONCENTRATION: 10 mmol

+ Add New Destination ▾

"This is very intuitive. I would have no problem using this."

- Medicinal Chemist at Top 10 Pharmaceutical Company

REACTION TYPE: Amide Coupling

ELN Number: 301853

TARGET AMOUNT: 4mmol

REACTIONS: --

EST. COMPLETION: --

EST. COST: --

Previous Next

Launching A New Synthesis

Destinations for Synthesized Product

Send Purified Product will store the specified amount of final compound in automated storage.

Receive Excess will allocate extra material at the end of synthesis to this destination.

Submit to Bio-Assay will ensure enough product is synthesized to run the selected assay.

Ship To Address will dispatch a shipment of the desired amount to the specified address following synthesis.

Amount to synthesize tallied below.

Projects > Fun Synthesis Times > New Synthesis

Reaction Type Set Destination Reaction Setup Materials Sourcing Review

Set Destinations For Your Final Product

Your synthesis requires materials to be provided directly, as well as sourced commercially.

Drag cards to set priority ⓘ

Store Purified Product Configuration Details

AMOUNT	mmol	RECEIVE EXCESS	TEMPERATURE	°C	FACILITY	FORM	VIAL	SOLVENT	CONCENTRATION
4	mmol	<input type="radio"/> No <input checked="" type="radio"/> Yes	4	°C	L2S2	<input checked="" type="radio"/> DMSO Stock <input type="radio"/> Solid	3x A1 vials	DMSO	10 mmol

Submit to Bioassay Configuration Details

VOLUME	CONCENTRATION	BIOASSAY	NEXT RUN
2mL	10 mmol	My Cool Assay 2	December 19, 2018

Ship to Address Configuration Details

AMOUNT	mmol	RECEIVE EXCESS	ADDRESS	TEMPERATURE	°C	FORM	VIAL	SOLVENT	CONCENTRATION
4	mmol	<input type="radio"/> No <input checked="" type="radio"/> Yes	3656 Haven Av. Suite 3 Menlo Park, CA 94025	4	°C	<input checked="" type="radio"/> DMSO Stock <input type="radio"/> Solid	3x A1 vials	DMSO	10 mmol

+ Add New Destination ▾

REACTION TYPE ELN Number TARGET AMOUNT REACTIONS EST. COMPLETION EST. COST

Amide Coupling 301853 14mmol -- -- --

Previous Next

Temperature, preferred facility, and desired form.

For the specified assay, the amount required is set, and not editable.

Specify the destination address, and form in which it should be sent (solubilized/purified).

Proceed to next step.

Launching A New Synthesis

Reaction Configuration

The screenshot shows the transcriptic software interface for launching a new synthesis. The top navigation bar includes links for Projects, Inventory, Shipments, and Packages. The main title is "Projects > Fun Synthesis Times > New Synthesis". Below the title is a progress bar with five steps: Reaction Type (green checkmark), Set Destination (green checkmark), Reaction Setup (purple circle), Materials Sourcing (grey circle), and Review (grey circle). The central area is titled "Specify Your Reaction Parameters" and contains a message: "Your synthesis requires materials to be provided directly, as well as sourced commercially." Below this is a "Reaction List" table with columns: AMINE VARIABLE, CARBOXYLIC ACID VARIABLE, REAGENTS & CONDITIONS, PRODUCT, LEAD TIME ▲, and CONFIDENCE. The table has three rows, each with a "Define" button. A green arrow points from the text "Click to define the Amine Variable for this reaction." to the first "Define" button. A red line connects the text "Template headers are specific to the selected reaction type." to the first row of the table. Another red line connects the text "Add another blank reaction template." to the "Add a New Reaction" button. A red line also connects the text "Previously set details documented for reference." to the bottom summary row. A large green arrow points from the "Add a New Reaction" button towards the "Define" button in the first row. A red line connects the "Upload a Compound List" button to the right side of the table. The bottom of the screen shows a summary row with fields: REACTION TYPE (Amide Coupling), ELN Number (301853), TARGET AMOUNT (14mmol), REACTIONS (--), EST. COMPLETION (--), and EST. COST (--). Navigation buttons "Previous" and "Next" are at the bottom right.

Template headers are specific to the selected reaction type.

Click to define the **Amine Variable** for this reaction.

Add another blank reaction template.

Previously set details documented for reference.

Blank reaction template.

Compound Explorer

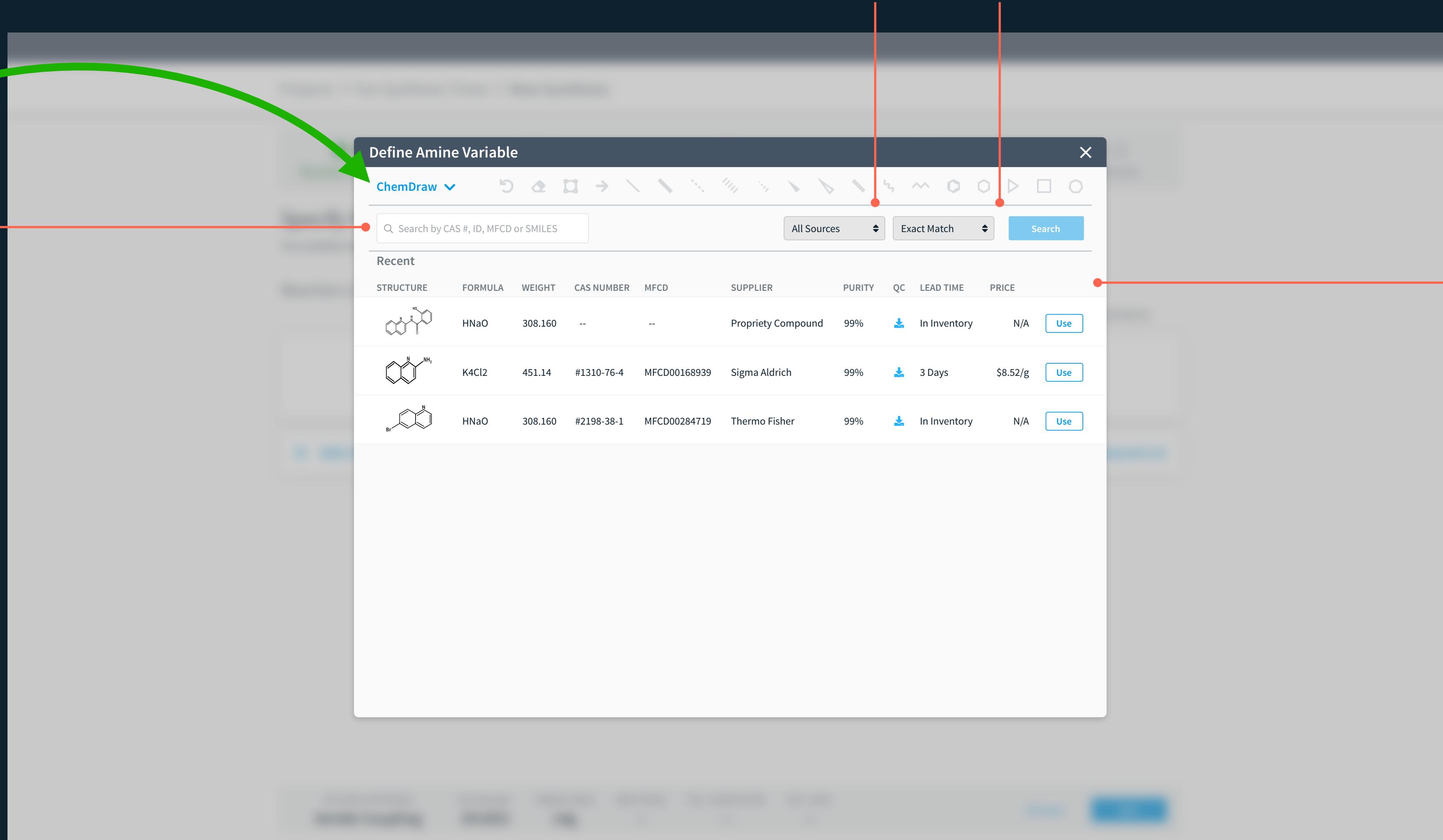
Default State

Click to open the
ChemDraw drawer.

Search with a CAS #,
Tx ID, MFCD, or SMILES
string.

Filter results to commercial compounds, compounds in Transcriptic inventory, or both.

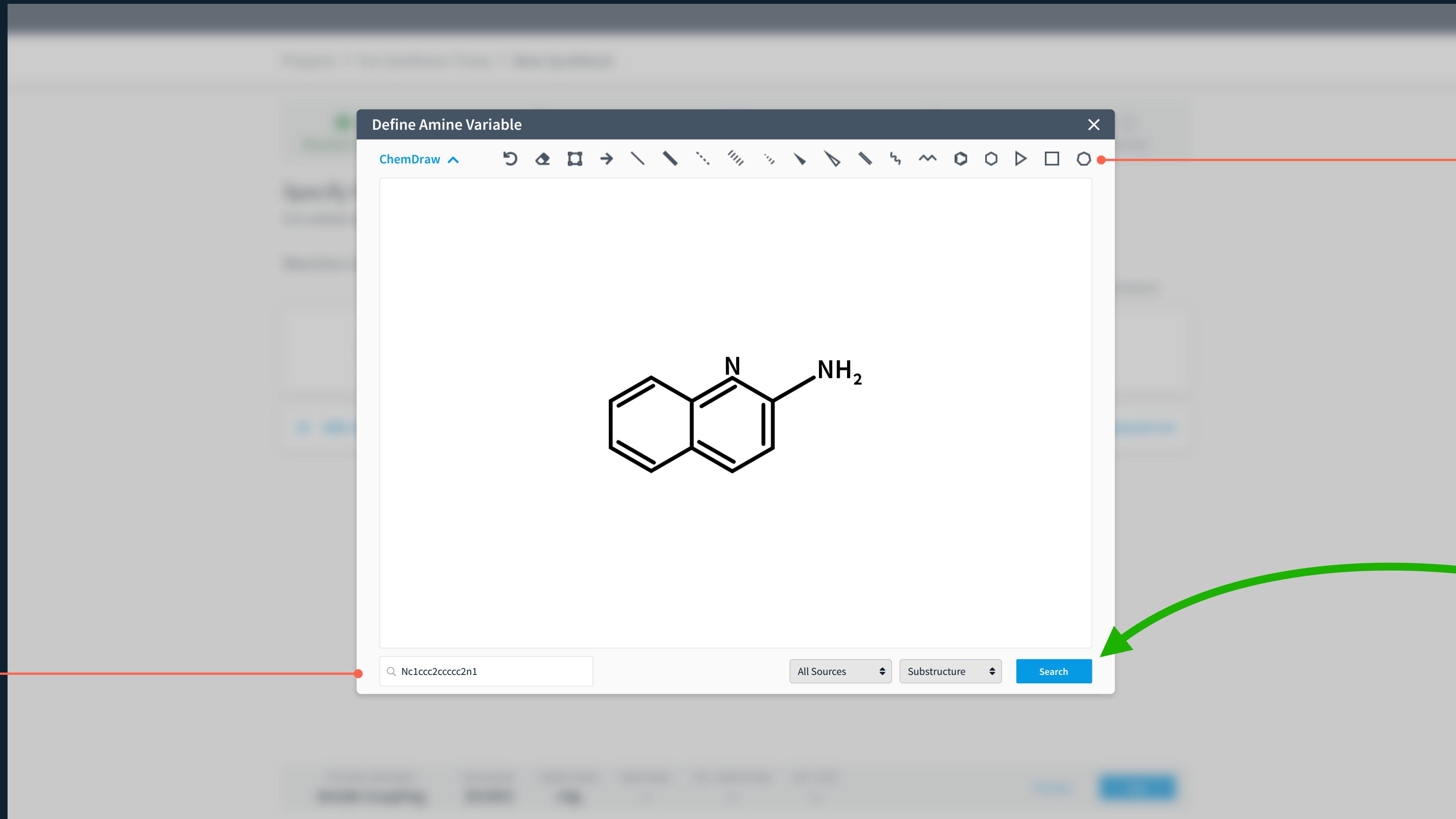
Search by **Substructure**, **Similarity**, or **Exact Match**



When no search query has been provided, recent results are shown for quick access.

Compound Explorer

Draw a Compound



Compound Explorer

Substructure Search Results

Results from Substructure search shown below.

Define Amine Variable

ChemDraw ▾

Substructure Matches

STRUCTURE	FORMULA	WEIGHT	CAS NUMBER	MFCD	SUPPLIER	PURITY	QC	LEAD TIME	PRICE
	HNaO	308.160	--	--	Proprietary Compound	99%		In Inventory	N/A
	K4Cl2	451.14	#1310-76-4	MFCD00168939	Sigma Aldrich	99%		3 Days	\$8.52/g
	HNaO	308.160	#2198-38-1	MFCD00284719	Thermo Fisher	91%		4 Days	\$12.19 / g
	HNaO	308.160	#2198-38-1	MFCD00284719	Carbosynth	95%		In Inventory	N/A
	HNaO	308.160	#2198-38-1	MFCD00284719	Thermo Fisher	99%		3 Days	\$54.24 / g
	HNaO	308.160	#2198-38-1	MFCD00284719	Sigma Aldrich	83%		5 Days	\$23.71 / g
	HNaO	308.160	#2198-38-1	MFCD00284719	Self Sourced	?		Please Ship	N/A
	HNaO	308.160	#2198-38-1	MFCD00284719	Matrix Scientific	88%		6 Days	\$12.42
	HNaO	308.160	#2198-38-1	MFCD00284719	Apollo Scientific	99%		2 Days	\$43.14
	HNaO	308.160	#2198-38-1	MFCD00284719	Thermo Fisher	99%		In Inventory	N/A

Click to switch to a Similarity search.

Click into a row to see alternative sources. All results can be self-sourced.

Compound Explorer

Similarity Search Results

If there is no exact structure match in a **Similarity** search, the exact structure will be shown separately.

The screenshot shows a modal window titled "Compound Explorer > Amine Variable". The search bar contains the SMILES string Nc1ccc2ccccc2n1. The search results are displayed under "Similarity Matches".

Exact Match:

- Structure:** N-(p-tolyl)quinolin-6-amine (represented by a chemical structure diagram)
- Empirical Formula:** C₁₆H₁₄N₂
- Molecular Weight:** 234.30
- Supplier:** Proprietary Compound
- Purity:** 97%
- QC:** In Inventory
- Lead Time:** N/A
- Price:** Use

Similarity Matches:

- Structure:** N-(p-tolyl)quinolin-6-amine (represented by a chemical structure diagram)
- Formula:** HNaO
- Weight:** 308.160
- CAS Number:** --
- MFCD:** --
- Supplier:** Proprietary Compound
- Purity:** 97%
- QC:** In Inventory
- Lead Time:** N/A
- Price:** Use

- Structure:** N-(p-tolyl)quinolin-6-amine (represented by a chemical structure diagram)
- Formula:** GeH8O2
- Weight:** 308.160
- CAS Number:** #1310-73-2
- MFCD:** MFCD00168939
- Supplier:** Sigma Aldrich
- Purity:** 97%
- QC:** 3 Days
- Lead Time:** \$54.24 / g
- Price:** Use

- Structure:** N-(p-tolyl)quinolin-6-amine (represented by a chemical structure diagram)
- Formula:** BrH2K4
- Weight:** 308.160
- CAS Number:** --
- MFCD:** --
- Supplier:** Proprietary Compound
- Purity:** ?
- QC:** Please Ship
- Lead Time:** N/A
- Price:** Use

- Structure:** N-(p-tolyl)quinolin-6-amine (represented by a chemical structure diagram)
- Formula:** HNaO
- Weight:** 308.160
- CAS Number:** --
- MFCD:** --
- Supplier:** Proprietary Compound
- Purity:** ?
- QC:** Please Ship
- Lead Time:** N/A
- Price:** Use

Click to register the compound in Transcriplic. It will be set as a self sourced compound for this part of the reaction template.

Similarity results are shown below.

Launching A New Synthesis

Reaction Configuration

Defined compound set in reaction template.

Click to define the product for the reaction template.

transcriptic

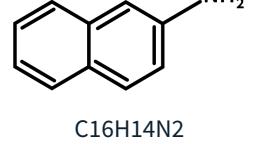
Projects > Fun Synthesis Times > New Synthesis

Reaction Type Set Destination Reaction Setup Materials Sourcing Review

Specify Your Reaction Parameters

Your synthesis requires materials to be provided directly, as well as sourced commercially.

Reaction List

AMINE VARIABLE	CARBOXYLIC ACID VARIABLE	REAGENTS & CONDITIONS	PRODUCT	LEAD TIME ▲	CONFIDENCE
 C ₁₆ H ₁₄ N ₂	+ Define	Define → Reaction Undefined	Define		
+ Add a New Reaction					

REACTION TYPE: Amide Coupling | ELN Number: 301853 | TARGET AMOUNT: 14mmol | REACTIONS: -- | EST. COMPLETION: -- | EST. COST: --

Previous Validate

Compound Explorer

Draw a Compound

The screenshot shows the 'Define Amine Variable' dialog box from ChemDraw. The main area displays a chemical structure consisting of a quinoline ring system connected to a benzylamino group, which is further connected to a phenol ring. Below the structure is a search bar containing the SMILES string `Nc1ccc2ccccc2n1`. At the bottom of the dialog are three buttons: 'All Sources', 'Substructure', and a blue 'Search' button. A red arrow points from the text 'Set an **Exact Match** search since we are looking for a specific structure.' to the 'Search' button. A green arrow points from the text 'Click to search for this structure.' to the same button.

Set an **Exact Match** search since we are looking for a specific structure.

Click to search for this structure.

Compound Explorer

Exact Match Search

When no result is found for an **Exact Match** search, details about the compound are shown instead.

Define Amine Variable

ChemDraw ▾

Search bar: Nc1ccc2ccccc2n1

Buttons: All Sources, Exact Match, Search

No Exact Matches Found. Register as a Proprietary Compound?

Registering your compound of interest as a proprietary compound will add the compound to your Transcriplic organization. It will appear in future searches and be tracked in your Transcriplic inventory.

Chemical structure: N-(p-tolyl)quinolin-6-amine

EMPERICAL FORMULA: C₁₆H₁₄N₂ MOLECULAR WEIGHT: 234.30

Buttons: Not Now, Register and Use

Click to register the compound in Transcriplic and set it as the desired product for this reaction.

Synthesis Management

Retro-Synthetic Planning Dialogue

The reactants necessary to produce this product can be computed using retro-synthetic planning.

A screenshot of a software interface titled "Define Amine Variable". It features a ChemDraw toolbar at the top. Below the toolbar is a chemical structure of a compound: 2-(2-hydroxyphenyl)-N-(naphthalen-1-yl)acetamide. A search bar below the structure contains the SMILES string Nc1ccc2ccccc2n1. To the right of the search bar are dropdown menus for "All Sources" and "Exact Match", and a "Search" button. A message below the search bar states "No Exact Matches Found. Register as a Proprietary Compound?" with a note about registering the compound for future searches and tracking in the inventory. At the bottom of the dialogue is a "Compute Reactants?" section with two buttons: "I'll Define It Myself" and "Generate Reactants". A green arrow points from the text on the left to the "Generate Reactants" button.

Click to use retro-synthetic planning to compute the reactants for this reaction.

Launching A New Synthesis

Retro-Synthetic Planning Loading State

When retro-synthetic planning has finished, the reaction card will resolve.

Projects > Fun Synthesis Times > New Synthesis

Reaction Type Set Destination Reaction Setup Materials Sourcing Review

Specify Your Reaction Parameters

Your synthesis requires materials to be provided directly, as well as sourced commercially.

Reaction List

AMINE VARIABLE	CARBOXYLIC ACID VARIABLE	REAGENTS & CONDITIONS	PRODUCT	LEAD TIME ▲	CONFIDENCE
		Define Reaction → Reaction Undefined	 C16H14N2	--	--

+ Add a New Reaction Upload a Compound List

REACTION TYPE Amide Coupling	ELN Number 301853	TARGET AMOUNT 14mmol	REACTIONS --	EST. COMPLETION --	EST. COST --
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Previous Validate

Launching A New Synthesis

Collapsed Reaction Group

Multiple possible reactant sets may be returned from retrosynthetic planning. If this occurs, they will be combined in a **Reaction Group**.

Note: All reactions with identical compounds will be grouped into a single **Reaction Group**, regardless of whether they were computed from the same retrosynthetic plan, or defined via other means.

The screenshot shows the transcriptic software interface for launching a new synthesis. The top navigation bar includes 'Projects', 'Inventory', 'Shipments', and 'Packages'. The main title is 'Projects > Fun Synthesis Times > New Synthesis'. A progress bar at the top indicates steps: 'Reaction Type' (green checkmark), 'Set Destination' (green checkmark), 'Reaction Setup' (purple circle), 'Materials Sourcing' (grey circle), and 'Review' (grey circle). Below the progress bar, the section 'Specify Your Reaction Parameters' is shown, with a note: 'Your synthesis requires materials to be provided directly, as well as sourced commercially.' The 'Reaction List' table has columns: AMINE VARIABLE, CARBOXYLIC ACID VARIABLE, REAGENTS & CONDITIONS, PRODUCT, LEAD TIME ▲, and CONFIDENCE. One reaction row is expanded, showing a reaction between 1-naphthylamine (C₁₆H₁₄N₂) and 2-hydroxy-3-oxobutanoic acid (C₁₆H₁₄N₂O₃) to produce 1-(2-hydroxy-3-oxobutyl)naphthalene (C₁₆H₁₄N₂O₂). The reaction is labeled 'Reaction Undefined'. A red arrow points to the '+ Add a New Reaction' button. A green curved arrow points to the 'Upload a Compound List' button. The bottom of the screen shows a summary table with fields: REACTION TYPE (Amide Coupling), ELN Number (301853), TARGET AMOUNT (14mmol), REACTIONS (--), EST. COMPLETION (--), and EST. COST (--). Buttons for 'Previous', 'Validate', and 'Next' are also present.

Click to expand the **Reaction Group**.

Launching A New Synthesis

Expanded Reaction Group

Reaction Groups are visually grouped together when in an expanded state. Here they can be edited and manipulated independently. Any modification that alters the final product will remove them from the reaction group.

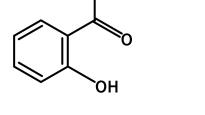
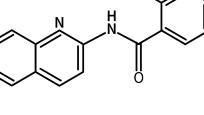
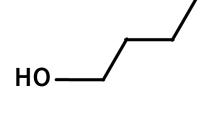
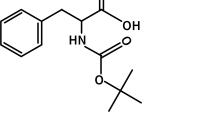
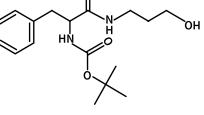
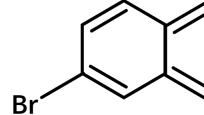
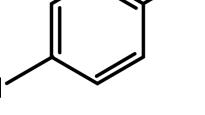
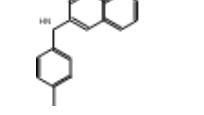
Projects > Fun Synthesis Times > New Synthesis

Reaction Type Set Destination Reaction Setup Materials Sourcing Review

Specify Your Reaction Parameters

Your synthesis requires materials to be provided directly, as well as sourced commercially.

Reaction List

AMINE VARIABLE	CARBOXYLIC ACID VARIABLE	REAGENTS & CONDITIONS	PRODUCT	LEAD TIME ▲	CONFIDENCE
 C16H14N2	 C16H14N2	<button>Define Reaction →</button> Reaction Undefined	 C16H14N2	3 Days	98% ⚡
 C16H14N2	 C16H14N2	<button>Define Reaction →</button> Reaction Undefined	 C16H14N2	3 Days	98% ⚡
 C16H14N2	 C16H14N2	<button>Define Reaction →</button> Reaction Undefined	 C16H14N2	3 Days	98% ⚡

PREDICTION GROUP

+ Add a New Reaction Upload a Compound List

REACTION TYPE: Amide Coupling ELN Number: 301853 TARGET AMOUNT: 14mmol REACTIONS: 3 EST. COMPLETION: -- EST. COST: --

Previous Validate

Launching A New Synthesis

Opened Reaction Inspector

The screenshot shows the transcriptic software interface for launching a new synthesis. At the top, there's a navigation bar with the logo, Projects, Inventory, Shipments, and Packages. Below the navigation is a progress bar with five steps: Reaction Type (green checkmark), Set Destination (green checkmark), Reaction Setup (purple circle), Materials Sourcing (grey circle), and Review (grey circle). The main area is titled "Specify Your Reaction Parameters" and includes a "Reaction List" section. In the Reaction List, there are four components: an Amine Variable (2-aminoquinoline, C₁₆H₁₄N₂), a Carboxylic Acid Variable (4-hydroxy-2-oxoquinoline, C₁₆H₁₄N₂), Reagents & Conditions (Reaction Undefined), and a Product (2-hydroxy-4-(2-aminoquinolin-2-yl)quinoline). Below the Reaction List are buttons for "+ Add a New Reaction" and "Upload a Compound List". A callout box with a green arrow points to the reaction card, containing the text: "Click into a Reaction Card to open the Reaction Inspector." To the right of the reaction card is the "Reaction Definition" panel, which lists five steps: 1. Dispense AMINE VARIABLE (2-aminoquinoline, Sigma Aldrich, 3 days lead time), 2. Dispense CARBOXYLIC ACID VARIABLE (4-hydroxy-2-oxoquinoline, Sigma Aldrich, 2 days lead time), 3. Dispense SOLVENT (empty), 4. Dispense COUPLING AGENT (empty), and 5. Dispense BASE (empty). Each step has a "Define" button. A red line and arrow point from the text "The Reaction Inspector provides a detailed view for configuring the reaction." to the "Reaction Definition" panel. At the bottom of the screen, there's a summary row with fields: REACTION TYPE (Amide Coupling), ELN Number (301853), TARGET AMOUNT (14mmol), REACTIONS (empty), EST. COMPLETION (empty), and EST. COST (empty). There are also "Previous" and "Validate" buttons.

Click into a Reaction Card to open the Reaction Inspector.

"This is perfect. It's very intuitive and straight forward."

- Medicinal Chemist at Top 10 Pharmaceutical Company

Projects > Fun Synthesis Times > New Synthesis

Reaction Type: Amide Coupling | ELN Number: 301853 | Target Amount: 14mmol | Reactions: -- | Est. Completion: -- | Est. Cost: --

Reaction Definition

Pre-charge Configuration

Template

3 days lead time.

Drag to rearrange steps *i* Auto Configure

1 DISPENSE AMINE VARIABLE
C₁₆H₁₄N₂ Sigma Aldrich 3 days lead time

2 DISPENSE CARBOXYLIC ACID VARIABLE
C₉H₈N₂ Sigma Aldrich 2 days lead time

3 DISPENSE SOLVENT
-- Define

4 DISPENSE COUPLING AGENT
-- Define

5 DISPENSE BASE
-- Define

Reaction Type: Amide Coupling | ELN Number: 301853 | Target Amount: 14mmol | Reactions: -- | Est. Completion: -- | Est. Cost: --

Previous | Validate

The **Reaction Inspector** provides a detailed view for configuring the reaction.

By default, Reagents are exposed in the **Reaction Inspector** based on the Reaction Type template. In this case we are configuring an Amide Coupling, so unique components such as Coupling Agents, as well as generic components such as Solvents, are exposed here.

Launching A New Synthesis

Reagent Definition

The screenshot shows the transcriptic software interface for launching a new synthesis. At the top, there's a navigation bar with 'Projects', 'Inventory', 'Shipments', and 'Packages'. Below it, a progress bar indicates the steps: 'Reaction Type' (green checkmark), 'Set Destination' (green checkmark), 'Reaction Setup' (purple circle), 'Materials Sourcing' (grey circle), and 'Review' (grey circle). The main area is titled 'Specify Your Reaction Parameters' and shows a 'Reaction List' with two reagents: 'AMINE VARIABLE' (2-aminoquinoline) and 'CARBOXYLIC ACID VARIABLE' (2-hydroxyacetophenone). A 'PRODUCT' structure is shown as the reaction undefined. Buttons for '+ Add a New Reaction' and 'Upload a Compound List' are available. To the right, a 'Reaction Definition' modal is open, detailing the pre-charge configuration with four steps: 1. Dispense AMINE VARIABLE (2-aminoquinoline), 2. Dispense CARBOXYLIC ACID VARIABLE (2-hydroxyacetophenone), 3. Dispense SOLVENT (dimethyl sulfoxide), 4. STIR (duration 120 seconds). A red arrow points from the 'STIR' step to a text box below. In the bottom left, a quote from a Lilly Medicinal Chemist is displayed, and in the bottom right, another quote from a medicinal chemist at a top pharmaceutical company. The bottom of the screen shows summary details: REACTION TYPE 'Amide Coupling', ELN Number '301853', TARGET AMOUNT '14mmol', and other metrics like REACTIONS, EST. COMPLETION, and EST. COST.

"Trust in the reaction assembly is critical. Right now, [for the] pre-charge instruction, I give a detailed account of how I want that to be assembled."

- Lilly Medicinal Chemist and ASL User

"This is very straight forward. I would have no issue using this."

- Medicinal Chemist at Top 10 Pharmaceutical Company

Pre-charge steps can also be added, such as stirring, heating, or simply a delay.

Launching A New Synthesis

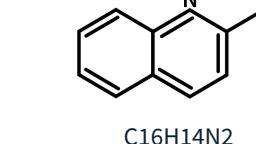
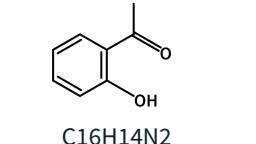
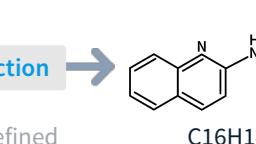
Reaction Conditions

The screenshot shows the transcriptic software interface for launching a new synthesis. The top navigation bar includes Projects, Inventory, Shipments, and Packages. The main workflow steps are Reaction Type (green checkmark), Set Destination (green checkmark), Reaction Setup (purple circle), Materials Sourcing (grey circle), and Review (grey circle). The current step is Reaction Setup.

Specify Your Reaction Parameters

Your synthesis requires materials to be provided directly, as well as sourced commercially.

Reaction List

AMINE VARIABLE:  C16H14N2 + CARBOXYLIC ACID VARIABLE:  C16H14N2 REACTANTS & CONDITIONS: Define Reaction → PRODUCT:  C16H14N2

Reaction Definition

4 DISPENSE COUPLING AGENT
5 DISPENSE BASE

Start Reaction

Incubation Conditions
DURATION: 120 S TEMPERATURE: 4 °C

pH Sensitivity
Acidic

Prediction Yield
Specify the yield you anticipate for this reaction. If you're not sure, disable this field.
Graph: Predicted yield distribution (45% at 0%, 78% at 100%)

SUGGESTED SCALE
0.4 mmol

Previous Validate

REACTION TYPE: Amide Coupling **ELN Number**: 301853 **TARGET AMOUNT**: 14mmol **REACTIONS**: -- **EST. COMPLETION**: -- **EST. COST**: --

Changes are saved immediately as they are made.

Reaction conditions, such as incubation time and temperature are set below the pre-charge steps.

Purification sensitivity

Finally, predicted yield can be set, to inform the appropriate scale for the reaction.

"Let's say I have a set of 10 substrates, and it's the first time I've used this particular common intermediate. I'll take what I consider to be the least reactive component of those 10 and run the reaction. That'll set my worse scenario. That sets a lower bound for my predicted yield."

- Lilly Medicinal Chemist and ASL User

Launching A New Synthesis

Reaction Conditions

"If I'm just doing an Amide Coupling, I'll just literally duplicate a prior Amide Coupling step. I just change one of the components. Or even just change all the components, [and] just keep all the language the same."

- Medicinal Chemist at Top 10 Pharmaceutical Company

The screenshot shows the transcriptic software interface for launching a new synthesis. At the top, a navigation bar includes 'Projects', 'Inventory', 'Shipments', and 'Packages'. Below the navigation bar, a progress bar indicates steps: 'Reaction Type' (green checkmark), 'Set Destination' (green checkmark), 'Reaction Setup' (purple circle), 'Materials Sourcing' (grey circle), and 'Review' (grey circle). The main area is titled 'Specify Your Reaction Parameters' and displays a 'Reaction List' with two entries. Each entry shows a reaction scheme: an amine (C16H14N2) reacting with a carboxylic acid (C16H14N2) to produce a product. Both entries have a 'Define Reaction' button and are labeled 'Reaction Undefined'. A red line highlights the 'Template' dropdown in the 'Reaction Definition' dialog, which is overlaid on the right side of the screen. The dialog shows a sequence of four steps: 1. Dispense AMINE VARIABLE (C16H14N2, Sigma Aldrich, 3 days lead time), 2. Dispense CARBOXYLIC ACID VARIABLE (C9H8N2, Sigma Aldrich, 2 days lead time), 3. Dispense SOLVENT (C9H8N2, Custom Compound, Ship to L2S2), and 4. STIR (DURATION: 120 s). A green arrow points from the 'Upload a Compound List' button in the reaction list to the 'Reaction Definition' dialog. At the bottom, a summary table provides details: REACTION TYPE 'Amide Coupling', ELN Number '301853', TARGET AMOUNT '14mmol', and other fields like 'REACTIONS', 'EST. COMPLETION', and 'EST. COST' are shown as '--'.

REACTION TYPE	ELN Number	TARGET AMOUNT	REACTIONS	EST. COMPLETION	EST. COST
Amide Coupling	301853	14mmol	--	--	--

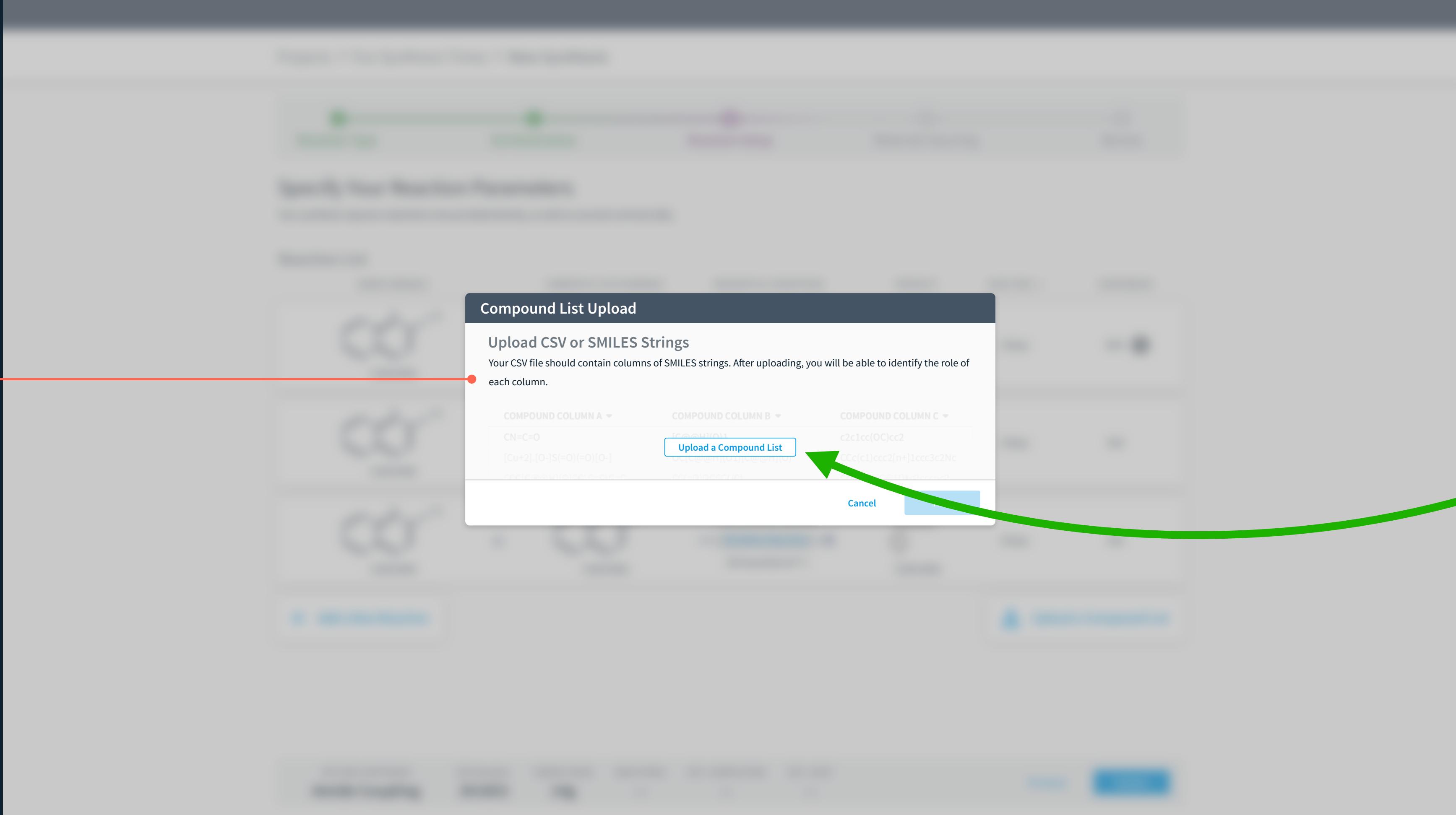
To build up parallel reactions, clone a reaction. Then edit only the aspects that need to be changed.

Add many reactions at once by uploading list of SMILES strings.

Launching A New Synthesis

CSV Compound List Upload

The required format for uploaded compound lists is described with example data.

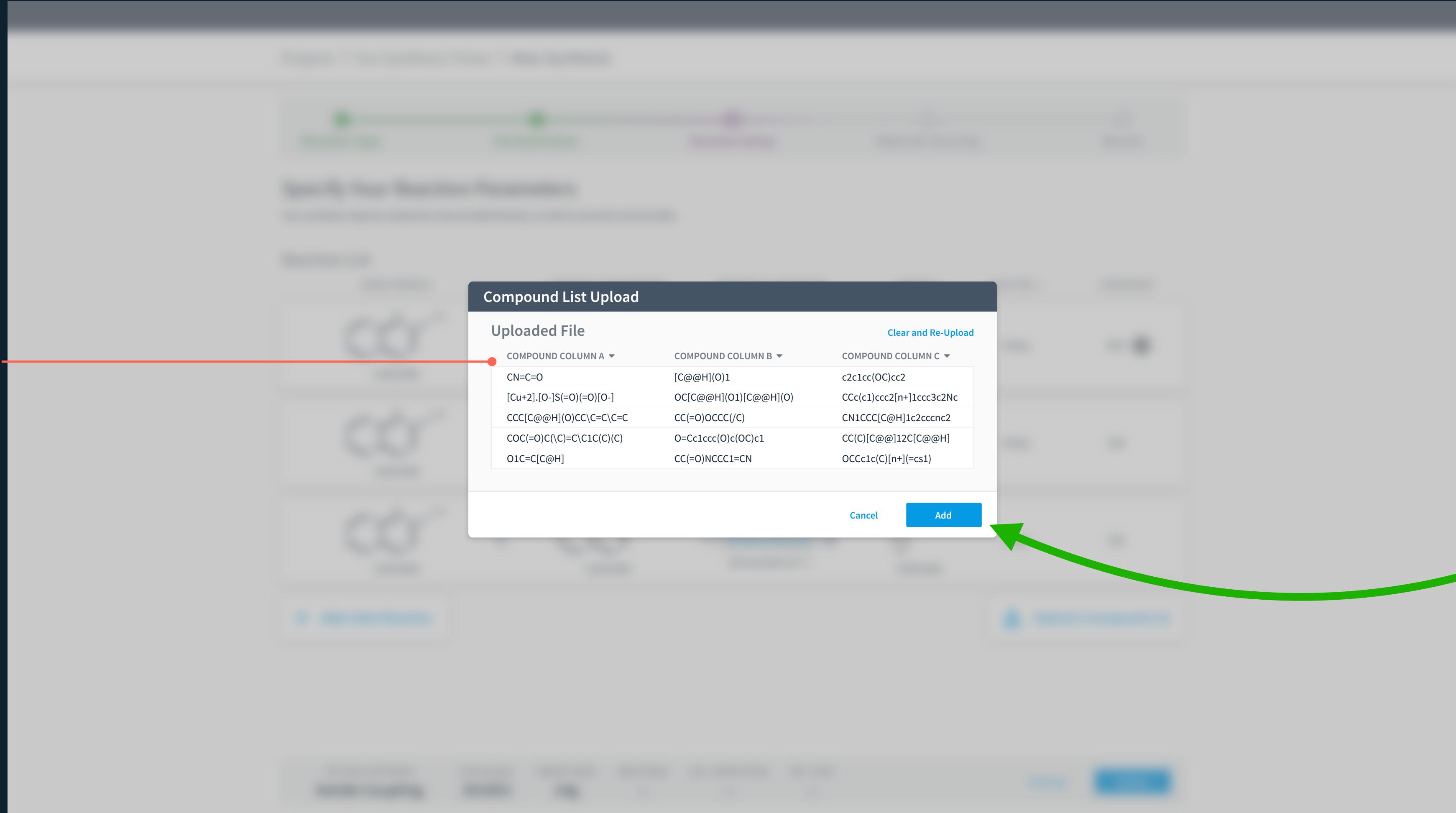


Upload a file in the specified format.

Launching A New Synthesis

CSV Compound List Upload

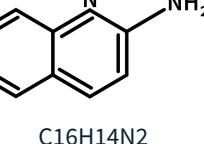
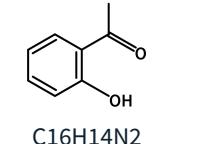
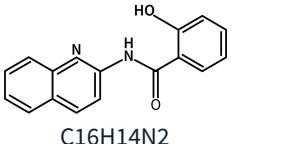
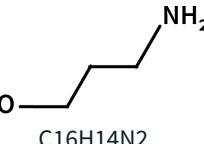
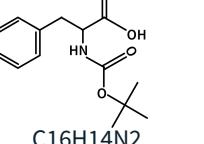
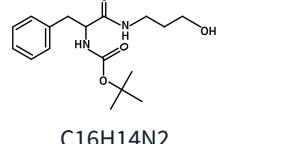
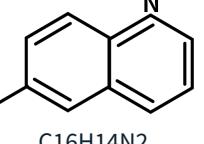
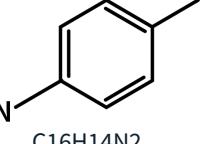
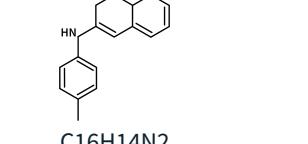
Specify which parameter of the reaction template the uploaded compounds represent.



Launching A New Synthesis

Full Reaction List Following CSV Upload

The screenshot shows the transcriptic software interface for launching a new synthesis. At the top, there's a navigation bar with the transcriptic logo, Projects, Inventory, Shipments, and Packages. Below the navigation is a progress bar with five steps: Reaction Type (green checkmark), Set Destination (green checkmark), Reaction Setup (purple circle), Materials Sourcing (grey circle), and Review (grey circle). The main area is titled "Specify Your Reaction Parameters" and includes a note: "Your synthesis requires materials to be provided directly, as well as sourced commercially." Below this is a "Reaction List" section with columns for AMINE VARIABLE, CARBOXYLIC ACID VARIABLE, REAGENTS & CONDITIONS, PRODUCT, LEAD TIME ▲, and CONFIDENCE.

AMINE VARIABLE	CARBOXYLIC ACID VARIABLE	REAGENTS & CONDITIONS	PRODUCT	LEAD TIME ▲	CONFIDENCE
 C ₁₆ H ₁₄ N ₂	 C ₁₆ H ₁₄ N ₂	HATU, DMSO, C ₁₀ H ₇ Br Define Reaction → 120 seconds at 4 °c	 C ₁₆ H ₁₄ N ₂	3 Days	98% ⚡
 C ₁₆ H ₁₄ N ₂	 C ₁₆ H ₁₄ N ₂	HATU, DMSO, C ₁₀ H ₇ Br Define Reaction → 120 seconds at 4 °c	 C ₁₆ H ₁₄ N ₂	3 Days	N/A
 C ₁₆ H ₁₄ N ₂	 C ₁₆ H ₁₄ N ₂	HATU, DMSO, C ₁₀ H ₇ Br Define Reaction → 120 seconds at 4 °c	 C ₁₆ H ₁₄ N ₂	3 Days	N/A

At the bottom left, there's a button to "Add a New Reaction" and another to "Upload a Compound List". A validation message box is visible: "Hang in there! We're validating your syntheses. We pass all submissions through a rigorous check to identify potential errors and safety hazards. We also estimate a synthesis time and cost." A progress bar shows "Validating...".

At the very bottom, there are buttons for "Previous", "Validate", and "Next".

A red arrow points from the text "Following a bulk compound list upload, the full reaction list is presented." to the reaction list area. Another red arrow points from the text "Validation progress is shown in real time." to the validation message box. A green arrow points from the text "Trigger a validation." to the "Validate" button.

Following a bulk compound list upload, the full reaction list is presented.

Validation progress is shown in real time.

Trigger a validation.

Launching A New Synthesis

Validation Failure

Following Reaction Setup, all reactions are validated and checked for invalid information, incompatible reaction processes, or the synthesis of dis-allowed compounds.

The screenshot shows the transcriptic software interface for launching a new synthesis. The top navigation bar includes 'Projects', 'Inventory', 'Shipments', and 'Packages'. The main workflow steps are 'Reaction Type' (green checkmark), 'Set Destination' (green checkmark), 'Reaction Setup' (purple circle), 'Materials Sourcing' (grey circle), and 'Review' (grey circle). The current step is 'Reaction Setup'. Below this, a progress bar indicates completion of the first two steps. The main area is titled 'Specify Your Reaction Parameters' and notes that materials must be provided directly or sourced commercially. A 'Reaction List' table displays four entries:

AMINE VARIABLE	CARBOXYLIC ACID VARIABLE	REAGENTS & CONDITIONS	PRODUCT	LEAD TIME ▲	CONFIDENCE
C16H14N2	C16H14N2	HATU, DMSO, C10H7Br 120 seconds at 4 °c		3 Days	98% ⚡
C16H14N2	C16H14N2	HATU, DMSO, C10H7Br 120 seconds at 4 °c		3 Days	N/A
C16H14N2	C16H14N2	HATU, DMSO, C10H7Br 120 seconds at 4 °c		3 Days	N/A

Below the table are buttons for 'Add a New Reaction' and 'Upload a Compound List'. A validation message box states: 'Hang in there! We're validating your syntheses. We pass all submissions through a rigorous check to identify potential errors and safety hazards. We also estimate a synthesis time and cost.' It shows a progress bar from 'In Progress' to 'Failed' with a red exclamation mark. The bottom of the screen shows summary details: 'REACTION TYPE Amide Coupling', 'ELN Number 301853', 'TARGET AMOUNT 14mmol', 'REACTIONS --', 'EST. COMPLETION --', 'EST. COST --', 'Previous', and a 'Validate' button.

Validation result is shown following validation completion.

Launching A New Synthesis

Validation Errors

The screenshot shows the transcriptic software interface for launching a new synthesis. The top navigation bar includes Projects, Inventory, Shipments, and Packages. The main workflow steps are Reaction Type (green checkmark), Set Destination (green checkmark), Reaction Setup (purple circle), Materials Sourcing (grey circle), and Review (grey circle). The current step is Reaction Setup.

Specify Your Reaction Parameters
Your synthesis requires materials to be provided directly, as well as sourced commercially.

Reaction List

AMINE VARIABLE	CARBOXYLIC ACID VARIABLE	REAGENTS & CONDITIONS	PRODUCT
		HATU, DMSO, C10H7Br 120 seconds at 4 °C	
		HATU, DMSO, C10H7Br 120 seconds at 4 °C	
		HATU, DMSO, C10H7Br 120 seconds at 4 °C	

Add a New Reaction | **Upload a Compound List**

REACTION TYPE: Amide Coupling | **ELN Number**: 301853 | **TARGET AMOUNT**: 14mmol | **REACTIONS**: -- | **EST. COMPLETION**: -- | **EST. COST**: --

Reaction Definition

Pre-charge Configuration **X**

Validation Errors ⓘ

Restricted Reagent Combination
You have chosen building blocks that cannot be used in combination with each other. Remove one or more.

Template: 3 days lead time.
Drag to rearrange steps ⓘ **Reset**

- 1 DISPENSE ⚡ AMINE VARIABLE
C16H14N2 Sigma Aldrich 3 days lead time
- 2 DISPENSE ⚡ CARBOXYLIC ACID VARIABLE
C9H8N2 Sigma Aldrich 2 days lead time
- 3 DISPENSE ⚡ SOLVENT
C9H8N2 Custom Compound ⓘ Ship to L2S2
- 4 STIR ⚡

A red arrow points from the text "Reactions that failed validation are flagged in red." to the third reaction row. A green arrow points from the text "Remove the problematic reaction to resolve this validation error." to the "Validation Errors" section. A red line connects the validation error message to the "Reaction Inspector" heading.

Remove the problematic reaction to resolve this validation error.

Specific validation errors are shown in the **Reaction Inspector**.

Launching A New Synthesis

Validation Success

The screenshot shows the transcriptic software interface for launching a new synthesis. The top navigation bar includes 'Projects', 'Inventory', 'Shipments', and 'Packages'. Below the navigation is a progress bar with five steps: 'Reaction Type' (green checkmark), 'Set Destination' (green checkmark), 'Reaction Setup' (purple circle), 'Materials Sourcing' (grey circle), and 'Review' (grey circle). The main section is titled 'Specify Your Reaction Parameters' and includes a note: 'Your synthesis requires materials to be provided directly, as well as sourced commercially.' The 'Reaction List' table has columns for 'AMINE VARIABLE', 'CARBOXYLIC ACID VARIABLE', 'REAGENTS & CONDITIONS', 'PRODUCT', 'LEAD TIME ▲', and 'CONFIDENCE'. Two reaction rows are shown:

AMINE VARIABLE	CARBOXYLIC ACID VARIABLE	REAGENTS & CONDITIONS	PRODUCT	LEAD TIME ▲	CONFIDENCE
C16H14N2	C16H14N2	HATU, DMSO, C10H7Br Define Reaction → 120 seconds at 4 °c	C16H14N2	3 Days	98% ⚡
C16H14N2	C16H14N2	HATU, DMSO, C10H7Br Define Reaction → 120 seconds at 4 °c	C16H14N2	3 Days	N/A

Buttons include '+ Add a New Reaction' and 'Upload a Compound List'. At the bottom, a summary table shows: REACTION TYPE 'Amide Coupling', ELN Number '301853', TARGET AMOUNT '14mmol', and other fields like 'REACTIONS', 'EST. COMPLETION', and 'EST. COST' with values '--'. A success message box says: 'Hang in there! We're validating your syntheses. We pass all submissions through a rigorous check to identify potential errors and safety hazards. We also estimate a synthesis time and cost.' with a green 'Success' button. A green arrow points from the 'Success' button to the 'Materials Sourcing' step in the progress bar.

Following a successful validation, proceed to materials sourcing.

Launching A New Synthesis

Material Sources Review

Projects > Fun Synthesis Times > New Synthesis

Reaction Type Set Destination Reaction Setup Materials Sourcing Review

Specify Your Material Sources

Your synthesis requires materials to be provided directly, as well as sourced commercially.

Materials that must be provided by the user are shown up top.

The Following Materials Need to Be Shipped By You

STRUCTURE	FORMULA	WEIGHT	ROLE
	C ₇ H ₈ NH	98.11	Amine Variable
	C ₇ H ₈ NH	98.11	Carboxylic Acid Variable
	C ₇ H ₈ NH	98.11	Solvent

At Your Bench?

If you have your pre-barcoded Transcriptic vials handy, you can create your shipment now. Otherwise, you can always take care of it later.

Need Vials? Order some more.

Create Shipment

Materials that will be sourced commercially are shown below.

The Following Materials Need to Be Shipped By You

STRUCTURE	FORMULA	WEIGHT	ROLE	SOURCE	LEAD TIME	FORM	AMOUNT	PURITY	QC DATA
	C ₇ H ₈ NH	98.11	Coupling Agent	Sigma Aldrich	Available Now	Powder	0.4g	89.2%	
	C ₇ H ₈ NH	98.11	Coupling Agent	Sigma Aldrich	Available Now	Powder	0.4g	89.2%	
	C ₇ H ₈ NH	98.11	Coupling Agent	Sigma Aldrich	Available Now	Powder	0.4g	89.2%	

REACTION TYPE ELN Number TARGET AMOUNT REACTIONS EST. COMPLETION EST. COST

Amide Coupling 301853 14mmol 3 Dec 19, 9:14am \$3565.03

Previous Next

Launching A New Synthesis

Shipment Creation

A simple checklist of materials to be provided are shown. They are marked as complete once all info is filled in.

Specify the concentration/% weight of the material.

Create Shipment

It Looks Like You Need To Send Us Some Things
Follow these simple steps to submit your custom compounds to Transcriptic.

Step 1
Specify the purity of your compounds for each entry below to calculate the mass required. Place the calculated mass in a pre-barcode Transcriptic vial, and specify the barcode of the vial.

STRUCTURE	FORMULA	WEIGHT	VIAL TYPE	FORM	TEMPERATURE	CONC./% WEIGHT	AMOUNT	BARCODE
	C7Br4H2	306.31	A1	Powder	4 °C	98 %	12.00g	579648
	C7Br4H2	306.31	A1	Powder	4 °C	98 %	12.00g	579648
	C7Br4H2	306.31	A1	Powder	4 °C	98 %	12.00g	579648

Step 2
Box up your vials and send them to the following address. Make sure you include the shipment intake code: **TMFX**

Transcriptic South
Shipping and Receiving
Shipment Code: **TMFX**
10290 Campus Point Dr.
San Diego, CA 92121

Step 3 (Optional)
Once you've generated a tracking code, provide it here to receive more accurate timing estimates for your syntheses.

Tracking Code

Cancel Create

Specify the type of vial that will be used to store the material.

Specify if the material is a solid or liquid.

Enter the barcode from the pre-barcoded vial that will be used to ship the material.

Make note of the shipping address to send the samples to.

If desired, enter the tracking code from the shipment.

Click to create the shipment.

Launching A New Synthesis

Review Synthesis Submission

Before submitting, review the syntheses that have been configured.

Review the destinations to which the final product will be dispatched.

Submission overview is displayed at the bottom.

Projects > Fun Synthesis Times > New Synthesis

Reaction Type Set Destination Reaction Setup Materials Sourcing Review

Review Synthesis Submissions

Your synthesis requires materials to be provided directly, as well as sourced commercially.

Configured Syntheses

STRUCTURE	FORMULA	WEIGHT	PREDICTED SCALE	EST. SYNTHESIS TIME	EST. START	EST. COMPLETION	PRICE
	HNaO	308.160	0.100 mmol	5 hours, 15 minutes	12/11/18 11:00 am	12/11/18 11:00 pm	\$519.73
	HNaO	308.160	0.100 mmol	5 hours, 15 minutes	12/11/18 11:00 am	12/11/18 11:00 pm	\$519.73
	HNaO	308.160	0.100 mmol	5 hours, 15 minutes	12/11/18 11:00 am	12/11/18 11:00 pm	\$519.73
	HNaO	308.160	0.100 mmol	5 hours, 15 minutes	12/11/18 11:00 am	12/11/18 11:00 pm	\$519.73

Downstream Destinations

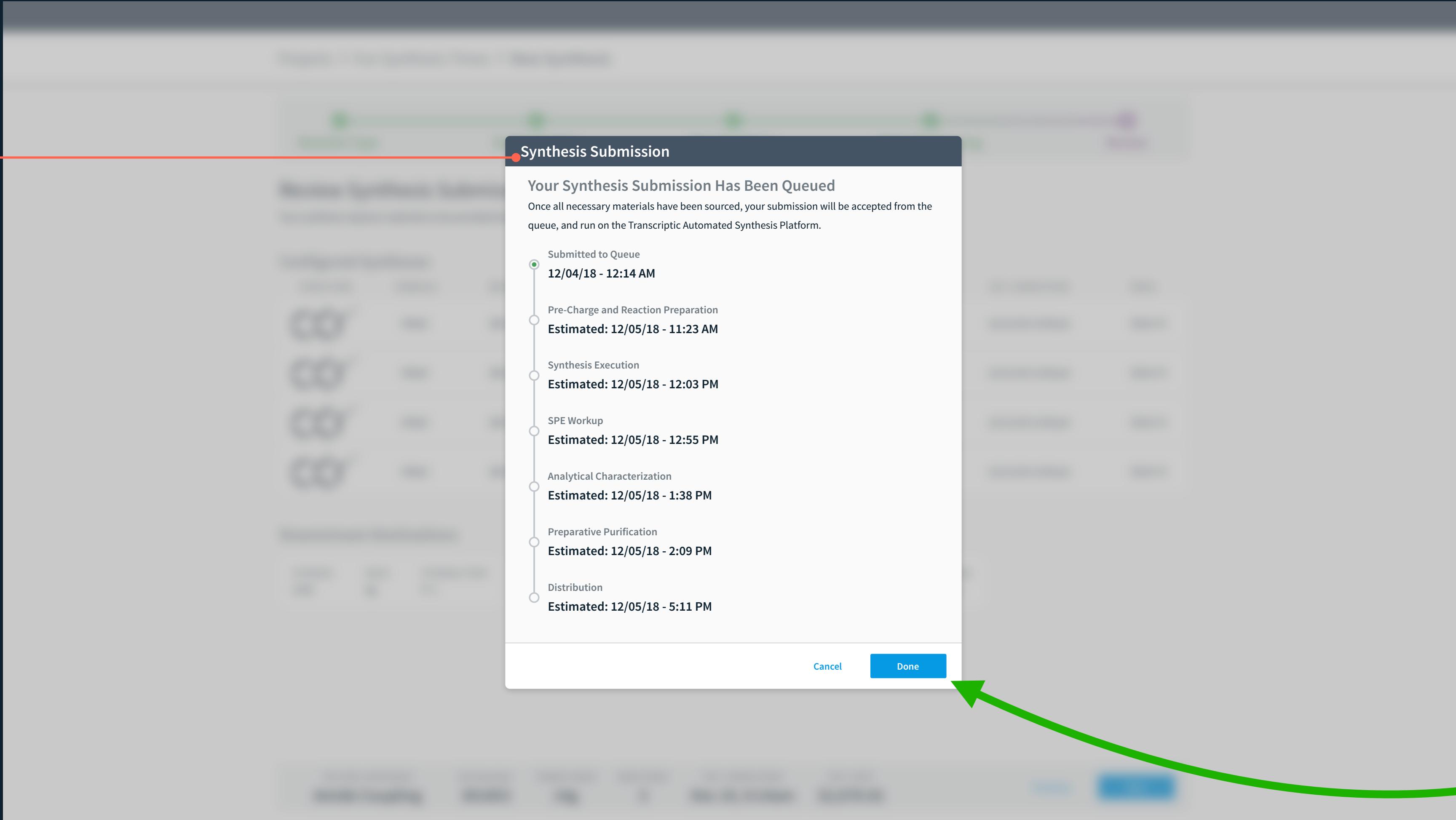
STORAGE L2S2	STORAGE TEMP 4 °C	AMOUNT 4mmol	BIOASSAY My Cool Assay 2	SCHEDULE Weekly	AMOUNT 6mmol	SHIP Menlo Park, CA	AMOUNT 4mmol
-----------------	----------------------	-----------------	-----------------------------	--------------------	-----------------	------------------------	-----------------

REACTION TYPE Amide Coupling	ELN Number 301853	TARGET AMOUNT 14mmol	REACTIONS 3	EST. COMPLETION Dec 19, 9:14am	EST. COST \$3565.03	Previous	Submit
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Launching A New Synthesis

Estimated Synthesis Timeline

Following submission, an estimated timeline of how the synthesis will execute is shown.



Click Done to return to the
[Project Page](#).

Synthesis Management

Project Page

New tasks from the synthesis have been added to my To Do list.

The screenshot shows the Synthesis Management Project Page. On the left, a sidebar lists 'New tasks from the synthesis have been added to my To Do list.' and 'The synthesis has been added to the list of syntheses waiting for building blocks.' A red line with arrows points from these text blocks to the 'Your Input Is Needed' and 'Waiting For Building Blocks' sections respectively.

Your Input Is Needed

- Complete the shipping info for the self sourced building blocks in **My Cool Reaction Library**. [Complete Shipment](#)
- Ship your samples for the following synthesis: **My Other Cool Reaction Library**. [Mark as Shipped](#)

Activity Since Last Login

Route Modified

Super Sulfonamide
Submitted by Todd de Collo on December 8th, 2018
Started: 12/10/18 at 9:02 AM
Incubation was extended at a higher temperature.

Completed

Urea Fo' Rea'
Submitted by Rick and Marty on December 8th, 2018
COMPLETED: 12/10/18 at 10:04 PM
The target mass of all desired products was successfully synthesized.

Syntheses

Waiting For Building Blocks

- My Cool Reaction Library**
Amide Coupling
r1234abcd5678efgh
Submitted by Todd de Collo on December 12th, 2018
Waiting for shipping information to be provided. [Edit](#)
- Nifty Synthesis Library**
Amide Coupling
r9876zyxw5432jdxk
Submitted by Alex Hadik Today at 10:54 AM
Waiting for 3 self sourced, and 2 commercial building blocks to arrive. [Edit](#)

In Queue

- What Even Is A Mide?**
Amide Coupling
r1234abcd5678efgh
Waiting for capacity to become available for automated synthesis. [Edit](#)

Syntheses that are waiting for materials to arrive are grouped at the top.

Syntheses for which all materials have arrived, but for which capacity is not yet available, are shown as being **In Queue**.

Syntheses that are currently in progress are grouped together, with a progress bar indicating how far along they have progressed.

Click to further inspect why this synthesis route was modified.

Syntheses that have completed are grouped as completed. Even if not all reaction succeeded, the overall synthesis is marked as Complete when there are no more reactions being run.

Syntheses

Waiting For Building Blocks ▾

My Cool Reaction Library

Amide Coupling
r1234abcd5678efgh

Submitted by Todd de Collo on December 12th, 2018

ⓘ Waiting for shipping information to be provided.

Library Size: 4 compounds

Target Product Mass: 14 milligrams

Estimated Start Date: 12/21/18

Nifty Synthesis Library

Amide Coupling
r9876zyxw5432jdkx

Submitted by Alex Hadik Today at 10:54 AM

ⓘ Waiting for 3 self sourced, and 2 commercial building blocks to arrive.

Library Size: 2 compounds

Target Product Mass: 14 milligrams

Estimated Start Date: 12/20/18

In Queue ▾

What Even Is A Mide?

Amide Coupling
r1234abcd5678efgh

Submitted by Alex Hadik on December 12th, 2018

ⓘ Waiting for capacity to become available for automated synthesis.

Library Size: 2 compounds

Target Product Mass: 10 milligrams

Estimated Start Date: 12/14/18

In Progress ▾

Let's Make Some Chemicals!

Suzuki Coupling
r1234abcd5678efgh

Submitted by Jim Beck on December 9th, 2018

45% Complete

Library Size: 2 compounds

Target Product Mass: 10 milligrams

Started: 12/11/18 at 9:02 AM

Current Step: Solid Phase Extraction

Super Sulfonamide

Sulfonamide Formation
r1234abcd5678efgh

Submitted by Todd de Collo on December 8th, 2018

⚠ Incubation was extended at a higher temperature.

Library Size: 120 compounds

Target Product Mass: 4 milligrams

Started: 12/10/18 at 9:02 AM

Current Step: Post Purification

87% Complete

Completed ▾

Urea Fo' Rea'

Urea Formation
r1234abcd5678efgh

Submitted by Rick and Marty on December 8th, 2018

ⓘ The target mass of all desired products was successfully synthesized.

Library Size: 1 compound

Target Product Mass: 10 milligrams

Started: 12/09/18 at 9:02 AM

Completed: 12/10/18 at 10:04 PM

Spooky Suzuki

Suzuki Coupling
r1234abcd5678efgh

Submitted by Mike Bem on December 1st, 2018

⚠ Not all desired products were successfully synthesized. Click to see more information.

Library Size: 16 compound

Target Product Mass: 9 milligrams

Started: 12/02/18 at 9:02 AM

Completed: 12/03/18 at 10:04 PM

The detailed status of the synthesis is shown at the top of the card.

Some syntheses will have been modified mid-flight. This is indicated directly on the card.

The degree to which the synthesis succeeded is indicated.

Synthesis Management

Synthesis Page

The progress of each reaction within the synthesis is shown. This reaction has fully completed.

Click into a reaction to see more detail.

Projects > Fun Synthesis Times > Super Sulfonamide

OVERVIEW CONTAINERS RESULTS QUOTE

Synthesis Summary

Sort by Percent Complete ▾ Filter by: Incomplete ▾

N-(p-tolyl)quinolin-6-amine

EMPERICAL FORMULA C16H14N2 MOLECULAR WEIGHT 234.30

Recent Activity

December 10th

9:02 AM Start

8:13 AM Analytical LCMS RESULT: Synthesis incomplete PERCENT COI: 43%

8:42 AM

9:08 AM Incubation

10:42 AM Route Intervention DURATION: 1 hour, 30 minutes TEMPERATURE: 120 °C

Expand 6 instructions

Expand 3 remaining instruction

Final product is reviewed at the top.

A collapsed view of the synthesis thus far is displayed by default.

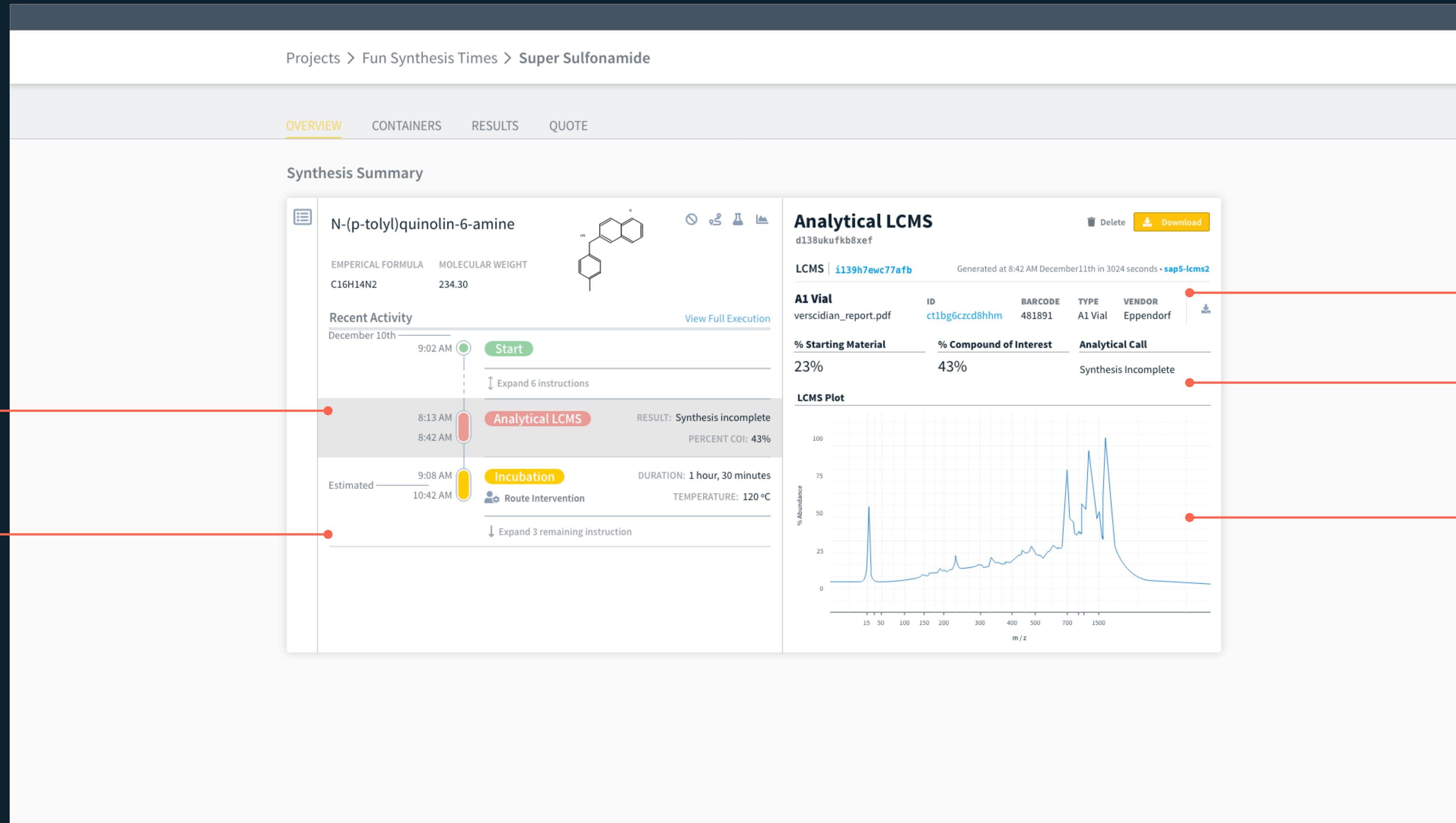
Each instruction can be further explored.

Synthesis Management

Analytical LCMS Visualization

Selected instruction is highlighted.

An additional incubation step has been added based on the results of the Analytical LCMS.



An overview of the containers of the instruction is shown up top.

A review of the data generated.

A visual plot of the raw LCMS data.

Synthesis Management

Incubation Instruction Visualization

Projects > Fun Synthesis Times > Super Sulfonamide

OVERVIEW CONTAINERS RESULTS QUOTE

Synthesis Summary

N-(p-tolyl)quinolin-6-amine

EMPERICAL FORMULA C16H14N2 MOLECULAR WEIGHT 234.30

Recent Activity

December 10th

9:02 AM Start

8:13 AM Analytical LCMS RESULT: Synthesis incomplete PERCENT COI: 43%

8:42 AM

Estimated 9:08 AM Incubation DURATION: 1 hour, 30 minutes TEMPERATURE: 120 °C

10:42 AM Route Intervention

↓ Expand 6 instructions

↓ Expand 3 remaining instruction

Incubation

i138ukufkb8xef Started at 9:08 AM December 11th • sap2-indigo1

A1 Vial ID ct1bg6czcd8hhm BARCODE 481891 TYPE A1 Vial VENDOR Eppendorf

This incubation was added automatically based on the analysis of LCMS. Do you agree with this decision?

Absolutely Not Not Really No Opinion Looks Fine Yes Absolutely

ANY COMMENTS?

I would probably have increased to 125 °C, but this is fine.

Submit

Incubation Time 1 hour, 30 minutes Incubation Temperature 120 °C Device Indigo Reactor

Temperature and Pressure Plot

Temperature (°C) Pressure

Instructions that have been modified or dynamically added are flagged as a **Route Intervention**.

Provide feedback on the modification that was made to the proposed synthesis route.

Time and pressure plotted over time.

Synthesis Management

Project Page

The full execution can be shown if desired. If the synthesis is in progress, the past steps are shown, as well as the predicted steps going forward.

Projects > Fun Synthesis Times > Super Sulfonamide

OVERVIEW CONTAINERS RESULTS QUOTE

Synthesis Summary

N-(p-tolyl)quinolin-6-amine

EMPERICAL FORMULA C16H14N2 MOLECULAR WEIGHT 234.30

Recent Activity

December 10th

- 9:02 AM Start
- 11:16 PM Accession NUMBER OF COMPOUNDS: 4 SOURCE: Verso Store
- 11:45 PM Dispense COMPOUND: Amine HRA1 MASS: 91.7 mg
- 11:52 PM Dispense COMPOUND: Carboxylic Acid HRA1 MASS: 106.0 mg
- Today
- 12:04 AM Dispense COMPOUND: DMSO VOLUME: 2 ml
- 12:13 AM Dispense COMPOUND: DMSO VOLUME: 2 ml
- 12:31 AM Dispense COMPOUND: DMSO VOLUME: 2 ml
- 12:52 AM Dispense COMPOUND: DMSO VOLUME: 2 ml
- 3:18 AM Stir DURATION: 5 minutes
- 3:25 AM Stir DURATION: 5 minutes
- 4:48 AM Incubation DURATION: 1 hour, 30 minutes TEMPERATURE: 120 °C
- 6:21 AM Analytical LCMS RESULT: Synthesis incomplete PERCENT COI: 43%
- 8:13 AM Estimated 9:08 AM Incubation DURATION: 1 hour, 30 minutes TEMPERATURE: 120 °C
- 10:42 AM Route Intervention
- Estimated 9:08 AM Incubation DURATION: 1 hour, 30 minutes TEMPERATURE: 120 °C
- 8:13 AM SPE Workup BLOWOFF TIME: 14 minutes BLOWOFF TEMPERATURE: 92 °C
- 8:42 AM Prep. Purification COI SOLVENT: -- COI VOLUME: 3 ml

Incubation

i138ukufkb8xef Started at 9:08 AM December 11th • sap2-indigo1

A1 Vial ID ct1bg6czcd8hhm BARCODE 481891 TYPE A1 Vial VENDOR Eppendorf

This incubation was added automatically based on the analysis of LCMS. Do you agree with this decision?

Absolutely Not Not Really No Opinion Looks Fine Yes Absolutely

ANY COMMENTS?

I would probably have increased to 125 °C, but this is fine.

Incubation Time 1 hour, 30 minutes Incubation Temperature 120 °C Device Indigo Reactor

Temperature and Pressure Plot

Temperature (°C) Pressure

Time 9:00 AM 9:05 AM 9:10 AM 9:15 AM 9:20 AM 9:25 AM 9:30 AM

Temperature Pressure