

From Molecules to Collective Intelligence: Connected Science for AI-Enhanced Chemical R&D

NextGen Chemicals and Petrochemicals Summit 2026

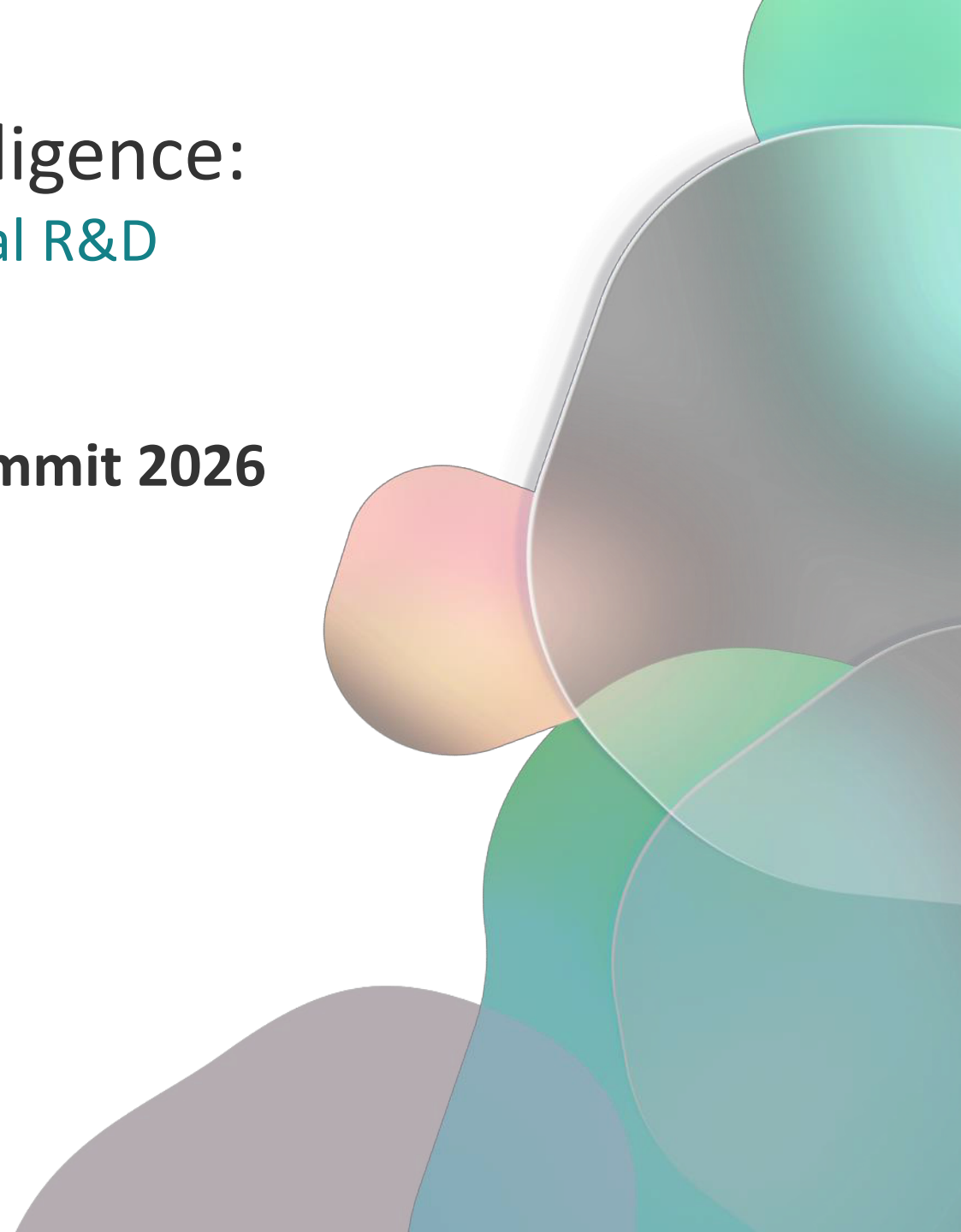
Presenter:

Manish M. Khandagale, PhD

Sr. Application Scientist, Revvity Signals

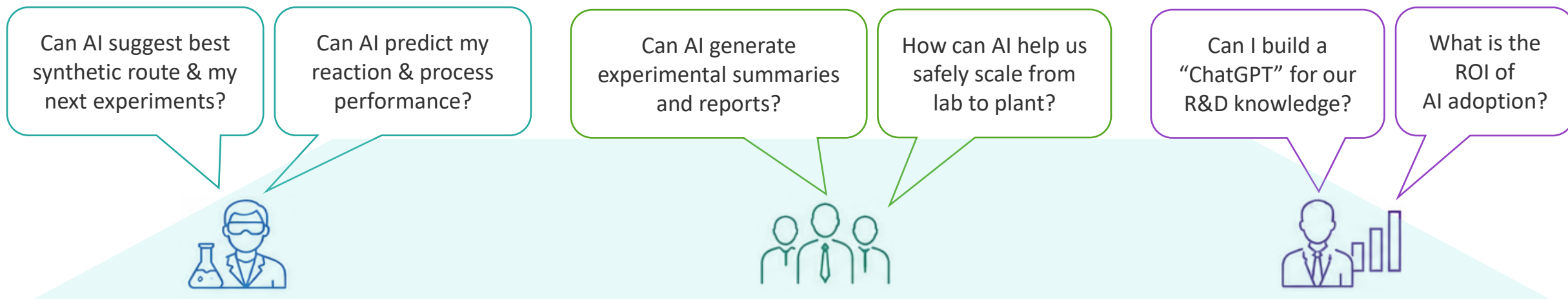


July 09, 2026



Common AI/ML Expectations

We Need AI/ML-Do you have it in your Software?



What is Usually missing



Historical data isn't structured or connected

Data isn't standardized across the projects

Integrated Tools & Workflows

R&D and plant data remain siloed

Unified scientific data platform or governance

The Journey Towards
AI-driven Innovation

CAPTURE

CONNECT

UNIFY

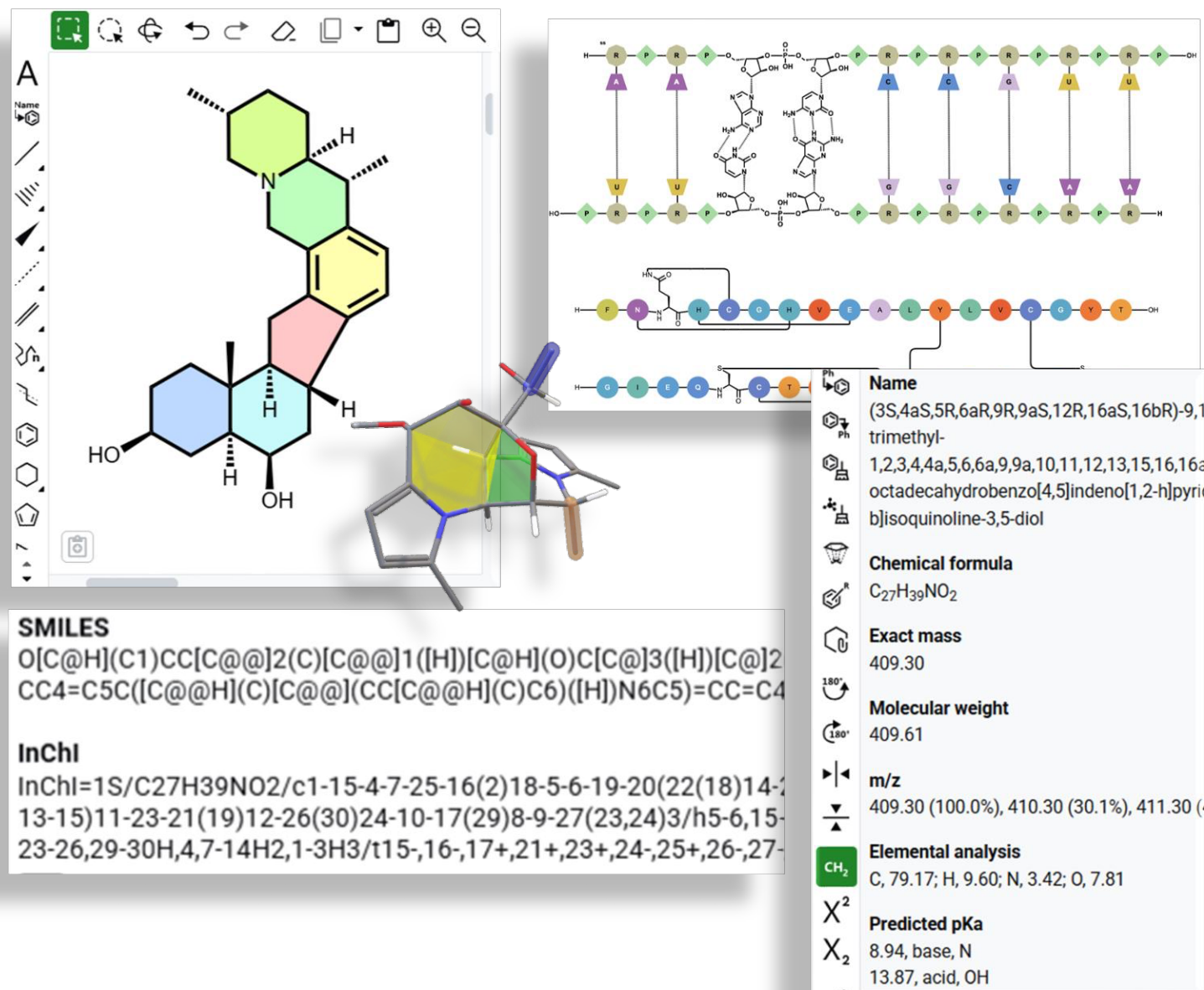
ANALYZE

INTELLECT

INNOVATE

- **Draw**- Capture Chemical structures digitally.
- **Standardize**- Nomenclature, representations, identifiers to ensure consistency.
- **Understand**- Calculate & visualize molecular properties
- **Communicate**- Clearly with accurate visual depictions

Create A Digital Language Of Chemistry
— Making It Machine Readable



Linking Structures to Physical Material and Inventory

Order / Internal request

SEARCH

MATERIAL CAS
= 138786-67-1

CONTAINER Contents Name
= sodium;5-(difluoromethoxy)-2-[...]

Chemical

match substructure

Order Material | Reagent

Search

121-57-3

Exact

Search

Results

Inventory System Suppliers ChemACX On Order Reorder

Internal Request

Sulfanilic acid

CAS 121-57-3 Properties

Type to filter...

Supplier	Size	Price	Purity	Catalog
A2B	5 g	\$10	95%	AB47060
A2B	25 g	\$15	95%	AB47060
A2B		\$40	95%	AB47060
A2B	500 g	\$150	95%	AB47060
ABCR			98%	AV15825

Supplier

Supplier Name* VWR International, LLC

Supplier Catalog Number* AAAL04115-30

Purity 98%

Supplier Concentration Enter Concentration

Price \$16.82

Size 250 g

Number of Containers 1

Supplier Website http://www.vwr.com

Request

Requestor* Manish K

Destination Location* /Thane GB Site/THA GB

Amount Requested 250 g

Register

0000000367

4-aminobenzenesulfonic acid

CAS: 121-57-3

Lot: Reagent-0057-001

Expires: Jul 02, 2026

Active Compounds
AC-0002 4/4
(2S)-2-(2-oxopyrrolidin-1-...

Active Compounds
AC-0002-04
(2S)-2-(2-oxopyrrolidin-1-...

Active Compounds
AC-0002-03
(2S)-2-(2-oxopyrrolidin-1-...

Active Compounds
AC-0002-02
(2S)-2-(2-oxopyrrolidin-1-...

Active Compounds
AC-0002-01
(2S)-2-(2-oxopyrrolidin-1-...

Track custody & Consumption

/ Thane GB Site / THA GB Chemistry Lab-801 / Container-000341

History

Sulfanilic Acid | IN_USE
[Reagent-0057-002](#)

Amount Available 500 g

Current User Arsha Rai

Barcode 0000000368

Expiration Date Jun 05, 2028, 12:00 AM

Check In/Out

Update Amount

Aliquot Container

Copy

Print Barcode

Request Container

Dispose

Safety & Properties

NONE GHS00 No Hazard	GHS01 Explosives	GHS02 Flammables	GHS03 Oxidizers
GHS04 Compressed Gases	GHS05 Corrosives	GHS06 Acute Toxicity	GHS07 Irritant

CONNECT

Building A Digital Thread - Integrated Workflow

signalsNotebook

Route of Synthesis
& Step ReactionMaterial selection
& StoichiometryRecord Process
Data-SheetSample & container
Creation

Registration

Analysis Request

Task Assignment

Results

Synthesis Route

General: 93% ... A · Ω, Bonds, Templates, Symbols, HELM, Structure

Reaction Scheme:

4-aminobenzenesulfonic acid [I] + sodium nitrite [II] $\xrightarrow{0-5^{\circ}\text{C}}$ 4-sulfobenzenediazonium chloride [III] + 5-oxo-1-(4-sulfophenyl)-2,5-dihydro-1H-pyrazole-3-carboxylic acid

5-oxo-1-(4-sulfophenyl)-2,5-dihydro-1H-pyrazole-3-carboxylic acid + NaOH / Na₂CO₃ $\xrightarrow{\text{NaOH / Na}_2\text{CO}_3}$ sodium 5-oxo-1-(4-sulfophenyl)-4-((E)-4-sulfonatophenyl)diazene-4,5-dihydro-1H-pyrazole-3-carboxylate [IV]

Step-1: Diazotization

Reaction Scheme:

4-aminobenzenesulfonic acid [I] + sodium nitrite [II] $\xrightarrow{0-5^{\circ}\text{C}}$ 4-sulfobenzenediazonium chloride [IV]

Reactants Table:

Run ID	Reactant	CAS Number	Barcode	Container ID	MF	MW	Limit?	Eq	Sample Mass	Moles	Vol	Grade	GHS Hazard Statements
I	Sulfanilic Acid	121-57-3	0000000368	Container-000341 1:1	C ₆ H ₇ NO ₃ S	173.19	✓	1	100.3 g	579.1 mmol		AR	H315, H317, H319
II	sodium nitrite	7632-00-0			NaNO ₂	68.99		1	39.95 g	579.1 mmol		GR	H272, H301, H400, H319, H341 + 7 more

Samples

Chemical Structure: 4-sulfobenzenediazonium chloride

ID: S000478

Created Date: Jul 03, 2026, 03:01 PM

Chemical Name: 4-sulfobenzenediazonium chloride

Create Tasks Test Request

Type: Analytical Testing

Required By: May 30, 2025, 10:00 AM

Analytical Test: In-process sample analysis, Purity by HPLC, Characterization

Samples Table References (1 row, count 3)

☐ Create 1 Task for each item (All | None)

☒ S00... ☒ AC... ☒ Cont...

Cancel Create

Task Assignment

Structures

Materials

Samples

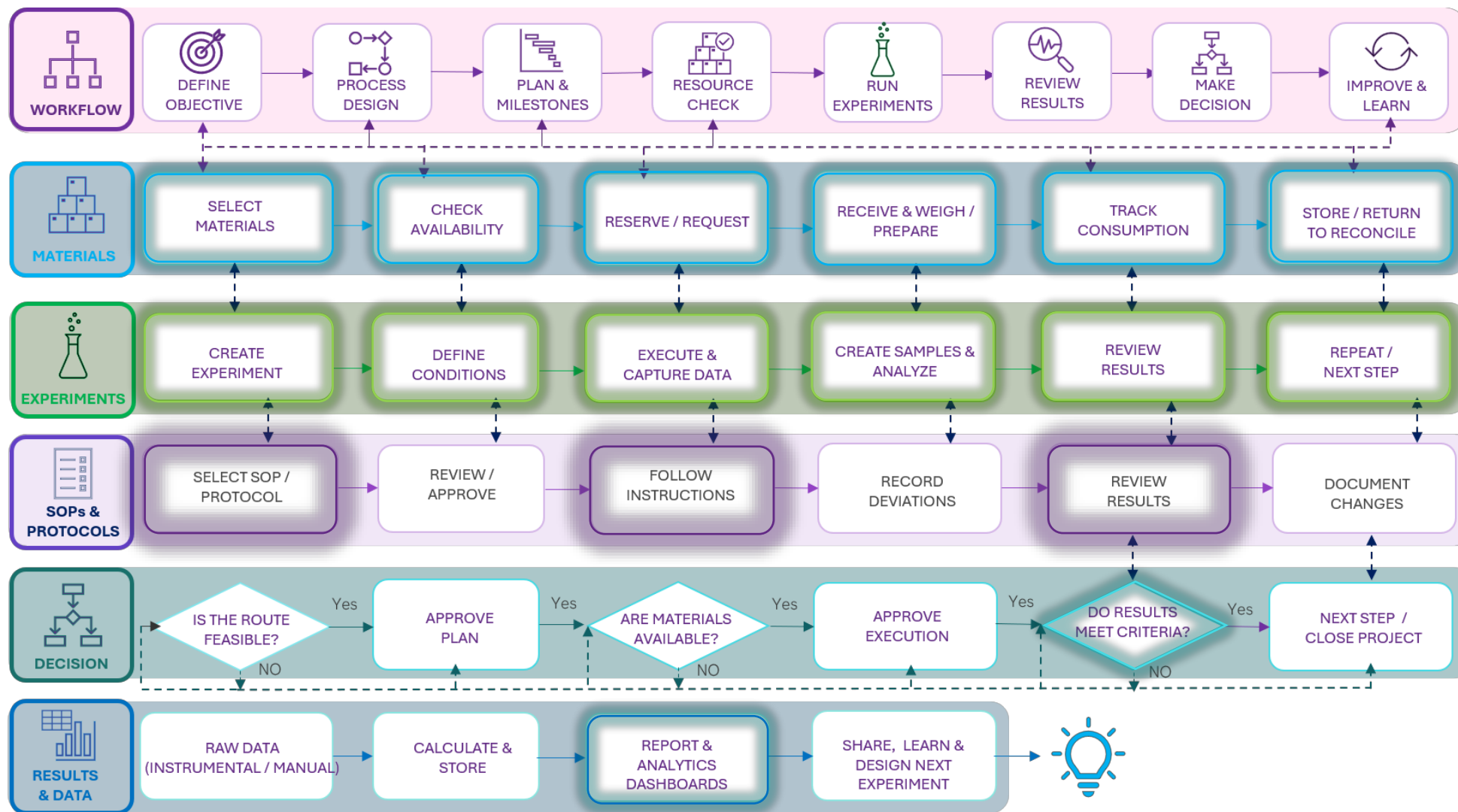
People

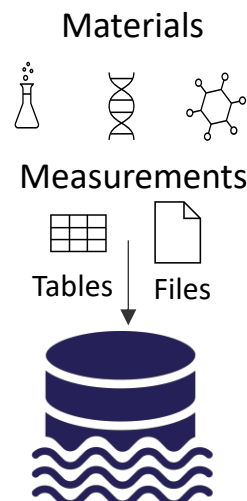
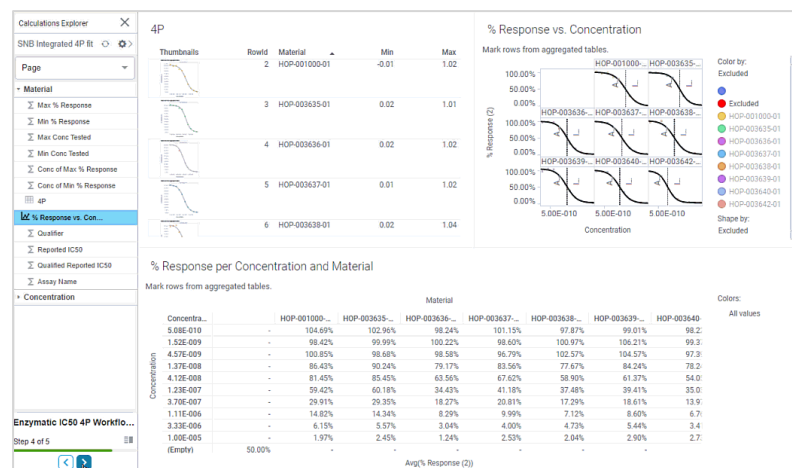
Tasks

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Revvity Proprietary Information

Towards an Orchestrated workflow: One connected Data Pipeline





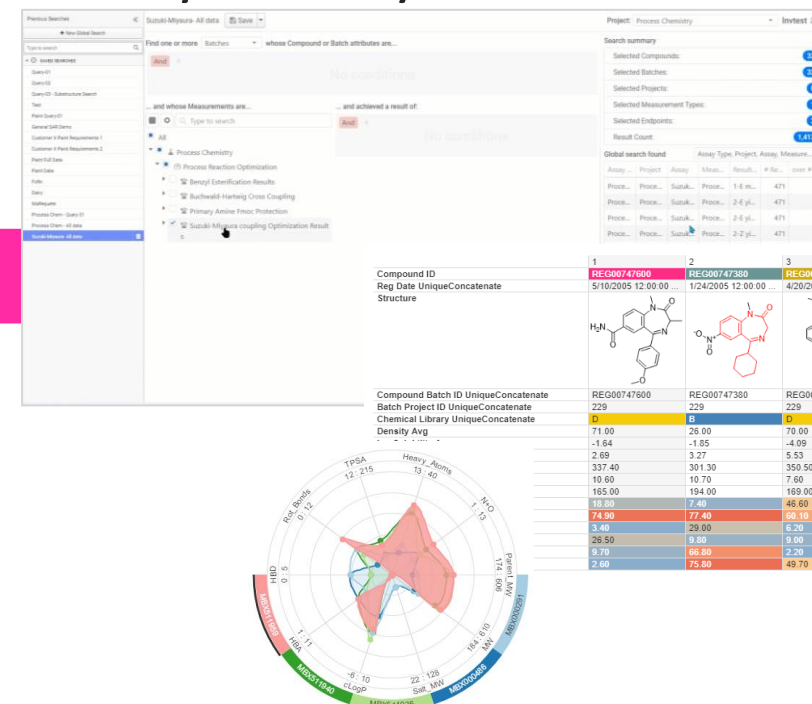
Central Data Lake

(unified Data Index)

Standardized | Indexed | Searchable

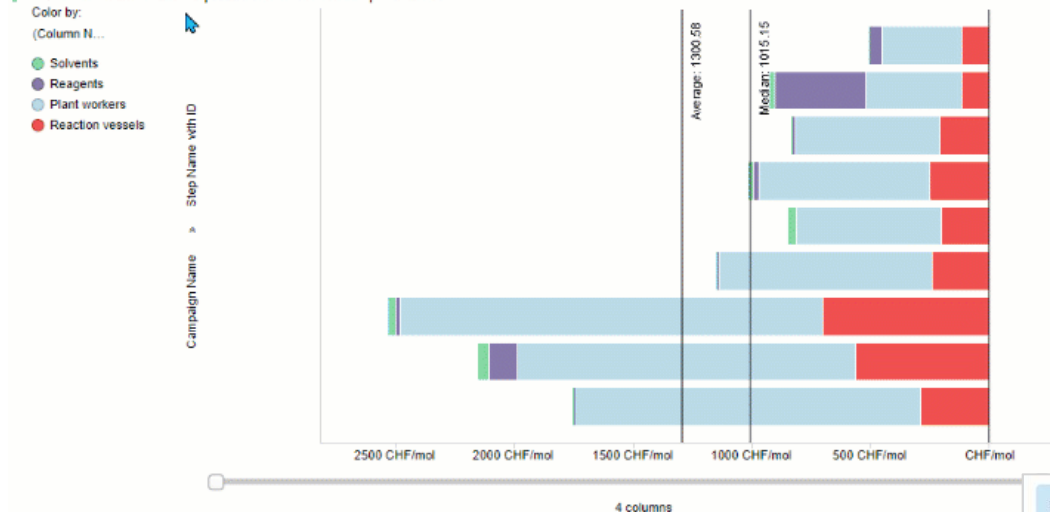


Query & Analyze



Process KPIs Solvents, costs and safety

How much does it cost to produce one mol of Step Product?



Cost Drivers

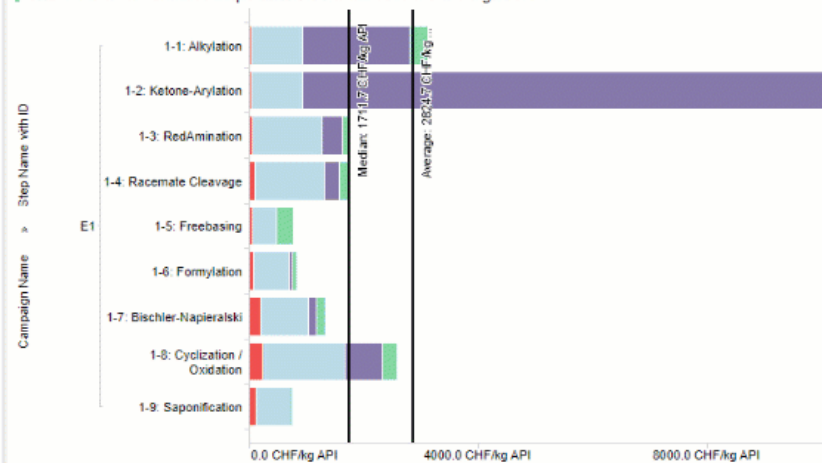
Campaign Name	Step Name with ID	Name	Unique Solvent/Reagent Amount per kg API	Unique Solvent/Reagent Amount per mol step...	Unique Solvent/Reagent...
E1	1-8: Cyclization / Oxidation	Water	75.92 kg/kg API	13.99 kg/mol	0.80 CHF/kg
E1	1-9: Saponification	Phosphoric Acid	0.44 kg/kg API	0.18 kg/mol	0.73 CHF/kg
E1	1-1: Alkylation	Water	71.57 kg/kg API	1.99 kg/mol	0.70 CHF/kg
E1	1-8: Cyclization / Oxidation	NaOH	0.43 kg/kg API	0.08 kg/mol	0.54 CHF/kg
E1	1-3: RedAmination	Water	42.94 kg/kg API	1.71 kg/mol	0.53 CHF/kg
E1	1-5: Freebasing	NaOH	0.53 kg/kg API	0.06 kg/mol	0.49 CHF/kg
E1	1-2: Ketone-Arylation	Water	42.94 kg/kg API	1.51 kg/mol	0.45 CHF/kg
E1	1-7: Bischler-Napieralski	Water	35.64 kg/kg API	6.56 kg/mol	0.43 CHF/kg
E1	1-9: Saponification	Active Carbon	0.12 kg/kg API	0.05 kg/mol	0.37 CHF/kg
E1	1-6: Formylation	Water	35.70 kg/kg API	4.92 kg/mol	0.30 CHF/kg
E1	1-5: Freebasing	Water	24.99 kg/kg API	2.91 kg/mol	0.23 CHF/kg
E1	1-9: Saponification	Water	22.35 kg/kg API	9.38 kg/mol	0.20 CHF/kg

ChemPager x Robustness x Economy x Safety x Greenness x Project Difficulty x Costs x Solvents x PMI x

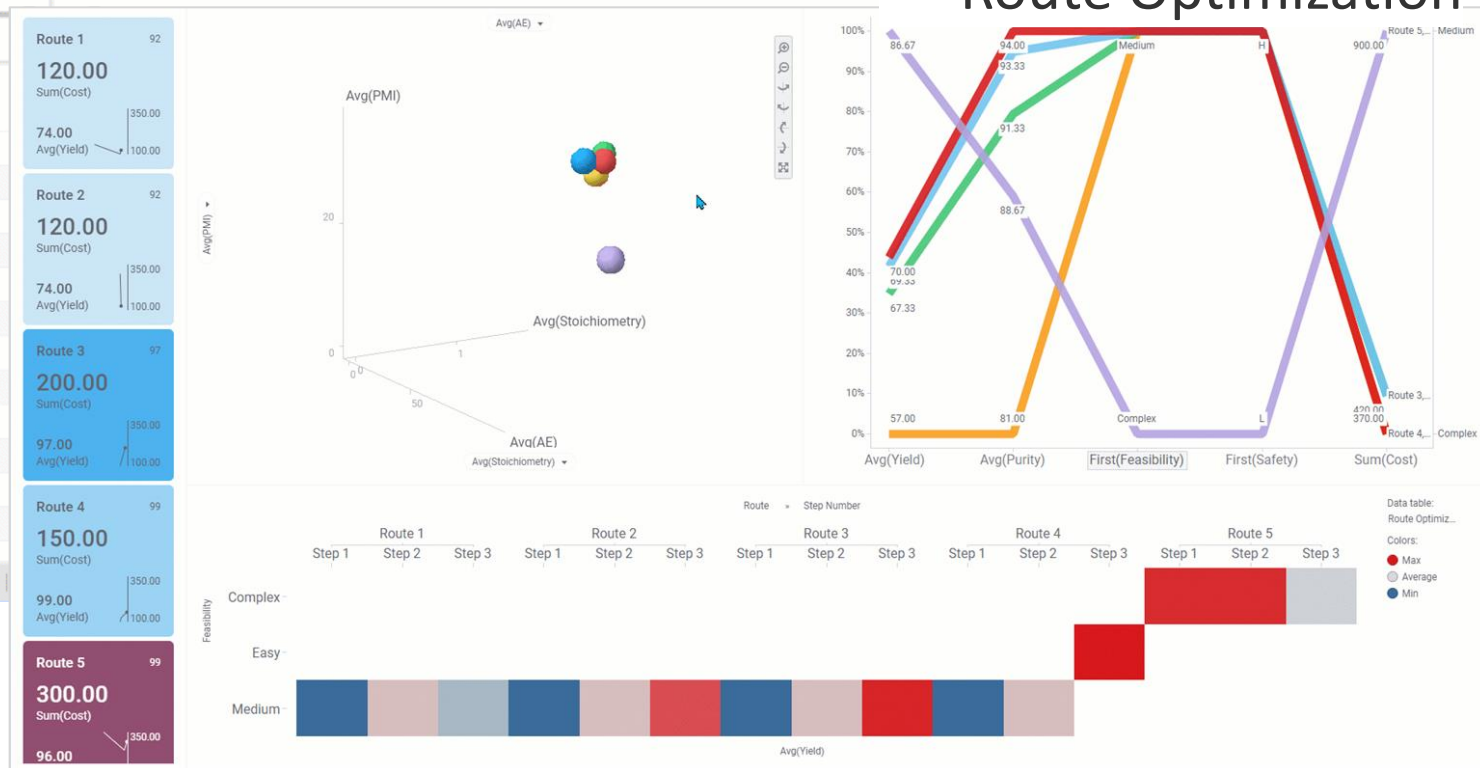
Ref: DOI: 10.1021/acs.oprd.8b00199

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How much do the different steps contribute to the cost of one kilogram API?



Route Optimization



Research Intelligence: Scientific insights & Summary

Language Intelligence: understands intent and context

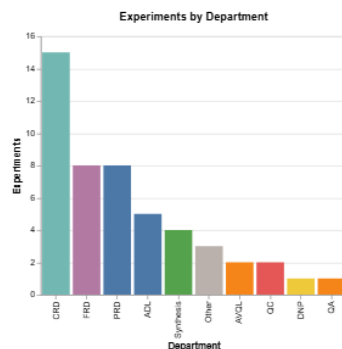
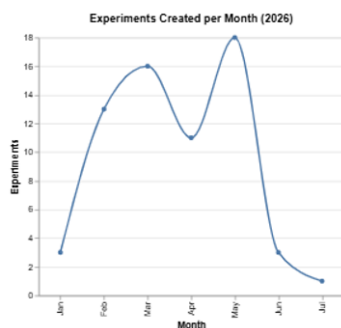
? Can you give me overall report of my Experiments this Year? include department, reactions, formulations and visual metrics on number of experiments performed and status

- » Identifying the current user to scope experiments
- » Counting my experiments created this year
- » Getting department distribution for my experiments this year
- » Getting state distribution for my experiments this year
- » Getting experiment type distribution this year
- » Counting reactions within my experiments this year
- » Counting formulation variation tables within my experiments this year
- » Retrieving my experiments this year for monthly trend
- » Retrieving next batch of my experiments this year
- » Retrieving final batch of my experiments this year
- » Computing monthly experiment counts from creation dates
- » Building the combined report visualization node
- » Building the combined report visualization node

Annual report of my experiments including departments, reactions, formulations, and visual metrics

My 2026 Experiment Report

You created 68 experiments so far this year (Jan 1 – Jul 7, 2026), spanning synthesis, formulation, and analytical work across 12 departments.



? drill into the reaction metrics

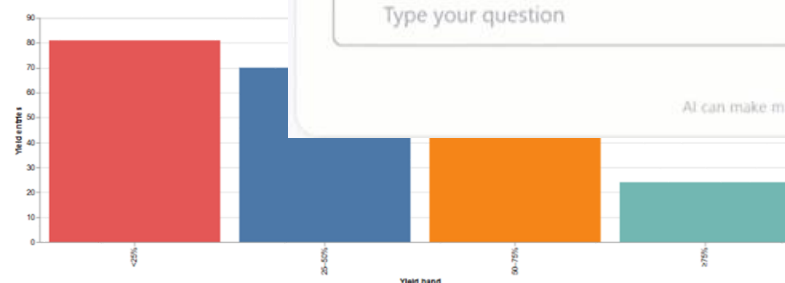
- » Counting my reactions this year with a recorded yield
- » Getting product success distribution for my reactions
- » Counting reactions with yield below 25 percent
- » Counting reactions with yield 25 to 50 percent
- » Counting reactions with yield 50 to 75 percent
- » Counting reactions with yield 75 percent or higher
- » Counting reactions with a positive recorded yield
- » Counting reactions with yield above 100 percent as
- » Building yield and success visualization node

Breakdown of my reactions this year by product

My Reactions — Yield & Success (2026)

Of the 251 reactions in your experiments this year, 105 reactions were successful.

Yield distribution



? for the Suzuki and Diels-Alder reactions in the project-Alpha notebook, render the reactant and product structures describe the bond formed and the functional-group changes, and name the reaction class

For the Suzuki and Diels-Alder reactions i... Jun 12, 9:19 AM

For the Suzuki and Diels-Alder reactions in the Project - Alpha notebook, render the reactant and product structures, describe the bond formed and the functional-group changes, and name the reaction class

... Thinking



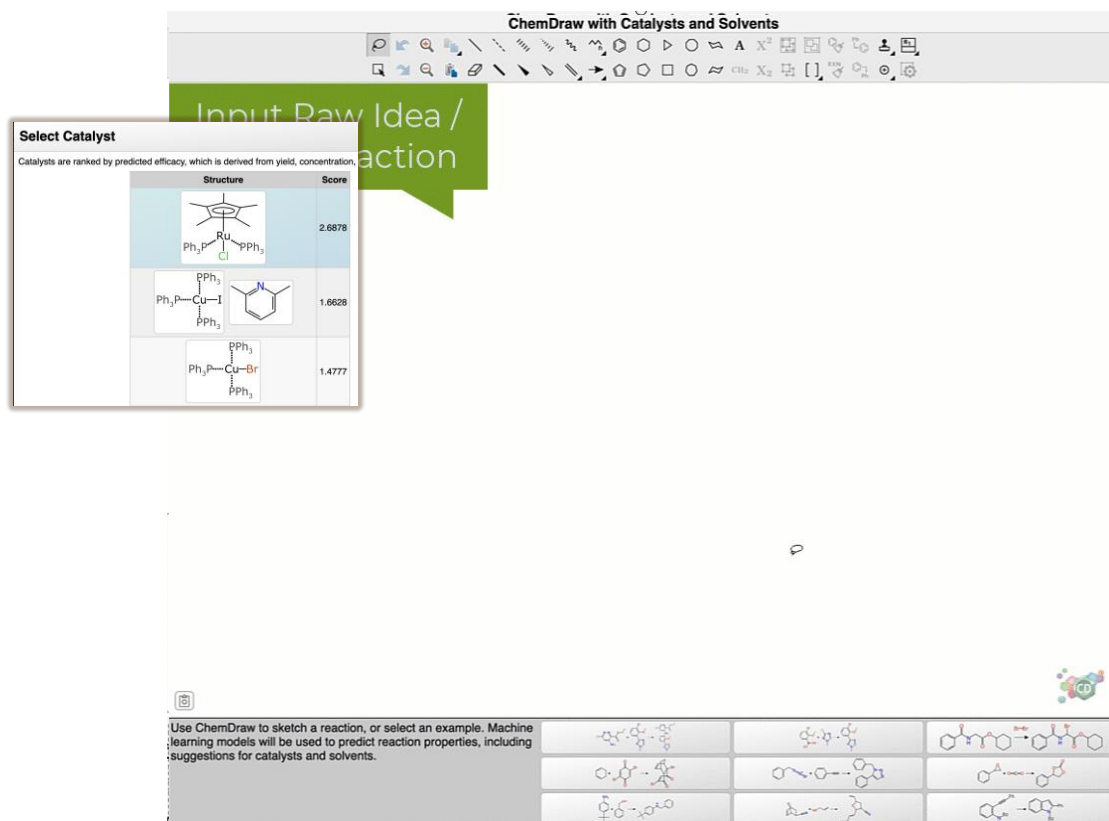
Type your question

AI can make mistakes. Double-check important information. ExplorerAI has access to all experiments, notebooks, and data in your account.

AI-Augmented Design – Predictive AI/ML

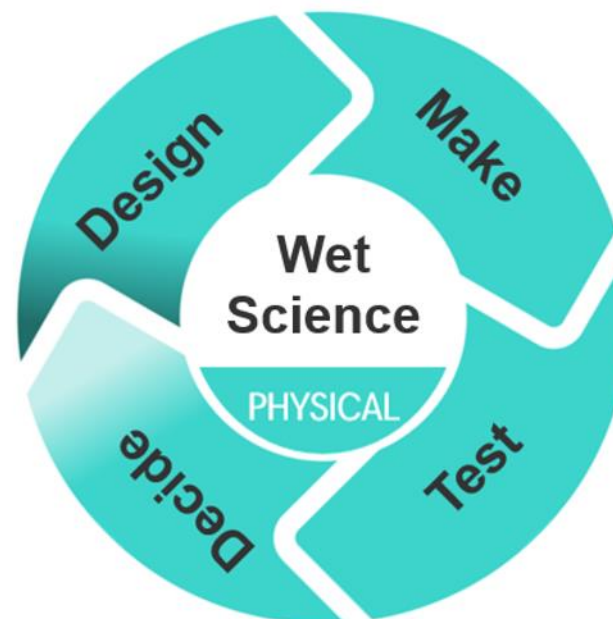
Chemical Reaction Recommendations

- suitable catalysts,
- solvents,
- key reaction parameters

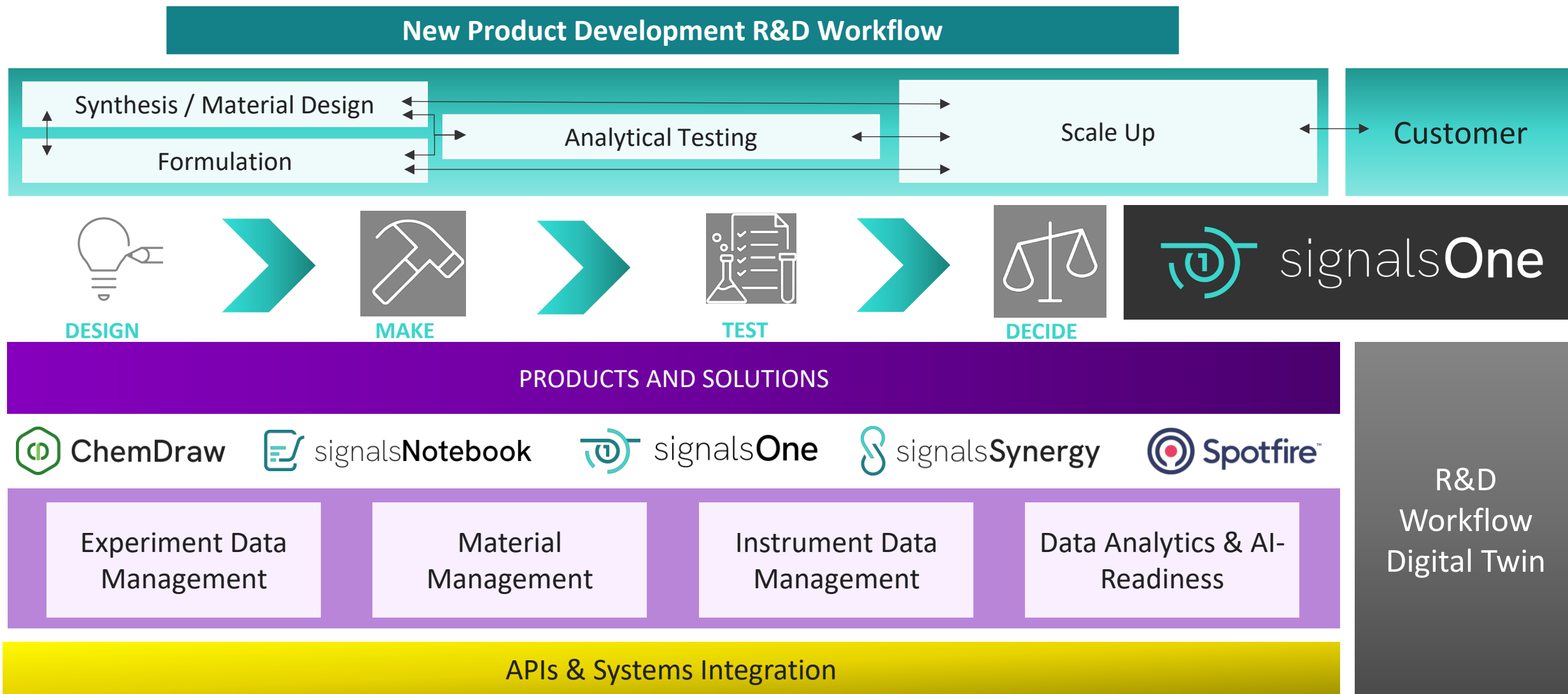


AI-Powered in-silico Design

- LLM Generates novel molecules
- ML models predict physchem properties
- Automated virtual compound screening
- Direct integration with experimental data



Enabling Connected R&D with the Signals Platform



Revvity Signals' Role as a Partner in Digital Transformation

1M+

Worldwide users

35+ years

Delivering Scientific Software

16 of Top 20

Chemical Companies

750+

Employees

4000+

Customers

6 of Top 20

Agrochemical Companies

Markets

- Life Sciences
- Specialty Chemicals
- Food
- Flavor & Fragrance
- Agrochemical
- Consumer Products



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Explore more about Revvity Signals at
<https://revvitysignals.com>

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