

LiveDesign™

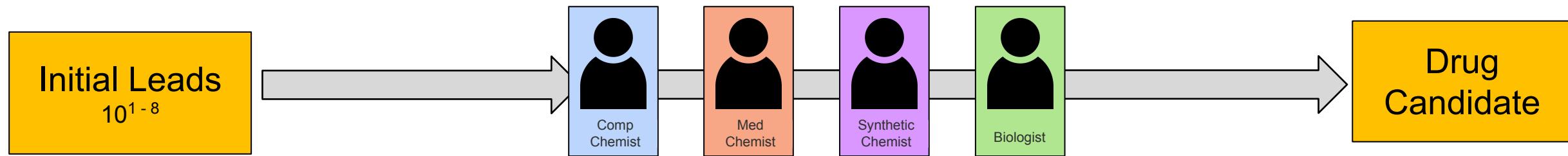
by SCHRÖDINGER®

Organize Data and Collaborate Effectively
in Drug Discovery

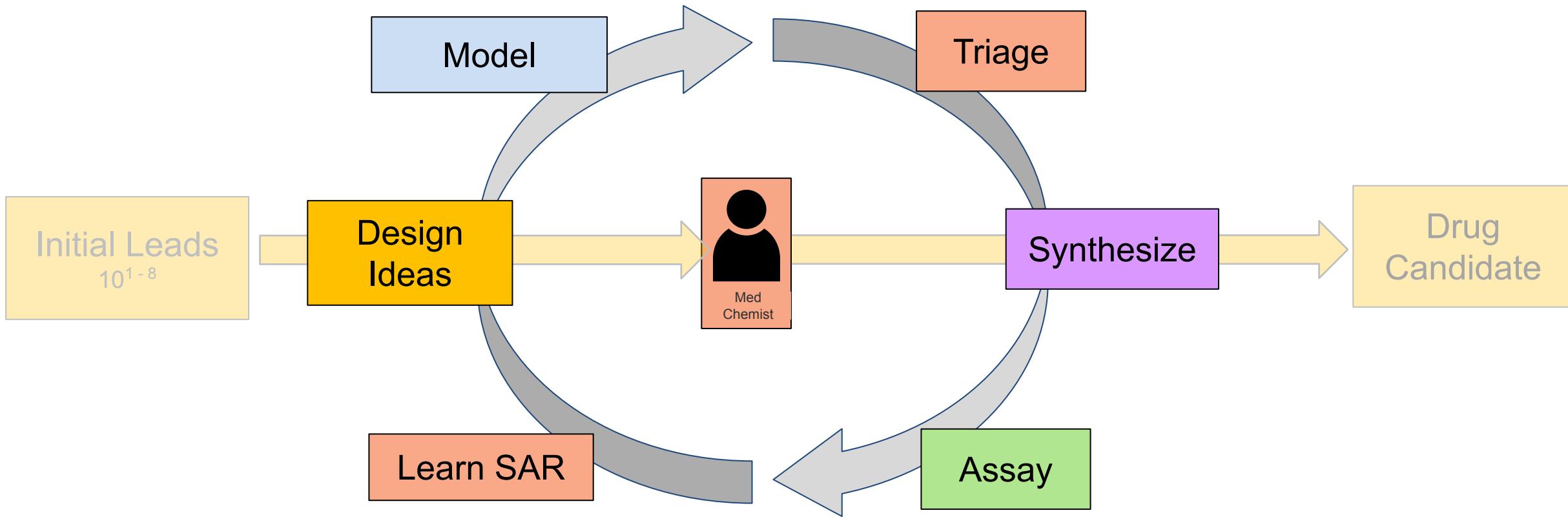
Introduction to LiveDesign

The image displays the LiveDesign software interface running on a laptop and a monitor. The software is designed for drug discovery, providing a centralized platform for organizing and analyzing experimental data. The dashboard on the laptop includes sections for 'Data Overview' (with tabs for 'Compound Structure (Aligned)', 'ID', 'Dose Response Curves', 'Novelty Score', and 'BP'), 'Quick Properties (Schrödinger PISA)', 'Quick Properties (Schrödinger Moog)', and 'ACME Predict'. Below these are tables for 'CMFDA-10056', 'CMFDA-10052', 'CMFDA-12381', and 'CMFDA-12389', each with associated plots and data. The monitor screen shows a detailed 3D visualization of a protein structure, likely a receptor or enzyme, with various regions highlighted in different colors (red, orange, yellow) and chemical residues labeled.

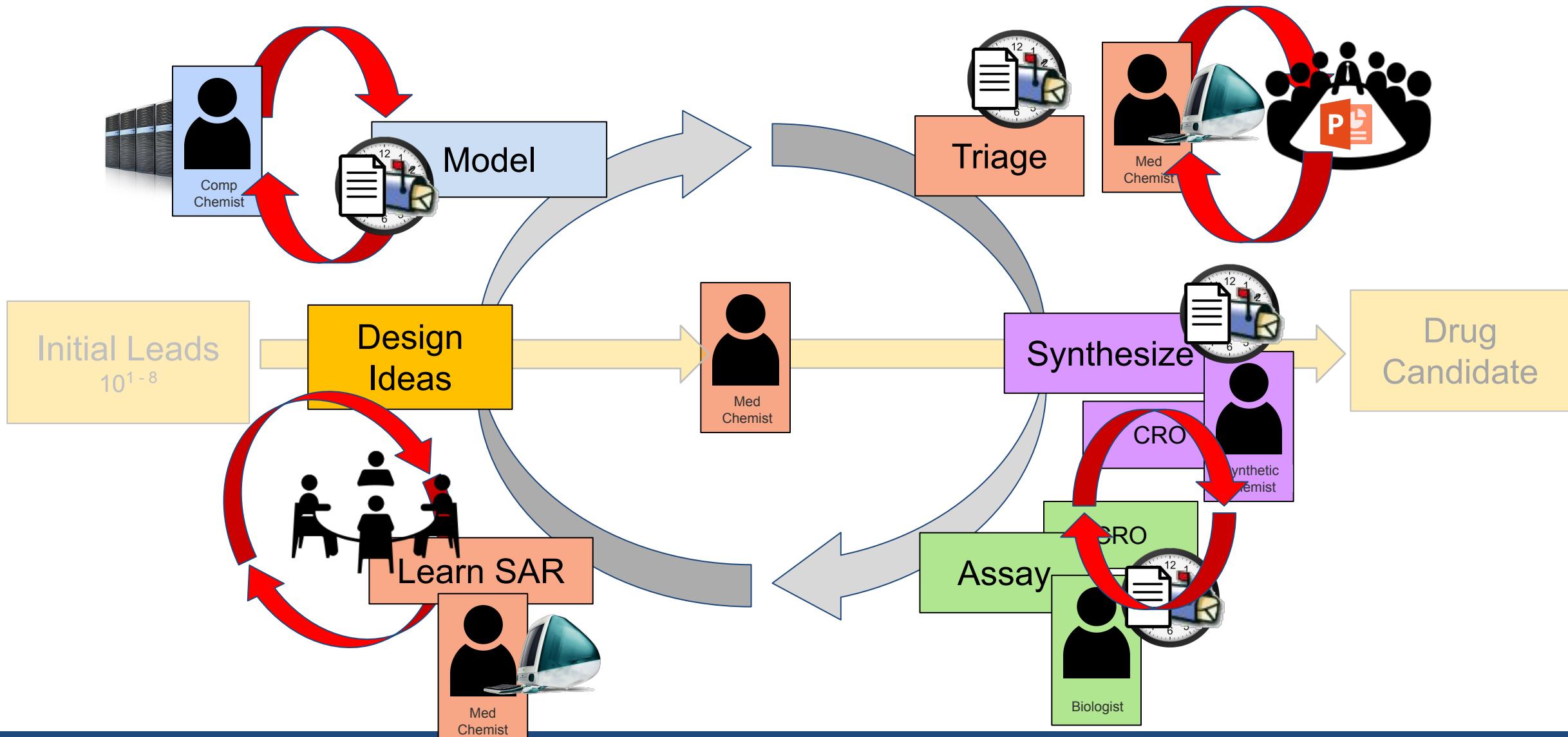
The idealized drug design cycle is simple and linear



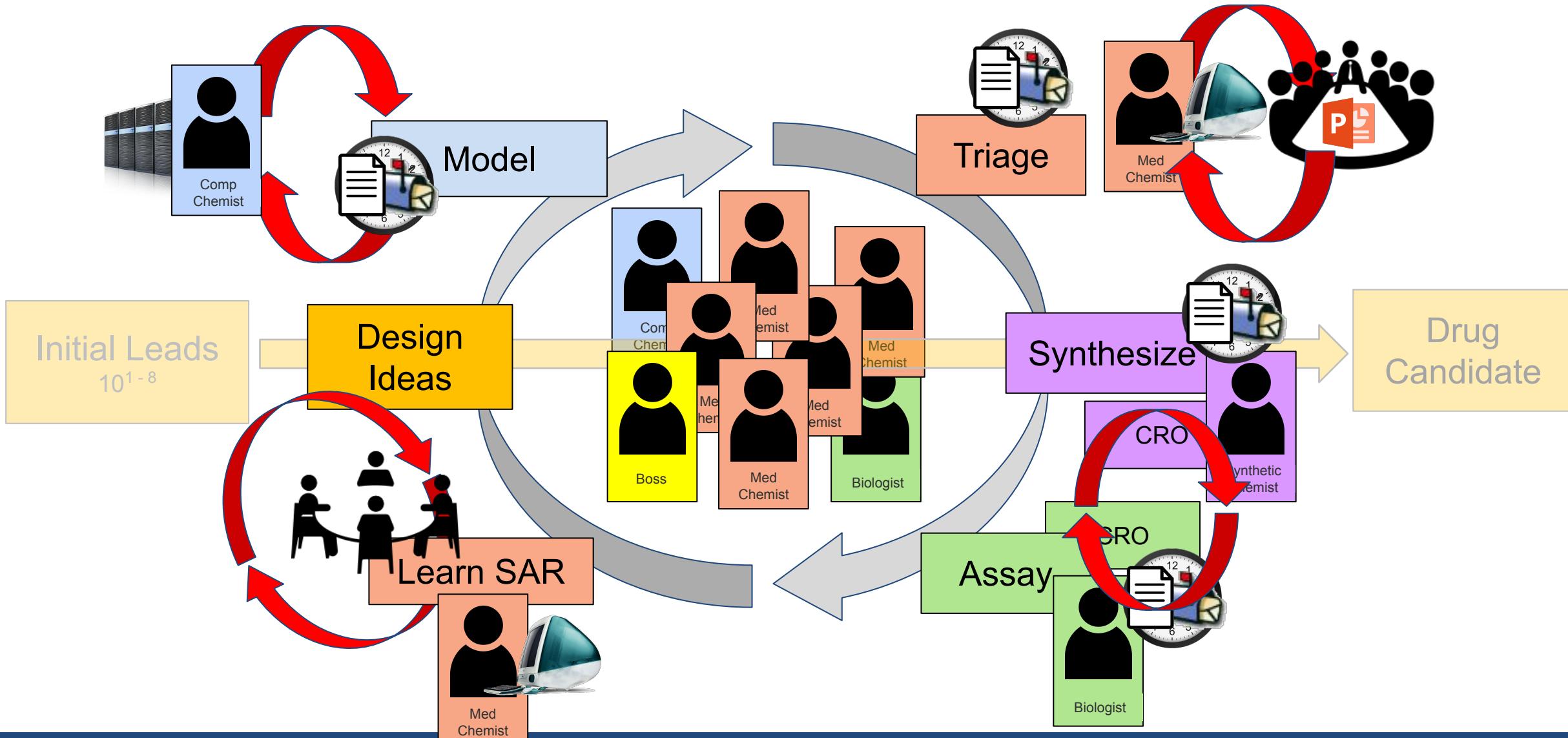
Except the drug design cycle is a cycle



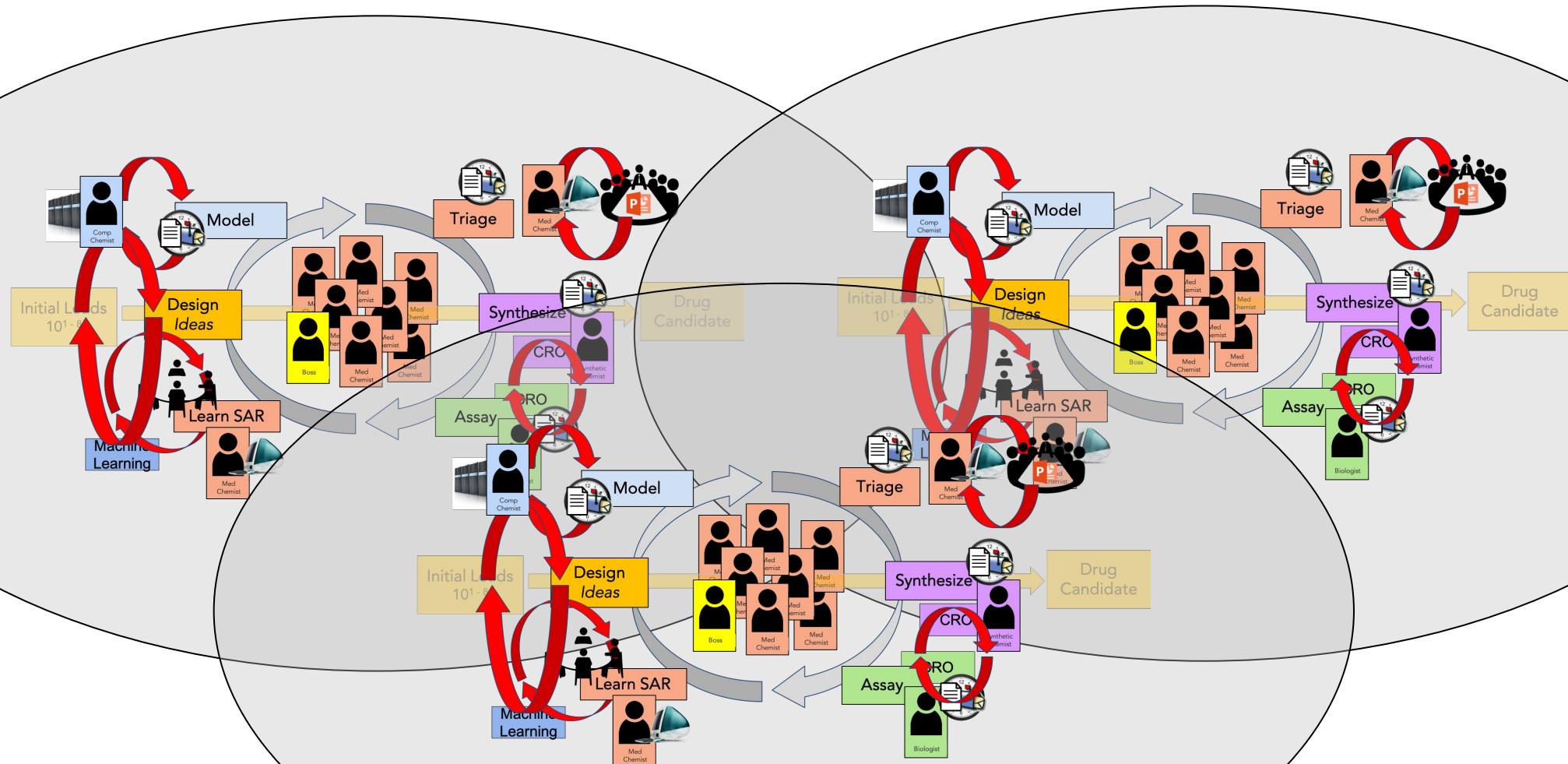
Each cycle requires extensive analytics, data sharing, hypothesis capture, meetings, meetings, meetings...



Multiple people are involved in the cycle



Most drug discovery involves multiple projects



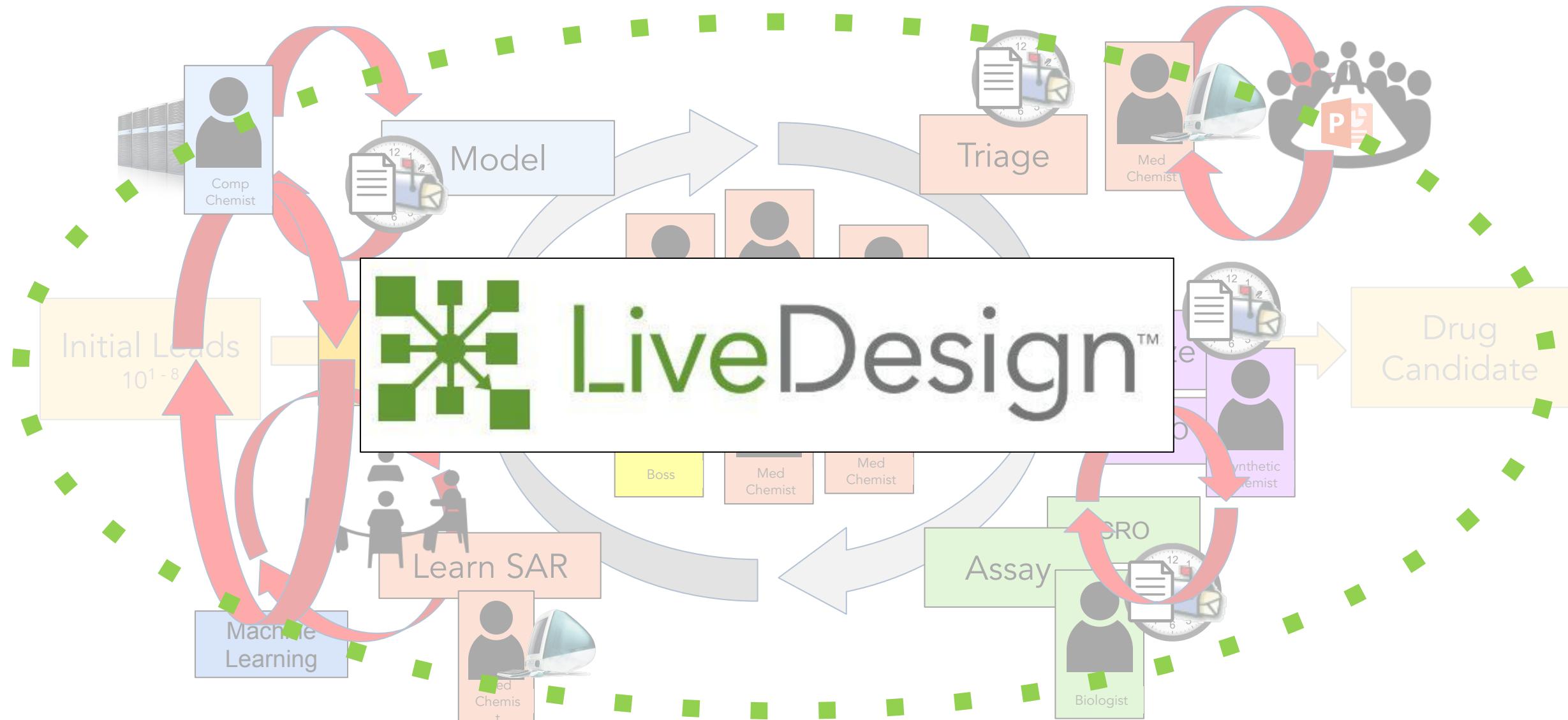
Connecting all the science is a huge challenge

- Applications are complex or disconnected
- Communication in and across teams (email, files)
- Data versioning (assay0561_finalFINAL_v2_thisone.xls)
- Disparate data sources
- Project management of compound progression
- People flux

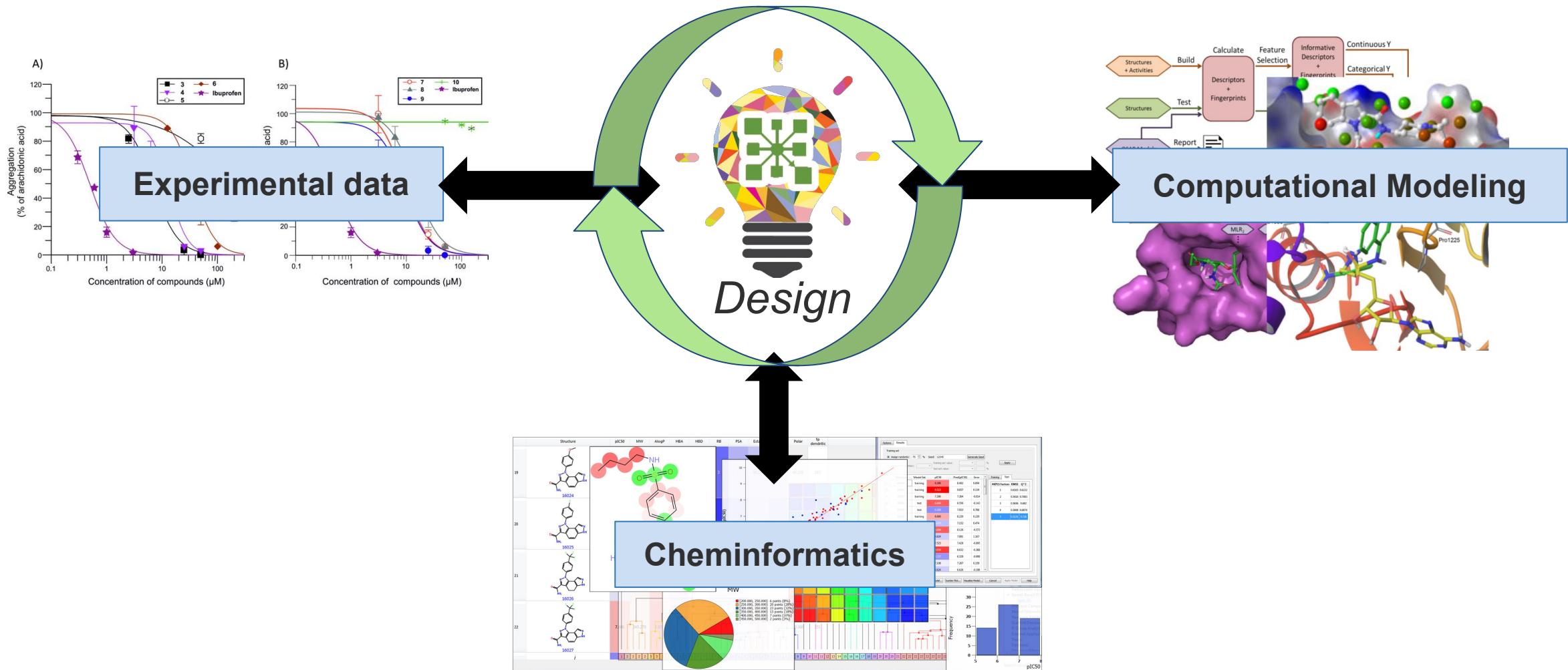
Lots of room for **error**, loss of **data**, loss of **time**

Research can be stalled for non-scientific reasons.

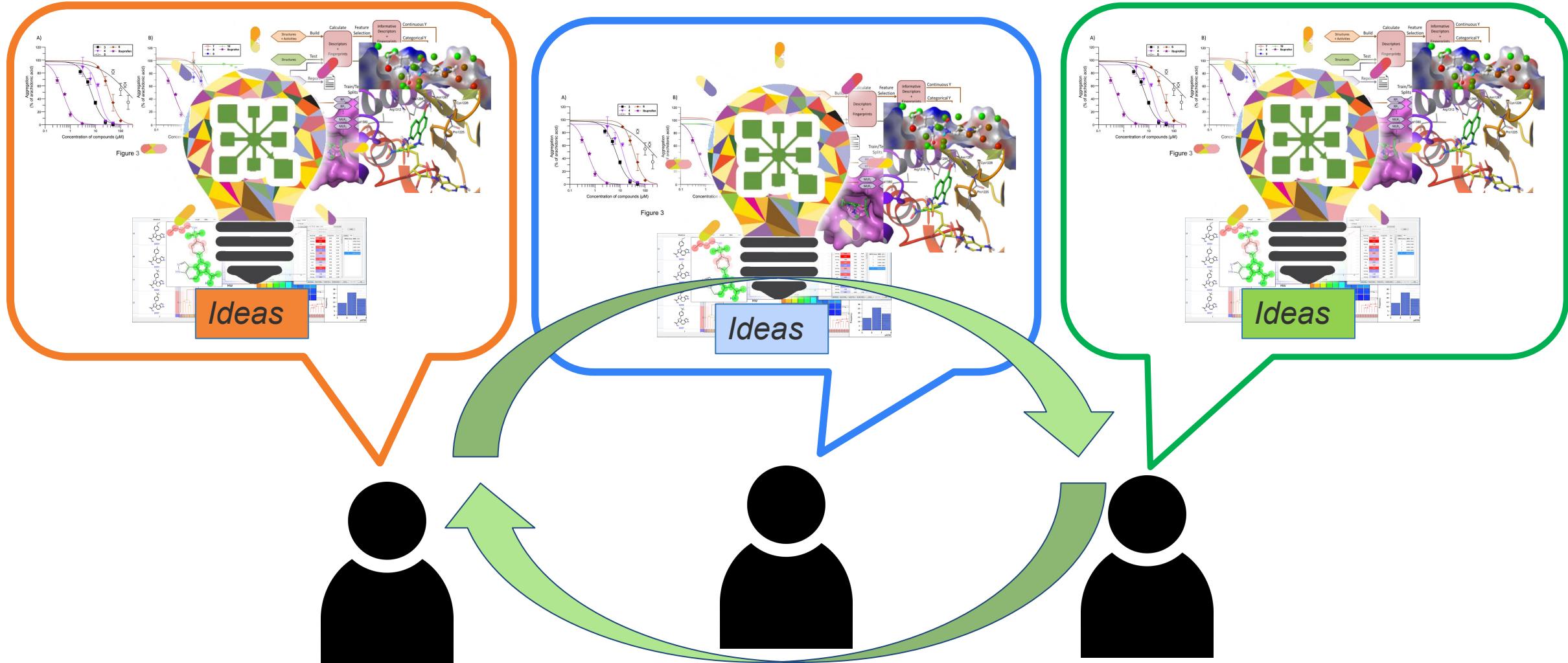
LiveDesign is an enterprise platform to facilitate discovery



Good design needs access to different kinds of data



Efficient design needs good knowledge transfer



LiveReports can quickly find and generate information on compounds



LiveReports are dynamically updated

A2A

2671

LiveReports... + A2A Data Review ▾

Compound Structure ID Adenosine Receptor (A2A Ki) [nM] Adenosine Receptor (A1 Ki) [nM] Selectivity Flag for Modeling follow-up Modeling Comment QuickProp MPO A2A Docking A2A Watermap (3D)

QuickPro ps (AlogP) QuickPro ps (Mol. Wt.) QuickPro ps (PSA) QuickPro ps (HBA(mae)) AD ME MP A2A Docking Model A2A Docking Model (3D) A2A Docking Model (Ligand Interaction)

1 CMPD-13442 0.9 15.4 SEL ✓ 4.0 393.4 93.8 4 0.851 -13.1 3D model 3D interaction 3D model

2 CMPD-13442 0.9 15.4 SEL ✓ 4.0 393.4 93.8 4 0.851 -13.1 3D model 3D interaction 3D model

3 CMPD-13442 0.9 15.4 SEL ✓ Alkyl chain could be optimized 3.0 399.4 101.2 6 0.889 -12.5 3D model 3D interaction 3D model

4 CMPD-13316 1 1.8 Non-selective 3.0 358.4 87.7 4 0.884 -12.1 3D model 3D interaction 3D model

5 CMPD-16874 105 6300 S 3.0 358.4 87.7 4 0.884 -12.1 3D model 3D interaction 3D model

LIVE!

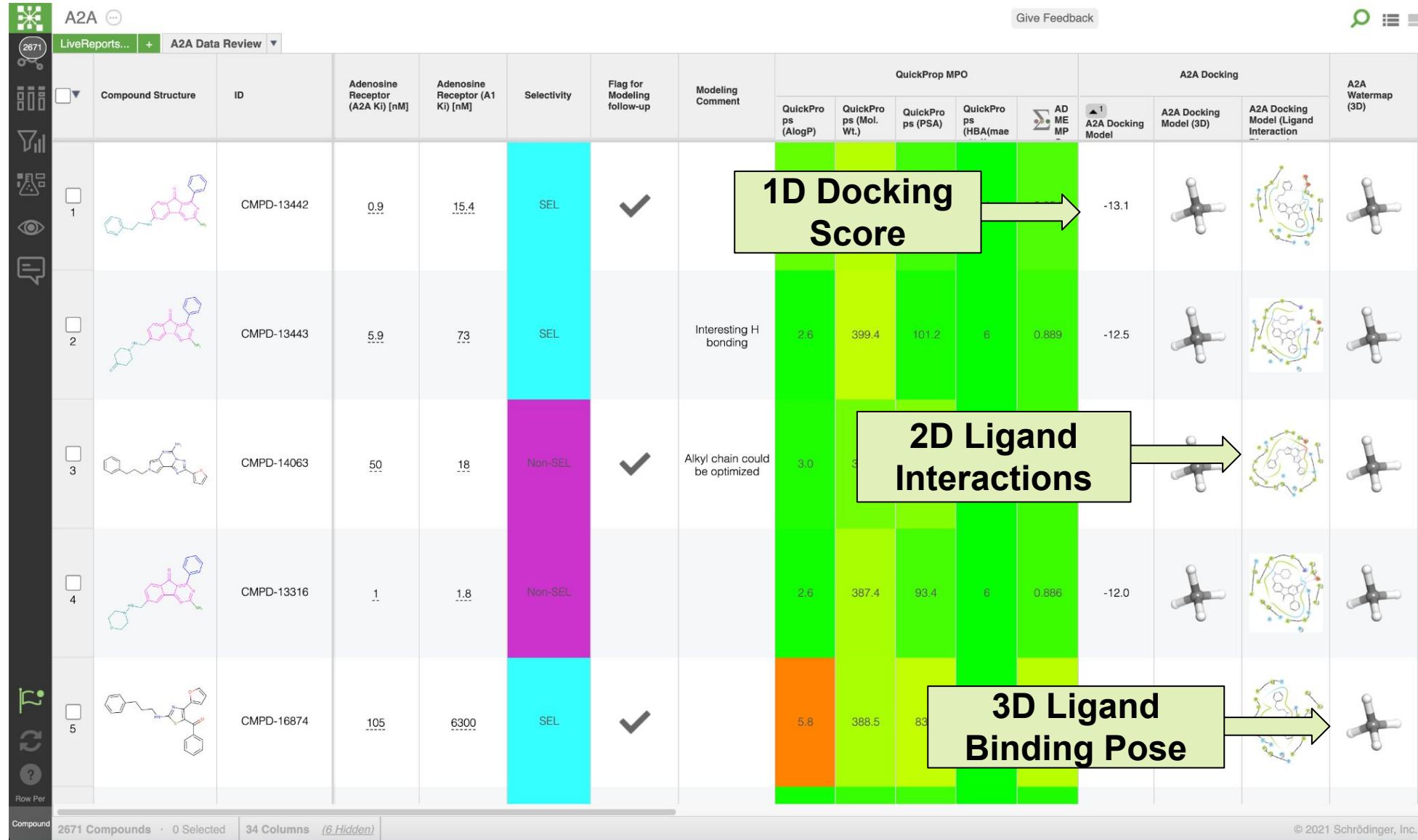
All data from database is automatically updated across LiveDesign when it is changed (assays, models, annotations, calculations, etc.)

Row Per

Compound 2671 Compounds 0 Selected 34 Columns (6 Hidden)

© 2021 Schrödinger, Inc.

LiveReports can contain 1D, 2D, and 3D information



LiveReports can contain 1D, 2D, and 3D information

Open Live Report | A2A Reference | A2A Data Review

Give Feedback

erin.davis (Logout)

A2A

Compound Structure ID Adenosine Receptor (A2A Ki) [nM] Adenosine Receptor (A1 Ki) [nM] Flag for modeling follow-up

2671

1 CHEMBL374760 16.1 141 ✓

2 CHEMBL2398480 22 160 ✓

3 CHEMBL506450 300 1100 ✓

4 CHEMBL2112157 10000 1600 ✓

5 CHEMBL205225 4963 558 ✓

6 CHEMBL223326 91 34 ✓

Row Per Compound

Compound Structure ID

QuickProp MPO

AD ME MP

A2A Docking Model

A2A Docking Model (3D)

Give Feedback

VISUALIZE + 3D

Contents Styles

APPLY TO: All Selected

COMPOUND

- Nonpolar H
- Surface

PROTEIN

- Nonpolar H
- Surface

BINDING SITE

- Distance: 6 Å
- Nonpolar H
- Surface

Residue Labels

WATER/METAL STYLES

BACKGROUND

INTERACTIONS

Reset Custom Styles

TOOLS:

Click to view in 3D

The screenshot displays three panels of the Schrödinger LiveDesign software. The left panel shows a 1D table of compound data with columns for ID, Adenosine Receptor (A2A Ki) [nM], and Adenosine Receptor (A1 Ki) [nM]. The middle panel shows a 2D heatmap of QuickProp MPO scores for various compounds, with an orange callout box containing the text "Click to view in 3D" pointing to the 3D visualization on the right. The right panel is a 3D visualization of a protein-ligand docking model, showing a protein structure with orange and yellow surface representations and a bound ligand shown as sticks and spheres. A legend on the right side of the 3D panel provides options for applying styles to different components like compound, protein, and binding site.

Use advanced database searching to populate your LiveReport

Basic Search

The screenshot shows the Marvin JS interface for化合物 (Compounds) search. The top navigation bar includes 'CDK2' and 'Design' (which is underlined, indicating it's the active tab), along with 'Search', 'Import', 'Advanced', and 'Enumerate'. Below the navigation is a toolbar with various icons for sketching, zooming, and selection. To the left is a sidebar with icons for 'CDK2', 'Design', 'Search', 'Import', 'Advanced', and 'Enumerate'. The main workspace features the Marvin JS logo and a ChemAxon watermark. On the right, there's a vertical panel with atomic symbols: H, C, N, O, S, F, P, Cl, Br, I, *, and A. At the bottom, there are buttons for 'PREVIEW PROPERTIES' (with a checked checkbox) and 'Add Idea To LiveReport'.

Design

CDK2

COMPOUNDS

Design Search Import Advanced Enumerate

Marvin JS by ChemAxon

PREVIEW PROPERTIES

Add Idea To LiveReport

To preview properties as you sketch, add some Property columns to your Live Report.

Use advanced database searching to populate your LiveReport

Basic Search

The screenshot shows the Marvin JS interface for a CDK2 database. At the top, there's a toolbar with icons for Design, Search, Import, Advanced, and Enumerate. Below the toolbar is a search bar with placeholder text "Add Query on...". Underneath the search bar are buttons for "TYPE: COMPOUND" and "R-GROUPS", and "COMPOUNDS: REAL" and "VIRTUAL". A checkbox labeled "Human CDK2 Inhibition (IC50)" is checked. On the left side, there's a vertical panel with chemical element symbols (H, C, N, O, S, F, P, Cl, Br) and their corresponding atomic numbers (1, 2, 3, 4, 5, 6, 7, 8). At the bottom, there are buttons for "PREVIEW PROPERTIES" and "Add Idea To LiveReport". A note at the bottom says: "To preview properties as you sketch, add some Property columns to your Live Report."

The screenshot shows the Marvin JS interface for a CDK2 database, specifically focusing on the "Advanced" tab. The search bar now has the placeholder text "Add Query on...". The "Advanced" tab is highlighted. Below the search bar are the same buttons for "TYPE: COMPOUND" and "R-GROUPS", and "COMPOUNDS: REAL" and "VIRTUAL". A checkbox labeled "Human CDK2 Inhibition (IC50)" is checked. On the left side, there's a vertical panel with chemical element symbols (H, C, N, O, S, F, P, Cl, Br) and their corresponding atomic numbers (1, 2, 3, 4, 5, 6, 7, 8). A large green box at the bottom contains the text "Advanced Searching by experimental detail". An orange arrow points from the text in this box towards the search bar.

Use advanced database searching to populate your LiveReport

Basic Search

The Marvin JS interface shows a basic search for CDK2 compounds. It includes a toolbar with various icons, a sidebar with element filters (H, C, N, O, S, F, P, Cl, Br), and a main area for sketching chemical structures. A green box labeled "Basic Search" highlights the top navigation bar.

The Marvin JS interface shows advanced searching by experimental detail. It includes a toolbar, a sidebar with element filters, and a main area for sketching chemical structures. A green box labeled "Advanced Searching by experimental detail" highlights the "Advanced" tab in the top navigation bar.

The Schrödinger LiveDesign interface shows advanced database searching. It features a search bar at the top, followed by sections for ID, Show Compounds (REAL and VIRTUAL checked), and experimental conditions (DHFR T. gondii (IC50) and DHFR Human (IC50)). Below these are numerical filters (e.g., 1000, -11). A green box labeled "Combine advanced searching with modeling, annotations, and structural restrictions" points to the search bar.

Combine advanced searching with modeling, annotations, and structural restrictions

The Schrödinger LiveDesign interface shows graphical representation for larger queries. It displays a complex query structure with AND, OR operators, and subqueries involving compound structures (e.g., thiophene, pyridine). A green box labeled "Graphical representation for larger queries" points to a chemical structure of a thiophene ring.

Graphical representation for larger queries

Use advanced database searching to populate your LiveReport

Basic Search

The Marvin JS interface shows a basic search for CDK2 compounds. It includes a toolbar with various sketching and selection tools, a central workspace for drawing chemical structures, and a menu bar with options like Design, Search, Import, Advanced, and Enumerate. A green box labeled "Basic Search" is overlaid on the top left.

The Marvin JS interface shows an advanced search for CDK2 compounds, specifically targeting Human CDK2 Inhibition (IC50). The search criteria include a minimum IC50 value of 0 and a maximum value of 100. A green box labeled "Advanced Searching by experimental detail" is overlaid on the middle section.

Combine advanced searching with modeling, annotations, and structural restrictions

The Marvin JS interface shows a complex search query combining multiple conditions. It includes filters for DHFR T. gondii (IC50), DHFR Human (IC50), Run FEP, and Compound Structure. The search results are visualized using chemical structures and operators like AND, OR, and parentheses. A green box labeled "Graphical representation for larger queries" is overlaid on the bottom right.

Graphical representation for larger queries

Quickly capture information on design ideas

A2A

Give Feedback

LiveReports... + Lead Analog ▾

Compound Structure ID All IDs A2A Docking Model (3D) A2A Docking Model (Ligand Interaction Diagram) A2A Docking Model (Run Status) A2A Docking Model (Score) Quick Properties RDKit (PSA) Quick Properties RDKit (MW) Quick Properties RDKit (HBA) Quick Properties RDKit (AlogP) ADME MPO

CMPD-17318 CMPD-17318 V46137

1

0.953

The screenshot shows a software interface for managing chemical compounds. On the left is a vertical toolbar with icons for search, filters, and other functions. The main area has a header with tabs like 'LiveReports...', '+', 'Lead Analog', and a dropdown. Below is a table with columns for Compound Structure, ID, All IDs, A2A Docking Model (3D), A2A Docking Model (Ligand Interaction Diagram), A2A Docking Model (Run Status), A2A Docking Model (Score), Quick Properties RDKit (PSA), Quick Properties RDKit (MW), Quick Properties RDKit (HBA), Quick Properties RDKit (AlogP), and ADME MPO. The first row is a header, and the second row contains data for a compound named CMPD-17318, version V46137. The 'Compound Structure' column shows a complex organic molecule. The 'A2A Docking Model (3D)' column shows a 3D ball-and-stick model of the molecule. The 'A2A Docking Model (Ligand Interaction Diagram)' column shows a 2D diagram with colored dots representing interactions. The 'Run Status' is 'Completed'. The 'Score' is -7.9. The 'PSA' is 103.3, 'MW' is 324.3, 'HBA' is 6, 'AlogP' is 2.3, and the 'ADME MPO' value is 0.953. A green highlight covers the last two columns.

Quickly capture information on design ideas

The screenshot shows the Schrödinger LiveDesign software interface. On the left, there's a sidebar with various icons and two tabs labeled "A2A". The main area has a header with "LiveReports..." and "Lead Analog". Below the header is a table with columns: Compound Structure, ID, All IDs, A2A Docking Model (3D), A2A Docking Model (Ligand Interaction Diagram), A2A Docking Model (Run Status), A2A Docking Model (Score), Quick Properties RDKit (PSA), Quick Properties RDKit (MW), Quick Properties RDKit (HBA), and Quick Properties RDKit. The first row of the table is highlighted in green and shows a chemical structure of a compound (17318, 137), its 3D model, and its docking interaction diagram. To the right of the table is a green bar labeled "ADME MPO" with a value of "0.942". On the far left, there's a pink box with a white molecular sketcher icon and the text "DRAG & DROP COMPOUND STRUCTURE". An orange arrow points from this box to the chemical structure in the table. A callout box with a black border and light green background contains the text "Drag compounds to the sketcher for editing". At the bottom left, there are buttons for "PREVIEW PROPERTIES" and "Add Idea To LiveReport". A note below says "To preview properties as you sketch, add some Property columns to your Live Report."

Give Feedback

LiveReports... + Lead Analog

Compound Structure ID All IDs A2A Docking Model (3D) A2A Docking Model (Ligand Interaction Diagram) A2A Docking Model (Run Status) A2A Docking Model (Score) Quick Properties RDKit (PSA) Quick Properties RDKit (MW) Quick Properties RDKit (HBA) Quick Properties RDKit

17318 137

Completed -7.9 103.3 324.3 6 2.

ADME MPO 0.942

DRAG & DROP COMPOUND STRUCTURE

PREVIEW PROPERTIES Add Idea To LiveReport

To preview properties as you sketch, add some Property columns to your Live Report.

Drag compounds to the sketcher for editing

Quickly capture information on design ideas

A2A

Open Live Report + March 2019 Ideas x p38 2D3D Builder - Uridine Lead x Scaffold Explore x Lead Analog ▾ Give Feedback

Compound Structure ID All IDs ADVANCED « Open Live Report + March 2019 Ideas p38 2D3D Builder - Uridine Lead Scaffold Explore Lead Analog ▾ ADME MPO demo

To preview properties as you sketch, add some Property columns to your Live Report.

Docking Give Feedback ADME MPO

Compound Structure ID All IDs A2A Docking Model (Score) A2A Docking Model (3D) A2A Docking Model (Ligand Interaction) Quick Properties (PSA) Quick Properties (Mol Wt.) Quick Properties (HBA/maestro) Quick Properties (HBA/maestro) Quick Docking (AloP) ADME MPO

Design Search Import Advanced Enumerate

LiveReports... + Lead Analog ▾ Give Feedback

Sketch analog from the starting compound

Add new compound to LiveReport as a new row

PREVIEW PROPERTIES Add Idea To LiveReport

Chemical structure of CMPD-17318: 2-(4-methoxyphenyl)-N-(2-(5-methyl-2-oxo-4-pyrimidinyl)phenyl)acetamide

Compound Structure	ID	All IDs	A2A Docking Model (3D)	A2A Docking Model (Ligand Interaction Diagram)	A2A Docking Model (Run Status)	A2A Docking Model (Score)	Quick Properties RDKit (PSA)	Quick Properties RDKit (MW)	Quick Properties RDKit (HBA)
	CMPD-17318 V46137				Completed	-7.9	103.3	324.3	6

SAR: View your data in different manners to learn more

A2A

LiveReports... A2A Data Review

Give Feedback

Compound Structure ID Adenosine Receptor (A2A K_i) [nM] Adenosine Receptor (A1 K_i) [nM] Selectivity Flag for Modeling follow-up Modeling Comment QuickProp ps (AlogP) QuickProp ps (Mol. WL) QuickProp ps (PSA) QuickProp ps (HBA/mee) AD > ME MP A2A Docking Model A2A Docking Model (3D) A2A Docking Model (Lipid Interaction) A2A Watermap (3D)

Compound Structure	ID	Adenosine Receptor (A2A K _i) [nM]	Adenosine Receptor (A1 K _i) [nM]	Selectivity	Flag for Modeling follow-up	Modeling Comment	QuickProp ps (AlogP)	QuickProp ps (Mol. WL)	QuickProp ps (PSA)	QuickProp ps (HBA/mee)	AD > ME MP	A2A Docking Model	A2A Docking Model (3D)	A2A Docking Model (Lipid Interaction)	A2A Watermap (3D)
	CMPD-13442	0.9	15.4	SEL	✓		4.0	393.4	05.8	8	0.861	-13.1			
	CMPD-13443	5.9	73	SEL		Interesting H bonding	2.6	399.4	101.2	9	0.869	-12.5			
	CMPD-14063	50	18	Non SEL	✓	Alkyl chain could be optimized	3.0	398.4	67.7	9	0.894	-12.1			
	CMPD-13316	1	1.8	Non SEL	✓		2.8	387.4	93.4	9	0.896	-12.0			
	5						5.8	388.5	83.4	9	0.837	-11.9			

Spreadsheets

2671 Compounds · 1 Selected · 34 Columns (8 Hidden)

© 2021 Schrödinger, Inc.

SAR: View your data in different manners to learn more

A2A

LiveReports... A2A Data Review

Give Feedback

Compound Structure ID Adenosine Receptor (A2A K_i) [nM] Adenosine Receptor (A1 K_i) [nM] Selectivity Flag for Modeling follow-up Modeling Comment QuickProp ps (AlogP) QuickProp ps (Mol_WL) QuickProp ps (PSA) QuickProp ps (HBA/mes) AD → ME → MP A2A Docking Model (3D) A2A Docking Model (Ligand Interaction) A2A Watermap (3D)

1	CMPD-13442	0.9	15.4	SEL	✓		4.0	399.4	05.8	3	0.861	-13.1			
2	CMPD-13443	5.9	73	SEL		Interesting H bonding	2.6	399.4	101.2	9	0.869	-12.5			
3	CMPD-14063	50	18	Non-SEL	✓	Alkyl chain could be optimized	3.0	398.4	67.7	9	0.894	-12.1			
4	CMPD-13316	1	1.8	Non-SEL			2.8	387.4	93.4	9	0.890	-12.0			
5					✓		5.8	388.5	83.4	9	0.837	-11.9			

Spreadsheets

2671 Compounds · 1 Selected | 34 Columns (8 Hidden)

© 2021 Schrödinger, Inc.

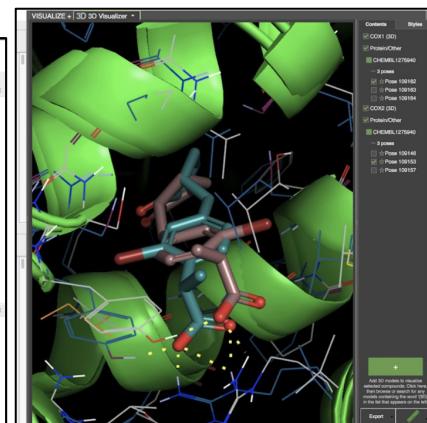
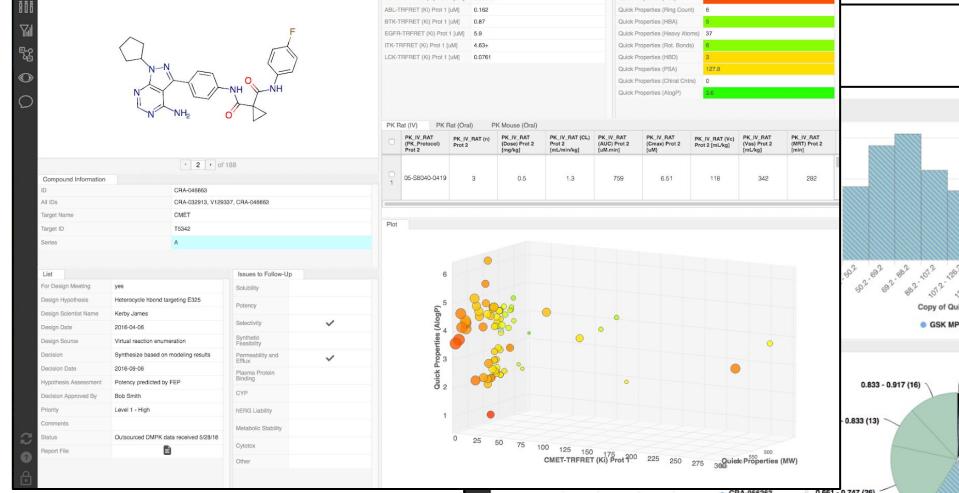
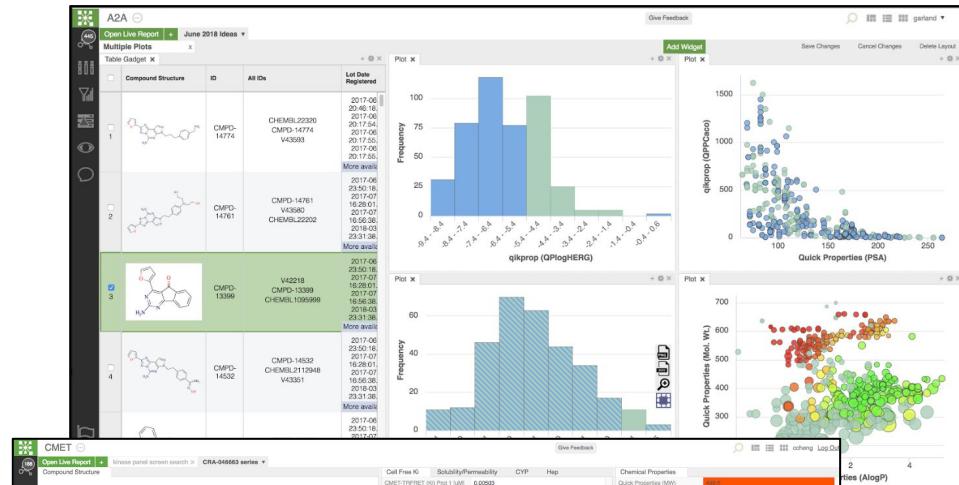
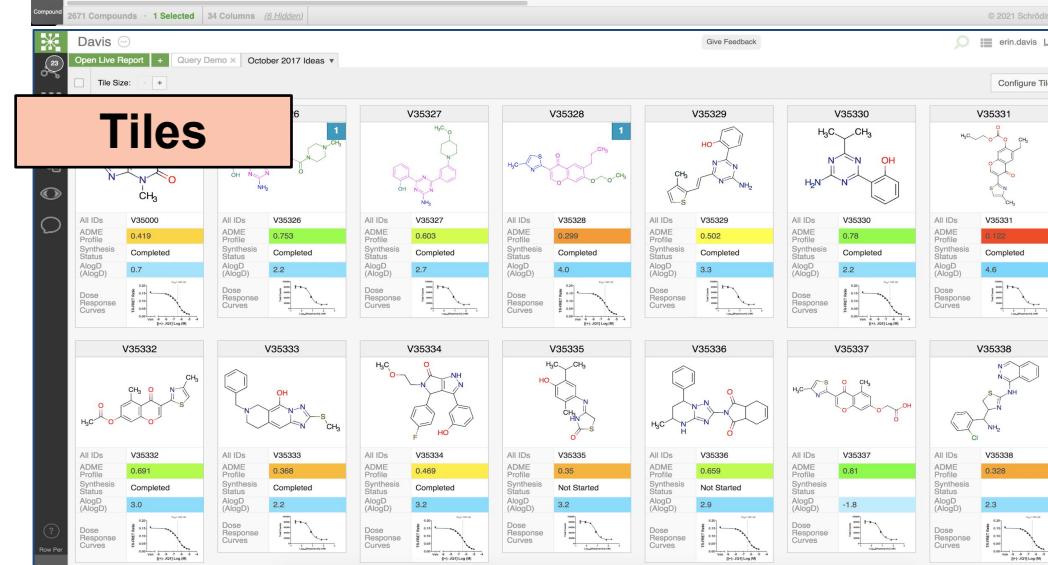
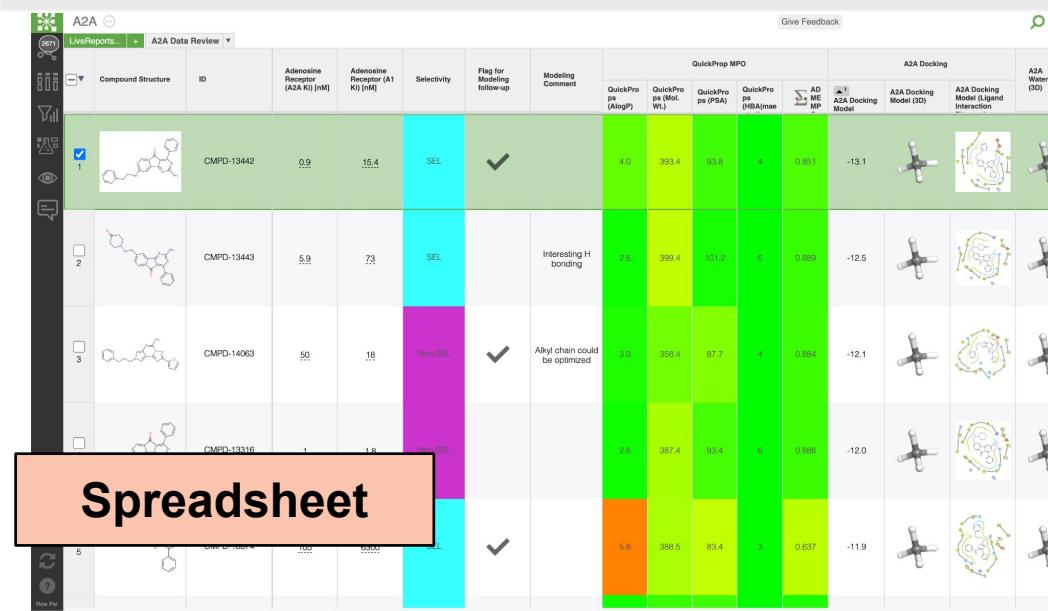
Open Live Report + Query Demo × October 2017 Ideas

Tiles

Configure Tiles...

V35000	V35327	V35328	V35329	V35330	V35331	
All IDs ADME Profile Synthesis Status AlogD (AlogD) Completed 0.419 0.7	All IDs ADME Profile Synthesis Status AlogD (AlogD) Completed 0.753 2.2	All IDs ADME Profile Synthesis Status AlogD (AlogD) Completed 0.803 2.7	All IDs ADME Profile Synthesis Status AlogD (AlogD) Completed 0.299 4.0	All IDs ADME Profile Synthesis Status AlogD (AlogD) Completed 0.502 3.3	All IDs ADME Profile Synthesis Status AlogD (AlogD) Completed 0.78 2.2	All IDs ADME Profile Synthesis Status AlogD (AlogD) Completed 0.612 4.6
Dose Response Curves	Dose Response Curves	Dose Response Curves	Dose Response Curves	Dose Response Curves	Dose Response Curves	Dose Response Curves
V35332	V35333	V35334	V35335	V35336	V35337	V35338
All IDs ADME Profile Synthesis Status AlogD (AlogD) Completed 0.691 3.0	All IDs ADME Profile Synthesis Status AlogD (AlogD) Completed 0.368 2.2	All IDs ADME Profile Synthesis Status AlogD (AlogD) Completed 0.469 3.2	All IDs ADME Profile Synthesis Status AlogD (AlogD) Not Started 0.35 3.2	All IDs ADME Profile Synthesis Status AlogD (AlogD) Not Started 0.659 2.9	All IDs ADME Profile Synthesis Status AlogD (AlogD) Not Started 0.61 1.8	All IDs ADME Profile Synthesis Status AlogD (AlogD) Not Started 0.328 2.3
Dose Response Curves	Dose Response Curves	Dose Response Curves	Dose Response Curves	Dose Response Curves	Dose Response Curves	Dose Response Curves

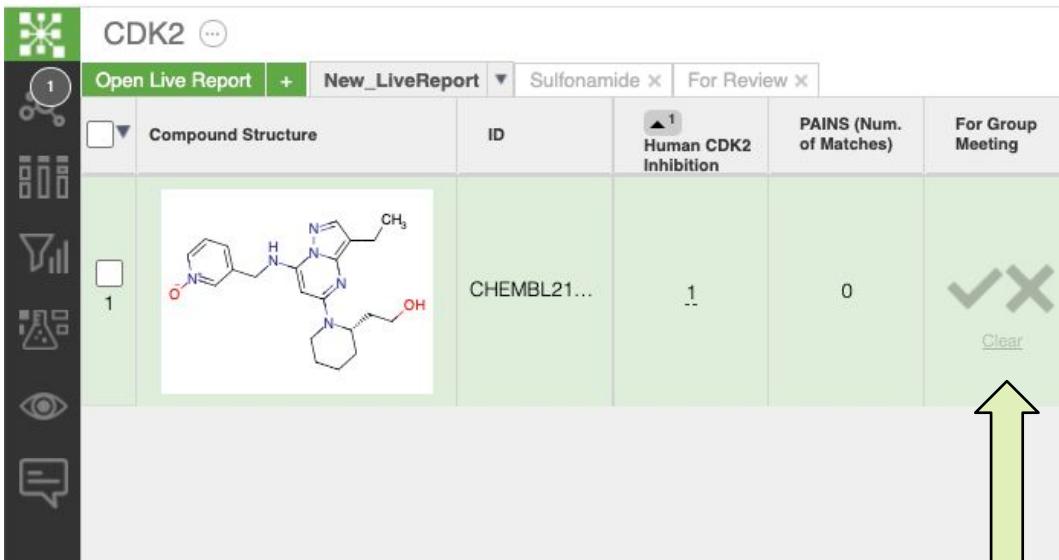
SAR: View your data in different manners to learn more



Customized Forms



Continually monitor your database and be alerted to new data



The screenshot shows the CDK2 interface with the "Advanced" tab selected. A search query "true" is entered under "For Group Meeting". A green arrow points upwards from the bottom of the slide towards this interface. A red box highlights the "Search and Add Compounds" button at the bottom right of the interface. To the right, there are four cards for adding compounds:

- Add compounds By Structure
- Add compounds By ID
- Add compounds & data From File
- Add more Data Columns

At the bottom right, it says "0 Compounds · 0 Selected · 13 Columns (4 Hidden)".

LiveReport will automatically update whenever the query condition is met: monitoring the database

Continually monitor your database and be alerted to new data

The screenshot shows the Schrödinger LiveDesign interface. On the left, there's a sidebar with various icons. The main area displays a table with a single row of data:

	Compound Structure	ID	Human CDK2 Inhibition	PAINS (Num. of Matches)	For Group Meeting
1		CHEMBL2103840	1	0	<input checked="" type="checkbox"/>

A large green arrow points from a text box in the foreground to the "For Group Meeting" checkbox in the table header.

Set this value to True and it will appear in the monitoring LiveReport

In the background, another window of the same interface is shown, also displaying the same table with the same data. This indicates that the setting being demonstrated is active across multiple sessions or tabs.

Continually monitor your database and be alerted to new data

Open Live Report + New_LiveReport x Sulfonamide x For Review ▾

Compound Structure

1

CN1C=NC2=C1C(=O)N(c3ccccc3)C(C)C2C3CCCO3

Close
Rename...
Move to Folder...
Duplicate...
Copy to Project...
Delete
Edit Default Rationale...
Show Hidden Compounds
Make Private
Make Read-Only
Subscribe to Notifications
Manage Templates ▾
Export Report ▾

Quick Properties (AER)
Quick Properties (HBA)
Quick Properties (HBD)

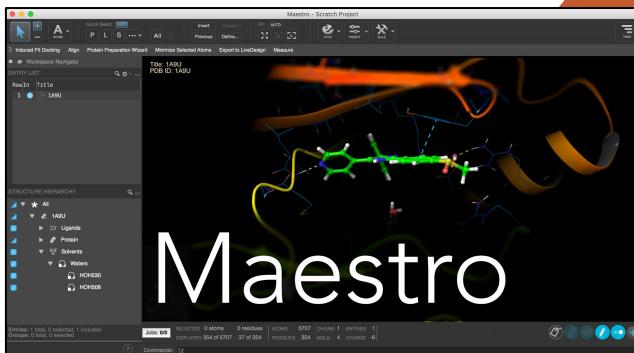
Subscribe to notifications to get digest email of whenever new data is available in your LiveReport.

You've got new data!
Click [here](#) to see
your updated
LiveReport

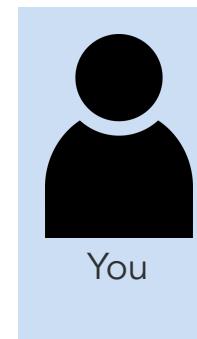


Data can be pushed/pulled between Maestro and LiveDesign

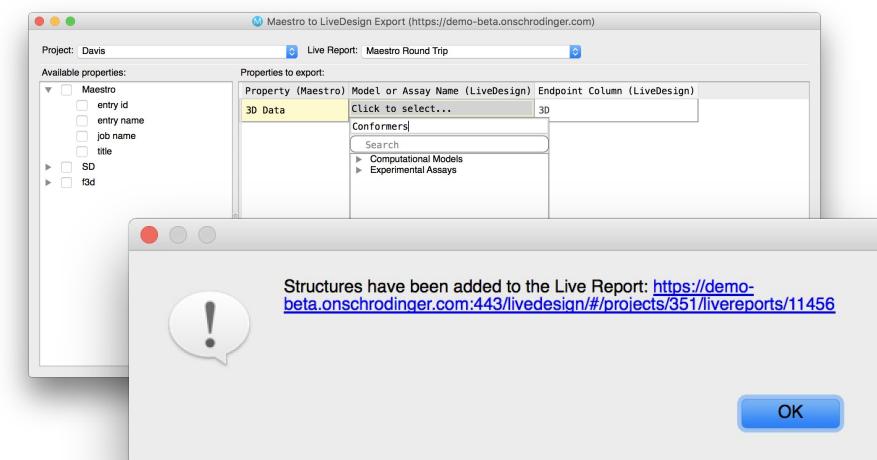
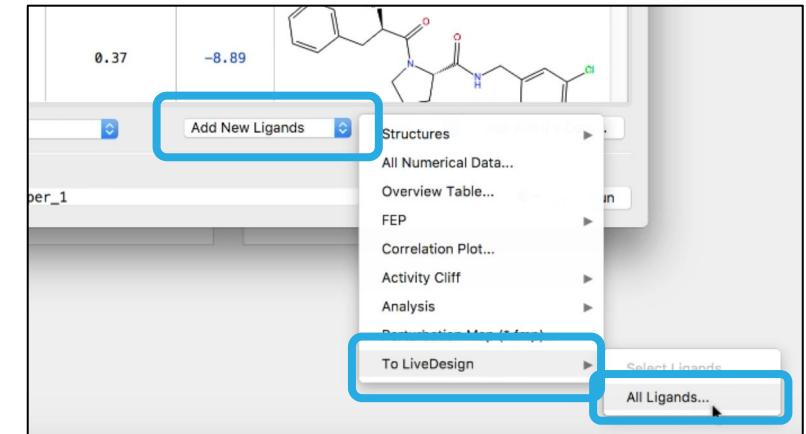
Direct connection with
Maestro



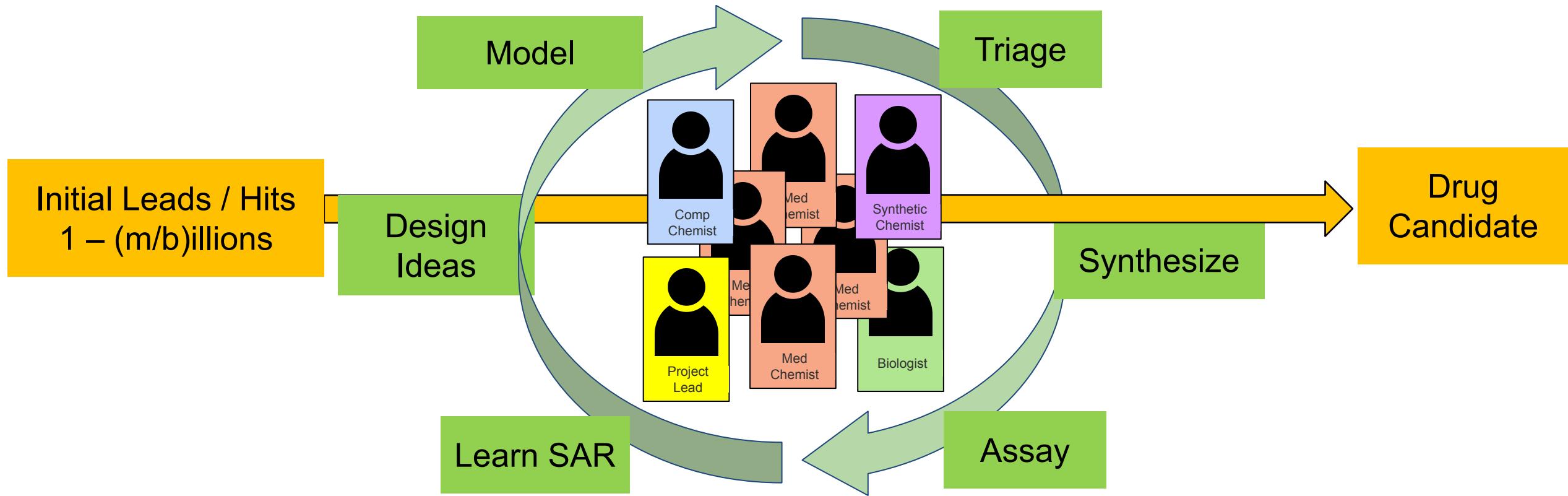
Maestro



LiveDesign™



LiveDesign gives research teams more control



Questions? Email us at online-learning@schrodinger.com