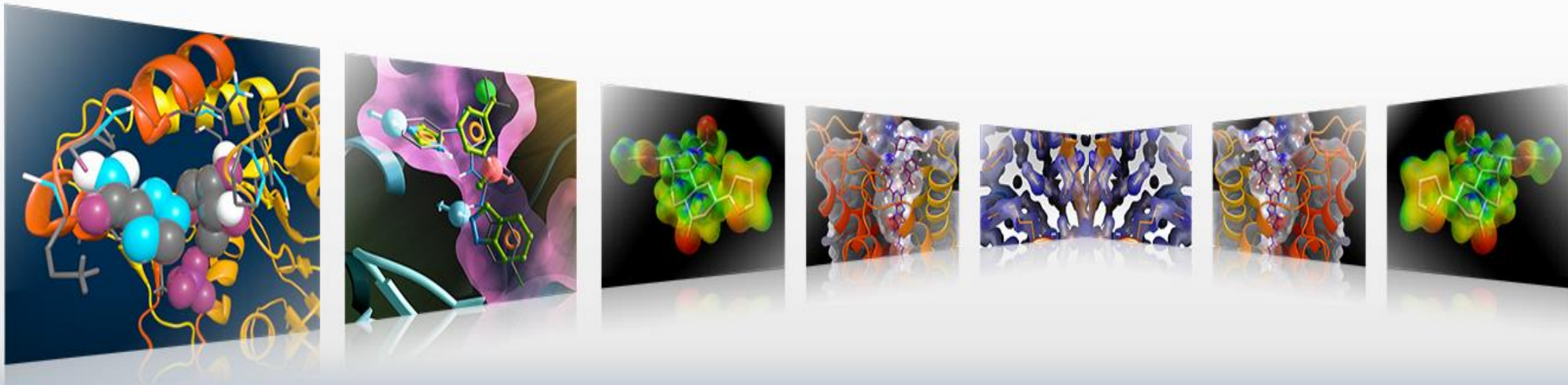


LiveDesign – Schrödinger's Next Generation Platform for Collaborative Drug Design

Andreas Witte
Schrödinger

Schrödinger

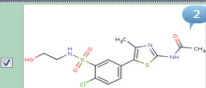
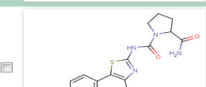
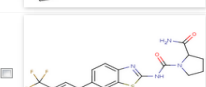
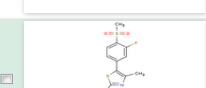
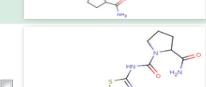
Empower researchers to achieve their goals of improving human health and quality of life through advanced computational techniques that transform the way chemists design compounds and materials.



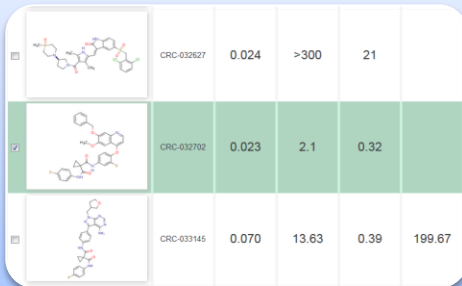
An online informatics platform

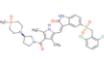
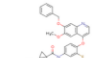
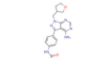
- LiveDesign™ is a browser-based enterprise platform
- Online, centralized hub for communication

The screenshot displays the LiveDesign™ interface for a PI3K project. The main window is titled "X-ray screening hit" and contains a table of results. The table has columns for Compound Structure, ID, AlogP (), Heavy Atom Count (), PSA (), and Predicted Solubility B (pH 7.4) (mol/L). The first row is highlighted in green and has a "2" in a blue circle next to its structure. To the right of the table is a "Structure Visualizer" window showing a 3D molecular model of a protein-ligand complex. The protein backbone is shown in cyan, and the ligand is shown in stick representation with various atoms colored (carbon in grey, oxygen in red, nitrogen in blue, sulfur in yellow). The Schrodinger logo is visible at the bottom of the visualization window.

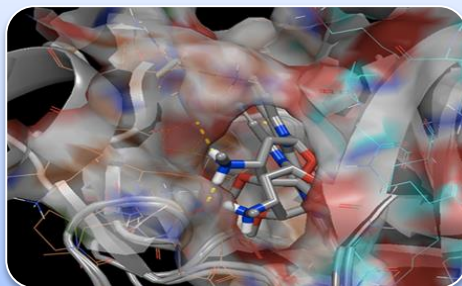
Compound Structure	ID	AlogP ()	Heavy Atom Count ()	PSA ()	Predicted Solubility B (pH 7.4) (mol/L)
	CRA-035000	1.03	24	145	102
	V35385	2.37	28	134	98
	V35389	3.25	31	155	49
	V35387	2.34	28	159	79
	V35386	2.14	27	159	97

Ideation – Create and manage Ideas



	CRC-032627	0.024	>300	21	
	CRC-032702	0.023	2.1	0.32	
	CRC-033145	0.070	13.63	0.39	199.67

Data – assays, physchem, adme,



Modeling – Lipinsky, SAR, 3D, ...



PK3kg MWQSA (dL3km)	PK3kg MWQSA (D)	P110 alpha (p1C3)	P110 gamma (p1C3)
-69.78			
-53.53			

Comments (2)

Enter a comment for the selected compound(s). Use [Link Title | Link URL] to include hyperlinks in your comment. Please be clear, concise, and focus on the facts when commenting. Use company values as a guide.

View Comments From
Selected Compound(s) All Compounds

Compound V35085

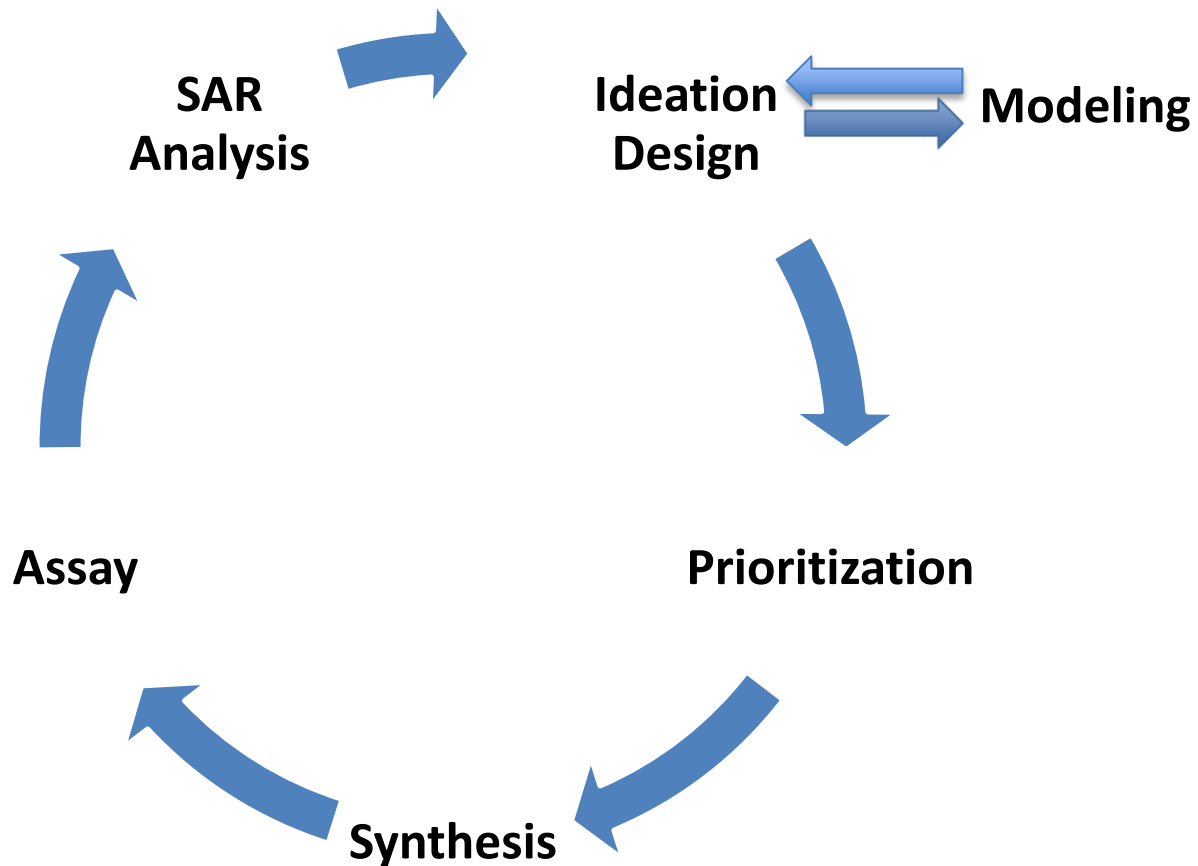
scott.becker 6/1/15 2:06:38 PM EDT
PSA is too high

mark.brewer 6/1/15 2:07:14 PM EDT
But I think we should analyze this further.

Communication – interactive, store, ...

Current Workflow

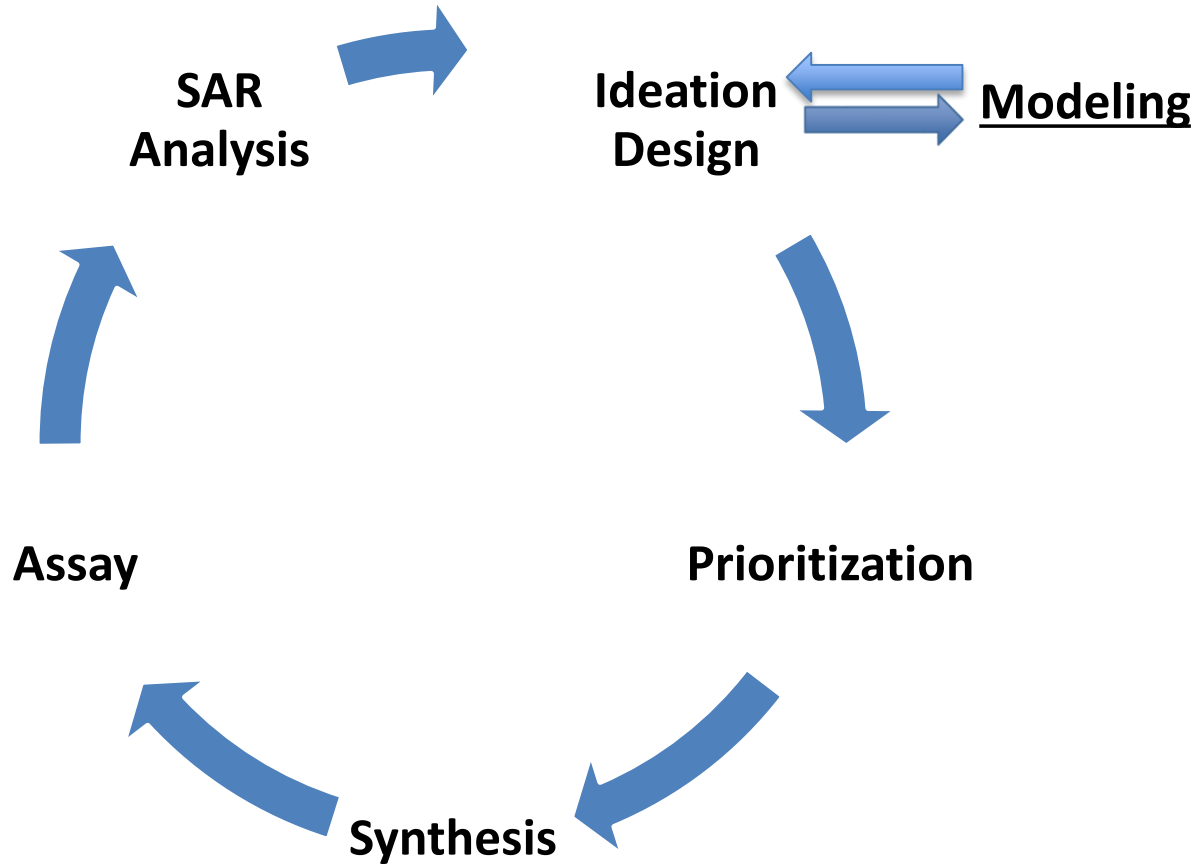
- Without LiveDesign:



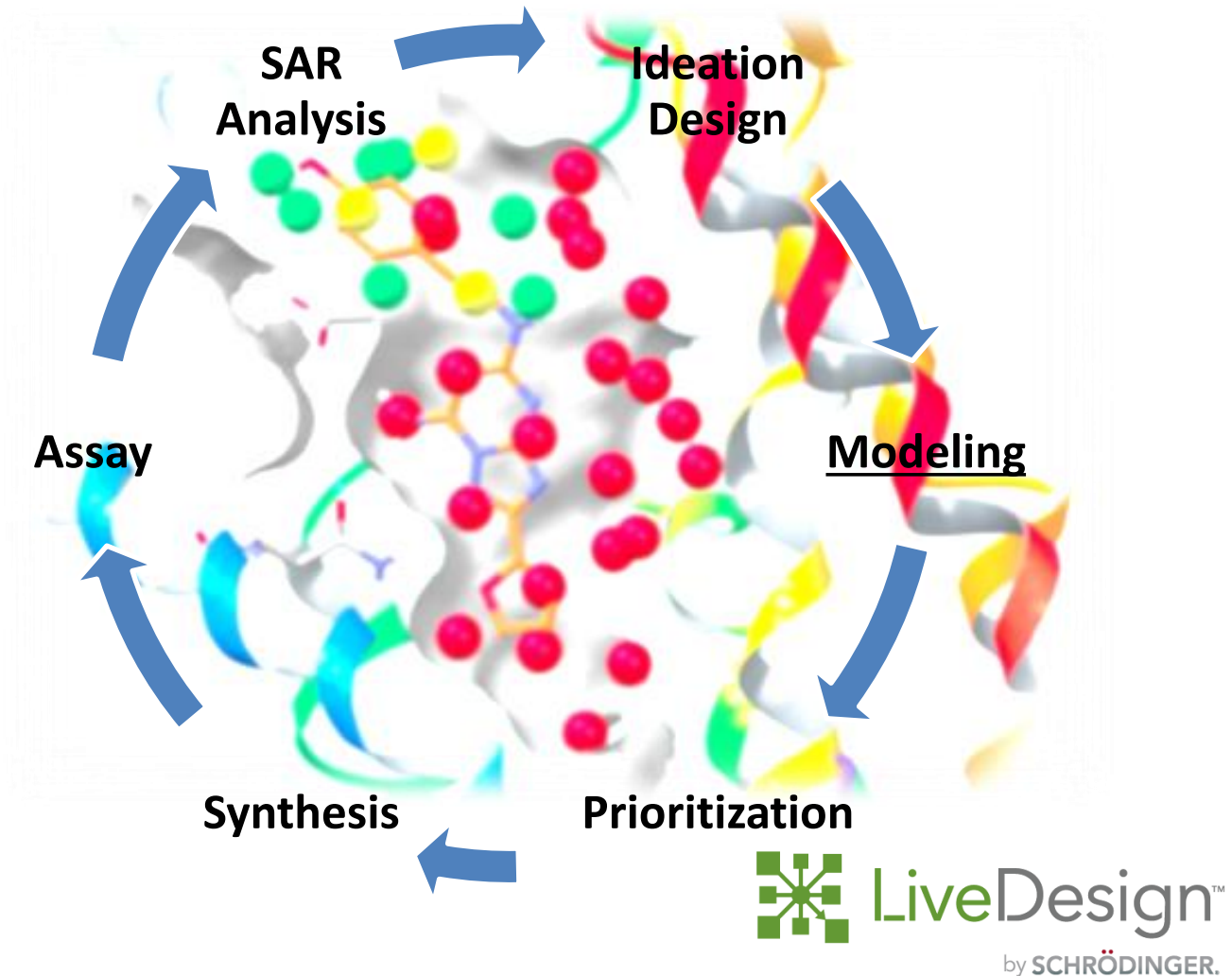
- Many compounds are insufficiently exposed to modeling
- Prioritization is not rigorously tracked
- Many disparate tools for analysis and design cause import/export overhead

Fundamental change in workflow

- Without LiveDesign:

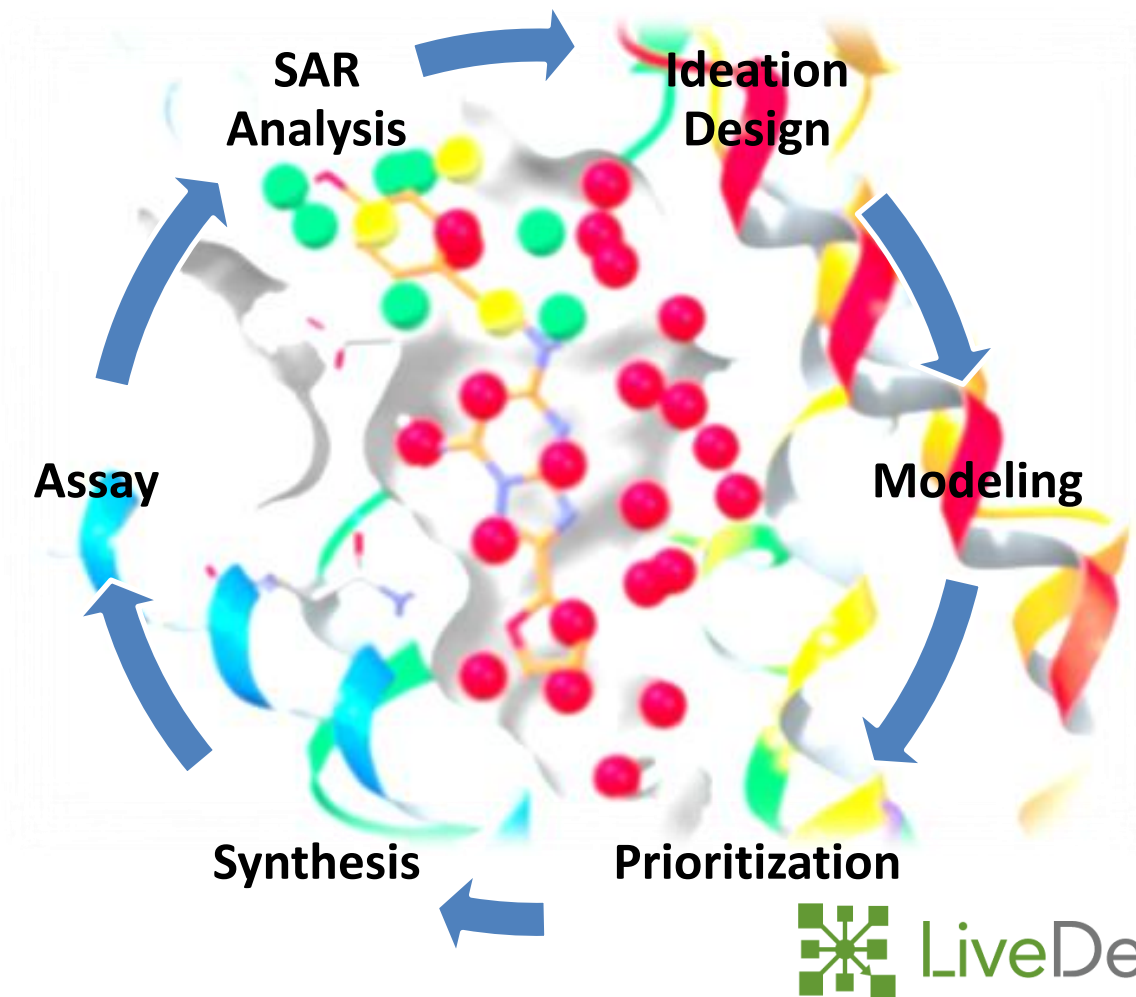


- With LiveDesign:



With LiveDesign: Fundamental change in workflow

- Tight integration of modeling
- All compounds are modeled
- Prioritization is rigorously tracked
- One centralized hub for all design and SAR work.



ChemAxon tools

- JChem
- MarvinJS
- Plexus enumeration (optional)
- ChemAxon property calculators (optional)

What does this actually mean?

- **We built LiveDesign to...**
 - Capture ideas on the fly from everyone on the team
 - Provide instantaneous feedback on ideas
 - Enable real-time sharing of ideas across sites
 - Enable computation in both structure- and ligand-based contexts
 - Enable scientists of all backgrounds to access project data