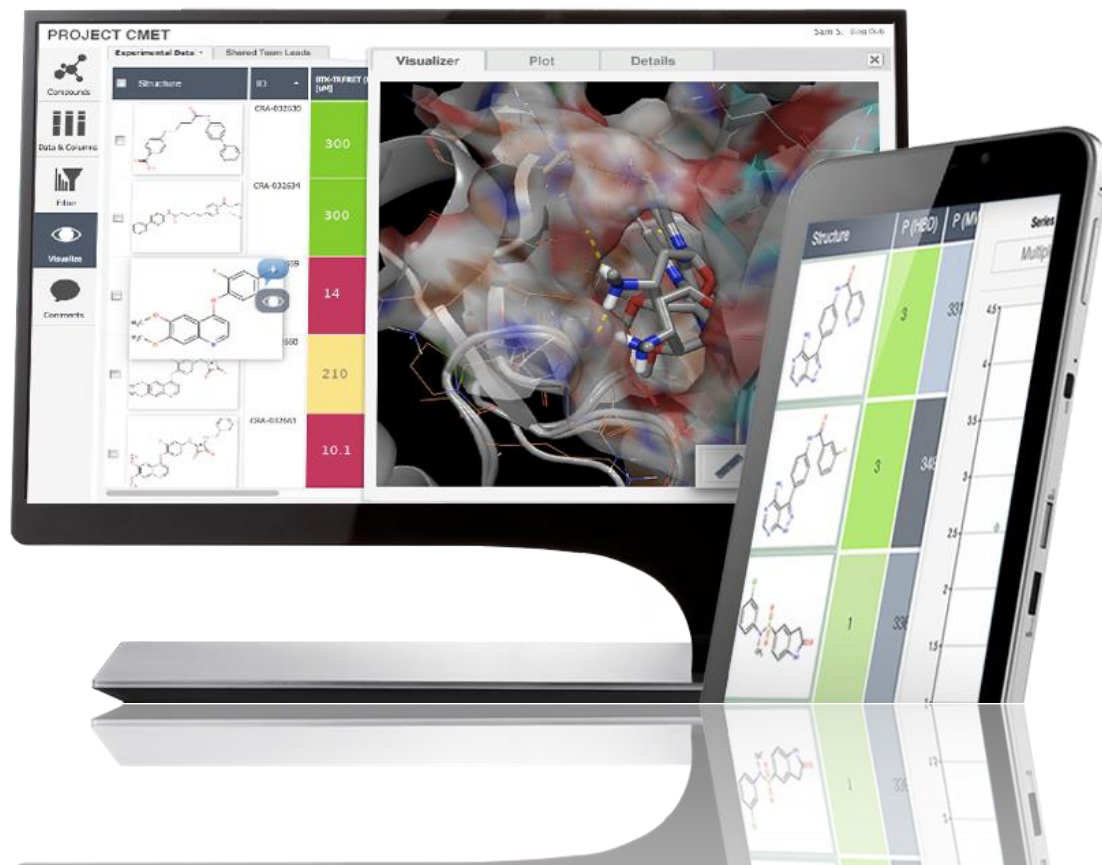
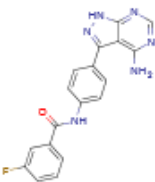
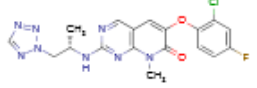
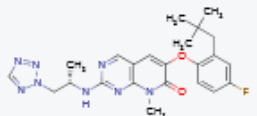
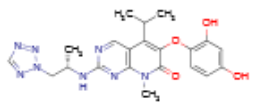




Real-time Collaborative Drug Design



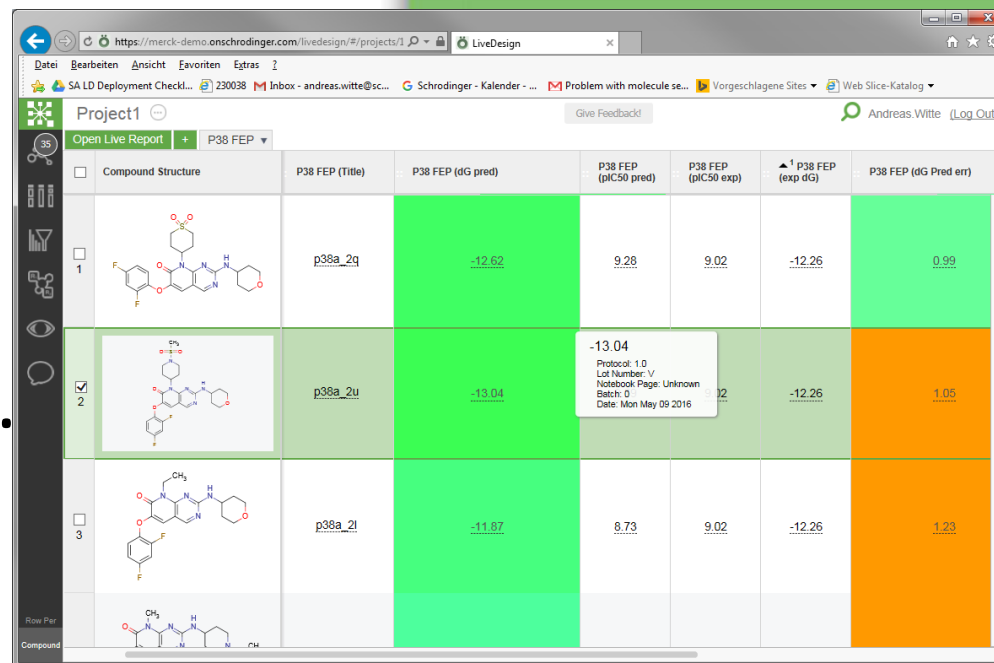
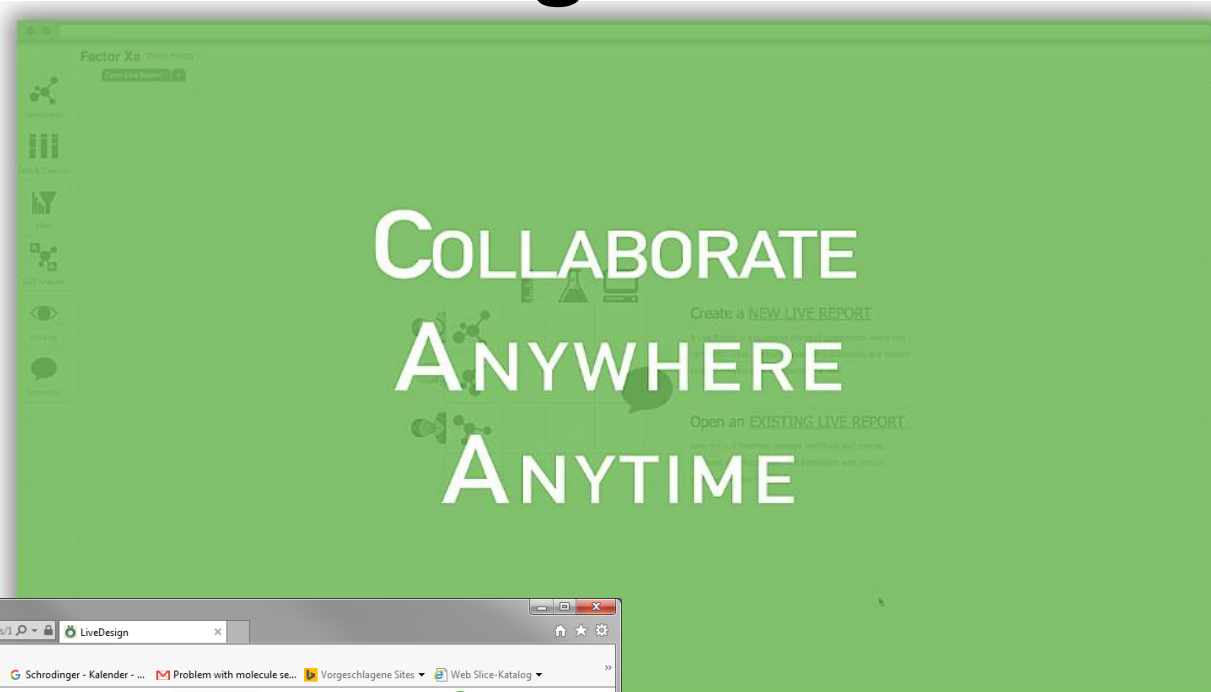
Open Live Report +		P38 FEP x	Latest Ideas v
<input type="checkbox"/>	Compound Structure	▲ ¹ ID	Series Tag
<input type="checkbox"/>		CRA-032432	Series A
<input type="checkbox"/>		V036478	Series B
<input type="checkbox"/>		V036479	Series B
<input type="checkbox"/>		V047107	Series B

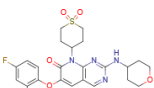
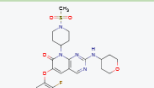
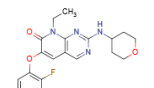
Ideation

- LiveDesign tracks ideas from the entire project team.
- Capture every new idea.
- Analyzed and prioritize new idea.
- Add property predictions.

Real-time Collaborative Design

- Collaborative spreadsheets streamline entire design process.
- Entire project team can work co-operatively from wherever they are.
- Live reporting eliminates the risk of duplicated efforts.

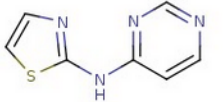

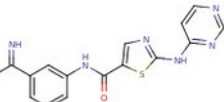

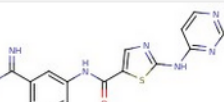

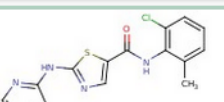



Compound Structure	P38 FEP (Title)	P38 FEP (dG pred)	P38 FEP (pIC50 pred)	P38 FEP (pIC50 exp)	P38 FEP (exp dG)	P38 FEP (dG Pred err)
	p38a_2q	-12.62	9.28	9.02	-12.26	0.99
	p38a_2u	-13.04	-13.04	12	-12.26	1.05
	p38a_2l	-11.87	8.73	9.02	-12.26	1.23

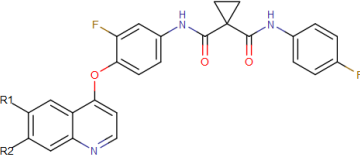
Plexus, Marvin JS & JChem





https://demo.bb.schrodinger.com/lived LiveDesign



CMET (change) + Create | Open Live Report

Compound Structure	Corporate ID	ABL (IC50)	Predicted ABL [Complex]
	CRA-035010	523	
	CRA-035013	435	
	CRA-035011		
	CRA-035012		

Scaffold

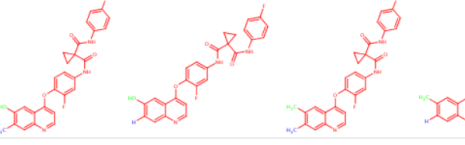


R1     Add

R2   Add

Add R3

Preview



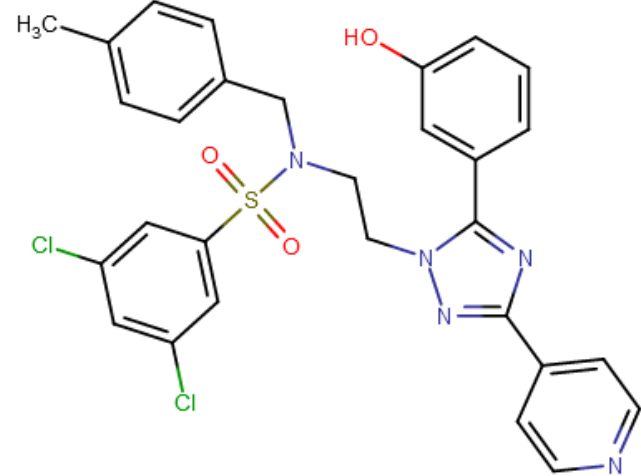
9999

AlogP 5.7078 HBA 6 HBD 1

Mol. Wt. 594.5115 Heavy Atoms 40 PSA 109.5900

Ring Count 5 Rot. Bonds 9

ADVANCED



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*

ADD
AND
OR
ANXOR

Add Idea Substructure Search Similarity Search Search Exact Match

Preview Properties Add Idea to Live Report


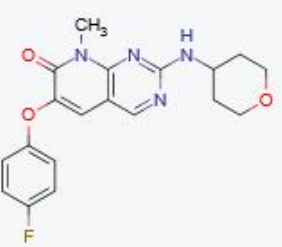





Use modeling data

- Computational models can be added by mouse click.
- Lipinsky-type calculations, project-specific ADME models ,
- and make 3D models available to the chemists ...

Open Live Report +		Compound Progression Tracker aw x		Tall x		Project ideas aw ▾					
<input type="checkbox"/>	Compound Structure	▲ ¹ ID	Quick Properties (AlogP)	Quick Properties (HBA)	Quick Properties (HBD)	Quick Properties (Mol. Wt.)	Quick Properties (Heavy)	Quick Properties (PSA)	Quick Properties (Ring Count)	Quick Properties (Rot. Bonds)	Lead Like
<input checked="" type="checkbox"/>		V42258	5.4	6.0	1.0	598.5	40.0	109.6	5.0	9.0	0.244
<input type="checkbox"/>		V42259	8.6	5.0	1.0	713.1	47.0	99.9	5.0	13.0	0.027

LiveDesign

The screenshot displays the LiveDesign web interface. The browser address bar shows the URL <https://merck-demo.onschrodinger.com/livedesign/#/projects/1>. The page title is "Project1". The main content area features a table with columns for "Compound Structure", "(dG Pred err)", "P38 FEP (3D)", and "p38 docking (3D)".

Compound Structure	(dG Pred err)	P38 FEP (3D)	p38 docking (3D)
			
	1.15		
	1.84		

On the right side, a "VISUALIZE + 3D 3D Visualizer" window is open, showing a 3D molecular model of a ligand bound to a protein. The protein surface is colored in various shades of green, red, and orange, while the ligand is shown in a stick representation with blue, red, and yellow atoms. The Schrodinger logo is visible at the bottom of the visualization window.

LiveDesign – Summary

- **Enterprise Solution**
Web-based interface is easy to use and intuitive to learn, while the data engine is built to support large data sets securely without compromising performance.
- **Ideation**
LiveDesign tracks ideas from the entire project team, allowing every new idea to be captured, analyzed, and prioritized. Real-time selectivity and property predictions update as you sketch.
- **Real-time Collaboration**
Collaborative spreadsheets and change notifications streamlines the entire design process, and allows the entire project team to work cooperatively from wherever they are. Live reporting eliminates the chance of duplicated efforts.
- **Maximize Modeling Benefits**
Validated structure- and ligand-based models in LiveDesign provide quick feedback on initial ideas, accelerating the selection of the best path forward. 3D visualization of simulation results elucidates key interactions and offers insights for further improvements.
- **Seamless Integration**
LiveDesign accesses the corporate database, and brings together tools for idea generation, SAR analysis, assay data viewing, enumeration, plotting, and in-browser PyMOL 3D visualization. LiveDesign can pull in models and computed properties from anywhere, facilitating analysis.