

LiveDesign – A Next Generation Platform for Collaborative Drug Discovery Informatics

Enterprise Informatics – what are we trying to solve?

- **Three pillars of functionality:**

- Enable med chemists to do basic modeling
- Track compound ideas; track compound status
- Facilitate communication across project teams

LiveDesign™ is a browser-based collaboration platform

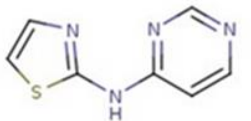
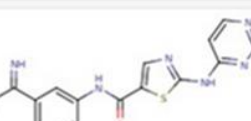
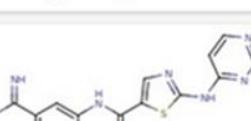
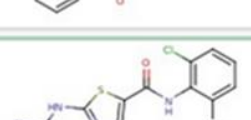
“Google docs for Chemistry”

The screenshot displays the LiveDesign interface for a project named "PI3K". The left sidebar contains navigation options: Compounds, Data & Columns, Filter, SAR Analysis, Visualize, and Comments. The "Data & Columns" panel shows a search for columns and a list of project favorites including AlogP, ChEMBL Info, Heavy Atom Count, and various P110 subtypes. The main area features a table of X-ray screening hits with columns for Compound Structure, ID, AlogP, Heavy Atom Count, PSA, and Predicted Solubility. The table lists five compounds, with the first one (CRA-035000) highlighted in green. To the right, the "Structure Visualizer" window shows a 3D molecular model of a protein-ligand complex, with the protein backbone in cyan and the ligand in stick representation. The Schrodinger logo is visible at the bottom of the visualizer.

Compound Structure	ID	AlogP ()	Heavy Atom Count ()	PSA ()	Predicted Solubility @ 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

LiveDesign integrates data visualization and predictive modeling

The screenshot displays the LiveDesign web interface. On the left is a navigation sidebar with icons for Compounds, Data/Columns, Filters & Sort, Sharing, Comments, and View. The main area features a table titled 'CMET' with columns for Compound Structure, Corporate ID, Predicted ABL [Complex], Predicted Solubility (pH 7.4), and Solubility (pH 7.4). The table contains four rows of data. To the right of the table is a 3D molecular model of a protein-ligand complex. Three red callout boxes with arrows point to specific data points in the table: the first points to the Solubility (pH 7.4) value of 51 for CRA-000343; the second points to the Predicted ABL [Complex] value of 52 for Virtual-000534; and the third points to the Predicted ABL [Complex] value of 24 for Virtual-000535.

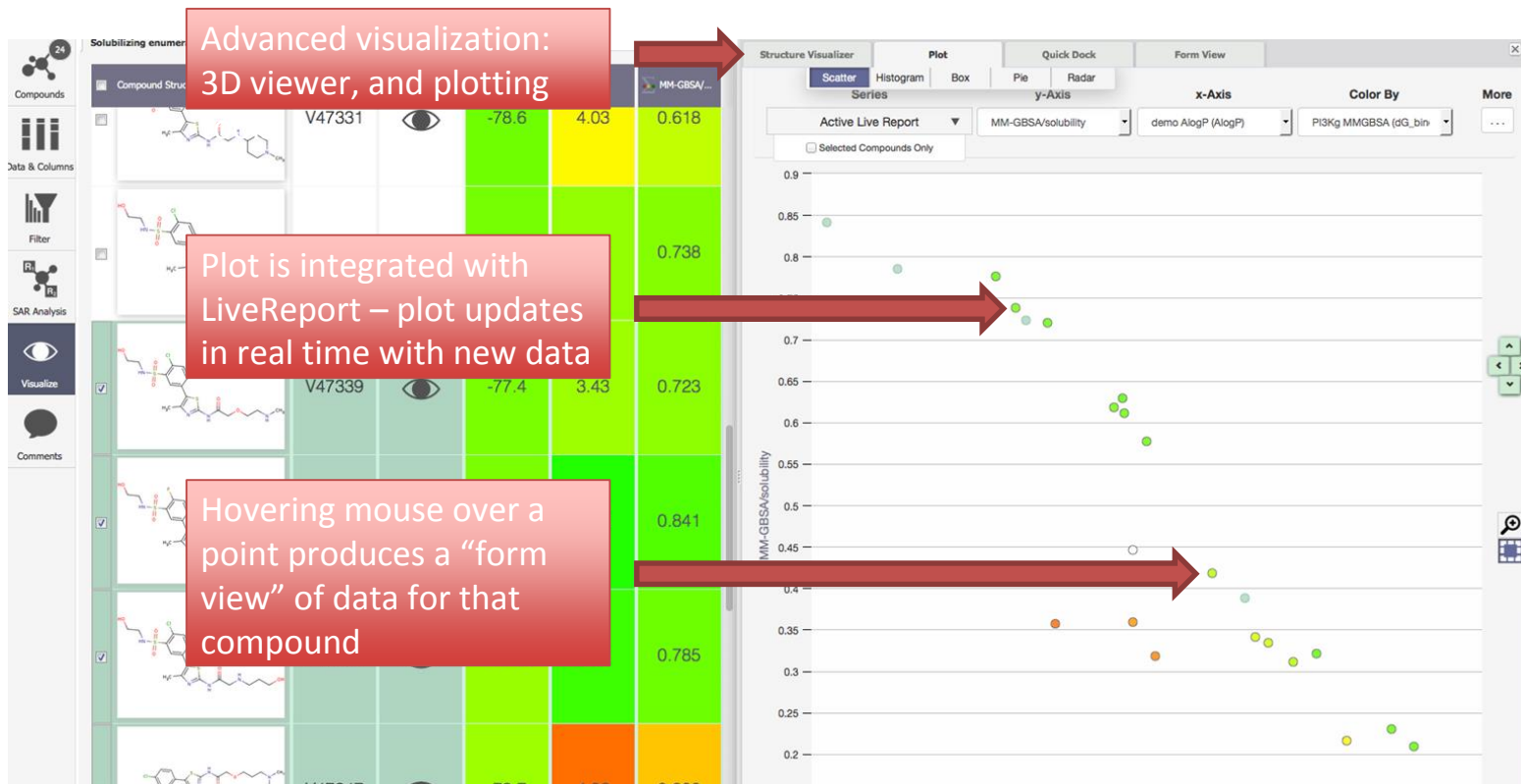
Compound Structure	Corporate ID	Predicted ABL [Complex]	Predicted Solubility (pH 7.4)	Solubility (pH 7.4)
	CRA-000343	View Complex	55.6	51
	CRA-000453	View Complex	42	45
	Virtual-000534	View Complex	52	
	Virtual-000535	View Complex	24	

Full access to both experimental and computational data

Easily calculate 2D and 3D model predictions for real and virtual compounds

Run models in a single click

LiveDesign's visualization tools enable facile analysis



Advantages of the platform

- Online collaboration, thin client; “digital whiteboard”
- Accessibility / usability
- Seamless integration with Schrödinger’s modeling software

How does ChemAxon fit into this?

- **Functionality to support UI:**
 - MarvinSketch
 - Plexus Enumeration
- **Functionality to support backend:**
 - JChemBase for standardization and searching
 - Modeling tools for property prediction

Vision for the future

- **Current paradigm:**
 1. Human generates idea
 2. Computer offers computational feedback
 3. Human iterates on design

Vision for the future

- **Our vision:**
 1. Human poses problem
 2. Computer offers design suggestions, along with computational evidence
 3. Human prioritizes designs

