LiveDesign – A Next Generation Platform for Collaborative Drug Discovery Informatics

LiveDesign™ by SCHRÖDINGER.

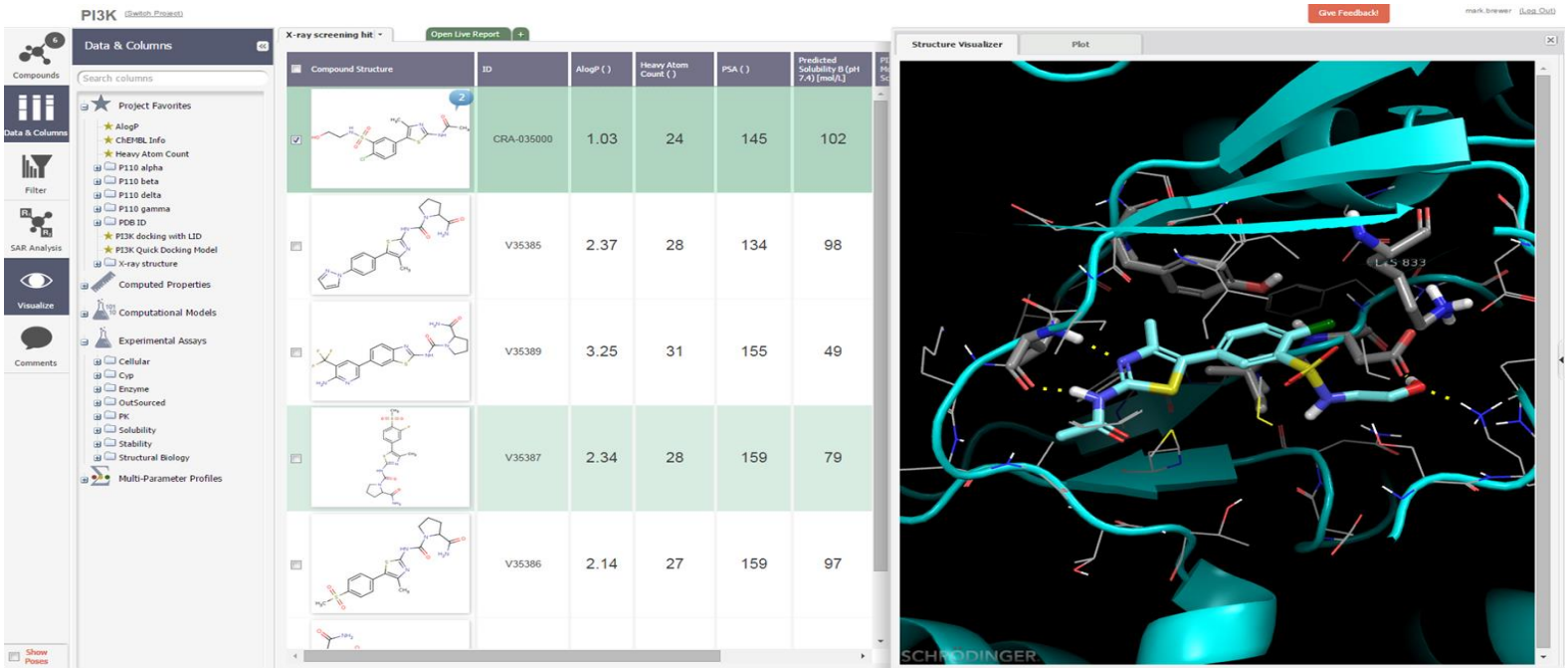
Enterprise Informatics – what are we trying to solve?

- **Three pillars of functionality:**
  - Enable med chemists to do basic modeling
  - Track compound ideas; track compound status
  - Facilitate communication across project teams

LiveDesign™ by SCHRÖDINGER.

LiveDesign™ is a browser-based collaboration platform

"Google docs for Chemistry"



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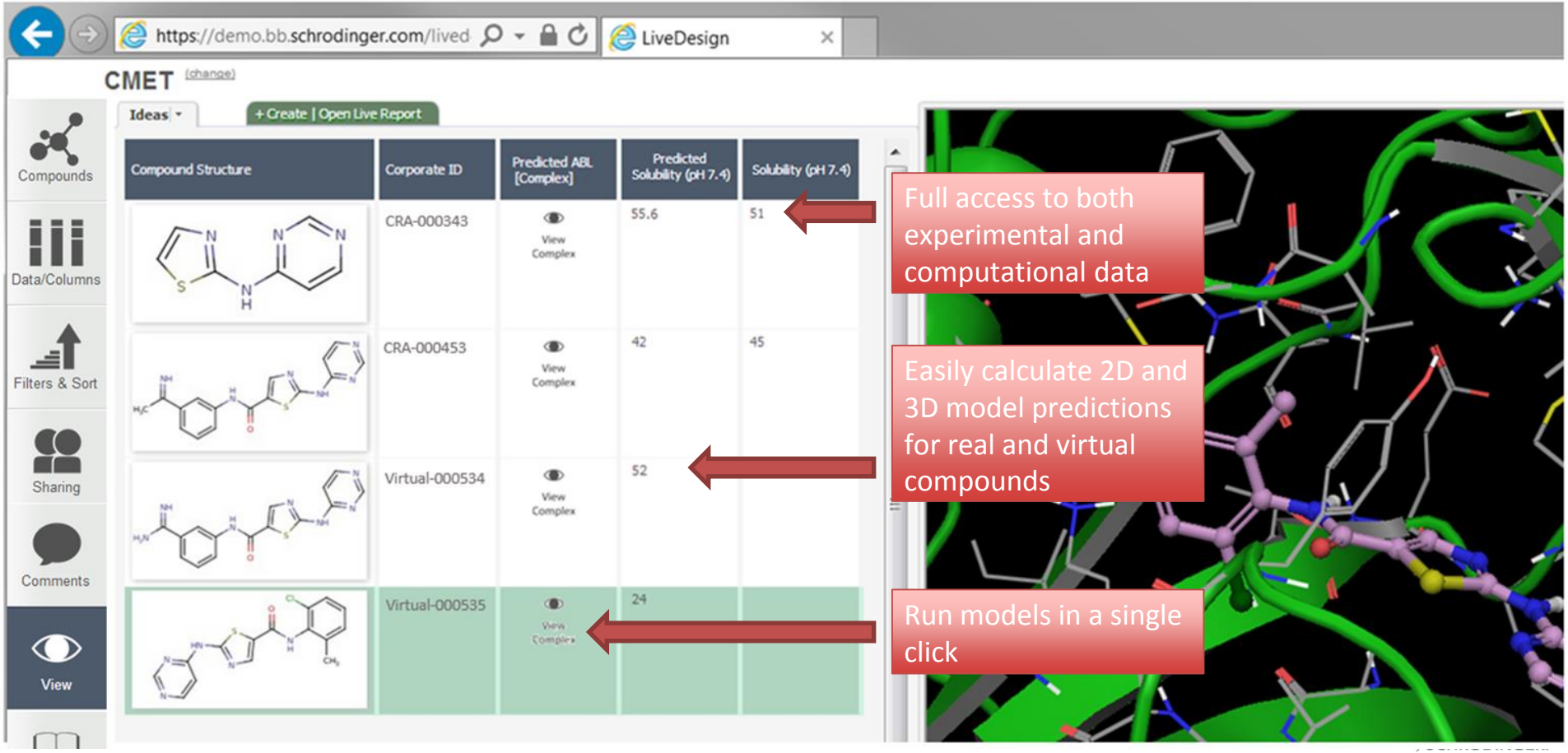
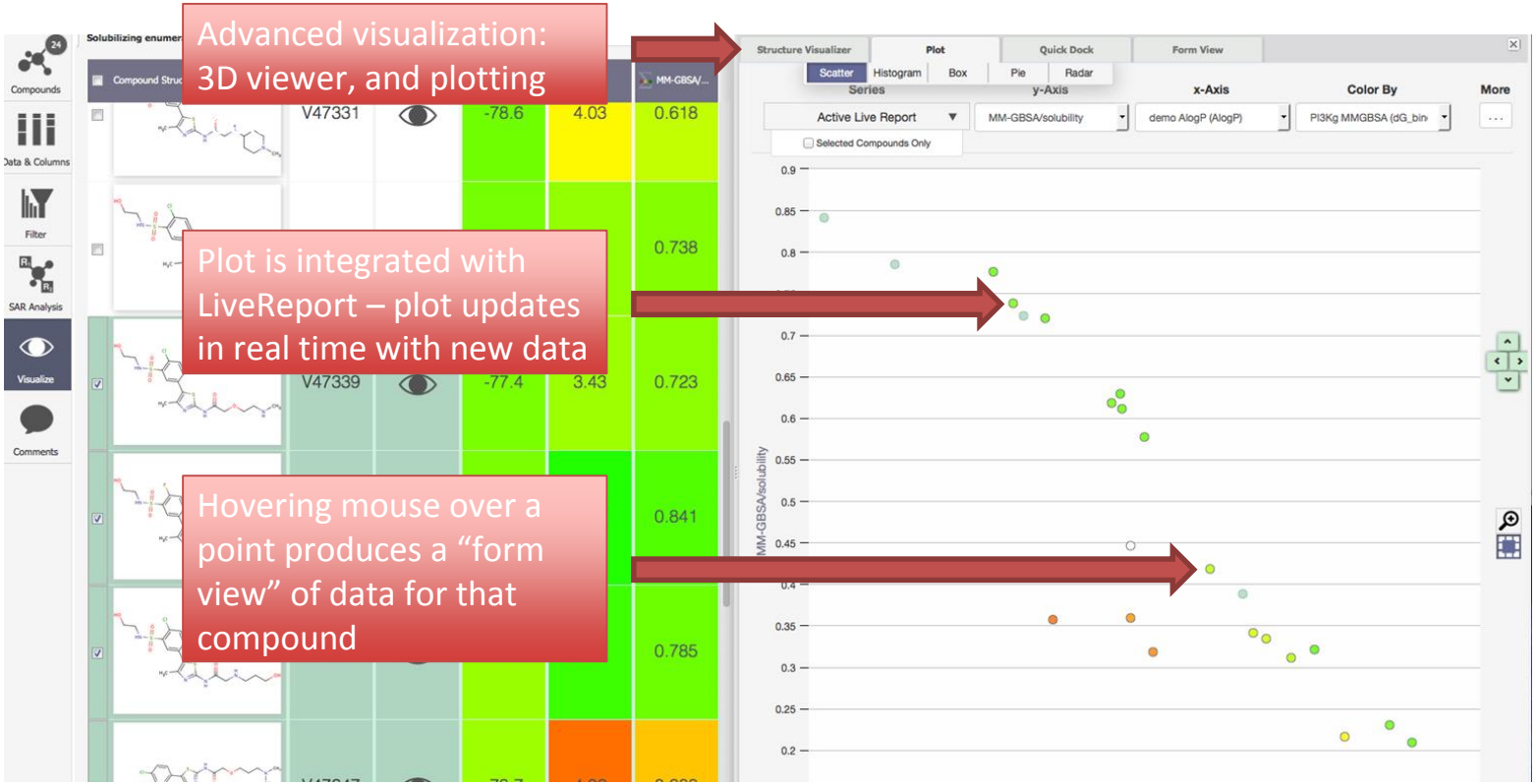
LiveDesign integrates data visualization and predictive modeling



LiveDesign's visualization tools enable facile analysis



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Advantages of the platform

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

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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