

Self-Service Data Access, SAR Analysis, and Molecular Design

Why do more than 5,000 discovery scientists use D360?

1. Self-service Access to All of Your Data

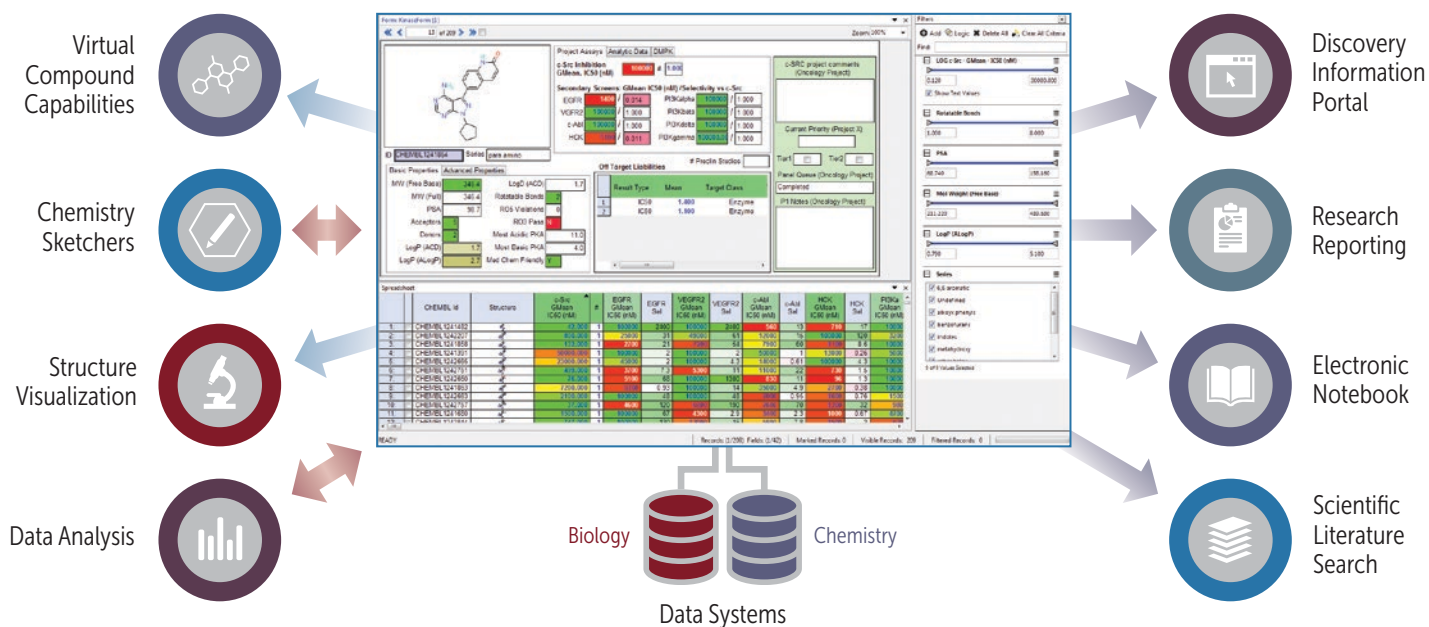
- Access all of your project data with one click, regardless of where and how it is stored
- Easily create your own queries with an intuitive interface to investigate scientific hypotheses
- Get near real-time access to new assays and assay data

2. Embedded SAR Analysis and Molecular Design Tools

- Use a spreadsheet for easy SAR or a form view to examine detailed data for individual compounds
- Understand your data quickly with graphs, charts, equations, and a host of analysis capabilities
- Leverage SAR tools like Chemical series, R-group, and matched series analysis for timely decision-making
- Apply your knowledge to molecular design through virtual compound addition and enumeration

D360 amplifies the impact of the investments that you have already made without disrupting your current infrastructure. It can be deployed quickly with standard connectors for chemical registration systems and commercial data sources from IDBS, Core Informatics, BIOVIA and more. Customized connectors are also available.

D360 Self-service Informatics Platform



- Annotate your compounds with sharable, searchable text, numerical data and external files
- Work together within and across teams with a robust sharing environment that includes queries and datasets
- Integrate seamlessly with Excel®, PowerPoint®, Spotfire®, JMP®, and other applications to span the entire workflow
- Collaborate with external research partners using D360 Partner Access while maintaining essential data security

– Scientist, Biochemistry
and Enzymology at Agios

The screenshot shows the 'Open a Dataset' window in the Certara Partner software. The window is divided into three main sections:

- Dataset List:** A table listing 32 datasets with columns for CHEMBL ID, Structure, C-DB (GMax), FQDB (GMax), VQFQDB (GMax), A-DB (GMax), HCK (GMax), PDB (GMax), PDB (GMax), PDB (GMax), and PDB (GMax). The datasets are numbered 1 through 32.
- Histogram:** A bar chart showing the distribution of selected fragments. The x-axis is labeled 'Selected fragments' and the y-axis is labeled 'Count'. The histogram shows a distribution of fragment counts across different categories.
- 3D Molecular Model:** A 3D visualization of a protein-ligand complex. The protein is shown as a green surface, and the ligand is shown as a red sphere. The model is labeled 'Structure (MolSrv) Structure 31'.

The Certara Partner logo is visible in the bottom left corner of the window.

– Scientist at Medivir

Coming soon! Web D360 that extends D360 capabilities online for anywhere, anytime access.

Certara is a leading provider of decision support technology and consulting services for optimizing drug development and improving health outcomes. Certara's solutions, which span the drug development and patient care lifecycle, help increase the probability of regulatory and commercial success by using the most scientifically advanced modeling and simulation technologies and regulatory strategies. Its clients include hundreds of global biopharmaceutical companies, leading academic institutions and key regulatory agencies.

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